



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:12 PM UTC

PDB ID : 8ZIR / pdb\_00008zir  
EMDB ID : EMD-60127  
Title : DUF4297-HerA complex  
Authors : Yu, Y.; Chen, Q.  
Deposited on : 2024-05-14  
Resolution : 3.08 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:

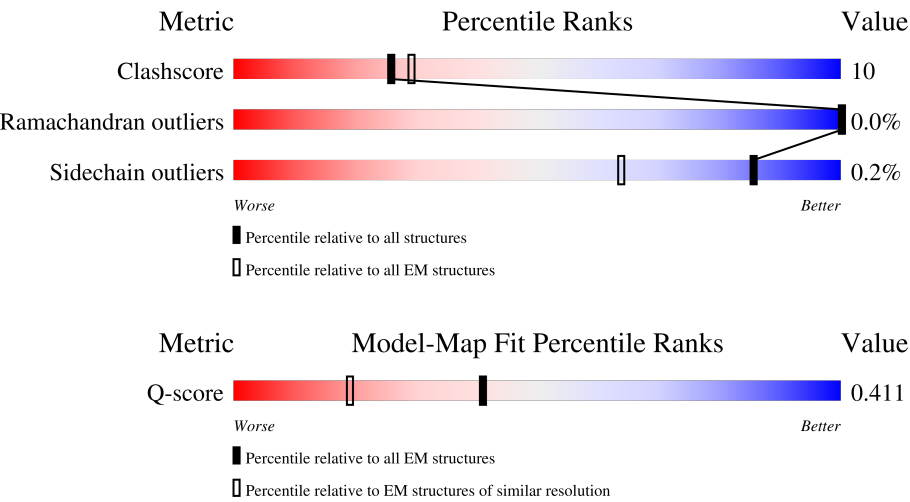
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 3.08 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.



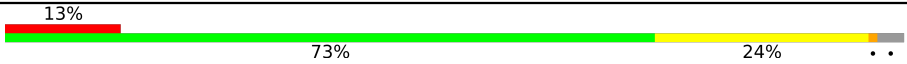
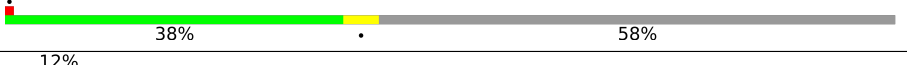
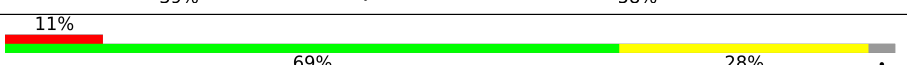
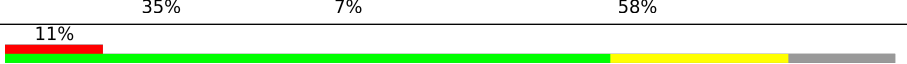
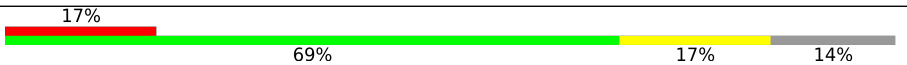
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14000 ( 2.58 - 3.58 )                                    |

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     | 397    |                  |
| 1   | B     | 397    |                  |
| 1   | C     | 397    |                  |
| 1   | D     | 397    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 397    |    |
| 1   | F     | 397    |    |
| 1   | G     | 397    |    |
| 1   | H     | 397    |    |
| 1   | I     | 397    |    |
| 1   | J     | 397    |    |
| 1   | K     | 397    |    |
| 1   | L     | 397    |    |
| 2   | M     | 617    |    |
| 2   | N     | 617    |   |
| 2   | O     | 617    |  |
| 2   | P     | 617    |  |
| 2   | Q     | 617    |  |
| 2   | R     | 617    |  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 102988 atoms, of which 50586 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 DUF4297.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 1   | A     | 388      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5985  | 2005 | 2851 | 545 | 576 | 8 |         |       |
| 1   | B     | 167      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2789  | 889  | 1400 | 251 | 245 | 4 |         |       |
| 1   | C     | 386      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 6002  | 1990 | 2890 | 541 | 573 | 8 |         |       |
| 1   | D     | 169      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2827  | 902  | 1418 | 253 | 250 | 4 |         |       |
| 1   | E     | 387      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5977  | 1993 | 2859 | 544 | 573 | 8 |         |       |
| 1   | F     | 167      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2794  | 889  | 1405 | 251 | 245 | 4 |         |       |
| 1   | G     | 380      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5931  | 1965 | 2856 | 537 | 565 | 8 |         |       |
| 1   | H     | 168      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2806  | 893  | 1409 | 252 | 248 | 4 |         |       |
| 1   | I     | 385      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5959  | 1988 | 2851 | 542 | 570 | 8 |         |       |
| 1   | J     | 169      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2827  | 902  | 1418 | 253 | 250 | 4 |         |       |
| 1   | K     | 384      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5948  | 1985 | 2846 | 541 | 568 | 8 |         |       |
| 1   | L     | 168      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2806  | 893  | 1409 | 252 | 248 | 4 |         |       |

- Molecule 2 is a protein called HerA.

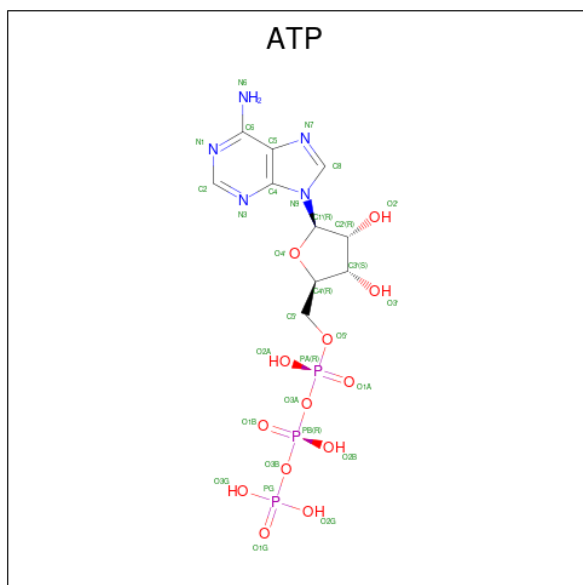
| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | M     | 546      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8430  | 2709 | 4189 | 713 | 806 | 13 |         |       |
| 2   | N     | 531      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8172  | 2619 | 4065 | 694 | 781 | 13 |         |       |
| 2   | O     | 543      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8390  | 2697 | 4168 | 710 | 802 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | P     | 553      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8479  | 2719 | 4211 | 724 | 812 | 13 |         |       |
| 2   | Q     | 546      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8401  | 2703 | 4168 | 708 | 809 | 13 |         |       |
| 2   | R     | 543      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8333  | 2675 | 4137 | 707 | 801 | 13 |         |       |

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

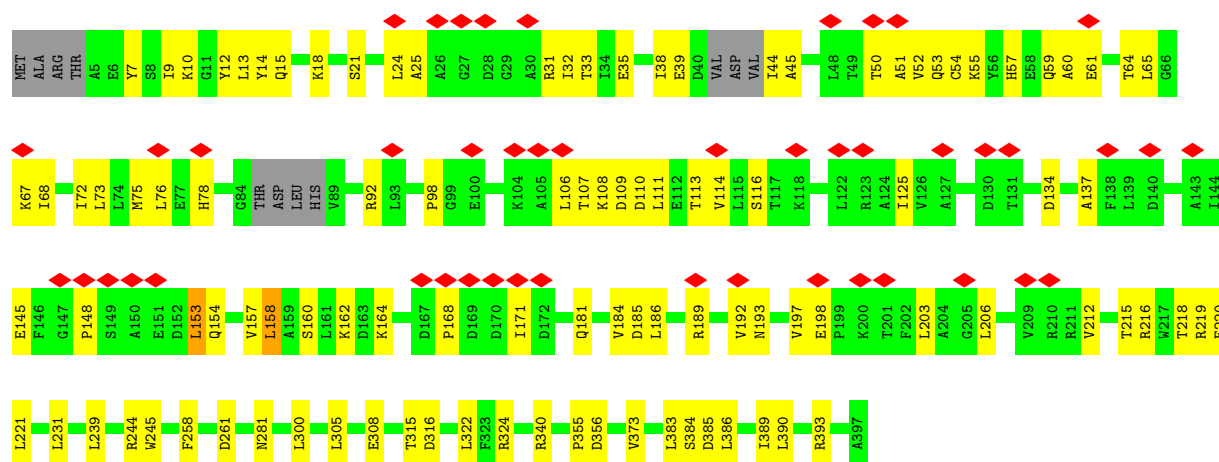


| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 3   | M     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 3   | O     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 3   | Q     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |

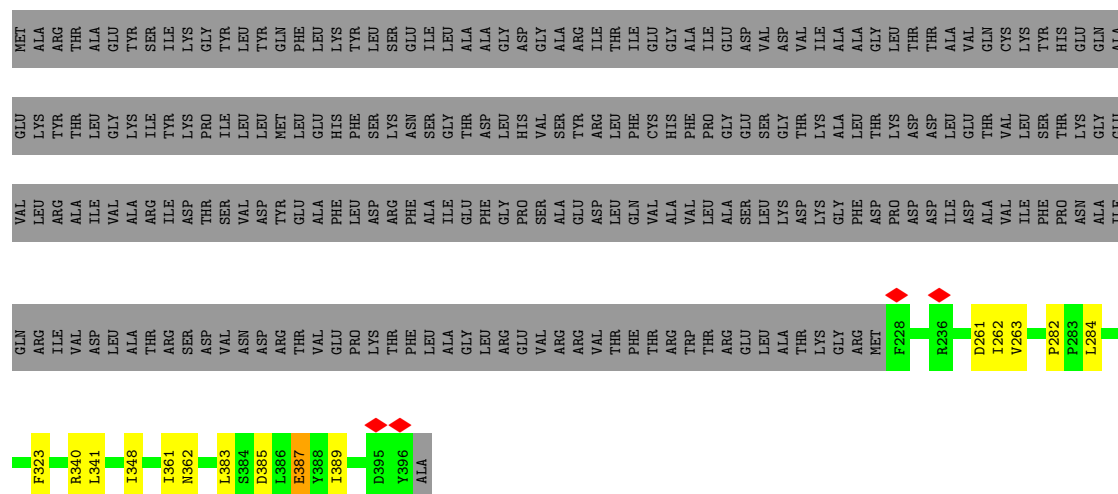
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | O     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | Q     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

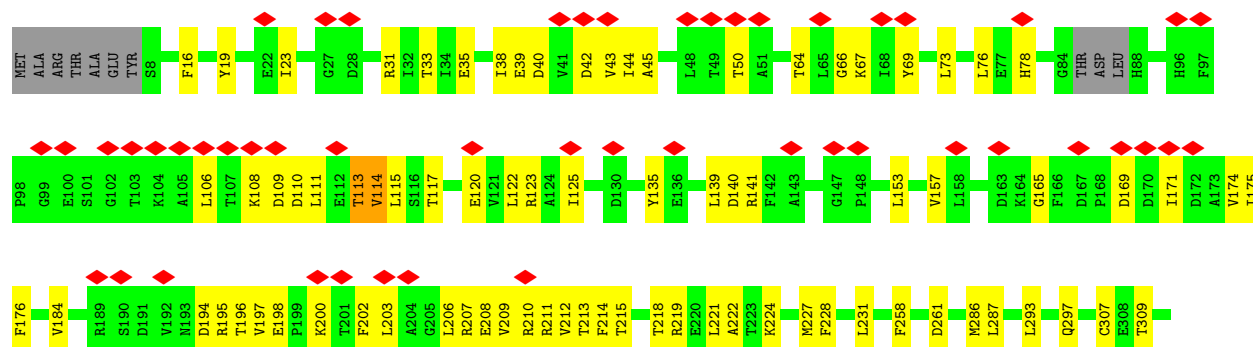
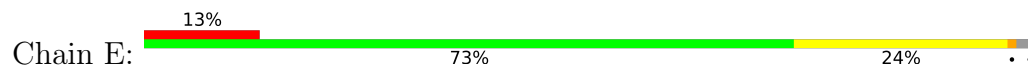




• Molecule 1: DUF4297



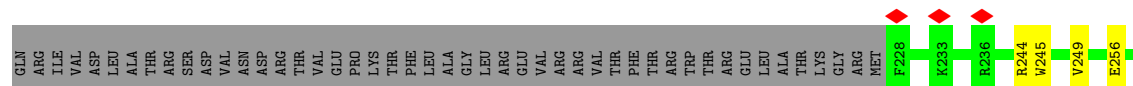
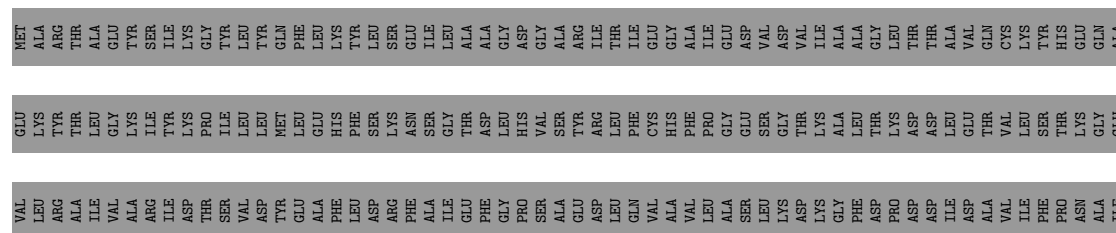
• Molecule 1: DUF4297





• Molecule 1: DUF4297

Chain F: 38% 58%



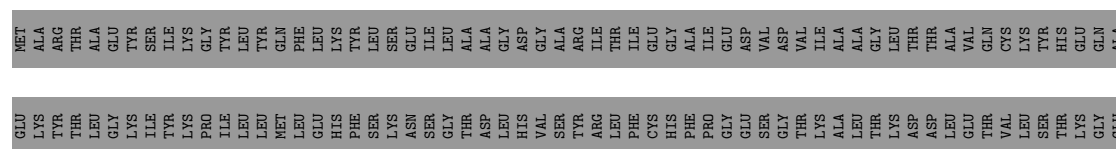
• Molecule 1: DUF4297

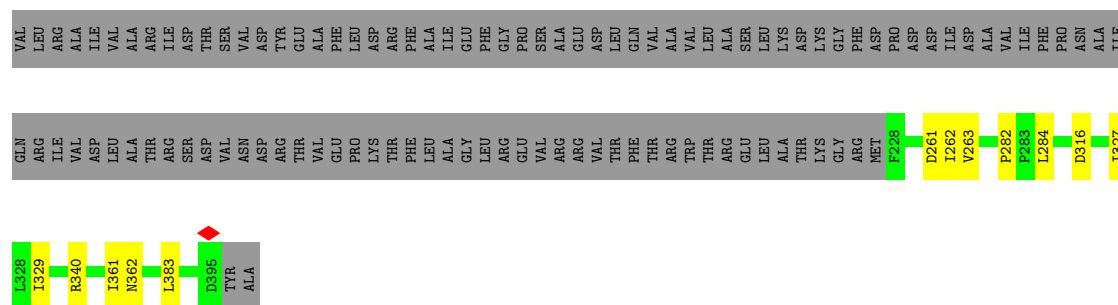
Chain G: 12% 72% 24%



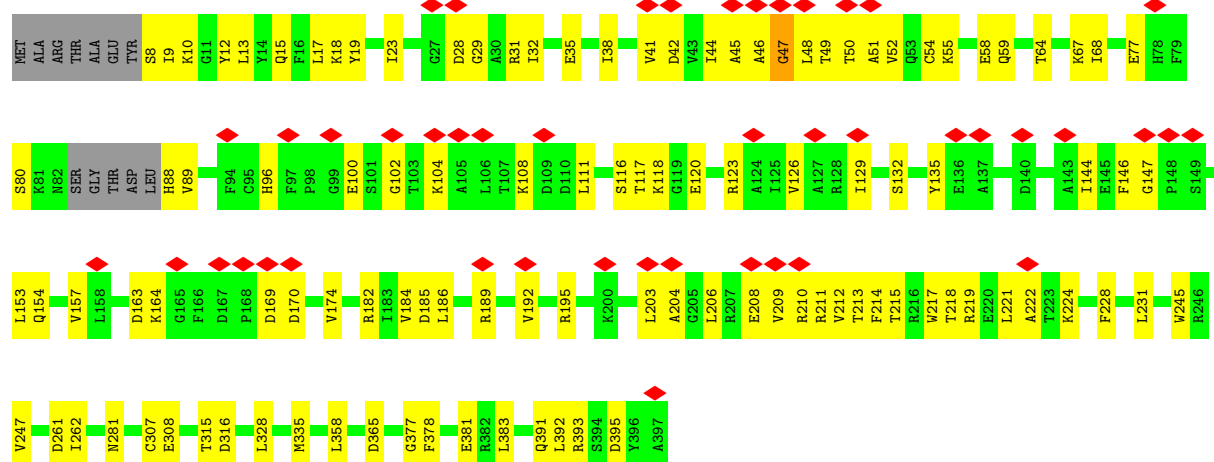
• Molecule 1: DUF4297

Chain H: 39% 58%

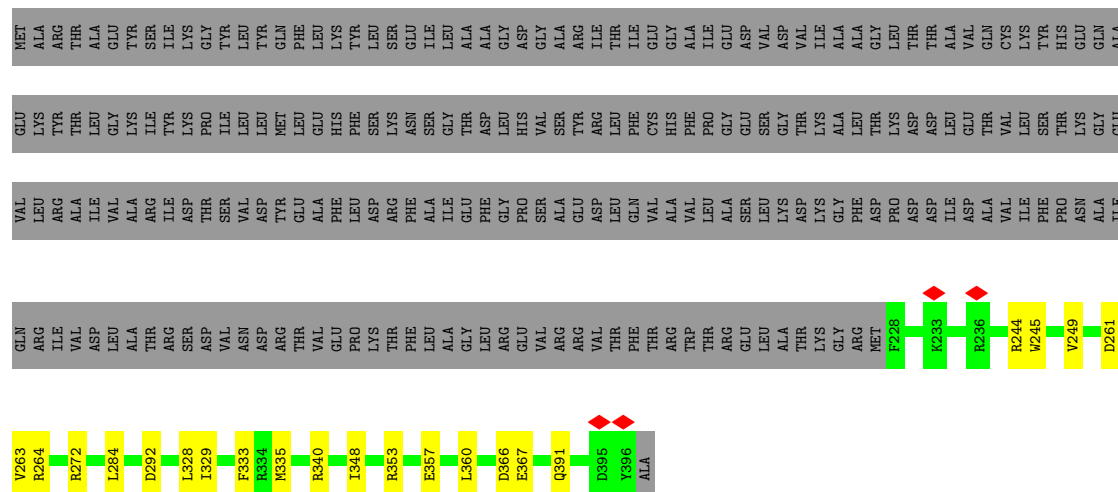
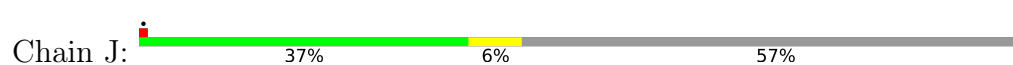




• Molecule 1: DUF4297

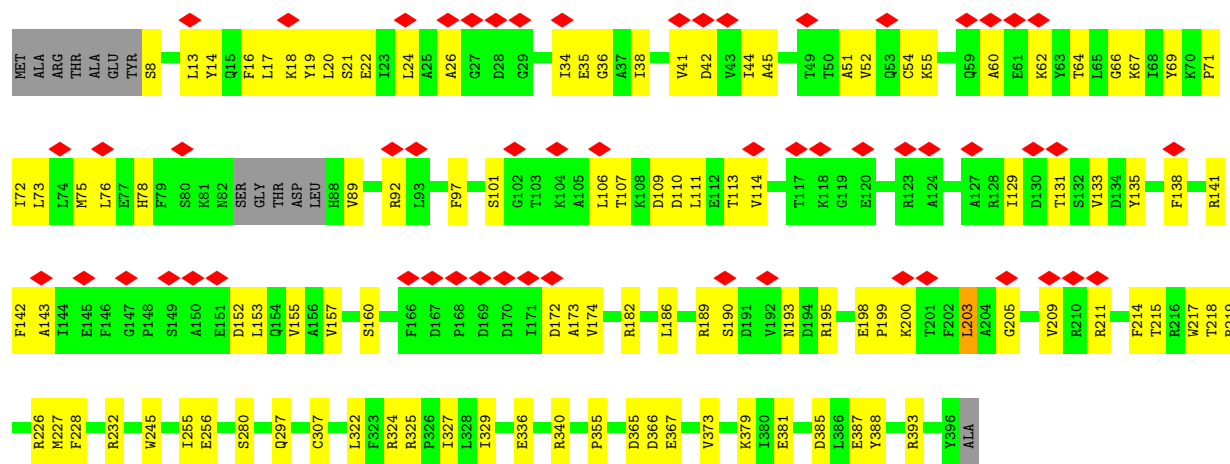


• Molecule 1: DUF4297



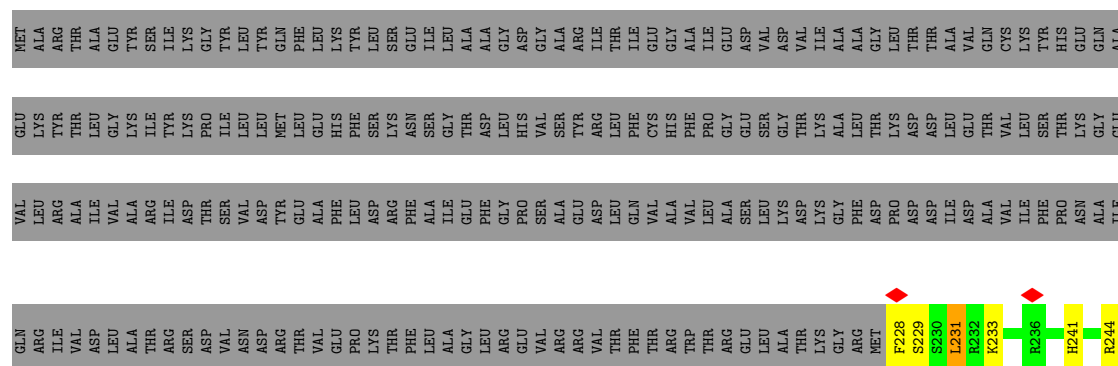
• Molecule 1: DUF4297





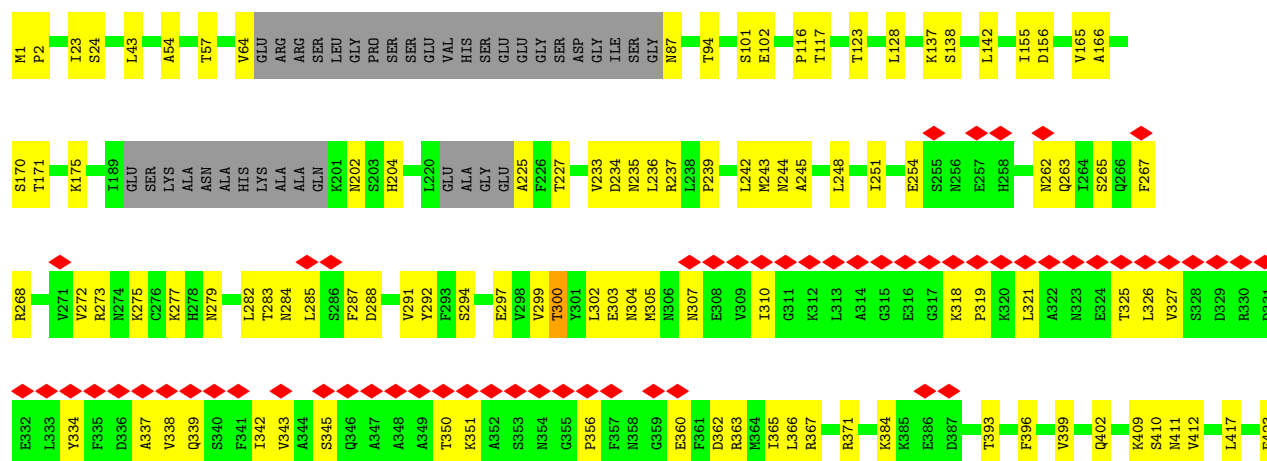
• Molecule 1: DUF4297

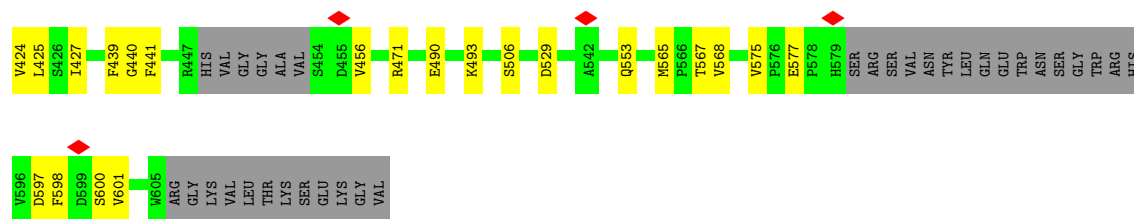
Chain L: 35% 7% 58%



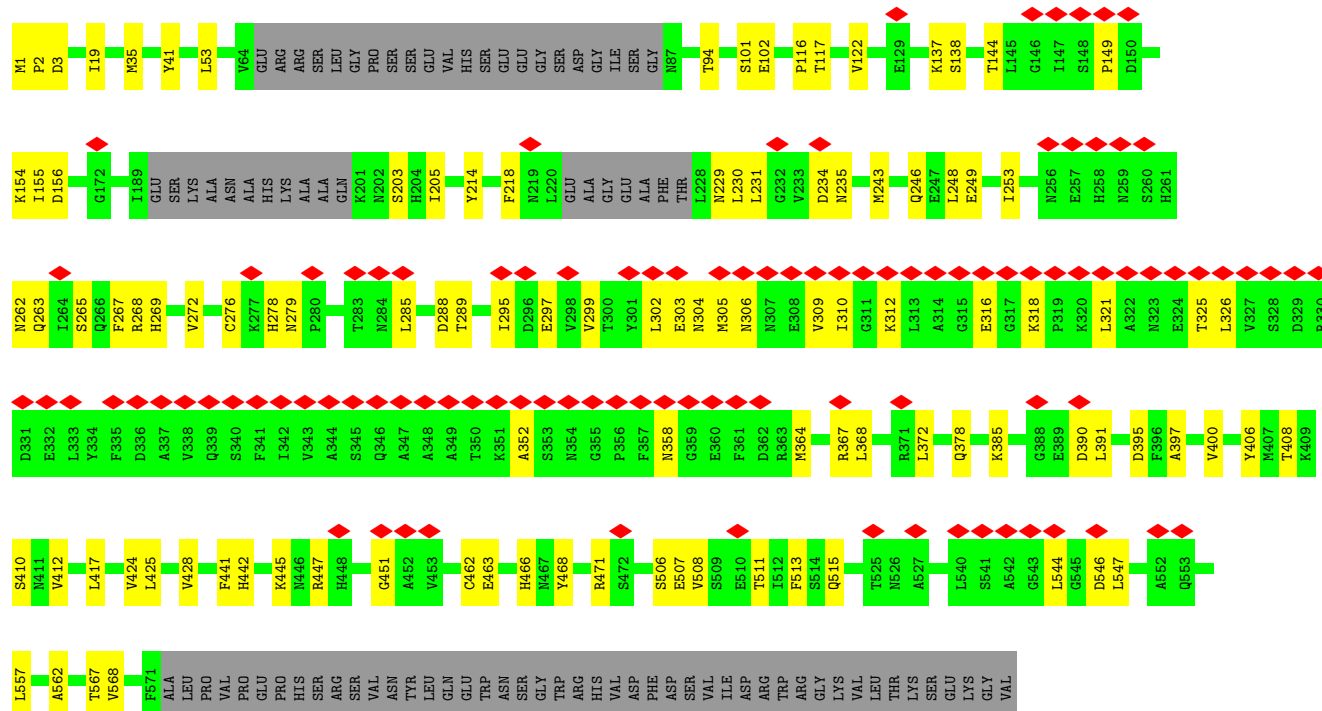
• Molecule 2: HerA

Chain M: 11% 68% 20% 12%

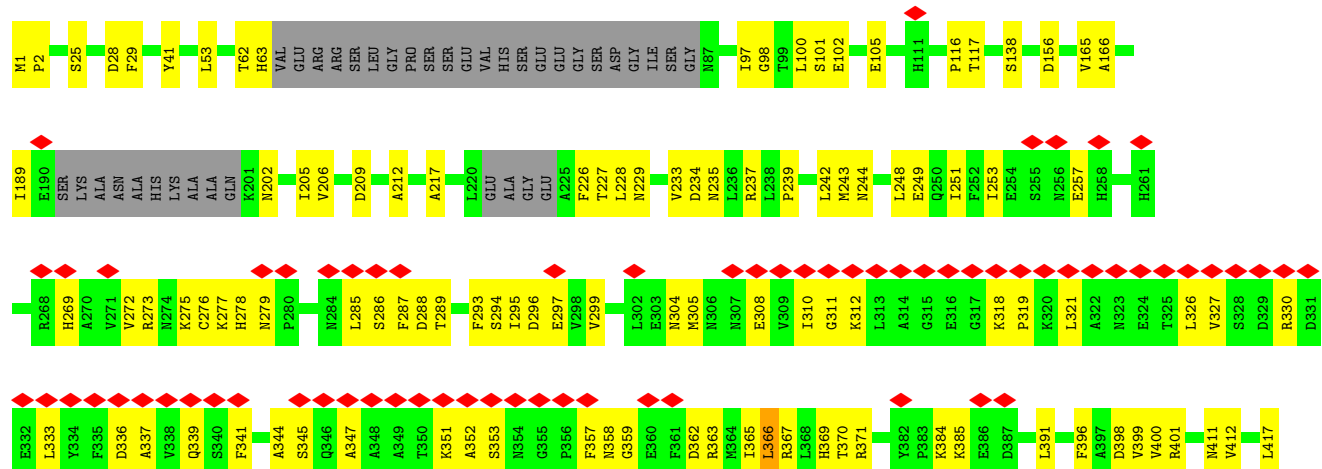


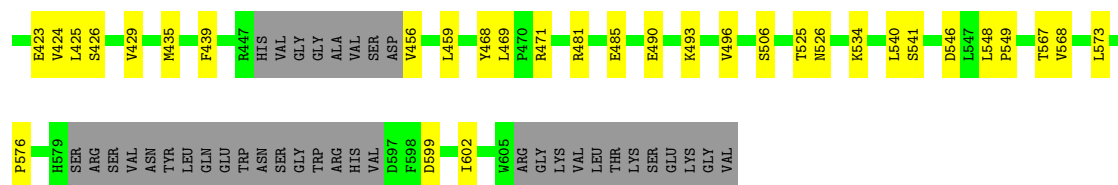


• Molecule 2: HerA

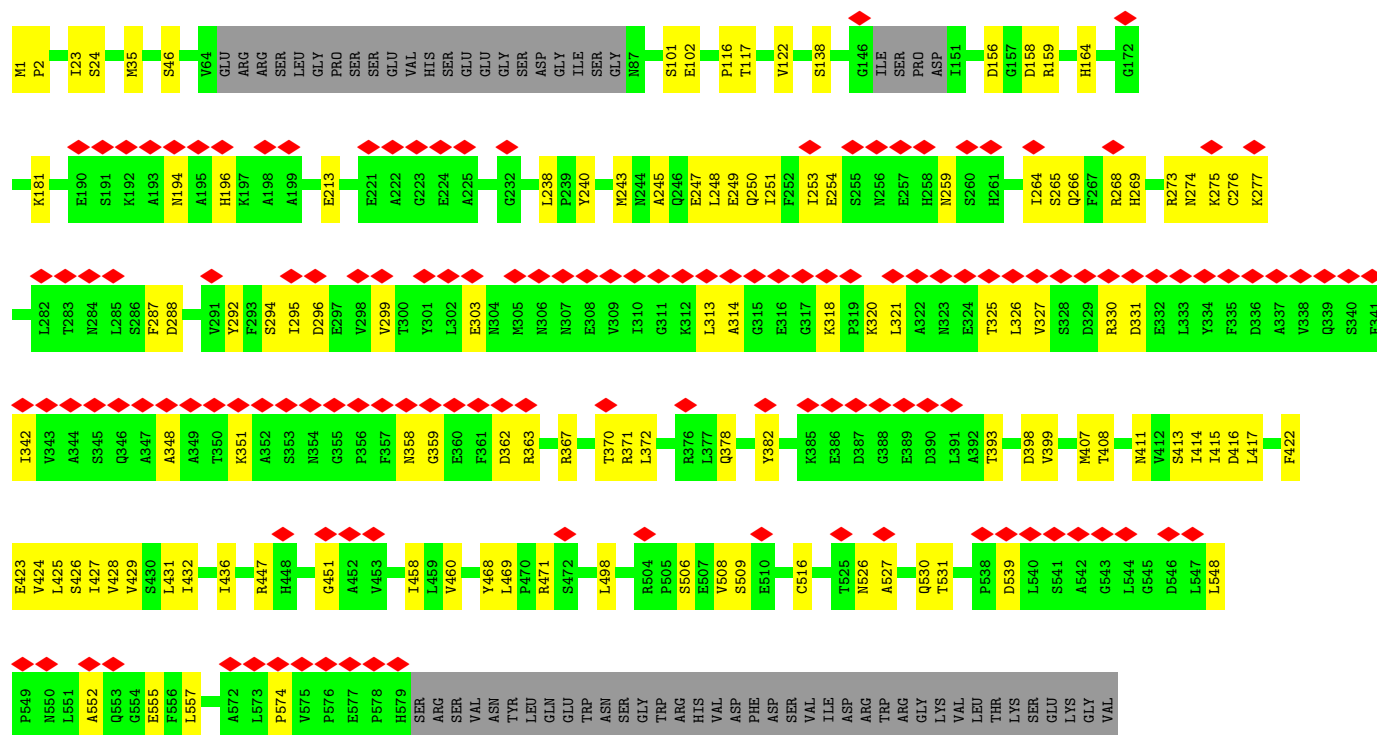


• Molecule 2: HerA



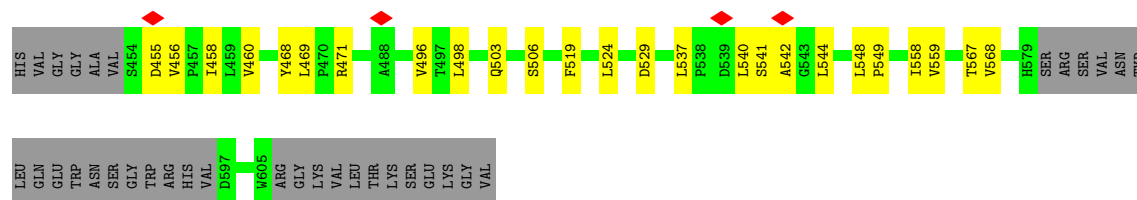


• Molecule 2: HerA

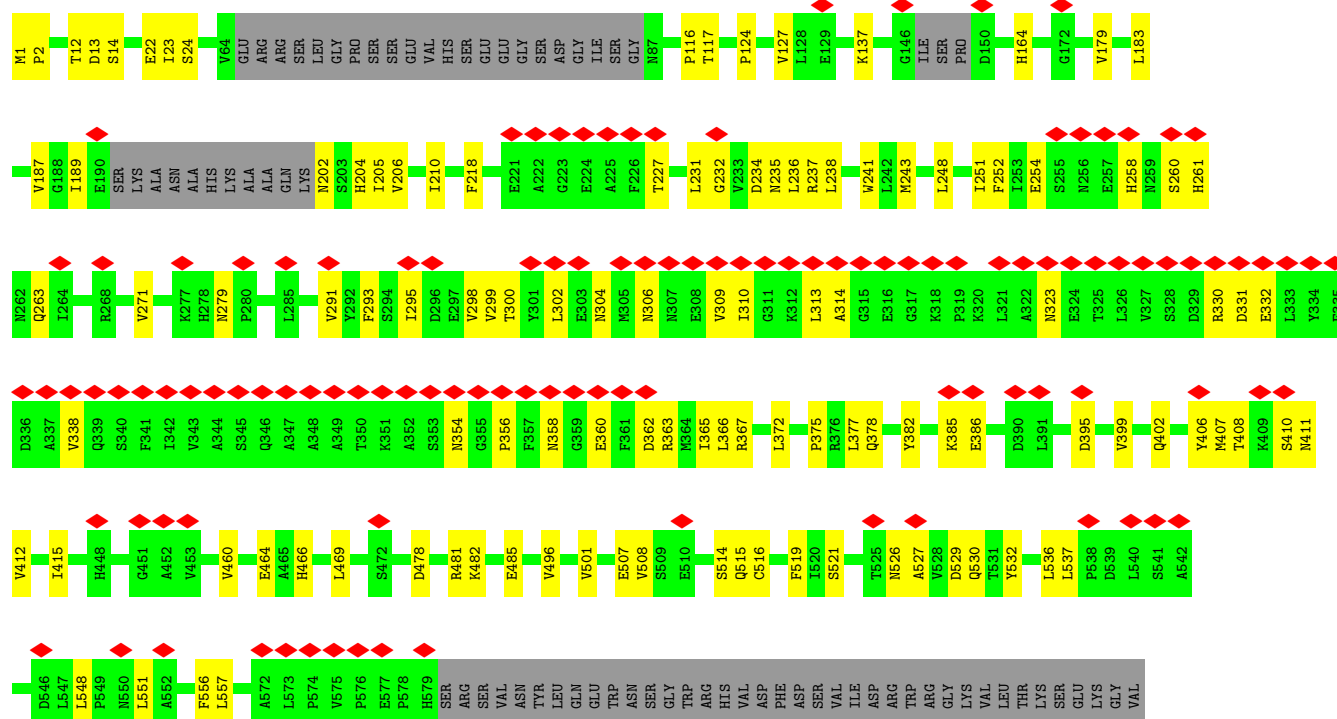


• Molecule 2: HerA





### • Molecule 2: HerA



## 4 Experimental information

| Property                             | Value                      | Source    |
|--------------------------------------|----------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE            | Depositor |
| Imposed symmetry                     | POINT, Not provided        |           |
| Number of particles used             | 158570                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF          | Depositor |
| CTF correction method                | NONE                       | Depositor |
| Microscope                           | FEI TITAN KRIOS            | Depositor |
| Voltage (kV)                         | 300                        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 65.58                      | Depositor |
| Minimum defocus (nm)                 | 328                        | Depositor |
| Maximum defocus (nm)                 | 5899                       | Depositor |
| Magnification                        | Not provided               |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value                    | 1.780                      | Depositor |
| Minimum map value                    | -0.022                     | Depositor |
| Average map value                    | 0.001                      | Depositor |
| Map value standard deviation         | 0.019                      | Depositor |
| Recommended contour level            | 0.05                       | Depositor |
| Map size ( $\text{\AA}$ )            | 484.0, 484.0, 484.0        | wwPDB     |
| Map dimensions                       | 440, 440, 440              | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0           | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.1, 1.1, 1.1              | 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

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     | 0.43         | 0/3196  | 0.44        | 0/4316  |
| 1   | B     | 0.58         | 0/1419  | 0.44        | 0/1912  |
| 1   | C     | 0.44         | 0/3172  | 0.47        | 0/4280  |
| 1   | D     | 0.57         | 0/1440  | 0.45        | 0/1941  |
| 1   | E     | 0.44         | 0/3179  | 0.43        | 0/4292  |
| 1   | F     | 0.58         | 0/1419  | 0.47        | 0/1912  |
| 1   | G     | 0.45         | 0/3136  | 0.49        | 0/4232  |
| 1   | H     | 0.58         | 0/1427  | 0.46        | 0/1923  |
| 1   | I     | 0.43         | 0/3169  | 0.45        | 0/4279  |
| 1   | J     | 0.57         | 0/1440  | 0.45        | 0/1941  |
| 1   | K     | 0.44         | 0/3163  | 0.45        | 0/4272  |
| 1   | L     | 0.58         | 0/1427  | 0.46        | 0/1923  |
| 2   | M     | 0.42         | 0/4331  | 0.41        | 0/5875  |
| 2   | N     | 0.38         | 0/4192  | 0.44        | 0/5684  |
| 2   | O     | 0.42         | 0/4312  | 0.43        | 0/5848  |
| 2   | P     | 0.36         | 0/4359  | 0.44        | 0/5913  |
| 2   | Q     | 0.41         | 0/4324  | 0.42        | 0/5868  |
| 2   | R     | 0.37         | 0/4285  | 0.44        | 0/5814  |
| All | All   | 0.44         | 0/53390 | 0.44        | 0/72225 |

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   | E     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 113 | THR  | Peptide |
| 1   | I     | 47  | GLY  | 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     | 3134  | 2851     | 3150     | 70      | 0            |
| 1   | B     | 1389  | 1400     | 1404     | 8       | 0            |
| 1   | C     | 3112  | 2890     | 3128     | 79      | 0            |
| 1   | D     | 1409  | 1418     | 1417     | 11      | 0            |
| 1   | E     | 3118  | 2859     | 3138     | 84      | 0            |
| 1   | F     | 1389  | 1405     | 1404     | 11      | 0            |
| 1   | G     | 3075  | 2856     | 3089     | 68      | 0            |
| 1   | H     | 1397  | 1409     | 1408     | 8       | 0            |
| 1   | I     | 3108  | 2851     | 3130     | 85      | 0            |
| 1   | J     | 1409  | 1418     | 1417     | 15      | 0            |
| 1   | K     | 3102  | 2846     | 3125     | 84      | 0            |
| 1   | L     | 1397  | 1409     | 1408     | 19      | 0            |
| 2   | M     | 4241  | 4189     | 4201     | 95      | 0            |
| 2   | N     | 4107  | 4065     | 4082     | 76      | 0            |
| 2   | O     | 4222  | 4168     | 4181     | 99      | 0            |
| 2   | P     | 4268  | 4211     | 4234     | 81      | 0            |
| 2   | Q     | 4233  | 4168     | 4181     | 95      | 0            |
| 2   | R     | 4196  | 4137     | 4152     | 86      | 0            |
| 3   | M     | 31    | 12       | 12       | 2       | 0            |
| 3   | O     | 31    | 12       | 12       | 1       | 0            |
| 3   | Q     | 31    | 12       | 12       | 0       | 0            |
| 4   | M     | 1     | 0        | 0        | 0       | 0            |
| 4   | O     | 1     | 0        | 0        | 0       | 0            |
| 4   | Q     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52402 | 50586    | 52285    | 1063    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1063) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:107:THR:OG1  | 1:G:109:ASP:OD2  | 1.80                     | 0.97              |
| 1:K:38:ILE:HB    | 1:K:51:ALA:HB1   | 1.44                     | 0.96              |
| 1:A:14:TYR:OH    | 1:A:148:PRO:O    | 1.84                     | 0.95              |
| 1:B:322:LEU:O    | 1:B:340:ARG:NH1  | 2.00                     | 0.95              |
| 1:I:117:THR:O    | 1:I:123:ARG:NH1  | 2.00                     | 0.94              |
| 2:O:138:SER:OG   | 2:O:156:ASP:OD1  | 1.88                     | 0.91              |
| 2:P:251:ILE:O    | 2:P:371:ARG:NH2  | 2.05                     | 0.90              |
| 2:O:294:SER:OG   | 2:O:296:ASP:OD1  | 1.91                     | 0.87              |
| 1:C:212:VAL:HG11 | 1:C:231:LEU:HD11 | 1.56                     | 0.86              |
| 1:I:120:GLU:OE2  | 1:I:123:ARG:NH2  | 2.08                     | 0.86              |
| 1:C:113:THR:O    | 1:C:116:SER:OG   | 1.95                     | 0.85              |
| 1:E:324:ARG:O    | 1:E:340:ARG:NH2  | 2.09                     | 0.85              |
| 2:R:407:MET:SD   | 2:R:408:THR:OG1  | 2.35                     | 0.85              |
| 1:D:387:GLU:N    | 1:D:387:GLU:OE1  | 2.09                     | 0.84              |
| 2:M:304:ASN:ND2  | 2:M:339:GLN:OE1  | 2.10                     | 0.84              |
| 2:O:534:LYS:NZ   | 2:O:540:LEU:O    | 2.09                     | 0.84              |
| 1:I:212:VAL:HG11 | 1:I:231:LEU:HD11 | 1.60                     | 0.83              |
| 2:M:597:ASP:O    | 2:M:600:SER:OG   | 1.95                     | 0.83              |
| 2:N:138:SER:OG   | 2:N:156:ASP:OD2  | 1.94                     | 0.83              |
| 2:O:28:ASP:OD1   | 2:O:29:PHE:N     | 2.12                     | 0.83              |
| 2:N:214:TYR:OH   | 2:N:463:GLU:OE2  | 1.97                     | 0.81              |
| 1:I:393:ARG:NH1  | 1:I:395:ASP:O    | 2.12                     | 0.81              |
| 1:J:272:ARG:NH1  | 1:J:391:GLN:O    | 2.15                     | 0.80              |
| 1:K:387:GLU:OE1  | 1:K:393:ARG:NH2  | 2.15                     | 0.80              |
| 2:Q:309:VAL:O    | 2:Q:320:LYS:N    | 2.13                     | 0.80              |
| 1:I:185:ASP:OD1  | 1:I:186:LEU:N    | 2.15                     | 0.79              |
| 2:R:514:SER:OG   | 2:R:515:GLN:OE1  | 1.99                     | 0.79              |
| 2:Q:138:SER:OG   | 2:Q:156:ASP:OD2  | 2.00                     | 0.78              |
| 2:M:225:ALA:O    | 2:M:409:LYS:NZ   | 2.17                     | 0.78              |
| 2:Q:275:LYS:O    | 2:Q:285:LEU:HD12 | 1.84                     | 0.78              |
| 2:R:372:LEU:O    | 2:R:378:GLN:NE2  | 2.16                     | 0.77              |
| 2:R:116:PRO:O    | 2:R:117:THR:OG1  | 2.02                     | 0.77              |
| 1:E:120:GLU:OE1  | 1:E:123:ARG:NE   | 2.17                     | 0.76              |
| 2:O:278:HIS:NE2  | 2:O:297:GLU:OE1  | 2.18                     | 0.76              |
| 1:G:131:THR:O    | 1:G:133:VAL:HG13 | 1.87                     | 0.75              |
| 1:A:212:VAL:HG11 | 1:A:231:LEU:HD11 | 1.67                     | 0.75              |
| 2:M:490:GLU:OE1  | 2:M:493:LYS:NZ   | 2.19                     | 0.75              |
| 2:M:262:ASN:O    | 2:M:265:SER:OG   | 2.03                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:344:ALA:HB2  | 2:O:352:ALA:HB3  | 1.69                     | 0.75              |
| 1:G:324:ARG:O    | 1:G:340:ARG:NH2  | 2.20                     | 0.75              |
| 1:K:324:ARG:O    | 1:K:340:ARG:NH2  | 2.20                     | 0.75              |
| 2:M:254:GLU:OE2  | 2:M:367:ARG:NH1  | 2.19                     | 0.74              |
| 2:R:306:ASN:ND2  | 2:R:358:ASN:OD1  | 2.19                     | 0.74              |
| 2:O:363:ARG:O    | 2:O:366:LEU:HD23 | 1.87                     | 0.74              |
| 2:M:275:LYS:NZ   | 2:M:291:VAL:O    | 2.20                     | 0.74              |
| 2:O:275:LYS:NZ   | 2:O:289:THR:O    | 2.21                     | 0.73              |
| 2:O:1:MET:HB3    | 2:O:2:PRO:HD3    | 1.70                     | 0.73              |
| 2:P:411:ASN:OD1  | 2:P:413:SER:OG   | 2.07                     | 0.73              |
| 2:Q:1:MET:HB3    | 2:Q:2:PRO:HD3    | 1.70                     | 0.73              |
| 2:Q:344:ALA:HA   | 2:Q:352:ALA:HB3  | 1.70                     | 0.72              |
| 1:I:219:ARG:O    | 1:I:224:LYS:HG2  | 1.88                     | 0.72              |
| 1:I:186:LEU:O    | 1:I:195:ARG:NH1  | 2.23                     | 0.72              |
| 1:K:215:THR:HA   | 1:K:381:GLU:OE2  | 1.90                     | 0.71              |
| 2:O:116:PRO:O    | 2:O:117:THR:OG1  | 2.09                     | 0.71              |
| 2:P:358:ASN:OD1  | 2:P:359:GLY:N    | 2.23                     | 0.71              |
| 1:B:384:SER:O    | 1:B:393:ARG:NH2  | 2.24                     | 0.70              |
| 1:C:14:TYR:OH    | 1:C:148:PRO:O    | 2.08                     | 0.70              |
| 2:Q:219:ASN:OD1  | 2:Q:220:LEU:N    | 2.23                     | 0.70              |
| 2:M:1:MET:HB3    | 2:M:2:PRO:HD3    | 1.73                     | 0.70              |
| 2:N:385:LYS:NZ   | 2:N:395:ASP:OD1  | 2.17                     | 0.70              |
| 1:C:385:ASP:OD2  | 1:C:386:LEU:N    | 2.24                     | 0.70              |
| 1:A:214:PHE:HB2  | 1:A:380:ILE:HD13 | 1.73                     | 0.70              |
| 1:G:18:LYS:O     | 1:G:21:SER:OG    | 2.08                     | 0.70              |
| 1:C:220:GLU:O    | 1:C:221:LEU:HD12 | 1.92                     | 0.70              |
| 1:E:355:PRO:O    | 1:E:373:VAL:HG22 | 1.92                     | 0.70              |
| 1:G:80:SER:O     | 1:G:83:SER:OG    | 2.10                     | 0.69              |
| 2:P:138:SER:OG   | 2:P:156:ASP:OD1  | 2.10                     | 0.69              |
| 1:E:35:GLU:HB3   | 1:E:50:THR:O     | 1.91                     | 0.69              |
| 2:O:367:ARG:O    | 2:O:370:THR:OG1  | 2.09                     | 0.69              |
| 2:O:275:LYS:O    | 2:O:279:ASN:N    | 2.25                     | 0.69              |
| 1:C:300:LEU:HD22 | 1:C:305:LEU:HD12 | 1.75                     | 0.69              |
| 2:O:243:MET:HE1  | 2:O:251:ILE:HD12 | 1.75                     | 0.69              |
| 2:N:321:LEU:HD13 | 2:N:325:THR:O    | 1.93                     | 0.68              |
| 1:E:115:LEU:HD21 | 1:E:135:TYR:CE1  | 2.29                     | 0.68              |
| 1:E:153:LEU:O    | 1:E:157:VAL:HG23 | 1.93                     | 0.68              |
| 1:E:219:ARG:O    | 1:E:224:LYS:HG2  | 1.94                     | 0.68              |
| 1:I:42:ASP:OD2   | 1:I:44:ILE:N     | 2.27                     | 0.68              |
| 1:A:153:LEU:O    | 1:A:157:VAL:HG23 | 1.94                     | 0.68              |
| 1:G:174:VAL:HG12 | 1:G:212:VAL:HG22 | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:471:ARG:NH2  | 2:O:506:SER:O    | 2.28                     | 0.67              |
| 2:O:25:SER:OG    | 2:O:28:ASP:OD2   | 2.11                     | 0.67              |
| 2:R:202:ASN:OD1  | 2:R:410:SER:OG   | 2.12                     | 0.67              |
| 1:K:215:THR:HG22 | 1:K:218:THR:HG23 | 1.77                     | 0.67              |
| 2:O:365:ILE:O    | 2:O:369:HIS:ND1  | 2.27                     | 0.67              |
| 2:P:548:LEU:HD21 | 2:P:557:LEU:HD21 | 1.76                     | 0.67              |
| 2:Q:279:ASN:HB2  | 2:Q:285:LEU:HD11 | 1.75                     | 0.67              |
| 2:N:397:ALA:O    | 2:N:400:VAL:HG12 | 1.95                     | 0.67              |
| 1:C:215:THR:HG22 | 1:C:218:THR:HG23 | 1.76                     | 0.67              |
| 1:A:369:LYS:HZ3  | 1:A:375:VAL:HG11 | 1.61                     | 0.66              |
| 1:K:205:GLY:O    | 1:K:209:VAL:HG13 | 1.96                     | 0.66              |
| 2:P:1:MET:HB3    | 2:P:2:PRO:HD3    | 1.77                     | 0.66              |
| 1:I:163:ASP:OD2  | 1:I:164:LYS:N    | 2.29                     | 0.66              |
| 1:C:39:GLU:OE2   | 1:C:39:GLU:N     | 2.28                     | 0.66              |
| 2:O:233:VAL:HG13 | 2:O:234:ASP:H    | 1.61                     | 0.66              |
| 1:G:136:GLU:N    | 1:G:136:GLU:OE1  | 2.29                     | 0.66              |
| 2:O:358:ASN:OD1  | 2:O:359:GLY:N    | 2.29                     | 0.65              |
| 1:E:385:ASP:OD2  | 1:E:386:LEU:N    | 2.29                     | 0.65              |
| 1:L:344:ARG:NH2  | 1:L:366:ASP:OD1  | 2.28                     | 0.65              |
| 2:Q:171:THR:OG1  | 2:Q:503:GLN:NE2  | 2.28                     | 0.65              |
| 2:O:233:VAL:HG13 | 2:O:234:ASP:N    | 2.10                     | 0.65              |
| 2:O:228:LEU:O    | 2:O:228:LEU:HD23 | 1.97                     | 0.65              |
| 1:I:221:LEU:HD12 | 1:I:222:ALA:H    | 1.60                     | 0.65              |
| 2:M:239:PRO:HD2  | 2:M:242:LEU:HD12 | 1.79                     | 0.64              |
| 2:Q:116:PRO:O    | 2:Q:117:THR:OG1  | 2.10                     | 0.64              |
| 2:Q:292:TYR:OH   | 2:Q:390:ASP:OD2  | 2.09                     | 0.64              |
| 1:D:261:ASP:HB3  | 1:D:383:LEU:HD12 | 1.79                     | 0.64              |
| 1:E:111:LEU:HB2  | 1:E:139:LEU:HD21 | 1.80                     | 0.64              |
| 1:C:218:THR:O    | 1:C:221:LEU:HD13 | 1.97                     | 0.64              |
| 2:N:471:ARG:NH1  | 2:N:507:GLU:O    | 2.30                     | 0.64              |
| 1:C:384:SER:OG   | 1:C:393:ARG:NH1  | 2.31                     | 0.64              |
| 2:N:203:SER:N    | 2:N:410:SER:OG   | 2.31                     | 0.64              |
| 2:N:278:HIS:NE2  | 2:N:297:GLU:OE1  | 2.31                     | 0.64              |
| 1:C:109:ASP:O    | 1:C:113:THR:HG23 | 1.97                     | 0.64              |
| 1:G:109:ASP:OD2  | 1:G:110:ASP:N    | 2.30                     | 0.64              |
| 2:N:309:VAL:CG2  | 2:N:352:ALA:HB1  | 2.28                     | 0.64              |
| 1:E:176:PHE:HE2  | 1:E:221:LEU:HD11 | 1.63                     | 0.64              |
| 1:E:352:GLN:OE1  | 1:E:352:GLN:N    | 2.31                     | 0.63              |
| 1:G:215:THR:O    | 1:G:219:ARG:HG3  | 1.98                     | 0.63              |
| 2:M:233:VAL:HG13 | 2:M:234:ASP:N    | 2.13                     | 0.63              |
| 2:N:1:MET:HB2    | 2:N:2:PRO:HD3    | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:SER:OG    | 1:A:128:ARG:NH1  | 2.31                     | 0.63              |
| 1:K:72:ILE:O     | 1:K:76:LEU:N     | 2.27                     | 0.63              |
| 2:P:247:GLU:OE1  | 2:P:427:ILE:HG23 | 1.96                     | 0.63              |
| 2:P:259:ASN:ND2  | 2:Q:284:ASN:OD1  | 2.32                     | 0.63              |
| 2:R:507:GLU:N    | 2:R:507:GLU:OE1  | 2.32                     | 0.63              |
| 2:R:1:MET:HB3    | 2:R:2:PRO:HD3    | 1.81                     | 0.63              |
| 1:C:38:ILE:HG13  | 1:C:52:VAL:O     | 1.99                     | 0.63              |
| 2:P:275:LYS:NZ   | 2:P:287:PHE:O    | 2.32                     | 0.62              |
| 2:N:144:THR:OG1  | 2:N:149:PRO:O    | 2.16                     | 0.62              |
| 2:M:597:ASP:O    | 2:M:600:SER:N    | 2.33                     | 0.62              |
| 1:C:31:ARG:NH2   | 1:C:198:GLU:OE1  | 2.32                     | 0.62              |
| 2:R:243:MET:HE1  | 2:R:251:ILE:HD12 | 1.82                     | 0.62              |
| 2:M:577:GLU:N    | 2:M:577:GLU:OE1  | 2.31                     | 0.62              |
| 1:I:35:GLU:HB2   | 1:I:50:THR:OG1   | 2.00                     | 0.61              |
| 2:P:378:GLN:O    | 2:P:382:TYR:N    | 2.25                     | 0.61              |
| 1:C:38:ILE:HG12  | 1:C:51:ALA:HB1   | 1.82                     | 0.61              |
| 1:F:256:GLU:OE2  | 1:F:382:ARG:NE   | 2.32                     | 0.61              |
| 1:A:369:LYS:NZ   | 1:A:375:VAL:HG11 | 2.16                     | 0.61              |
| 1:G:31:ARG:NH2   | 1:G:196:THR:OG1  | 2.32                     | 0.61              |
| 1:G:163:ASP:OD1  | 1:G:164:LYS:N    | 2.34                     | 0.61              |
| 2:P:251:ILE:HD11 | 2:P:427:ILE:HD13 | 1.82                     | 0.61              |
| 1:A:219:ARG:HB3  | 1:A:224:LYS:HE2  | 1.81                     | 0.61              |
| 2:M:303:GLU:O    | 2:M:307:ASN:ND2  | 2.33                     | 0.61              |
| 1:D:282:PRO:O    | 1:D:340:ARG:NH1  | 2.34                     | 0.61              |
| 2:Q:443:TYR:OH   | 2:Q:455:ASP:OD1  | 2.12                     | 0.61              |
| 1:E:384:SER:OG   | 1:E:393:ARG:NH1  | 2.33                     | 0.61              |
| 2:N:302:LEU:HD13 | 2:N:364:MET:HE2  | 1.83                     | 0.61              |
| 2:R:362:ASP:HA   | 2:R:365:ILE:HD12 | 1.83                     | 0.61              |
| 2:Q:455:ASP:OD2  | 2:Q:456:VAL:N    | 2.34                     | 0.60              |
| 2:R:1:MET:HB3    | 2:R:2:PRO:CD     | 2.31                     | 0.60              |
| 2:O:344:ALA:CB   | 2:O:352:ALA:HB3  | 2.31                     | 0.60              |
| 2:P:348:ALA:O    | 2:P:351:LYS:HE3  | 2.01                     | 0.60              |
| 1:C:322:LEU:O    | 1:C:340:ARG:NE   | 2.34                     | 0.60              |
| 1:I:116:SER:OG   | 1:I:118:LYS:NZ   | 2.35                     | 0.60              |
| 2:Q:299:VAL:HA   | 2:Q:302:LEU:HD12 | 1.83                     | 0.60              |
| 1:I:31:ARG:O     | 1:I:32:ILE:HD13  | 2.01                     | 0.60              |
| 2:Q:537:LEU:HD23 | 2:Q:559:VAL:CG2  | 2.30                     | 0.60              |
| 1:K:232:ARG:NH1  | 1:K:388:TYR:O    | 2.34                     | 0.60              |
| 1:G:33:THR:HG23  | 1:G:195:ARG:O    | 2.01                     | 0.59              |
| 1:K:211:ARG:HH22 | 1:K:379:LYS:HD2  | 1.67                     | 0.59              |
| 1:I:41:VAL:O     | 1:I:41:VAL:HG13  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:44:ILE:HG13  | 1:K:45:ALA:N     | 2.17                     | 0.59              |
| 2:N:205:ILE:HB   | 2:N:412:VAL:HG13 | 1.85                     | 0.59              |
| 1:C:107:THR:OG1  | 1:C:109:ASP:OD1  | 2.07                     | 0.59              |
| 1:C:38:ILE:HD12  | 1:C:53:GLN:HB2   | 1.84                     | 0.59              |
| 2:N:390:ASP:OD1  | 2:N:391:LEU:N    | 2.36                     | 0.59              |
| 1:C:216:ARG:O    | 1:C:216:ARG:HD3  | 2.02                     | 0.59              |
| 2:O:234:ASP:O    | 2:O:237:ARG:NH1  | 2.36                     | 0.58              |
| 2:N:424:VAL:HG22 | 2:N:424:VAL:O    | 2.04                     | 0.58              |
| 1:C:12:TYR:O     | 1:C:15:GLN:HG3   | 2.03                     | 0.58              |
| 1:C:35:GLU:HB2   | 1:C:50:THR:O     | 2.03                     | 0.58              |
| 1:K:41:VAL:HG23  | 1:K:41:VAL:O     | 2.03                     | 0.58              |
| 1:K:199:PRO:O    | 1:K:203:LEU:HD13 | 2.04                     | 0.58              |
| 2:P:35:MET:SD    | 2:P:122:VAL:HG11 | 2.43                     | 0.58              |
| 1:E:43:VAL:HG22  | 1:E:43:VAL:O     | 2.02                     | 0.58              |
| 1:E:366:ASP:OD1  | 1:E:367:GLU:N    | 2.37                     | 0.58              |
| 1:K:60:ALA:HB3   | 1:K:97:PHE:CE1   | 2.39                     | 0.58              |
| 2:M:101:SER:OG   | 2:M:102:GLU:N    | 2.33                     | 0.58              |
| 2:M:116:PRO:O    | 2:M:117:THR:OG1  | 2.21                     | 0.58              |
| 2:M:350:THR:HG22 | 2:M:350:THR:O    | 2.02                     | 0.58              |
| 1:E:206:LEU:HA   | 1:E:209:VAL:HG12 | 1.85                     | 0.58              |
| 1:I:164:LYS:HE3  | 1:I:203:LEU:HD12 | 1.86                     | 0.58              |
| 1:C:157:VAL:O    | 1:C:160:SER:OG   | 2.19                     | 0.57              |
| 2:R:395:ASP:O    | 2:R:399:VAL:HG23 | 2.03                     | 0.57              |
| 1:K:44:ILE:HG13  | 1:K:45:ALA:H     | 1.69                     | 0.57              |
| 2:P:527:ALA:O    | 2:P:530:GLN:HG2  | 2.04                     | 0.57              |
| 1:C:324:ARG:O    | 1:C:340:ARG:NH2  | 2.38                     | 0.57              |
| 2:Q:150:ASP:OD2  | 2:Q:151:ILE:N    | 2.37                     | 0.57              |
| 1:C:220:GLU:C    | 1:C:221:LEU:HD12 | 2.29                     | 0.57              |
| 2:N:243:MET:HB2  | 2:N:248:LEU:HB2  | 1.87                     | 0.57              |
| 2:Q:411:ASN:OD1  | 2:Q:412:VAL:N    | 2.37                     | 0.57              |
| 2:M:138:SER:OG   | 2:M:156:ASP:OD1  | 2.22                     | 0.57              |
| 2:Q:209:ASP:OD1  | 2:Q:212:ALA:N    | 2.38                     | 0.57              |
| 1:I:218:THR:O    | 1:I:221:LEU:HB3  | 2.05                     | 0.57              |
| 1:I:108:LYS:HZ2  | 1:I:111:LEU:CD2  | 2.18                     | 0.57              |
| 2:R:243:MET:SD   | 2:R:251:ILE:HD12 | 2.45                     | 0.57              |
| 1:A:6:GLU:HA     | 1:A:6:GLU:OE1    | 2.05                     | 0.57              |
| 1:I:117:THR:HG21 | 1:I:126:VAL:HG21 | 1.87                     | 0.56              |
| 1:C:107:THR:OG1  | 1:C:110:ASP:OD2  | 2.23                     | 0.56              |
| 1:A:324:ARG:O    | 1:A:340:ARG:NH2  | 2.37                     | 0.56              |
| 1:K:327:ILE:HG21 | 1:L:327:ILE:HG21 | 1.86                     | 0.56              |
| 2:N:155:ILE:HG22 | 2:N:156:ASP:H    | 1.69                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:462:CYS:SG   | 2:N:468:TYR:OH   | 2.63                     | 0.56              |
| 2:P:238:LEU:HD12 | 2:P:238:LEU:O    | 2.05                     | 0.56              |
| 2:R:363:ARG:HA   | 2:R:366:LEU:HG   | 1.86                     | 0.56              |
| 1:C:24:LEU:HD13  | 1:C:160:SER:HB2  | 1.86                     | 0.56              |
| 2:M:204:HIS:NE2  | 2:M:456:VAL:HG11 | 2.20                     | 0.56              |
| 2:M:297:GLU:O    | 2:M:300:THR:HG22 | 2.05                     | 0.56              |
| 1:I:38:ILE:HG13  | 1:I:51:ALA:HB1   | 1.88                     | 0.56              |
| 2:Q:274:ASN:HD22 | 2:Q:298:VAL:HG23 | 1.71                     | 0.56              |
| 1:E:212:VAL:HG11 | 1:E:231:LEU:HD11 | 1.86                     | 0.56              |
| 1:I:391:GLN:C    | 1:I:392:LEU:HD12 | 2.30                     | 0.56              |
| 1:K:24:LEU:HD13  | 1:K:160:SER:HB2  | 1.86                     | 0.56              |
| 2:P:436:ILE:HD11 | 2:P:458:ILE:HG21 | 1.87                     | 0.56              |
| 2:Q:57:THR:O     | 2:Q:57:THR:HG22  | 2.06                     | 0.56              |
| 1:G:175:ILE:HG23 | 1:G:206:LEU:HD21 | 1.88                     | 0.55              |
| 1:K:214:PHE:HD2  | 1:K:385:ASP:OD2  | 1.89                     | 0.55              |
| 2:N:364:MET:O    | 2:N:368:LEU:HD13 | 2.04                     | 0.55              |
| 2:Q:268:ARG:O    | 2:Q:272:VAL:HG23 | 2.05                     | 0.55              |
| 1:A:272:ARG:NH1  | 1:A:391:GLN:O    | 2.39                     | 0.55              |
| 1:A:219:ARG:CB   | 1:A:224:LYS:HE2  | 2.37                     | 0.55              |
| 1:C:154:GLN:O    | 1:C:158:LEU:HD23 | 2.06                     | 0.55              |
| 1:C:355:PRO:O    | 1:C:373:VAL:HG22 | 2.07                     | 0.55              |
| 1:I:307:CYS:SG   | 1:I:308:GLU:N    | 2.79                     | 0.55              |
| 1:C:215:THR:CG2  | 1:C:218:THR:HG23 | 2.36                     | 0.55              |
| 2:R:206:VAL:CG2  | 2:R:460:VAL:HG22 | 2.36                     | 0.55              |
| 1:E:297:GLN:NE2  | 1:E:307:CYS:SG   | 2.80                     | 0.55              |
| 2:M:142:LEU:HD22 | 2:M:155:ILE:HD13 | 1.88                     | 0.55              |
| 2:N:316:GLU:OE2  | 2:N:326:LEU:HD11 | 2.07                     | 0.55              |
| 2:N:466:HIS:HA   | 2:N:508:VAL:HG22 | 1.88                     | 0.55              |
| 1:B:312:VAL:HG12 | 1:B:312:VAL:O    | 2.07                     | 0.55              |
| 1:A:315:THR:HG23 | 1:A:316:ASP:OD1  | 2.07                     | 0.55              |
| 1:C:212:VAL:HG21 | 1:C:231:LEU:HD21 | 1.88                     | 0.55              |
| 2:M:233:VAL:HG13 | 2:M:234:ASP:H    | 1.70                     | 0.55              |
| 2:O:362:ASP:OD1  | 2:O:363:ARG:N    | 2.39                     | 0.55              |
| 1:C:109:ASP:OD1  | 1:C:110:ASP:N    | 2.40                     | 0.55              |
| 1:H:282:PRO:O    | 1:H:340:ARG:NH1  | 2.40                     | 0.55              |
| 1:I:19:TYR:CE2   | 1:I:23:ILE:HD11  | 2.42                     | 0.55              |
| 2:O:272:VAL:HG22 | 2:O:286:SER:C    | 2.31                     | 0.55              |
| 1:E:115:LEU:HD21 | 1:E:135:TYR:HE1  | 1.71                     | 0.54              |
| 1:I:100:GLU:OE2  | 1:I:100:GLU:N    | 2.40                     | 0.54              |
| 1:I:132:SER:O    | 1:I:132:SER:OG   | 2.23                     | 0.54              |
| 2:O:417:LEU:HD13 | 2:O:425:LEU:HD11 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:320:LYS:HE3  | 2:P:342:ILE:HD11 | 1.89                     | 0.54              |
| 2:P:552:ALA:HB3  | 2:P:555:GLU:OE1  | 2.08                     | 0.54              |
| 1:C:65:LEU:HD23  | 1:C:65:LEU:O     | 2.07                     | 0.54              |
| 1:F:296:LEU:O    | 1:F:300:LEU:HD13 | 2.06                     | 0.54              |
| 2:O:286:SER:OG   | 2:O:288:ASP:OD2  | 2.24                     | 0.54              |
| 2:O:385:LYS:HZ3  | 2:O:391:LEU:HA   | 1.73                     | 0.54              |
| 1:A:232:ARG:NH1  | 1:A:388:TYR:O    | 2.41                     | 0.54              |
| 1:K:19:TYR:CD1   | 1:K:34:ILE:HD12  | 2.42                     | 0.54              |
| 1:A:219:ARG:O    | 1:A:224:LYS:HE3  | 2.07                     | 0.54              |
| 1:C:35:GLU:HG3   | 1:C:52:VAL:HB    | 1.89                     | 0.54              |
| 1:I:35:GLU:O     | 1:I:35:GLU:HG2   | 2.07                     | 0.54              |
| 1:K:38:ILE:HG22  | 1:K:52:VAL:O     | 2.08                     | 0.54              |
| 2:O:227:THR:HB   | 2:O:411:ASN:HB3  | 1.89                     | 0.54              |
| 1:J:261:ASP:OD1  | 1:J:264:ARG:NH2  | 2.40                     | 0.54              |
| 1:K:200:LYS:H    | 1:K:200:LYS:HD2  | 1.72                     | 0.54              |
| 1:A:327:ILE:HG21 | 1:B:327:ILE:HG21 | 1.90                     | 0.54              |
| 2:Q:158:ASP:OD1  | 2:Q:159:ARG:N    | 2.39                     | 0.54              |
| 1:E:211:ARG:HG3  | 1:E:211:ARG:HH11 | 1.72                     | 0.54              |
| 1:E:227:MET:HG3  | 1:E:228:PHE:HD1  | 1.73                     | 0.54              |
| 1:G:72:ILE:HA    | 1:G:75:MET:HE3   | 1.88                     | 0.54              |
| 1:I:9:ILE:HD11   | 1:I:217:TRP:NE1  | 2.22                     | 0.54              |
| 2:M:396:PHE:O    | 2:M:399:VAL:HG22 | 2.07                     | 0.54              |
| 1:G:38:ILE:HB    | 1:G:52:VAL:HG12  | 1.89                     | 0.54              |
| 2:O:363:ARG:HA   | 2:O:366:LEU:CD2  | 2.38                     | 0.54              |
| 2:Q:262:ASN:OD1  | 2:Q:263:GLN:N    | 2.41                     | 0.54              |
| 1:I:153:LEU:O    | 1:I:157:VAL:HG23 | 2.08                     | 0.53              |
| 1:K:76:LEU:HD23  | 1:K:129:ILE:HD11 | 1.91                     | 0.53              |
| 2:P:116:PRO:O    | 2:P:117:THR:OG1  | 2.20                     | 0.53              |
| 2:Q:519:PHE:CB   | 2:Q:537:LEU:HD21 | 2.37                     | 0.53              |
| 1:A:224:LYS:HD3  | 1:A:228:PHE:CE2  | 2.43                     | 0.53              |
| 1:L:228:PHE:HA   | 1:L:231:LEU:HD13 | 1.90                     | 0.53              |
| 2:M:304:ASN:O    | 2:M:307:ASN:N    | 2.42                     | 0.53              |
| 2:M:321:LEU:HD22 | 2:M:325:THR:HB   | 1.89                     | 0.53              |
| 2:Q:264:ILE:HG23 | 2:Q:265:SER:N    | 2.23                     | 0.53              |
| 1:C:215:THR:O    | 1:C:219:ARG:HG3  | 2.09                     | 0.53              |
| 1:K:355:PRO:O    | 1:K:373:VAL:HG22 | 2.08                     | 0.53              |
| 2:O:336:ASP:OD1  | 2:O:337:ALA:N    | 2.41                     | 0.53              |
| 2:Q:275:LYS:HE3  | 2:Q:291:VAL:HG23 | 1.90                     | 0.53              |
| 2:Q:233:VAL:HG13 | 2:Q:234:ASP:N    | 2.24                     | 0.53              |
| 1:A:219:ARG:HA   | 1:A:224:LYS:HG3  | 1.90                     | 0.53              |
| 2:Q:458:ILE:HD11 | 2:Q:496:VAL:HG12 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:205:GLY:O    | 1:G:209:VAL:HG23 | 2.09                     | 0.53              |
| 2:N:309:VAL:HG21 | 2:N:352:ALA:HB1  | 1.90                     | 0.53              |
| 2:P:238:LEU:HD13 | 2:P:431:LEU:HD23 | 1.90                     | 0.53              |
| 1:G:215:THR:CG2  | 1:G:218:THR:HG23 | 2.39                     | 0.53              |
| 1:I:185:ASP:O    | 1:I:189:ARG:N    | 2.41                     | 0.53              |
| 1:I:261:ASP:OD2  | 1:I:262:ILE:N    | 2.42                     | 0.53              |
| 2:N:303:GLU:OE2  | 2:N:303:GLU:N    | 2.41                     | 0.53              |
| 1:A:54:CYS:SG    | 1:A:55:LYS:N     | 2.81                     | 0.53              |
| 1:G:20:LEU:HD22  | 1:G:180:ILE:HD13 | 1.90                     | 0.53              |
| 2:O:347:ALA:O    | 2:O:351:LYS:N    | 2.42                     | 0.53              |
| 1:K:215:THR:O    | 1:K:219:ARG:HG3  | 2.10                     | 0.52              |
| 1:C:153:LEU:O    | 1:C:157:VAL:HG23 | 2.09                     | 0.52              |
| 1:K:172:ASP:CG   | 1:K:226:ARG:HH21 | 2.18                     | 0.52              |
| 2:M:237:ARG:NH1  | 2:M:384:LYS:O    | 2.41                     | 0.52              |
| 1:C:192:VAL:O    | 1:C:193:ASN:ND2  | 2.43                     | 0.52              |
| 1:D:284:LEU:HD12 | 1:D:340:ARG:HB2  | 1.90                     | 0.52              |
| 2:M:273:ARG:O    | 2:M:277:LYS:NZ   | 2.42                     | 0.52              |
| 1:C:35:GLU:HG3   | 1:C:52:VAL:CG1   | 2.40                     | 0.52              |
| 1:E:215:THR:HG23 | 1:E:218:THR:H    | 1.75                     | 0.52              |
| 1:G:202:PHE:CD2  | 1:G:203:LEU:HD23 | 2.45                     | 0.52              |
| 1:G:355:PRO:O    | 1:G:373:VAL:HG22 | 2.09                     | 0.52              |
| 2:O:310:ILE:O    | 2:O:352:ALA:HB1  | 2.09                     | 0.52              |
| 2:P:294:SER:OG   | 2:P:296:ASP:OD1  | 2.20                     | 0.52              |
| 2:P:447:ARG:O    | 2:P:451:GLY:N    | 2.43                     | 0.52              |
| 2:Q:519:PHE:HB2  | 2:Q:537:LEU:HD21 | 1.90                     | 0.52              |
| 2:R:469:LEU:HD23 | 2:R:481:ARG:HB2  | 1.90                     | 0.52              |
| 1:A:37:ALA:HB1   | 1:A:39:GLU:OE1   | 2.10                     | 0.52              |
| 1:C:192:VAL:O    | 1:C:192:VAL:HG23 | 2.09                     | 0.52              |
| 1:K:64:THR:HG22  | 1:K:67:LYS:NZ    | 2.24                     | 0.52              |
| 2:O:272:VAL:HG22 | 2:O:287:PHE:N    | 2.24                     | 0.52              |
| 2:O:327:VAL:HG21 | 2:O:333:LEU:HD22 | 1.90                     | 0.52              |
| 1:E:174:VAL:HG11 | 1:E:210:ARG:HH12 | 1.75                     | 0.52              |
| 2:M:175:LYS:NZ   | 3:M:1501:ATP:O2B | 2.40                     | 0.52              |
| 2:P:508:VAL:HG12 | 2:P:509:SER:N    | 2.25                     | 0.52              |
| 2:Q:236:LEU:HD12 | 2:Q:237:ARG:H    | 1.74                     | 0.52              |
| 1:A:66:GLY:HA2   | 1:A:69:TYR:CE1   | 2.45                     | 0.52              |
| 1:C:18:LYS:O     | 1:C:21:SER:OG    | 2.20                     | 0.52              |
| 1:E:165:GLY:O    | 1:E:207:ARG:NH1  | 2.42                     | 0.52              |
| 1:I:54:CYS:SG    | 1:I:55:LYS:N     | 2.83                     | 0.52              |
| 2:M:268:ARG:O    | 2:M:272:VAL:HG23 | 2.09                     | 0.52              |
| 1:E:327:ILE:HG21 | 1:F:327:ILE:HG21 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:385:LYS:HG2  | 2:R:386:GLU:N    | 2.25                     | 0.52              |
| 1:I:38:ILE:CG1   | 1:I:51:ALA:HB1   | 2.40                     | 0.52              |
| 1:K:14:TYR:O     | 1:K:18:LYS:NZ    | 2.33                     | 0.52              |
| 1:K:73:LEU:O     | 1:K:76:LEU:HB3   | 2.09                     | 0.52              |
| 2:N:41:TYR:CD1   | 2:N:53:LEU:HD21  | 2.45                     | 0.52              |
| 2:N:154:LYS:O    | 2:N:155:ILE:HD13 | 2.09                     | 0.51              |
| 2:N:544:LEU:HD21 | 2:N:557:LEU:HD11 | 1.91                     | 0.51              |
| 2:O:244:ASN:O    | 2:O:248:LEU:HD23 | 2.09                     | 0.51              |
| 1:K:71:PRO:HB2   | 1:K:75:MET:HE2   | 1.92                     | 0.51              |
| 2:N:372:LEU:O    | 2:N:378:GLN:NE2  | 2.42                     | 0.51              |
| 1:A:38:ILE:HD12  | 1:A:38:ILE:H     | 1.74                     | 0.51              |
| 1:I:214:PHE:HE1  | 1:I:228:PHE:CE1  | 2.28                     | 0.51              |
| 1:K:66:GLY:HA2   | 1:K:69:TYR:CE2   | 2.46                     | 0.51              |
| 1:L:293:LEU:HD11 | 1:L:343:LYS:HG3  | 1.93                     | 0.51              |
| 2:M:57:THR:HG23  | 2:M:57:THR:O     | 2.09                     | 0.51              |
| 2:O:53:LEU:HD22  | 2:O:97:ILE:HD11  | 1.91                     | 0.51              |
| 2:O:396:PHE:O    | 2:O:399:VAL:HG22 | 2.10                     | 0.51              |
| 2:R:254:GLU:N    | 2:R:254:GLU:OE1  | 2.43                     | 0.51              |
| 2:R:309:VAL:HG22 | 2:R:354:ASN:OD1  | 2.11                     | 0.51              |
| 1:A:41:VAL:HG23  | 1:A:41:VAL:O     | 2.09                     | 0.51              |
| 1:E:221:LEU:HD12 | 1:E:222:ALA:H    | 1.76                     | 0.51              |
| 2:M:275:LYS:O    | 2:M:285:LEU:HD12 | 2.10                     | 0.51              |
| 2:M:471:ARG:NH2  | 2:M:506:SER:O    | 2.40                     | 0.51              |
| 2:N:155:ILE:HG21 | 2:N:562:ALA:HB1  | 1.92                     | 0.51              |
| 2:N:218:PHE:HE1  | 2:N:412:VAL:HG21 | 1.76                     | 0.51              |
| 2:N:316:GLU:CD   | 2:N:326:LEU:HD11 | 2.34                     | 0.51              |
| 2:O:205:ILE:HG12 | 2:O:459:LEU:HD21 | 1.92                     | 0.51              |
| 2:O:400:VAL:HG22 | 2:O:435:MET:HE3  | 1.93                     | 0.51              |
| 2:O:534:LYS:NZ   | 2:O:541:SER:O    | 2.39                     | 0.51              |
| 1:I:64:THR:OG1   | 1:I:67:LYS:HE2   | 2.10                     | 0.51              |
| 1:K:38:ILE:CB    | 1:K:51:ALA:HB1   | 2.29                     | 0.51              |
| 2:Q:367:ARG:O    | 2:Q:371:ARG:HG2  | 2.11                     | 0.51              |
| 1:L:231:LEU:HD12 | 1:L:231:LEU:H    | 1.76                     | 0.51              |
| 2:M:137:LYS:H    | 2:M:137:LYS:HD2  | 1.76                     | 0.51              |
| 2:P:398:ASP:OD2  | 2:P:399:VAL:N    | 2.44                     | 0.51              |
| 2:Q:397:ALA:O    | 2:Q:401:ARG:N    | 2.39                     | 0.51              |
| 2:N:267:PHE:CZ   | 2:N:364:MET:HE3  | 2.46                     | 0.51              |
| 1:F:244:ARG:NE   | 1:F:357:GLU:OE1  | 2.43                     | 0.51              |
| 1:G:9:ILE:O      | 1:G:13:LEU:HD23  | 2.10                     | 0.51              |
| 2:P:416:ASP:OD1  | 2:P:417:LEU:N    | 2.44                     | 0.51              |
| 1:L:284:LEU:HD12 | 1:L:340:ARG:HB2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:155:ILE:HG22 | 2:N:156:ASP:N    | 2.26                     | 0.51              |
| 1:I:102:GLY:H    | 1:I:146:PHE:HB2  | 1.76                     | 0.51              |
| 1:F:249:VAL:HB   | 1:F:360:LEU:HD23 | 1.93                     | 0.50              |
| 2:O:239:PRO:HD2  | 2:O:242:LEU:HD12 | 1.93                     | 0.50              |
| 2:O:426:SER:O    | 2:O:429:VAL:HG22 | 2.12                     | 0.50              |
| 1:G:126:VAL:HA   | 1:G:129:ILE:HD12 | 1.92                     | 0.50              |
| 2:O:189:ILE:HD11 | 2:O:226:PHE:CZ   | 2.47                     | 0.50              |
| 2:P:407:MET:SD   | 2:P:408:THR:OG1  | 2.66                     | 0.50              |
| 1:C:54:CYS:SG    | 1:C:55:LYS:N     | 2.85                     | 0.50              |
| 2:Q:275:LYS:CE   | 2:Q:291:VAL:HG23 | 2.41                     | 0.50              |
| 1:E:31:ARG:NH2   | 1:E:198:GLU:OE2  | 2.44                     | 0.50              |
| 1:I:38:ILE:HD11  | 1:I:89:VAL:HG13  | 1.94                     | 0.50              |
| 1:K:322:LEU:O    | 1:K:340:ARG:NE   | 2.44                     | 0.50              |
| 2:P:253:ILE:HG21 | 2:P:264:ILE:CG1  | 2.42                     | 0.50              |
| 2:R:116:PRO:C    | 2:R:117:THR:HG1  | 2.13                     | 0.50              |
| 2:R:210:ILE:HD12 | 2:R:464:GLU:HB2  | 1.93                     | 0.50              |
| 1:E:208:GLU:O    | 1:E:210:ARG:HG2  | 2.11                     | 0.50              |
| 1:G:188:THR:HG23 | 1:G:188:THR:O    | 2.11                     | 0.50              |
| 1:G:60:ALA:HB3   | 1:G:97:PHE:CE1   | 2.47                     | 0.50              |
| 1:K:157:VAL:O    | 1:K:160:SER:OG   | 2.29                     | 0.50              |
| 2:N:262:ASN:OD1  | 2:N:265:SER:OG   | 2.29                     | 0.50              |
| 2:Q:54:ALA:HB1   | 2:Q:94:THR:HB    | 1.94                     | 0.50              |
| 2:N:137:LYS:N    | 2:N:137:LYS:HD2  | 2.26                     | 0.50              |
| 1:I:261:ASP:CG   | 1:I:383:LEU:HD12 | 2.36                     | 0.50              |
| 1:L:319:ILE:HD11 | 1:L:347:VAL:HG13 | 1.94                     | 0.50              |
| 2:N:406:TYR:HB3  | 2:N:408:THR:O    | 2.11                     | 0.50              |
| 2:N:447:ARG:O    | 2:N:451:GLY:N    | 2.44                     | 0.50              |
| 2:N:471:ARG:NH2  | 2:N:506:SER:O    | 2.40                     | 0.50              |
| 1:A:151:GLU:O    | 1:A:155:VAL:HG23 | 2.12                     | 0.49              |
| 1:E:215:THR:H    | 1:E:218:THR:CG2  | 2.24                     | 0.49              |
| 1:E:315:THR:HG23 | 1:E:316:ASP:N    | 2.27                     | 0.49              |
| 1:I:77:GLU:O     | 1:I:80:SER:OG    | 2.25                     | 0.49              |
| 1:I:174:VAL:HG12 | 1:I:174:VAL:O    | 2.11                     | 0.49              |
| 1:G:89:VAL:HG13  | 1:G:89:VAL:O     | 2.12                     | 0.49              |
| 2:O:318:LYS:HD2  | 2:O:326:LEU:HB3  | 1.93                     | 0.49              |
| 1:G:115:LEU:HD23 | 1:G:115:LEU:O    | 2.12                     | 0.49              |
| 1:J:245:TRP:CG   | 1:J:353:ARG:HH12 | 2.30                     | 0.49              |
| 1:E:16:PHE:CE2   | 1:E:184:VAL:HG22 | 2.47                     | 0.49              |
| 1:G:31:ARG:HH21  | 1:G:196:THR:HG1  | 1.61                     | 0.49              |
| 1:I:182:ARG:O    | 1:I:185:ASP:OD1  | 2.30                     | 0.49              |
| 2:O:101:SER:OG   | 2:O:102:GLU:N    | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:234:ASP:OD1  | 2:O:235:ASN:N    | 2.44                     | 0.49              |
| 2:O:100:LEU:HD12 | 2:O:105:GLU:O    | 2.11                     | 0.49              |
| 2:P:158:ASP:OD1  | 2:P:159:ARG:N    | 2.46                     | 0.49              |
| 2:Q:275:LYS:HD2  | 2:Q:293:PHE:HB2  | 1.95                     | 0.49              |
| 1:C:186:LEU:HD11 | 1:C:197:VAL:HG11 | 1.93                     | 0.49              |
| 1:I:212:VAL:HG21 | 1:I:231:LEU:HD21 | 1.94                     | 0.49              |
| 2:M:299:VAL:O    | 2:M:302:LEU:HG   | 2.13                     | 0.49              |
| 2:M:325:THR:O    | 2:M:326:LEU:HD23 | 2.13                     | 0.49              |
| 2:Q:423:GLU:OE1  | 2:Q:423:GLU:N    | 2.43                     | 0.49              |
| 2:R:466:HIS:HA   | 2:R:508:VAL:HG22 | 1.94                     | 0.49              |
| 1:B:244:ARG:NE   | 1:B:357:GLU:OE1  | 2.44                     | 0.49              |
| 1:G:122:LEU:HD23 | 1:G:125:ILE:HD12 | 1.95                     | 0.49              |
| 2:M:411:ASN:OD1  | 2:M:412:VAL:N    | 2.46                     | 0.49              |
| 2:O:243:MET:HB2  | 2:O:248:LEU:HD22 | 1.95                     | 0.49              |
| 2:P:423:GLU:HG3  | 2:P:424:VAL:HG13 | 1.94                     | 0.49              |
| 1:E:309:THR:HG22 | 1:E:309:THR:O    | 2.11                     | 0.49              |
| 1:G:34:ILE:HG22  | 1:G:35:GLU:N     | 2.28                     | 0.49              |
| 1:G:221:LEU:HB3  | 1:G:223:THR:HG22 | 1.95                     | 0.49              |
| 1:K:89:VAL:HG13  | 1:K:89:VAL:O     | 2.11                     | 0.49              |
| 2:N:229:ASN:OD1  | 2:N:230:LEU:N    | 2.46                     | 0.49              |
| 1:G:112:GLU:HA   | 1:G:115:LEU:HB3  | 1.95                     | 0.49              |
| 2:M:399:VAL:O    | 2:M:402:GLN:HG2  | 2.13                     | 0.49              |
| 2:Q:318:LYS:HE3  | 2:Q:328:SER:HA   | 1.94                     | 0.49              |
| 1:A:309:THR:HG22 | 1:A:309:THR:O    | 2.13                     | 0.48              |
| 1:E:194:ASP:OD2  | 1:E:196:THR:HG22 | 2.13                     | 0.48              |
| 1:K:365:ASP:OD1  | 1:K:366:ASP:N    | 2.46                     | 0.48              |
| 2:M:283:THR:OG1  | 2:M:284:ASN:N    | 2.46                     | 0.48              |
| 2:R:124:PRO:HG2  | 2:R:127:VAL:HG23 | 1.95                     | 0.48              |
| 2:R:313:LEU:HD23 | 2:R:314:ALA:N    | 2.28                     | 0.48              |
| 1:G:384:SER:OG   | 1:G:393:ARG:NH2  | 2.46                     | 0.48              |
| 1:K:193:ASN:O    | 1:K:195:ARG:NH1  | 2.46                     | 0.48              |
| 2:M:251:ILE:HG12 | 2:M:427:ILE:HD13 | 1.94                     | 0.48              |
| 2:O:296:ASP:OD1  | 2:O:296:ASP:N    | 2.46                     | 0.48              |
| 2:O:310:ILE:HG22 | 2:O:311:GLY:N    | 2.27                     | 0.48              |
| 2:Q:101:SER:OG   | 2:Q:102:GLU:N    | 2.45                     | 0.48              |
| 2:Q:468:TYR:O    | 2:Q:469:LEU:HG   | 2.14                     | 0.48              |
| 2:R:529:ASP:OD2  | 2:R:530:GLN:N    | 2.45                     | 0.48              |
| 2:M:325:THR:HG22 | 2:M:326:LEU:H    | 1.77                     | 0.48              |
| 2:N:230:LEU:O    | 2:N:231:LEU:HD12 | 2.13                     | 0.48              |
| 2:P:265:SER:O    | 2:P:269:HIS:ND1  | 2.36                     | 0.48              |
| 2:R:187:VAL:HG12 | 2:R:187:VAL:O    | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:106:LEU:O    | 1:A:139:LEU:HD22 | 2.14                     | 0.48              |
| 1:A:162:LYS:HD3  | 1:A:162:LYS:O    | 2.13                     | 0.48              |
| 1:C:216:ARG:HD3  | 1:C:216:ARG:C    | 2.38                     | 0.48              |
| 2:M:236:LEU:HD12 | 2:M:237:ARG:H    | 1.78                     | 0.48              |
| 1:I:184:VAL:HG21 | 1:I:217:TRP:CD2  | 2.48                     | 0.48              |
| 1:K:215:THR:HG23 | 1:K:217:TRP:H    | 1.79                     | 0.48              |
| 2:N:299:VAL:O    | 2:N:303:GLU:OE2  | 2.31                     | 0.48              |
| 2:N:310:ILE:HG22 | 2:N:312:LYS:CE   | 2.43                     | 0.48              |
| 2:P:213:GLU:N    | 2:P:213:GLU:OE2  | 2.46                     | 0.48              |
| 2:R:243:MET:HE1  | 2:R:251:ILE:CD1  | 2.43                     | 0.48              |
| 2:R:243:MET:CE   | 2:R:251:ILE:HD12 | 2.43                     | 0.48              |
| 2:M:283:THR:HG22 | 2:R:360:GLU:HG3  | 1.96                     | 0.48              |
| 2:M:318:LYS:HB2  | 2:M:326:LEU:HD22 | 1.94                     | 0.48              |
| 2:N:511:THR:O    | 2:N:515:GLN:NE2  | 2.43                     | 0.48              |
| 2:Q:254:GLU:OE2  | 2:Q:254:GLU:HA   | 2.14                     | 0.48              |
| 1:A:39:GLU:H     | 1:A:39:GLU:CD    | 2.19                     | 0.48              |
| 2:M:279:ASN:ND2  | 2:M:292:TYR:O    | 2.47                     | 0.48              |
| 2:M:417:LEU:HD23 | 2:M:425:LEU:HD11 | 1.96                     | 0.48              |
| 1:A:70:LYS:N     | 1:A:71:PRO:CD    | 2.77                     | 0.48              |
| 1:E:174:VAL:HG12 | 1:E:174:VAL:O    | 2.13                     | 0.48              |
| 1:E:215:THR:H    | 1:E:218:THR:HG22 | 1.78                     | 0.48              |
| 1:G:329:ILE:HD11 | 1:H:327:ILE:HG23 | 1.94                     | 0.48              |
| 2:P:320:LYS:CE   | 2:P:342:ILE:HD11 | 2.43                     | 0.48              |
| 2:Q:471:ARG:NH2  | 2:Q:506:SER:O    | 2.43                     | 0.48              |
| 1:A:35:GLU:HB2   | 1:A:50:THR:O     | 2.14                     | 0.48              |
| 1:K:13:LEU:O     | 1:K:17:LEU:HG    | 2.14                     | 0.48              |
| 1:K:226:ARG:HG3  | 1:K:226:ARG:HH11 | 1.79                     | 0.48              |
| 2:M:302:LEU:O    | 2:M:305:MET:HG2  | 2.13                     | 0.48              |
| 1:I:206:LEU:O    | 1:I:209:VAL:HG12 | 2.14                     | 0.47              |
| 1:I:365:ASP:OD2  | 1:I:365:ASP:N    | 2.47                     | 0.47              |
| 1:K:42:ASP:HB2   | 1:K:44:ILE:HG12  | 1.96                     | 0.47              |
| 2:P:243:MET:HE3  | 2:P:248:LEU:HB2  | 1.95                     | 0.47              |
| 1:A:164:LYS:C    | 1:A:164:LYS:HD3  | 2.39                     | 0.47              |
| 1:C:244:ARG:HD2  | 1:C:356:ASP:HB2  | 1.95                     | 0.47              |
| 1:G:82:ASN:OD1   | 1:G:82:ASN:N     | 2.45                     | 0.47              |
| 1:L:345:ASP:OD1  | 1:L:346:GLU:N    | 2.47                     | 0.47              |
| 2:R:295:ILE:O    | 2:R:298:VAL:N    | 2.45                     | 0.47              |
| 1:C:258:PHE:HA   | 1:C:261:ASP:OD2  | 2.14                     | 0.47              |
| 1:I:28:ASP:OD1   | 1:I:29:GLY:N     | 2.48                     | 0.47              |
| 1:I:215:THR:HA   | 1:I:381:GLU:CG   | 2.44                     | 0.47              |
| 2:M:64:VAL:O     | 2:M:87:ASN:N     | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:204:HIS:CD2  | 2:M:456:VAL:HG11 | 2.49                     | 0.47              |
| 2:N:295:ILE:O    | 2:N:299:VAL:HG13 | 2.14                     | 0.47              |
| 2:P:181:LYS:HE2  | 2:P:574:PRO:HB3  | 1.95                     | 0.47              |
| 1:G:66:GLY:O     | 1:G:69:TYR:CG    | 2.68                     | 0.47              |
| 2:M:337:ALA:O    | 2:M:339:GLN:NE2  | 2.43                     | 0.47              |
| 2:N:101:SER:OG   | 2:N:102:GLU:N    | 2.47                     | 0.47              |
| 2:O:249:GLU:O    | 2:O:253:ILE:HB   | 2.14                     | 0.47              |
| 2:O:273:ARG:HA   | 2:O:276:CYS:SG   | 2.54                     | 0.47              |
| 2:P:253:ILE:HG21 | 2:P:264:ILE:HG12 | 1.95                     | 0.47              |
| 1:D:348:ILE:O    | 1:D:348:ILE:HG13 | 2.15                     | 0.47              |
| 1:E:108:LYS:HE2  | 1:E:135:TYR:HB3  | 1.96                     | 0.47              |
| 1:E:211:ARG:HH12 | 1:E:213:THR:HG22 | 1.77                     | 0.47              |
| 1:I:96:HIS:ND1   | 1:I:147:GLY:O    | 2.42                     | 0.47              |
| 2:R:313:LEU:HD23 | 2:R:314:ALA:O    | 2.15                     | 0.47              |
| 1:E:176:PHE:CE2  | 1:E:221:LEU:HD11 | 2.45                     | 0.47              |
| 2:P:245:ALA:HB2  | 2:P:288:ASP:HB3  | 1.96                     | 0.47              |
| 1:A:215:THR:H    | 1:A:218:THR:CG2  | 2.28                     | 0.47              |
| 1:E:33:THR:HG23  | 1:E:195:ARG:HB3  | 1.97                     | 0.47              |
| 2:P:243:MET:HG3  | 2:P:247:GLU:HB3  | 1.95                     | 0.47              |
| 2:Q:267:PHE:O    | 2:Q:271:VAL:HG23 | 2.15                     | 0.47              |
| 2:M:128:LEU:HD21 | 2:M:565:MET:HE1  | 1.95                     | 0.47              |
| 2:Q:243:MET:HE2  | 2:Q:248:LEU:N    | 2.29                     | 0.47              |
| 2:Q:274:ASN:HD21 | 2:Q:297:GLU:CG   | 2.27                     | 0.47              |
| 1:G:32:ILE:HG22  | 1:G:33:THR:N     | 2.30                     | 0.47              |
| 2:N:557:LEU:HD13 | 2:N:568:VAL:HG12 | 1.97                     | 0.47              |
| 2:R:378:GLN:O    | 2:R:382:TYR:N    | 2.46                     | 0.47              |
| 2:R:548:LEU:HD21 | 2:R:557:LEU:HD21 | 1.97                     | 0.47              |
| 1:C:315:THR:HG23 | 1:C:316:ASP:N    | 2.30                     | 0.47              |
| 1:I:19:TYR:HE2   | 1:I:23:ILE:HD11  | 1.80                     | 0.47              |
| 1:I:204:ALA:O    | 1:I:208:GLU:OE1  | 2.33                     | 0.47              |
| 1:J:348:ILE:O    | 1:J:348:ILE:HG13 | 2.15                     | 0.47              |
| 1:K:16:PHE:O     | 1:K:20:LEU:HD23  | 2.14                     | 0.47              |
| 2:P:299:VAL:HG12 | 2:P:303:GLU:OE2  | 2.14                     | 0.47              |
| 1:E:76:LEU:HD12  | 1:E:76:LEU:H     | 1.80                     | 0.46              |
| 2:M:356:PRO:O    | 2:M:360:GLU:OE2  | 2.33                     | 0.46              |
| 2:O:41:TYR:CD1   | 2:O:53:LEU:HD21  | 2.50                     | 0.46              |
| 2:R:243:MET:HE2  | 2:R:248:LEU:N    | 2.30                     | 0.46              |
| 1:G:327:ILE:HG23 | 1:H:329:ILE:HD11 | 1.97                     | 0.46              |
| 1:H:284:LEU:HD13 | 1:H:340:ARG:HB2  | 1.97                     | 0.46              |
| 1:I:35:GLU:HG3   | 1:I:52:VAL:HG23  | 1.97                     | 0.46              |
| 1:I:221:LEU:HD12 | 1:I:222:ALA:N    | 2.28                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:245:TRP:HE3  | 1:I:281:ASN:HD21 | 1.64                     | 0.46              |
| 1:K:173:ALA:HB2  | 1:K:227:MET:HA   | 1.98                     | 0.46              |
| 1:G:107:THR:OG1  | 1:G:110:ASP:OD2  | 2.33                     | 0.46              |
| 1:K:106:LEU:HD23 | 1:K:107:THR:O    | 2.15                     | 0.46              |
| 1:L:274:SER:O    | 1:L:274:SER:OG   | 2.28                     | 0.46              |
| 1:A:117:THR:CG2  | 1:A:123:ARG:HB3  | 2.46                     | 0.46              |
| 1:E:171:ILE:HD13 | 1:E:175:ILE:HD11 | 1.96                     | 0.46              |
| 1:J:249:VAL:HB   | 1:J:360:LEU:HD23 | 1.96                     | 0.46              |
| 2:M:243:MET:HE3  | 2:M:251:ILE:CD1  | 2.46                     | 0.46              |
| 2:N:269:HIS:HA   | 2:N:272:VAL:HG12 | 1.96                     | 0.46              |
| 1:A:96:HIS:HB2   | 1:A:147:GLY:O    | 2.16                     | 0.46              |
| 1:C:7:TYR:CD1    | 1:C:39:GLU:HG2   | 2.50                     | 0.46              |
| 1:I:35:GLU:N     | 1:I:35:GLU:OE1   | 2.48                     | 0.46              |
| 1:I:58:GLU:HG2   | 1:I:59:GLN:H     | 1.79                     | 0.46              |
| 2:O:367:ARG:O    | 2:O:371:ARG:HG2  | 2.15                     | 0.46              |
| 2:P:318:LYS:HE2  | 2:P:326:LEU:HB3  | 1.98                     | 0.46              |
| 1:E:175:ILE:HG13 | 1:E:176:PHE:N    | 2.31                     | 0.46              |
| 1:E:211:ARG:HH12 | 1:E:213:THR:CG2  | 2.29                     | 0.46              |
| 1:G:8:SER:O      | 1:G:12:TYR:HD2   | 1.98                     | 0.46              |
| 1:G:71:PRO:O     | 1:G:74:LEU:HD23  | 2.15                     | 0.46              |
| 2:M:54:ALA:HB1   | 2:M:94:THR:HB    | 1.97                     | 0.46              |
| 2:P:530:GLN:CG   | 2:P:531:THR:N    | 2.78                     | 0.46              |
| 2:R:385:LYS:HG2  | 2:R:386:GLU:H    | 1.80                     | 0.46              |
| 1:C:9:ILE:HG21   | 1:C:216:ARG:CZ   | 2.46                     | 0.46              |
| 1:I:38:ILE:HG22  | 1:I:38:ILE:O     | 2.16                     | 0.46              |
| 2:M:367:ARG:O    | 2:M:371:ARG:HG2  | 2.15                     | 0.46              |
| 2:N:267:PHE:O    | 2:N:268:ARG:C    | 2.58                     | 0.46              |
| 2:Q:362:ASP:OD1  | 2:Q:362:ASP:N    | 2.48                     | 0.46              |
| 2:Q:524:LEU:HD21 | 2:Q:529:ASP:HB2  | 1.97                     | 0.46              |
| 2:R:137:LYS:HD2  | 2:R:137:LYS:N    | 2.31                     | 0.46              |
| 1:A:212:VAL:HG21 | 1:A:231:LEU:HD21 | 1.98                     | 0.46              |
| 1:C:75:MET:O     | 1:C:78:HIS:HB3   | 2.15                     | 0.46              |
| 1:E:108:LYS:HA   | 1:E:139:LEU:HD11 | 1.98                     | 0.46              |
| 1:E:140:ASP:OD2  | 1:E:141:ARG:N    | 2.49                     | 0.46              |
| 1:H:261:ASP:HB2  | 1:H:383:LEU:HD12 | 1.97                     | 0.46              |
| 1:I:169:ASP:OD2  | 1:I:170:ASP:N    | 2.49                     | 0.46              |
| 2:M:165:VAL:HG12 | 2:M:166:ALA:N    | 2.31                     | 0.46              |
| 2:M:234:ASP:OD2  | 2:M:235:ASN:N    | 2.48                     | 0.46              |
| 2:Q:170:SER:OG   | 2:Q:171:THR:N    | 2.49                     | 0.46              |
| 2:R:279:ASN:ND2  | 2:R:291:VAL:HG21 | 2.30                     | 0.46              |
| 2:R:330:ARG:HD2  | 2:R:330:ARG:N    | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:406:TYR:CD2  | 2:R:408:THR:O    | 2.69                     | 0.46              |
| 1:A:60:ALA:HB3   | 1:A:97:PHE:CZ    | 2.51                     | 0.46              |
| 1:I:15:GLN:O     | 1:I:18:LYS:HG3   | 2.15                     | 0.46              |
| 1:K:327:ILE:HD12 | 1:K:336:GLU:OE2  | 2.16                     | 0.46              |
| 2:N:253:ILE:HG12 | 2:N:267:PHE:CE2  | 2.51                     | 0.46              |
| 1:E:38:ILE:HG12  | 1:E:78:HIS:NE2   | 2.31                     | 0.46              |
| 1:I:104:LYS:O    | 1:I:144:ILE:HG22 | 2.16                     | 0.46              |
| 1:J:262:ILE:HG23 | 1:J:263:VAL:N    | 2.31                     | 0.46              |
| 1:A:39:GLU:OE1   | 1:A:39:GLU:N     | 2.29                     | 0.45              |
| 2:P:240:TYR:O    | 2:P:243:MET:HB3  | 2.16                     | 0.45              |
| 2:R:238:LEU:HG   | 2:R:238:LEU:O    | 2.17                     | 0.45              |
| 2:M:294:SER:OG   | 2:M:297:GLU:OE2  | 2.32                     | 0.45              |
| 2:O:400:VAL:HG22 | 2:O:435:MET:CE   | 2.46                     | 0.45              |
| 2:O:423:GLU:HG2  | 2:O:424:VAL:HG13 | 1.99                     | 0.45              |
| 1:G:15:GLN:O     | 1:G:19:TYR:CD2   | 2.70                     | 0.45              |
| 1:I:48:LEU:HD12  | 1:I:50:THR:HG23  | 1.98                     | 0.45              |
| 1:K:227:MET:HG3  | 1:K:228:PHE:N    | 2.30                     | 0.45              |
| 2:O:481:ARG:O    | 2:O:485:GLU:HG2  | 2.17                     | 0.45              |
| 2:P:417:LEU:HB3  | 2:P:425:LEU:HD11 | 1.98                     | 0.45              |
| 2:R:243:MET:HB2  | 2:R:248:LEU:HD12 | 1.97                     | 0.45              |
| 1:E:174:VAL:HG11 | 1:E:210:ARG:NH1  | 2.32                     | 0.45              |
| 1:E:286:MET:C    | 1:E:287:LEU:HD23 | 2.42                     | 0.45              |
| 2:O:345:SER:O    | 2:O:351:LYS:HA   | 2.17                     | 0.45              |
| 2:M:310:ILE:HA   | 2:M:319:PRO:HA   | 1.98                     | 0.45              |
| 2:R:260:SER:HA   | 2:R:263:GLN:HB2  | 1.97                     | 0.45              |
| 1:E:176:PHE:CD2  | 1:E:221:LEU:HD21 | 2.51                     | 0.45              |
| 1:F:284:LEU:HD12 | 1:F:340:ARG:HB2  | 1.98                     | 0.45              |
| 1:G:14:TYR:OH    | 1:G:148:PRO:O    | 2.34                     | 0.45              |
| 1:I:315:THR:HG23 | 1:I:316:ASP:N    | 2.32                     | 0.45              |
| 2:M:43:LEU:HG    | 2:M:123:THR:HG22 | 1.99                     | 0.45              |
| 2:M:423:GLU:OE1  | 2:M:423:GLU:N    | 2.43                     | 0.45              |
| 2:N:35:MET:SD    | 2:N:122:VAL:HG11 | 2.56                     | 0.45              |
| 2:N:218:PHE:CE1  | 2:N:412:VAL:HG21 | 2.52                     | 0.45              |
| 2:P:46:SER:O     | 2:P:46:SER:OG    | 2.30                     | 0.45              |
| 2:Q:283:THR:OG1  | 2:Q:284:ASN:N    | 2.50                     | 0.45              |
| 2:R:13:ASP:OD1   | 2:R:14:SER:N     | 2.49                     | 0.45              |
| 2:R:330:ARG:HD2  | 2:R:330:ARG:H    | 1.81                     | 0.45              |
| 1:C:44:ILE:HG23  | 1:C:45:ALA:N     | 2.31                     | 0.45              |
| 1:C:64:THR:HG22  | 1:C:67:LYS:HE2   | 1.98                     | 0.45              |
| 1:C:72:ILE:HG22  | 1:C:76:LEU:HD13  | 1.98                     | 0.45              |
| 1:C:162:LYS:C    | 1:C:162:LYS:HD3  | 2.41                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:203:LEU:HA   | 1:C:206:LEU:HG   | 1.99                     | 0.45              |
| 1:E:39:GLU:OE2   | 1:E:39:GLU:N     | 2.49                     | 0.45              |
| 1:E:169:ASP:OD1  | 1:E:169:ASP:N    | 2.50                     | 0.45              |
| 1:E:212:VAL:HG21 | 1:E:231:LEU:HD21 | 1.97                     | 0.45              |
| 1:G:35:GLU:CD    | 1:G:92:ARG:HH12  | 2.24                     | 0.45              |
| 1:K:211:ARG:NH2  | 1:K:379:LYS:HB2  | 2.31                     | 0.45              |
| 2:Q:541:SER:OG   | 2:Q:542:ALA:N    | 2.50                     | 0.45              |
| 2:R:237:ARG:NH1  | 2:R:402:GLN:OE1  | 2.50                     | 0.45              |
| 2:R:258:HIS:O    | 2:R:258:HIS:ND1  | 2.50                     | 0.45              |
| 1:A:34:ILE:HG22  | 1:A:35:GLU:N     | 2.32                     | 0.45              |
| 1:E:106:LEU:N    | 1:E:106:LEU:HD12 | 2.31                     | 0.45              |
| 1:K:73:LEU:O     | 1:K:76:LEU:CB    | 2.65                     | 0.45              |
| 2:O:273:ARG:O    | 2:O:277:LYS:HG2  | 2.16                     | 0.45              |
| 2:P:101:SER:OG   | 2:P:102:GLU:N    | 2.50                     | 0.45              |
| 2:M:204:HIS:CE1  | 2:M:410:SER:HA   | 2.52                     | 0.45              |
| 2:N:249:GLU:O    | 2:N:253:ILE:HB   | 2.17                     | 0.45              |
| 2:N:310:ILE:HG22 | 2:N:312:LYS:HE3  | 1.99                     | 0.45              |
| 2:N:316:GLU:HG3  | 2:N:316:GLU:O    | 2.17                     | 0.45              |
| 2:O:308:GLU:OE2  | 2:O:330:ARG:NH2  | 2.50                     | 0.45              |
| 2:P:539:ASP:O    | 2:P:539:ASP:OD2  | 2.35                     | 0.45              |
| 2:R:232:GLY:O    | 2:R:236:LEU:HG   | 2.17                     | 0.45              |
| 1:I:68:ILE:O     | 1:I:68:ILE:HG22  | 2.17                     | 0.45              |
| 1:I:185:ASP:OD1  | 1:I:185:ASP:C    | 2.60                     | 0.45              |
| 2:P:362:ASP:OD1  | 2:P:363:ARG:N    | 2.50                     | 0.45              |
| 2:R:241:TRP:CB   | 2:R:293:PHE:HE1  | 2.29                     | 0.45              |
| 2:R:482:LYS:O    | 2:R:485:GLU:HG3  | 2.17                     | 0.45              |
| 2:R:496:VAL:O    | 2:R:496:VAL:HG13 | 2.17                     | 0.45              |
| 1:A:9:ILE:HG23   | 1:A:10:LYS:N     | 2.31                     | 0.44              |
| 1:A:125:ILE:O    | 1:A:128:ARG:N    | 2.43                     | 0.44              |
| 1:B:262:ILE:HG23 | 1:B:263:VAL:N    | 2.32                     | 0.44              |
| 1:E:215:THR:O    | 1:E:218:THR:HG22 | 2.17                     | 0.44              |
| 1:G:215:THR:HG22 | 1:G:218:THR:HG23 | 1.98                     | 0.44              |
| 1:K:71:PRO:O     | 1:K:72:ILE:C     | 2.60                     | 0.44              |
| 2:R:227:THR:OG1  | 2:R:411:ASN:ND2  | 2.46                     | 0.44              |
| 1:E:38:ILE:O     | 1:E:38:ILE:HG13  | 2.16                     | 0.44              |
| 1:K:131:THR:O    | 1:K:133:VAL:HG13 | 2.18                     | 0.44              |
| 1:K:280:SER:O    | 1:K:325:ARG:NH2  | 2.50                     | 0.44              |
| 1:L:327:ILE:C    | 1:L:328:LEU:HD12 | 2.42                     | 0.44              |
| 1:A:133:VAL:HG13 | 1:A:133:VAL:O    | 2.17                     | 0.44              |
| 1:A:152:ASP:N    | 1:A:152:ASP:OD1  | 2.49                     | 0.44              |
| 1:C:245:TRP:HE3  | 1:C:281:ASN:HD21 | 1.63                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:340:ARG:C    | 1:D:341:LEU:HD12 | 2.42                     | 0.44              |
| 1:E:212:VAL:HG12 | 1:E:213:THR:N    | 2.32                     | 0.44              |
| 1:I:67:LYS:HD3   | 1:I:67:LYS:N     | 2.32                     | 0.44              |
| 1:K:297:GLN:NE2  | 1:K:307:CYS:SG   | 2.90                     | 0.44              |
| 2:Q:320:LYS:HG3  | 2:Q:324:GLU:OE1  | 2.17                     | 0.44              |
| 2:Q:320:LYS:NZ   | 2:Q:351:LYS:O    | 2.48                     | 0.44              |
| 1:C:125:ILE:HD12 | 1:C:125:ILE:H    | 1.81                     | 0.44              |
| 1:E:113:THR:O    | 1:E:114:VAL:C    | 2.60                     | 0.44              |
| 1:E:206:LEU:O    | 1:E:209:VAL:HG12 | 2.18                     | 0.44              |
| 1:K:329:ILE:HD11 | 1:L:327:ILE:HG23 | 1.98                     | 0.44              |
| 2:N:3:ASP:OD2    | 2:N:3:ASP:N      | 2.51                     | 0.44              |
| 2:P:321:LEU:HD13 | 2:P:325:THR:O    | 2.18                     | 0.44              |
| 2:R:204:HIS:CE1  | 2:R:410:SER:OG   | 2.71                     | 0.44              |
| 1:A:111:LEU:HB2  | 1:A:139:LEU:HD11 | 2.00                     | 0.44              |
| 1:C:185:ASP:O    | 1:C:189:ARG:HD2  | 2.17                     | 0.44              |
| 1:I:10:LYS:O     | 1:I:13:LEU:HG    | 2.17                     | 0.44              |
| 1:J:353:ARG:HG3  | 1:J:353:ARG:HH11 | 1.82                     | 0.44              |
| 2:M:202:ASN:HB2  | 2:M:456:VAL:HG22 | 1.98                     | 0.44              |
| 1:A:7:TYR:O      | 1:A:8:SER:C      | 2.60                     | 0.44              |
| 1:G:108:LYS:O    | 1:G:111:LEU:HB3  | 2.17                     | 0.44              |
| 1:J:284:LEU:HD12 | 1:J:340:ARG:HB2  | 1.99                     | 0.44              |
| 1:J:329:ILE:O    | 1:J:333:PHE:HA   | 2.18                     | 0.44              |
| 2:M:362:ASP:OD1  | 2:M:362:ASP:N    | 2.51                     | 0.44              |
| 2:N:306:ASN:OD1  | 2:N:358:ASN:OD1  | 2.35                     | 0.44              |
| 2:O:312:LYS:NZ   | 2:O:352:ALA:O    | 2.44                     | 0.44              |
| 2:P:164:HIS:HB2  | 2:P:516:CYS:HA   | 2.00                     | 0.44              |
| 2:P:194:ASN:OD1  | 2:P:196:HIS:N    | 2.50                     | 0.44              |
| 2:P:253:ILE:HG22 | 2:P:254:GLU:N    | 2.31                     | 0.44              |
| 2:P:372:LEU:O    | 2:P:378:GLN:NE2  | 2.51                     | 0.44              |
| 2:Q:245:ALA:HA   | 2:Q:287:PHE:CE2  | 2.53                     | 0.44              |
| 2:R:302:LEU:HD22 | 2:R:365:ILE:HD11 | 1.99                     | 0.44              |
| 1:C:61:GLU:O     | 1:C:98:PRO:HG2   | 2.18                     | 0.44              |
| 1:E:200:LYS:O    | 1:E:200:LYS:HD3  | 2.18                     | 0.44              |
| 2:P:468:TYR:O    | 2:P:469:LEU:HG   | 2.17                     | 0.44              |
| 2:Q:296:ASP:HB3  | 2:Q:382:TYR:OH   | 2.18                     | 0.44              |
| 2:R:23:ILE:HG22  | 2:R:24:SER:N     | 2.33                     | 0.44              |
| 1:F:245:TRP:HD1  | 1:F:355:PRO:HA   | 1.82                     | 0.44              |
| 1:G:73:LEU:O     | 1:G:76:LEU:HB2   | 2.18                     | 0.44              |
| 1:J:292:ASP:OD1  | 1:J:292:ASP:N    | 2.47                     | 0.44              |
| 1:K:69:TYR:O     | 1:K:73:LEU:HD13  | 2.18                     | 0.44              |
| 2:N:321:LEU:HD22 | 2:N:325:THR:HB   | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:412:VAL:O    | 2:Q:412:VAL:HG13 | 2.18                     | 0.44              |
| 2:R:304:ASN:OD1  | 2:R:338:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:24:LEU:HD12  | 1:C:25:ALA:N     | 2.33                     | 0.44              |
| 1:C:60:ALA:CB    | 1:C:67:LYS:HE3   | 2.48                     | 0.44              |
| 1:C:134:ASP:CG   | 1:C:137:ALA:HB3  | 2.43                     | 0.44              |
| 1:E:109:ASP:OD1  | 1:E:110:ASP:N    | 2.50                     | 0.44              |
| 1:H:262:ILE:HG23 | 1:H:263:VAL:N    | 2.33                     | 0.44              |
| 1:K:66:GLY:O     | 1:K:69:TYR:CD2   | 2.71                     | 0.44              |
| 2:M:529:ASP:OD1  | 2:M:529:ASP:N    | 2.51                     | 0.44              |
| 2:O:321:LEU:HD13 | 2:O:341:PHE:HE1  | 1.83                     | 0.44              |
| 2:O:321:LEU:HD13 | 2:O:341:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:215:THR:H    | 1:A:218:THR:HG22 | 1.82                     | 0.43              |
| 1:E:16:PHE:CD2   | 1:E:184:VAL:HG22 | 2.52                     | 0.43              |
| 1:E:44:ILE:HG23  | 1:E:45:ALA:N     | 2.33                     | 0.43              |
| 1:K:198:GLU:N    | 1:K:198:GLU:OE2  | 2.51                     | 0.43              |
| 2:M:423:GLU:HG2  | 2:M:424:VAL:HG13 | 1.99                     | 0.43              |
| 2:M:439:PHE:CD2  | 2:M:439:PHE:C    | 2.95                     | 0.43              |
| 2:O:573:LEU:HD21 | 3:O:1501:ATP:C2  | 2.53                     | 0.43              |
| 2:P:460:VAL:HG23 | 2:P:460:VAL:O    | 2.18                     | 0.43              |
| 2:R:323:ASN:O    | 2:R:323:ASN:ND2  | 2.51                     | 0.43              |
| 1:G:181:GLN:NE2  | 1:G:215:THR:HG21 | 2.33                     | 0.43              |
| 2:M:233:VAL:CG1  | 2:M:234:ASP:N    | 2.80                     | 0.43              |
| 2:M:267:PHE:C    | 2:M:267:PHE:CD2  | 2.96                     | 0.43              |
| 2:M:297:GLU:OE2  | 2:M:297:GLU:N    | 2.40                     | 0.43              |
| 2:N:19:ILE:HB    | 2:N:94:THR:OG1   | 2.18                     | 0.43              |
| 2:N:116:PRO:O    | 2:N:117:THR:OG1  | 2.32                     | 0.43              |
| 2:O:567:THR:HG22 | 2:O:568:VAL:N    | 2.33                     | 0.43              |
| 2:P:295:ILE:HG13 | 2:P:296:ASP:N    | 2.34                     | 0.43              |
| 2:Q:263:GLN:HA   | 2:Q:266:GLN:HB2  | 2.01                     | 0.43              |
| 2:Q:304:ASN:O    | 2:Q:307:ASN:N    | 2.51                     | 0.43              |
| 2:Q:359:GLY:O    | 2:R:261:HIS:HD2  | 2.01                     | 0.43              |
| 2:R:234:ASP:OD1  | 2:R:235:ASN:N    | 2.51                     | 0.43              |
| 1:A:206:LEU:O    | 1:A:209:VAL:HG12 | 2.19                     | 0.43              |
| 1:C:181:GLN:HA   | 1:C:184:VAL:HG12 | 2.01                     | 0.43              |
| 1:E:40:ASP:OD2   | 1:E:42:ASP:N     | 2.51                     | 0.43              |
| 1:E:120:GLU:O    | 1:E:123:ARG:HG3  | 2.17                     | 0.43              |
| 1:F:284:LEU:CD2  | 1:F:286:MET:SD   | 3.07                     | 0.43              |
| 1:G:35:GLU:OE1   | 1:G:51:ALA:O     | 2.36                     | 0.43              |
| 1:H:361:ILE:O    | 1:H:362:ASN:HB2  | 2.18                     | 0.43              |
| 1:I:126:VAL:O    | 1:I:129:ILE:HG12 | 2.18                     | 0.43              |
| 2:M:363:ARG:O    | 2:M:366:LEU:HG   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:440:GLY:O    | 2:M:441:PHE:C    | 2.61                     | 0.43              |
| 2:O:362:ASP:O    | 2:O:365:ILE:HG12 | 2.18                     | 0.43              |
| 2:O:363:ARG:HA   | 2:O:366:LEU:HD22 | 1.99                     | 0.43              |
| 2:Q:264:ILE:HG23 | 2:Q:265:SER:H    | 1.83                     | 0.43              |
| 2:Q:331:ASP:N    | 2:Q:331:ASP:OD1  | 2.52                     | 0.43              |
| 2:R:377:LEU:N    | 2:R:377:LEU:HD12 | 2.32                     | 0.43              |
| 2:R:521:SER:O    | 2:R:556:PHE:HA   | 2.19                     | 0.43              |
| 1:C:308:GLU:OE2  | 1:C:324:ARG:NH2  | 2.51                     | 0.43              |
| 1:D:383:LEU:O    | 1:D:387:GLU:OE1  | 2.36                     | 0.43              |
| 1:K:138:PHE:O    | 1:K:141:ARG:N    | 2.52                     | 0.43              |
| 1:L:387:GLU:HG3  | 1:L:392:LEU:HD12 | 2.01                     | 0.43              |
| 2:M:285:LEU:HD13 | 2:M:291:VAL:CG2  | 2.48                     | 0.43              |
| 2:Q:165:VAL:HG12 | 2:Q:166:ALA:N    | 2.33                     | 0.43              |
| 2:Q:456:VAL:O    | 2:Q:456:VAL:HG23 | 2.18                     | 0.43              |
| 2:Q:540:LEU:HB2  | 2:Q:544:LEU:HD23 | 1.99                     | 0.43              |
| 2:R:532:TYR:CE2  | 2:R:536:LEU:HD11 | 2.53                     | 0.43              |
| 1:A:18:LYS:O     | 1:A:18:LYS:HD3   | 2.19                     | 0.43              |
| 1:B:307:CYS:SG   | 1:B:339:LEU:HD21 | 2.57                     | 0.43              |
| 1:G:15:GLN:NE2   | 1:G:16:PHE:CE1   | 2.86                     | 0.43              |
| 1:G:22:GLU:C     | 1:G:22:GLU:OE2   | 2.62                     | 0.43              |
| 1:K:18:LYS:HZ2   | 1:K:153:LEU:HD21 | 1.82                     | 0.43              |
| 2:N:441:PHE:O    | 2:N:445:LYS:HG2  | 2.18                     | 0.43              |
| 2:O:269:HIS:O    | 2:O:273:ARG:HG2  | 2.19                     | 0.43              |
| 2:O:439:PHE:CD1  | 2:O:439:PHE:C    | 2.96                     | 0.43              |
| 2:O:496:VAL:HG13 | 2:O:496:VAL:O    | 2.18                     | 0.43              |
| 2:R:12:THR:HG21  | 2:R:22:GLU:OE1   | 2.18                     | 0.43              |
| 1:A:224:LYS:HD3  | 1:A:228:PHE:HE2  | 1.83                     | 0.43              |
| 1:A:366:ASP:OD1  | 1:A:367:GLU:N    | 2.47                     | 0.43              |
| 1:C:65:LEU:HG    | 1:C:68:ILE:HD11  | 1.99                     | 0.43              |
| 1:E:258:PHE:HA   | 1:E:261:ASP:OD1  | 2.18                     | 0.43              |
| 1:I:215:THR:HA   | 1:I:381:GLU:HG2  | 2.01                     | 0.43              |
| 1:I:247:VAL:HB   | 1:I:358:LEU:HD12 | 1.99                     | 0.43              |
| 2:M:338:VAL:HG12 | 2:M:339:GLN:N    | 2.32                     | 0.43              |
| 2:N:318:LYS:HD2  | 2:N:326:LEU:HD13 | 1.99                     | 0.43              |
| 2:N:417:LEU:HD13 | 2:N:425:LEU:HD11 | 2.01                     | 0.43              |
| 2:O:546:ASP:C    | 2:O:546:ASP:OD2  | 2.61                     | 0.43              |
| 2:Q:259:ASN:O    | 2:Q:263:GLN:HG2  | 2.18                     | 0.43              |
| 1:D:262:ILE:HG23 | 1:D:263:VAL:N    | 2.33                     | 0.43              |
| 1:G:113:THR:O    | 1:G:116:SER:OG   | 2.36                     | 0.43              |
| 1:I:212:VAL:HB   | 1:I:378:PHE:HD1  | 1.84                     | 0.43              |
| 1:K:92:ARG:HA    | 1:K:92:ARG:HH11  | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:398:ASP:HA   | 2:O:401:ARG:HG2  | 2.00                     | 0.43              |
| 2:P:526:ASN:OD1  | 2:P:527:ALA:N    | 2.52                     | 0.43              |
| 1:A:5:ALA:HA     | 1:A:7:TYR:CE1    | 2.53                     | 0.43              |
| 1:A:73:LEU:O     | 1:A:76:LEU:HD12  | 2.19                     | 0.43              |
| 1:C:106:LEU:HG   | 1:C:107:THR:N    | 2.34                     | 0.43              |
| 1:C:168:PRO:HA   | 1:C:171:ILE:HD12 | 2.01                     | 0.43              |
| 1:C:261:ASP:CG   | 1:C:383:LEU:HD12 | 2.44                     | 0.43              |
| 1:E:286:MET:O    | 1:E:287:LEU:HD23 | 2.18                     | 0.43              |
| 1:I:117:THR:OG1  | 1:I:123:ARG:HB2  | 2.19                     | 0.43              |
| 1:J:328:LEU:CD2  | 1:J:335:MET:HG2  | 2.49                     | 0.43              |
| 2:O:490:GLU:HG3  | 2:O:493:LYS:HE3  | 2.01                     | 0.43              |
| 2:P:269:HIS:O    | 2:P:273:ARG:HG2  | 2.19                     | 0.43              |
| 2:P:422:PHE:N    | 2:P:422:PHE:CD1  | 2.84                     | 0.43              |
| 2:R:526:ASN:O    | 2:R:530:GLN:HB2  | 2.19                     | 0.43              |
| 1:I:108:LYS:HZ2  | 1:I:111:LEU:HD23 | 1.81                     | 0.43              |
| 1:J:353:ARG:HG3  | 1:J:353:ARG:NH1  | 2.34                     | 0.43              |
| 2:M:227:THR:HG23 | 2:M:411:ASN:CG   | 2.43                     | 0.43              |
| 2:M:300:THR:OG1  | 2:M:338:VAL:HG22 | 2.19                     | 0.43              |
| 2:M:342:ILE:HG22 | 2:M:343:VAL:N    | 2.34                     | 0.43              |
| 2:O:233:VAL:CG1  | 2:O:234:ASP:N    | 2.78                     | 0.43              |
| 2:P:243:MET:HG3  | 2:P:247:GLU:CB   | 2.49                     | 0.43              |
| 2:P:264:ILE:O    | 2:P:268:ARG:HG3  | 2.19                     | 0.43              |
| 1:L:231:LEU:H    | 1:L:231:LEU:CD1  | 2.31                     | 0.43              |
| 2:M:553:GLN:HG2  | 3:M:1501:ATP:C2  | 2.53                     | 0.43              |
| 2:N:424:VAL:O    | 2:N:428:VAL:HG23 | 2.19                     | 0.43              |
| 2:O:165:VAL:HG12 | 2:O:166:ALA:N    | 2.34                     | 0.43              |
| 2:O:295:ILE:O    | 2:O:299:VAL:HG23 | 2.18                     | 0.43              |
| 2:O:305:MET:HB3  | 2:O:357:PHE:HB3  | 2.01                     | 0.43              |
| 2:R:375:PRO:HA   | 2:R:378:GLN:CG   | 2.49                     | 0.43              |
| 1:C:300:LEU:CD2  | 1:C:305:LEU:HD12 | 2.45                     | 0.42              |
| 1:G:211:ARG:O    | 1:G:211:ARG:HG3  | 2.18                     | 0.42              |
| 2:N:234:ASP:OD1  | 2:N:235:ASN:N    | 2.52                     | 0.42              |
| 2:N:546:ASP:OD1  | 2:N:547:LEU:N    | 2.52                     | 0.42              |
| 2:O:202:ASN:HB3  | 2:O:456:VAL:HG13 | 2.01                     | 0.42              |
| 2:P:265:SER:OG   | 2:P:266:GLN:N    | 2.52                     | 0.42              |
| 2:P:416:ASP:C    | 2:P:417:LEU:HD12 | 2.44                     | 0.42              |
| 2:Q:142:LEU:HG   | 2:Q:142:LEU:O    | 2.19                     | 0.42              |
| 1:A:164:LYS:HE2  | 1:A:203:LEU:HD11 | 2.01                     | 0.42              |
| 1:E:293:LEU:HD11 | 1:E:343:LYS:HG3  | 2.01                     | 0.42              |
| 1:G:38:ILE:HB    | 1:G:52:VAL:CG1   | 2.49                     | 0.42              |
| 2:M:287:PHE:CD1  | 2:M:288:ASP:N    | 2.87                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:292:TYR:HB2  | 2:M:393:THR:OG1  | 2.19                     | 0.42              |
| 2:O:243:MET:CB   | 2:O:248:LEU:HD22 | 2.48                     | 0.42              |
| 2:O:304:ASN:ND2  | 2:O:339:GLN:OE1  | 2.52                     | 0.42              |
| 2:P:471:ARG:NH1  | 2:P:506:SER:O    | 2.52                     | 0.42              |
| 2:Q:268:ARG:HG3  | 2:Q:287:PHE:CD1  | 2.54                     | 0.42              |
| 2:Q:318:LYS:O    | 2:Q:319:PRO:C    | 2.61                     | 0.42              |
| 1:B:249:VAL:HB   | 1:B:360:LEU:HD23 | 2.00                     | 0.42              |
| 1:C:57:HIS:CE1   | 1:C:59:GLN:OE1   | 2.72                     | 0.42              |
| 1:E:66:GLY:O     | 1:E:69:TYR:HB2   | 2.19                     | 0.42              |
| 1:E:110:ASP:O    | 1:E:113:THR:HB   | 2.18                     | 0.42              |
| 1:J:328:LEU:HD23 | 1:J:335:MET:HG2  | 2.01                     | 0.42              |
| 2:N:395:ASP:OD2  | 2:N:395:ASP:N    | 2.51                     | 0.42              |
| 2:O:209:ASP:OD1  | 2:O:212:ALA:N    | 2.51                     | 0.42              |
| 2:P:331:ASP:OD2  | 2:P:331:ASP:N    | 2.51                     | 0.42              |
| 2:Q:276:CYS:SG   | 2:Q:285:LEU:O    | 2.77                     | 0.42              |
| 2:Q:303:GLU:OE1  | 2:Q:365:ILE:HD12 | 2.18                     | 0.42              |
| 2:Q:321:LEU:HD13 | 2:Q:325:THR:O    | 2.20                     | 0.42              |
| 2:R:526:ASN:OD1  | 2:R:527:ALA:N    | 2.52                     | 0.42              |
| 1:C:385:ASP:O    | 1:C:389:ILE:HG13 | 2.20                     | 0.42              |
| 1:K:8:SER:CB     | 1:K:54:CYS:O     | 2.67                     | 0.42              |
| 1:K:62:LYS:O     | 1:K:67:LYS:NZ    | 2.52                     | 0.42              |
| 1:K:109:ASP:N    | 1:K:109:ASP:OD1  | 2.50                     | 0.42              |
| 1:L:348:ILE:O    | 1:L:348:ILE:HG13 | 2.19                     | 0.42              |
| 2:M:597:ASP:O    | 2:M:598:PHE:C    | 2.62                     | 0.42              |
| 2:O:333:LEU:O    | 2:O:339:GLN:NE2  | 2.52                     | 0.42              |
| 2:R:179:VAL:HG21 | 2:R:501:VAL:HG21 | 2.01                     | 0.42              |
| 2:R:271:VAL:HG13 | 2:R:293:PHE:CE2  | 2.54                     | 0.42              |
| 2:R:478:ASP:HA   | 2:R:481:ARG:HG3  | 2.02                     | 0.42              |
| 2:R:519:PHE:CD1  | 2:R:537:LEU:HD11 | 2.54                     | 0.42              |
| 1:K:21:SER:O     | 1:K:24:LEU:HG    | 2.19                     | 0.42              |
| 2:M:262:ASN:OD1  | 2:M:263:GLN:N    | 2.53                     | 0.42              |
| 2:N:276:CYS:HA   | 2:N:285:LEU:HD22 | 2.00                     | 0.42              |
| 2:N:304:ASN:OD1  | 2:N:305:MET:N    | 2.52                     | 0.42              |
| 2:R:231:LEU:O    | 2:R:231:LEU:HD12 | 2.19                     | 0.42              |
| 1:C:32:ILE:HG22  | 1:C:33:THR:N     | 2.33                     | 0.42              |
| 1:K:153:LEU:O    | 1:K:157:VAL:HG23 | 2.19                     | 0.42              |
| 1:K:255:ILE:HG22 | 1:K:256:GLU:N    | 2.35                     | 0.42              |
| 2:O:257:GLU:N    | 2:O:363:ARG:NH2  | 2.68                     | 0.42              |
| 2:Q:243:MET:HE1  | 2:Q:251:ILE:CD1  | 2.50                     | 0.42              |
| 2:Q:460:VAL:CG1  | 2:Q:498:LEU:HD23 | 2.49                     | 0.42              |
| 2:R:218:PHE:CE2  | 2:R:412:VAL:HG11 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:10:LYS:O     | 1:C:13:LEU:HG    | 2.20                     | 0.42              |
| 1:I:108:LYS:HZ1  | 1:I:135:TYR:HB3  | 1.85                     | 0.42              |
| 1:I:224:LYS:HD2  | 1:I:224:LYS:O    | 2.20                     | 0.42              |
| 1:K:38:ILE:HG13  | 1:K:38:ILE:O     | 2.18                     | 0.42              |
| 2:P:243:MET:HE3  | 2:P:248:LEU:CB   | 2.50                     | 0.42              |
| 2:P:327:VAL:HB   | 2:P:330:ARG:HH21 | 1.85                     | 0.42              |
| 2:P:428:VAL:O    | 2:P:432:ILE:HG13 | 2.20                     | 0.42              |
| 2:Q:228:LEU:C    | 2:Q:228:LEU:HD23 | 2.45                     | 0.42              |
| 2:Q:537:LEU:HD12 | 2:Q:537:LEU:N    | 2.35                     | 0.42              |
| 2:R:189:ILE:HD12 | 2:R:189:ILE:H    | 1.84                     | 0.42              |
| 2:R:231:LEU:HD11 | 2:R:415:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:210:ARG:NE   | 1:A:210:ARG:HA   | 2.35                     | 0.42              |
| 1:C:134:ASP:OD1  | 1:C:137:ALA:HB3  | 2.20                     | 0.42              |
| 1:E:197:VAL:HG13 | 1:E:202:PHE:CE1  | 2.55                     | 0.42              |
| 1:E:211:ARG:HG3  | 1:E:211:ARG:NH1  | 2.35                     | 0.42              |
| 1:G:9:ILE:HA     | 1:G:12:TYR:CD2   | 2.54                     | 0.42              |
| 1:G:9:ILE:HA     | 1:G:12:TYR:HD2   | 1.85                     | 0.42              |
| 1:G:58:GLU:HG3   | 1:G:96:HIS:O     | 2.20                     | 0.42              |
| 1:J:366:ASP:OD1  | 1:J:367:GLU:N    | 2.48                     | 0.42              |
| 1:K:367:GLU:HG3  | 1:K:367:GLU:O    | 2.20                     | 0.42              |
| 2:M:342:ILE:CG2  | 2:M:343:VAL:N    | 2.83                     | 0.42              |
| 2:N:288:ASP:O    | 2:N:289:THR:C    | 2.63                     | 0.42              |
| 2:O:206:VAL:HG23 | 2:O:206:VAL:O    | 2.19                     | 0.42              |
| 2:O:312:LYS:HE3  | 2:O:353:SER:HB3  | 2.01                     | 0.42              |
| 2:P:548:LEU:CD2  | 2:P:557:LEU:HD21 | 2.46                     | 0.42              |
| 2:R:183:LEU:HD22 | 2:R:205:ILE:HD13 | 2.02                     | 0.42              |
| 1:A:109:ASP:OD1  | 1:A:110:ASP:OD1  | 2.38                     | 0.42              |
| 1:D:385:ASP:O    | 1:D:389:ILE:HG13 | 2.20                     | 0.42              |
| 1:G:32:ILE:CG2   | 1:G:33:THR:N     | 2.83                     | 0.42              |
| 1:I:49:THR:O     | 1:I:88:HIS:HB3   | 2.19                     | 0.42              |
| 1:I:58:GLU:O     | 1:I:59:GLN:HB2   | 2.19                     | 0.42              |
| 1:I:108:LYS:NZ   | 1:I:135:TYR:HB3  | 2.35                     | 0.42              |
| 1:K:110:ASP:O    | 1:K:114:VAL:HG23 | 2.19                     | 0.42              |
| 1:K:182:ARG:O    | 1:K:186:LEU:HD23 | 2.20                     | 0.42              |
| 1:L:319:ILE:HG23 | 1:L:323:PHE:CE2  | 2.54                     | 0.42              |
| 2:M:575:VAL:O    | 2:M:575:VAL:HG13 | 2.19                     | 0.42              |
| 2:N:246:GLN:O    | 2:N:249:GLU:HB3  | 2.20                     | 0.42              |
| 2:P:23:ILE:HG22  | 2:P:24:SER:N     | 2.34                     | 0.42              |
| 2:P:243:MET:SD   | 2:P:248:LEU:HA   | 2.60                     | 0.42              |
| 2:Q:279:ASN:OD1  | 2:Q:279:ASN:N    | 2.51                     | 0.42              |
| 2:R:375:PRO:HA   | 2:R:378:GLN:HG2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:60:ALA:HB3   | 1:A:97:PHE:CE1   | 2.55                     | 0.42              |
| 1:A:297:GLN:NE2  | 1:A:307:CYS:SG   | 2.93                     | 0.42              |
| 1:C:73:LEU:HD23  | 1:C:125:ILE:HD13 | 2.01                     | 0.42              |
| 1:E:73:LEU:HB3   | 1:E:125:ILE:HG21 | 2.02                     | 0.42              |
| 1:G:102:GLY:O    | 1:G:146:PHE:HB2  | 2.20                     | 0.42              |
| 2:M:304:ASN:HB3  | 2:M:334:TYR:CD1  | 2.55                     | 0.42              |
| 2:P:251:ILE:CD1  | 2:P:427:ILE:HD13 | 2.49                     | 0.42              |
| 2:Q:233:VAL:HG13 | 2:Q:234:ASP:H    | 1.83                     | 0.42              |
| 2:Q:234:ASP:OD1  | 2:Q:235:ASN:N    | 2.53                     | 0.42              |
| 2:Q:342:ILE:HG22 | 2:Q:343:VAL:N    | 2.34                     | 0.42              |
| 2:R:206:VAL:O    | 2:R:206:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:60:ALA:O     | 1:A:97:PHE:CD1   | 2.73                     | 0.41              |
| 1:E:211:ARG:HG3  | 1:E:211:ARG:O    | 2.19                     | 0.41              |
| 1:E:212:VAL:HG12 | 1:E:213:THR:H    | 1.85                     | 0.41              |
| 1:G:159:ALA:O    | 1:G:162:LYS:HB3  | 2.20                     | 0.41              |
| 1:L:229:SER:O    | 1:L:233:LYS:NZ   | 2.53                     | 0.41              |
| 1:L:241:HIS:CG   | 1:L:244:ARG:HH21 | 2.38                     | 0.41              |
| 1:L:261:ASP:HB2  | 1:L:383:LEU:HD12 | 2.02                     | 0.41              |
| 2:M:23:ILE:HG22  | 2:M:24:SER:N     | 2.35                     | 0.41              |
| 2:O:62:THR:HG22  | 2:O:63:HIS:N     | 2.34                     | 0.41              |
| 2:R:231:LEU:HD13 | 2:R:236:LEU:CD2  | 2.50                     | 0.41              |
| 1:A:117:THR:O    | 1:A:117:THR:HG23 | 2.20                     | 0.41              |
| 1:E:117:THR:OG1  | 1:E:122:LEU:HB3  | 2.19                     | 0.41              |
| 1:I:328:LEU:HD21 | 1:I:335:MET:HE3  | 2.01                     | 0.41              |
| 1:K:19:TYR:OH    | 1:K:35:GLU:HB3   | 2.20                     | 0.41              |
| 2:O:279:ASN:HB2  | 2:O:285:LEU:HD21 | 2.03                     | 0.41              |
| 2:O:293:PHE:CD2  | 2:O:294:SER:N    | 2.88                     | 0.41              |
| 2:O:384:LYS:HD2  | 2:O:384:LYS:C    | 2.44                     | 0.41              |
| 2:Q:243:MET:HE1  | 2:Q:251:ILE:HD12 | 2.02                     | 0.41              |
| 2:R:248:LEU:HD21 | 2:R:252:PHE:CE2  | 2.54                     | 0.41              |
| 1:A:286:MET:O    | 1:A:287:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:355:PRO:O    | 1:A:373:VAL:HG22 | 2.20                     | 0.41              |
| 1:C:35:GLU:HG3   | 1:C:52:VAL:CB    | 2.50                     | 0.41              |
| 1:D:319:ILE:HG23 | 1:D:323:PHE:CE2  | 2.55                     | 0.41              |
| 1:G:139:LEU:O    | 1:G:139:LEU:HD23 | 2.21                     | 0.41              |
| 1:K:54:CYS:SG    | 1:K:55:LYS:N     | 2.93                     | 0.41              |
| 2:O:525:THR:HG23 | 2:O:526:ASN:N    | 2.35                     | 0.41              |
| 1:C:65:LEU:HD21  | 1:C:114:VAL:HG21 | 2.03                     | 0.41              |
| 1:C:108:LYS:O    | 1:C:111:LEU:HB3  | 2.20                     | 0.41              |
| 1:E:171:ILE:HA   | 1:E:175:ILE:HD11 | 2.02                     | 0.41              |
| 1:G:91:TYR:C     | 1:G:92:ARG:HG3   | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:213:THR:O    | 1:I:213:THR:HG23 | 2.20                     | 0.41              |
| 1:K:35:GLU:HG2   | 1:K:36:GLY:N     | 2.35                     | 0.41              |
| 1:K:110:ASP:O    | 1:K:113:THR:OG1  | 2.28                     | 0.41              |
| 2:N:263:GLN:NE2  | 2:N:364:MET:SD   | 2.94                     | 0.41              |
| 2:N:265:SER:HA   | 2:N:268:ARG:HB3  | 2.02                     | 0.41              |
| 2:P:414:ILE:HG22 | 2:P:415:ILE:N    | 2.36                     | 0.41              |
| 1:A:211:ARG:HG3  | 1:A:212:VAL:H    | 1.86                     | 0.41              |
| 1:E:171:ILE:CD1  | 1:E:175:ILE:HD11 | 2.49                     | 0.41              |
| 1:I:45:ALA:O     | 1:I:47:GLY:N     | 2.53                     | 0.41              |
| 1:I:212:VAL:HB   | 1:I:378:PHE:CD1  | 2.55                     | 0.41              |
| 2:M:345:SER:O    | 2:M:351:LYS:HA   | 2.21                     | 0.41              |
| 2:N:367:ARG:HA   | 2:N:367:ARG:NE   | 2.34                     | 0.41              |
| 2:O:468:TYR:O    | 2:O:469:LEU:HG   | 2.19                     | 0.41              |
| 2:P:292:TYR:HB2  | 2:P:393:THR:HG23 | 2.03                     | 0.41              |
| 2:R:164:HIS:HB2  | 2:R:516:CYS:HA   | 2.01                     | 0.41              |
| 1:A:245:TRP:HD1  | 1:A:355:PRO:HA   | 1.85                     | 0.41              |
| 1:A:315:THR:HG23 | 1:A:316:ASP:N    | 2.36                     | 0.41              |
| 1:C:92:ARG:HH22  | 1:C:145:GLU:HB3  | 1.86                     | 0.41              |
| 1:D:361:ILE:O    | 1:D:362:ASN:HB2  | 2.20                     | 0.41              |
| 1:F:315:THR:HG23 | 1:F:316:ASP:N    | 2.36                     | 0.41              |
| 1:G:108:LYS:O    | 1:G:112:GLU:OE2  | 2.39                     | 0.41              |
| 1:K:34:ILE:HG22  | 1:K:35:GLU:N     | 2.35                     | 0.41              |
| 1:K:72:ILE:HA    | 1:K:75:MET:HE3   | 2.02                     | 0.41              |
| 2:M:170:SER:OG   | 2:M:171:THR:N    | 2.52                     | 0.41              |
| 2:M:243:MET:HB3  | 2:M:248:LEU:HB2  | 2.02                     | 0.41              |
| 2:M:282:LEU:HD11 | 2:M:285:LEU:HG   | 2.03                     | 0.41              |
| 2:M:283:THR:HG22 | 2:R:360:GLU:CG   | 2.50                     | 0.41              |
| 2:P:274:ASN:O    | 2:P:277:LYS:HB3  | 2.21                     | 0.41              |
| 2:P:426:SER:O    | 2:P:429:VAL:HG12 | 2.21                     | 0.41              |
| 2:R:548:LEU:HD23 | 2:R:551:LEU:HD11 | 2.01                     | 0.41              |
| 1:C:35:GLU:HG3   | 1:C:52:VAL:HG11  | 2.03                     | 0.41              |
| 1:G:212:VAL:HG12 | 1:G:213:THR:N    | 2.35                     | 0.41              |
| 1:G:232:ARG:NH1  | 1:G:388:TYR:O    | 2.53                     | 0.41              |
| 1:K:101:SER:O    | 1:K:101:SER:OG   | 2.38                     | 0.41              |
| 1:K:245:TRP:HD1  | 1:K:355:PRO:HA   | 1.84                     | 0.41              |
| 2:N:557:LEU:HD12 | 2:N:567:THR:O    | 2.21                     | 0.41              |
| 2:Q:269:HIS:CE1  | 2:Q:273:ARG:HG3  | 2.56                     | 0.41              |
| 2:Q:397:ALA:HA   | 2:Q:400:VAL:HG12 | 2.01                     | 0.41              |
| 1:A:96:HIS:O     | 1:A:97:PHE:CD1   | 2.73                     | 0.41              |
| 1:F:309:THR:O    | 1:F:309:THR:HG22 | 2.19                     | 0.41              |
| 1:G:73:LEU:HG    | 1:G:122:LEU:HD22 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:548:LEU:HB2  | 2:O:549:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:290:ASP:OD1  | 1:A:290:ASP:N    | 2.46                     | 0.41              |
| 1:E:64:THR:OG1   | 1:E:67:LYS:NZ    | 2.51                     | 0.41              |
| 1:G:23:ILE:O     | 1:G:26:ALA:HB3   | 2.21                     | 0.41              |
| 1:G:33:THR:CG2   | 1:G:195:ARG:HB3  | 2.51                     | 0.41              |
| 1:I:17:LEU:HD21  | 1:I:154:GLN:HB3  | 2.02                     | 0.41              |
| 1:I:211:ARG:HG3  | 1:I:377:GLY:C    | 2.46                     | 0.41              |
| 1:J:244:ARG:NH2  | 1:J:357:GLU:OE2  | 2.52                     | 0.41              |
| 1:K:22:GLU:O     | 1:K:26:ALA:N     | 2.54                     | 0.41              |
| 1:K:174:VAL:O    | 1:K:174:VAL:HG12 | 2.20                     | 0.41              |
| 1:L:280:SER:O    | 1:L:282:PRO:HD3  | 2.21                     | 0.41              |
| 2:M:318:LYS:CE   | 2:M:327:VAL:O    | 2.69                     | 0.41              |
| 2:M:409:LYS:HA   | 2:M:409:LYS:HD2  | 1.84                     | 0.41              |
| 2:M:601:VAL:HG13 | 2:N:442:HIS:HB3  | 2.02                     | 0.41              |
| 2:P:327:VAL:O    | 2:P:330:ARG:NH2  | 2.44                     | 0.41              |
| 2:P:460:VAL:CG2  | 2:P:498:LEU:HD23 | 2.49                     | 0.41              |
| 2:Q:244:ASN:OD1  | 2:Q:247:GLU:HG2  | 2.20                     | 0.41              |
| 2:Q:294:SER:OG   | 2:Q:296:ASP:OD1  | 2.39                     | 0.41              |
| 2:Q:356:PRO:O    | 2:Q:360:GLU:OE2  | 2.38                     | 0.41              |
| 2:Q:407:MET:O    | 2:Q:407:MET:HG2  | 2.21                     | 0.41              |
| 2:Q:441:PHE:CD2  | 2:Q:441:PHE:C    | 2.99                     | 0.41              |
| 2:Q:558:ILE:O    | 2:Q:558:ILE:HG23 | 2.20                     | 0.41              |
| 2:R:299:VAL:HG13 | 2:R:300:THR:N    | 2.36                     | 0.41              |
| 2:R:309:VAL:HG12 | 2:R:310:ILE:N    | 2.36                     | 0.41              |
| 1:K:203:LEU:CD1  | 1:K:203:LEU:N    | 2.84                     | 0.41              |
| 2:M:244:ASN:OD1  | 2:M:245:ALA:N    | 2.54                     | 0.41              |
| 2:Q:260:SER:O    | 2:Q:261:HIS:C    | 2.64                     | 0.41              |
| 1:A:11:GLY:O     | 1:A:15:GLN:OE1   | 2.38                     | 0.40              |
| 1:A:158:LEU:HD11 | 1:A:171:ILE:HD12 | 2.03                     | 0.40              |
| 1:E:176:PHE:CE2  | 1:E:221:LEU:HD21 | 2.56                     | 0.40              |
| 1:E:203:LEU:HD23 | 1:E:203:LEU:O    | 2.21                     | 0.40              |
| 1:F:245:TRP:CH2  | 1:F:340:ARG:NH2  | 2.89                     | 0.40              |
| 2:O:97:ILE:HG13  | 2:O:98:GLY:N     | 2.36                     | 0.40              |
| 2:O:217:ALA:HA   | 2:O:576:PRO:HG2  | 2.04                     | 0.40              |
| 2:O:229:ASN:OD1  | 2:O:412:VAL:O    | 2.39                     | 0.40              |
| 2:O:233:VAL:CG1  | 2:O:234:ASP:H    | 2.30                     | 0.40              |
| 2:O:599:ASP:HA   | 2:O:602:ILE:HG12 | 2.04                     | 0.40              |
| 2:R:238:LEU:HD23 | 2:R:238:LEU:H    | 1.86                     | 0.40              |
| 2:R:331:ASP:O    | 2:R:332:GLU:C    | 2.64                     | 0.40              |
| 1:A:109:ASP:O    | 1:A:113:THR:OG1  | 2.33                     | 0.40              |
| 1:C:239:LEU:HD11 | 1:C:390:LEU:HD23 | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:64:THR:OG1   | 1:E:67:LYS:HE2   | 2.21                     | 0.40              |
| 1:E:221:LEU:HD12 | 1:E:222:ALA:N    | 2.36                     | 0.40              |
| 1:I:8:SER:O      | 1:I:12:TYR:HD2   | 2.04                     | 0.40              |
| 1:I:192:VAL:HG23 | 1:I:192:VAL:O    | 2.22                     | 0.40              |
| 1:K:189:ARG:HD3  | 1:K:190:SER:N    | 2.36                     | 0.40              |
| 2:N:508:VAL:HB   | 2:N:513:PHE:CE2  | 2.56                     | 0.40              |
| 2:O:310:ILE:HD13 | 2:O:319:PRO:HA   | 2.03                     | 0.40              |
| 2:P:367:ARG:HA   | 2:P:370:THR:OG1  | 2.22                     | 0.40              |
| 2:P:408:THR:O    | 2:P:408:THR:HG22 | 2.20                     | 0.40              |
| 2:Q:258:HIS:O    | 2:Q:258:HIS:CG   | 2.74                     | 0.40              |
| 2:Q:383:PRO:HG2  | 2:Q:391:LEU:HD22 | 2.02                     | 0.40              |
| 1:A:114:VAL:O    | 1:A:115:LEU:C    | 2.63                     | 0.40              |
| 1:C:164:LYS:C    | 1:C:164:LYS:HD3  | 2.46                     | 0.40              |
| 1:E:19:TYR:O     | 1:E:23:ILE:HG13  | 2.21                     | 0.40              |
| 1:I:12:TYR:O     | 1:I:15:GLN:HG3   | 2.21                     | 0.40              |
| 1:I:214:PHE:HE1  | 1:I:228:PHE:HE1  | 1.70                     | 0.40              |
| 1:K:16:PHE:HA    | 1:K:19:TYR:HD2   | 1.87                     | 0.40              |
| 1:K:152:ASP:HA   | 1:K:155:VAL:HG12 | 2.03                     | 0.40              |
| 2:O:244:ASN:OD1  | 2:O:244:ASN:C    | 2.64                     | 0.40              |
| 2:Q:43:LEU:HD22  | 2:Q:51:TYR:HB3   | 2.03                     | 0.40              |
| 2:Q:385:LYS:HG3  | 2:Q:391:LEU:HD12 | 2.03                     | 0.40              |
| 1:H:316:ASP:OD2  | 1:H:316:ASP:N    | 2.52                     | 0.40              |
| 1:I:58:GLU:CG    | 1:I:59:GLN:H     | 2.33                     | 0.40              |
| 1:K:111:LEU:CD2  | 1:K:135:TYR:HB3  | 2.52                     | 0.40              |
| 2:M:302:LEU:HD13 | 2:M:365:ILE:CD1  | 2.52                     | 0.40              |
| 2:P:273:ARG:HA   | 2:P:276:CYS:SG   | 2.62                     | 0.40              |
| 2:Q:137:LYS:H    | 2:Q:137:LYS:HD2  | 1.87                     | 0.40              |
| 2:Q:236:LEU:HD12 | 2:Q:237:ARG:N    | 2.36                     | 0.40              |
| 2:Q:548:LEU:HB2  | 2:Q:549:PRO:HD3  | 2.03                     | 0.40              |
| 2:Q:567:THR:HG22 | 2:Q:568:VAL:N    | 2.35                     | 0.40              |
| 2:R:366:LEU:HD12 | 2:R:367:ARG:NE   | 2.37                     | 0.40              |
| 1:A:34:ILE:O     | 1:A:195:ARG:HG2  | 2.21                     | 0.40              |
| 1:E:40:ASP:OD2   | 1:E:40:ASP:C     | 2.65                     | 0.40              |
| 1:E:214:PHE:HE2  | 1:E:228:PHE:CE1  | 2.39                     | 0.40              |
| 1:G:13:LEU:O     | 1:G:14:TYR:C     | 2.64                     | 0.40              |
| 1:K:75:MET:O     | 1:K:78:HIS:HB3   | 2.22                     | 0.40              |
| 1:K:142:PHE:CD1  | 1:K:143:ALA:N    | 2.89                     | 0.40              |
| 2:M:567:THR:HG22 | 2:M:568:VAL:N    | 2.37                     | 0.40              |
| 2:N:279:ASN:HB2  | 2:N:285:LEU:HD21 | 2.04                     | 0.40              |
| 2:P:249:GLU:OE1  | 2:P:250:GLN:N    | 2.55                     | 0.40              |
| 2:P:313:LEU:HD23 | 2:P:314:ALA:O    | 2.22                     | 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     | 384/397 (97%)   | 364 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | B     | 165/397 (42%)   | 161 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 1   | C     | 380/397 (96%)   | 358 (94%)  | 22 (6%)  | 0        | 100         | 100 |
| 1   | D     | 167/397 (42%)   | 160 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 1   | E     | 383/397 (96%)   | 372 (97%)  | 10 (3%)  | 1 (0%)   | 36          | 64  |
| 1   | F     | 165/397 (42%)   | 158 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 1   | G     | 376/397 (95%)   | 360 (96%)  | 16 (4%)  | 0        | 100         | 100 |
| 1   | H     | 166/397 (42%)   | 157 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 1   | I     | 381/397 (96%)   | 363 (95%)  | 17 (4%)  | 1 (0%)   | 36          | 64  |
| 1   | J     | 167/397 (42%)   | 160 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 1   | K     | 380/397 (96%)   | 365 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | L     | 166/397 (42%)   | 161 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 2   | M     | 534/617 (86%)   | 506 (95%)  | 28 (5%)  | 0        | 100         | 100 |
| 2   | N     | 523/617 (85%)   | 500 (96%)  | 23 (4%)  | 0        | 100         | 100 |
| 2   | O     | 531/617 (86%)   | 505 (95%)  | 26 (5%)  | 0        | 100         | 100 |
| 2   | P     | 547/617 (89%)   | 518 (95%)  | 29 (5%)  | 0        | 100         | 100 |
| 2   | Q     | 536/617 (87%)   | 508 (95%)  | 28 (5%)  | 0        | 100         | 100 |
| 2   | R     | 535/617 (87%)   | 512 (96%)  | 22 (4%)  | 1 (0%)   | 43          | 71  |
| All | All   | 6486/8466 (77%) | 6188 (95%) | 295 (4%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 46  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 114 | VAL  |
| 2   | R     | 356 | PRO  |

### 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     | 337/346 (97%)   | 337 (100%)  | 0        | 100         | 100 |
| 1   | B     | 154/346 (44%)   | 154 (100%)  | 0        | 100         | 100 |
| 1   | C     | 334/346 (96%)   | 332 (99%)   | 2 (1%)   | 78          | 81  |
| 1   | D     | 156/346 (45%)   | 155 (99%)   | 1 (1%)   | 78          | 81  |
| 1   | E     | 336/346 (97%)   | 336 (100%)  | 0        | 100         | 100 |
| 1   | F     | 154/346 (44%)   | 154 (100%)  | 0        | 100         | 100 |
| 1   | G     | 332/346 (96%)   | 330 (99%)   | 2 (1%)   | 78          | 81  |
| 1   | H     | 155/346 (45%)   | 155 (100%)  | 0        | 100         | 100 |
| 1   | I     | 335/346 (97%)   | 334 (100%)  | 1 (0%)   | 86          | 85  |
| 1   | J     | 156/346 (45%)   | 156 (100%)  | 0        | 100         | 100 |
| 1   | K     | 335/346 (97%)   | 334 (100%)  | 1 (0%)   | 86          | 85  |
| 1   | L     | 155/346 (45%)   | 153 (99%)   | 2 (1%)   | 61          | 74  |
| 2   | M     | 470/525 (90%)   | 469 (100%)  | 1 (0%)   | 87          | 87  |
| 2   | N     | 454/525 (86%)   | 454 (100%)  | 0        | 100         | 100 |
| 2   | O     | 467/525 (89%)   | 466 (100%)  | 1 (0%)   | 87          | 87  |
| 2   | P     | 468/525 (89%)   | 468 (100%)  | 0        | 100         | 100 |
| 2   | Q     | 468/525 (89%)   | 466 (100%)  | 2 (0%)   | 84          | 84  |
| 2   | R     | 462/525 (88%)   | 462 (100%)  | 0        | 100         | 100 |
| All | All   | 5728/7302 (78%) | 5715 (100%) | 13 (0%)  | 85          | 87  |

All (13) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 153 | LEU  |
| 1   | C     | 158 | LEU  |
| 1   | D     | 387 | GLU  |
| 1   | G     | 82  | ASN  |
| 1   | G     | 153 | LEU  |
| 1   | I     | 210 | ARG  |
| 1   | K     | 203 | LEU  |
| 1   | L     | 231 | LEU  |
| 1   | L     | 393 | ARG  |
| 2   | M     | 300 | THR  |
| 2   | O     | 366 | LEU  |
| 2   | Q     | 279 | ASN  |
| 2   | Q     | 313 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | HIS  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 297 | GLN  |
| 1   | B     | 376 | HIS  |
| 1   | C     | 96  | HIS  |
| 1   | C     | 154 | GLN  |
| 1   | C     | 193 | ASN  |
| 1   | C     | 281 | ASN  |
| 1   | D     | 271 | GLN  |
| 1   | E     | 59  | GLN  |
| 1   | E     | 154 | GLN  |
| 1   | E     | 297 | GLN  |
| 1   | E     | 331 | ASN  |
| 1   | F     | 241 | HIS  |
| 1   | F     | 279 | HIS  |
| 1   | F     | 331 | ASN  |
| 1   | F     | 374 | ASN  |
| 1   | G     | 154 | GLN  |
| 1   | G     | 181 | GLN  |
| 1   | I     | 57  | HIS  |
| 1   | I     | 181 | GLN  |
| 1   | I     | 279 | HIS  |
| 1   | I     | 281 | ASN  |
| 1   | I     | 331 | ASN  |
| 1   | J     | 374 | ASN  |
| 1   | J     | 391 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 178 | ASN  |
| 1   | K     | 257 | ASN  |
| 1   | K     | 297 | GLN  |
| 2   | M     | 63  | HIS  |
| 2   | M     | 235 | ASN  |
| 2   | M     | 250 | GLN  |
| 2   | M     | 304 | ASN  |
| 2   | M     | 306 | ASN  |
| 2   | M     | 307 | ASN  |
| 2   | M     | 354 | ASN  |
| 2   | M     | 579 | HIS  |
| 2   | N     | 48  | ASN  |
| 2   | N     | 134 | HIS  |
| 2   | N     | 258 | HIS  |
| 2   | N     | 259 | ASN  |
| 2   | N     | 263 | GLN  |
| 2   | N     | 269 | HIS  |
| 2   | N     | 279 | ASN  |
| 2   | N     | 284 | ASN  |
| 2   | N     | 354 | ASN  |
| 2   | N     | 466 | HIS  |
| 2   | N     | 530 | GLN  |
| 2   | N     | 570 | HIS  |
| 2   | O     | 48  | ASN  |
| 2   | O     | 95  | GLN  |
| 2   | O     | 202 | ASN  |
| 2   | O     | 354 | ASN  |
| 2   | O     | 466 | HIS  |
| 2   | O     | 515 | GLN  |
| 2   | O     | 518 | ASN  |
| 2   | O     | 570 | HIS  |
| 2   | O     | 579 | HIS  |
| 2   | P     | 48  | ASN  |
| 2   | P     | 63  | HIS  |
| 2   | P     | 91  | GLN  |
| 2   | P     | 250 | GLN  |
| 2   | P     | 258 | HIS  |
| 2   | P     | 266 | GLN  |
| 2   | P     | 278 | HIS  |
| 2   | P     | 307 | ASN  |
| 2   | P     | 339 | GLN  |
| 2   | P     | 354 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 442 | HIS  |
| 2   | P     | 550 | ASN  |
| 2   | P     | 570 | HIS  |
| 2   | Q     | 48  | ASN  |
| 2   | Q     | 111 | HIS  |
| 2   | Q     | 204 | HIS  |
| 2   | Q     | 258 | HIS  |
| 2   | Q     | 263 | GLN  |
| 2   | Q     | 274 | ASN  |
| 2   | Q     | 278 | HIS  |
| 2   | Q     | 369 | HIS  |
| 2   | Q     | 378 | GLN  |
| 2   | Q     | 503 | GLN  |
| 2   | Q     | 550 | ASN  |
| 2   | Q     | 570 | HIS  |
| 2   | R     | 202 | ASN  |
| 2   | R     | 204 | HIS  |
| 2   | R     | 244 | ASN  |
| 2   | R     | 258 | HIS  |
| 2   | R     | 262 | ASN  |
| 2   | R     | 278 | HIS  |
| 2   | R     | 279 | ASN  |
| 2   | R     | 323 | ASN  |
| 2   | R     | 369 | HIS  |
| 2   | R     | 550 | ASN  |

### 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

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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  | O     | 1501 | 4    | 32,33,33     | 1.33 | 5 (15%)  | 48,52,52    | 1.75 | 11 (22%) |
| 3   | ATP  | Q     | 1501 | 4    | 32,33,33     | 1.33 | 4 (12%)  | 48,52,52    | 1.73 | 7 (14%)  |
| 3   | ATP  | M     | 1501 | -    | 32,33,33     | 1.33 | 4 (12%)  | 48,52,52    | 1.77 | 9 (18%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 3   | ATP  | O     | 1501 | 4    | -       | 3/22/38/38  | 0/3/3/3 |
| 3   | ATP  | Q     | 1501 | 4    | -       | 5/22/38/38  | 0/3/3/3 |
| 3   | ATP  | M     | 1501 | -    | -       | 10/22/38/38 | 0/3/3/3 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | M     | 1501 | ATP  | C5-C4 | 4.48  | 1.47        | 1.39     |
| 3   | Q     | 1501 | ATP  | C5-C4 | 4.47  | 1.47        | 1.39     |
| 3   | O     | 1501 | ATP  | C5-C4 | 4.42  | 1.47        | 1.39     |
| 3   | M     | 1501 | ATP  | C5-N7 | -2.56 | 1.34        | 1.39     |
| 3   | Q     | 1501 | ATP  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 3   | O     | 1501 | ATP  | C5-N7 | -2.53 | 1.34        | 1.39     |
| 3   | M     | 1501 | ATP  | C5-C6 | 2.51  | 1.48        | 1.41     |
| 3   | O     | 1501 | ATP  | C5-C6 | 2.44  | 1.47        | 1.41     |
| 3   | Q     | 1501 | ATP  | C5-N7 | -2.44 | 1.34        | 1.39     |
| 3   | O     | 1501 | ATP  | C8-N7 | 2.33  | 1.36        | 1.31     |
| 3   | Q     | 1501 | ATP  | C8-N7 | 2.30  | 1.36        | 1.31     |
| 3   | M     | 1501 | ATP  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 3   | O     | 1501 | ATP  | C4-N9 | -2.07 | 1.33        | 1.37     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | M     | 1501 | ATP  | C5-C4-N3    | -6.25 | 118.12      | 126.72   |
| 3   | Q     | 1501 | ATP  | C5-C4-N3    | -6.02 | 118.43      | 126.72   |
| 3   | O     | 1501 | ATP  | C5-C4-N3    | -5.71 | 118.86      | 126.72   |
| 3   | M     | 1501 | ATP  | N3-C4-N9    | 4.77  | 135.28      | 127.17   |
| 3   | Q     | 1501 | ATP  | N3-C4-N9    | 4.66  | 135.10      | 127.17   |
| 3   | O     | 1501 | ATP  | N3-C4-N9    | 4.48  | 134.78      | 127.17   |
| 3   | Q     | 1501 | ATP  | C2-N3-C4    | 3.89  | 121.32      | 111.83   |
| 3   | M     | 1501 | ATP  | C2-N3-C4    | 3.83  | 121.19      | 111.83   |
| 3   | O     | 1501 | ATP  | C2-N3-C4    | 3.79  | 121.08      | 111.83   |
| 3   | O     | 1501 | ATP  | N3-C2-N1    | -3.69 | 123.00      | 128.58   |
| 3   | Q     | 1501 | ATP  | N3-C2-N1    | -3.66 | 123.05      | 128.58   |
| 3   | M     | 1501 | ATP  | C4-C5-N7    | -3.46 | 106.63      | 110.58   |
| 3   | Q     | 1501 | ATP  | C4-C5-N7    | -3.42 | 106.68      | 110.58   |
| 3   | O     | 1501 | ATP  | C4-C5-N7    | -3.35 | 106.75      | 110.58   |
| 3   | M     | 1501 | ATP  | N3-C2-N1    | -3.34 | 123.53      | 128.58   |
| 3   | O     | 1501 | ATP  | C4-N9-C8    | 2.72  | 108.59      | 105.74   |
| 3   | Q     | 1501 | ATP  | C5-N7-C8    | 2.49  | 107.36      | 103.45   |
| 3   | O     | 1501 | ATP  | C5-N7-C8    | 2.48  | 107.35      | 103.45   |
| 3   | Q     | 1501 | ATP  | C4-N9-C8    | 2.41  | 108.27      | 105.74   |
| 3   | M     | 1501 | ATP  | C5-N7-C8    | 2.36  | 107.16      | 103.45   |
| 3   | M     | 1501 | ATP  | O4'-C1'-C2' | -2.24 | 101.82      | 106.62   |
| 3   | O     | 1501 | ATP  | N9-C8-N7    | -2.10 | 110.96      | 113.94   |
| 3   | M     | 1501 | ATP  | C4-N9-C8    | 2.06  | 107.91      | 105.74   |
| 3   | O     | 1501 | ATP  | C2-N1-C6    | 2.06  | 122.12      | 118.73   |
| 3   | O     | 1501 | ATP  | O4'-C1'-N9  | 2.04  | 112.01      | 108.09   |
| 3   | O     | 1501 | ATP  | C6-C5-N7    | 2.03  | 136.01      | 132.09   |
| 3   | M     | 1501 | ATP  | O2A-PA-O1A  | 2.03  | 121.88      | 112.44   |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | M     | 1501 | ATP  | C5'-O5'-PA-O3A  |
| 3   | M     | 1501 | ATP  | C4'-C5'-O5'-PA  |
| 3   | O     | 1501 | ATP  | C5'-O5'-PA-O2A  |
| 3   | O     | 1501 | ATP  | C5'-O5'-PA-O3A  |
| 3   | Q     | 1501 | ATP  | C5'-O5'-PA-O3A  |
| 3   | Q     | 1501 | ATP  | O4'-C4'-C5'-O5' |
| 3   | Q     | 1501 | ATP  | C3'-C4'-C5'-O5' |
| 3   | M     | 1501 | ATP  | O4'-C4'-C5'-O5' |
| 3   | M     | 1501 | ATP  | C3'-C4'-C5'-O5' |

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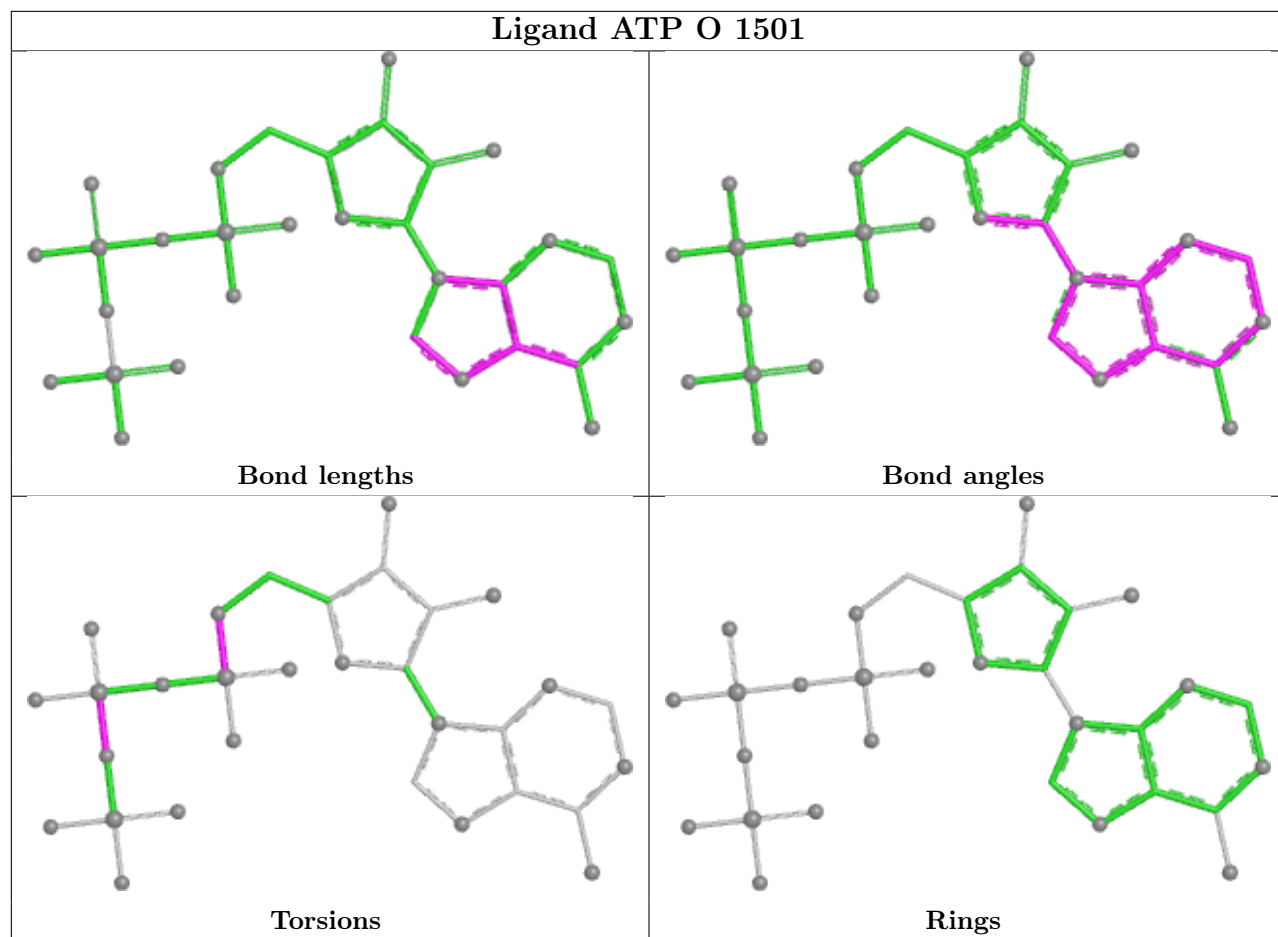
| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | M     | 1501 | ATP  | PB-O3B-PG-O1G  |
| 3   | M     | 1501 | ATP  | PB-O3B-PG-O2G  |
| 3   | M     | 1501 | ATP  | C2'-C1'-N9-C8  |
| 3   | M     | 1501 | ATP  | C5'-O5'-PA-O1A |
| 3   | Q     | 1501 | ATP  | C5'-O5'-PA-O1A |
| 3   | M     | 1501 | ATP  | C2'-C1'-N9-C4  |
| 3   | M     | 1501 | ATP  | O4'-C1'-N9-C8  |
| 3   | O     | 1501 | ATP  | PG-O3B-PB-O2B  |
| 3   | Q     | 1501 | ATP  | PA-O3A-PB-O2B  |

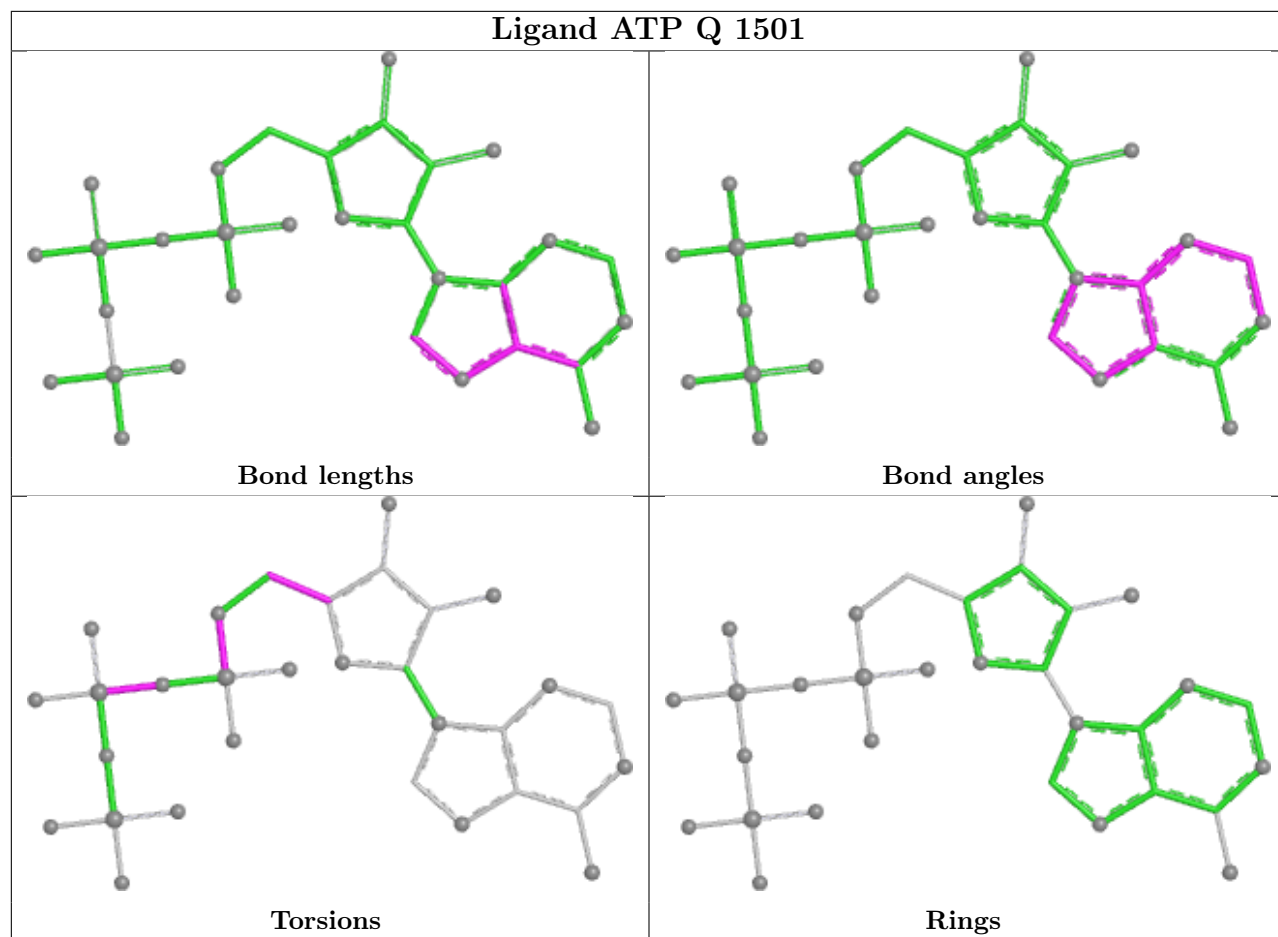
There are no ring outliers.

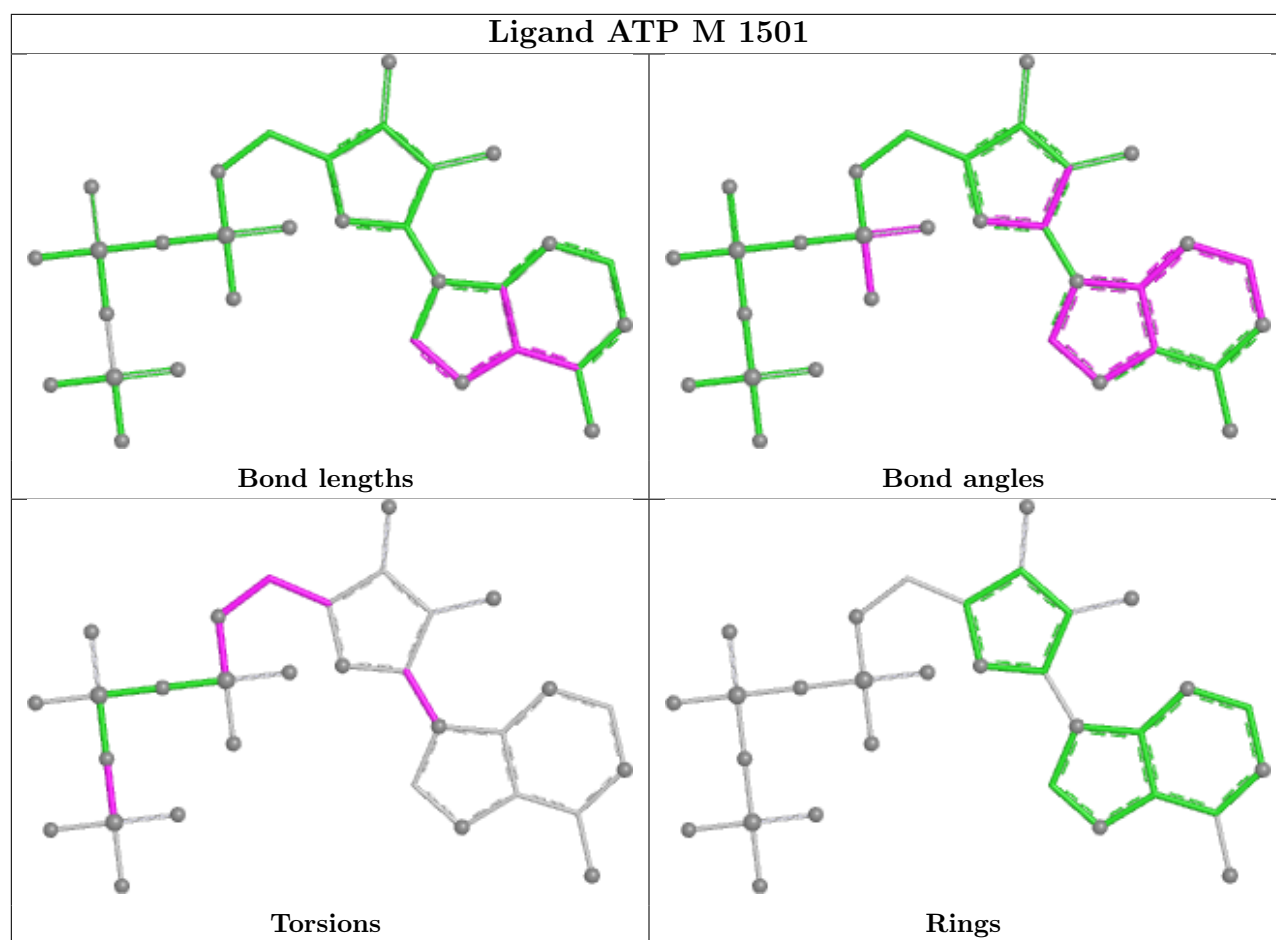
2 monomers are involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | O     | 1501 | ATP  | 1       | 0            |
| 3   | M     | 1501 | ATP  | 2       | 0            |

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

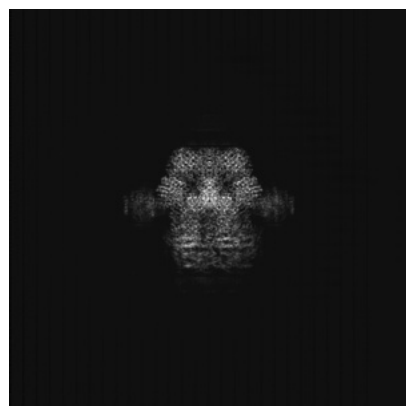
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60127. These allow visual inspection of the internal detail of the map and identification of artifacts.

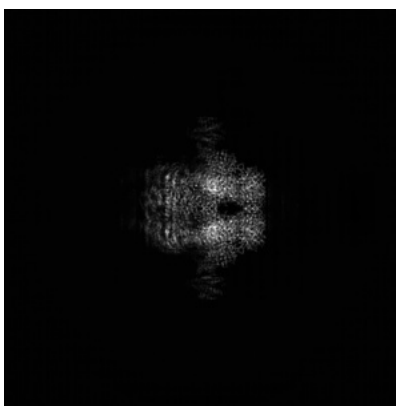
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

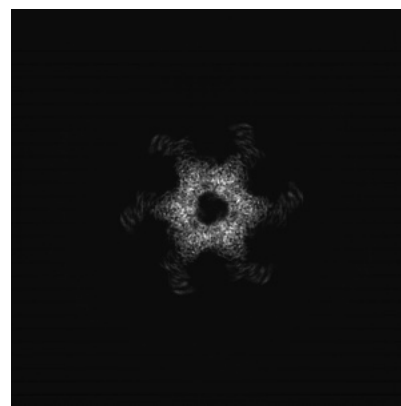
#### 6.1.1 Primary map



X

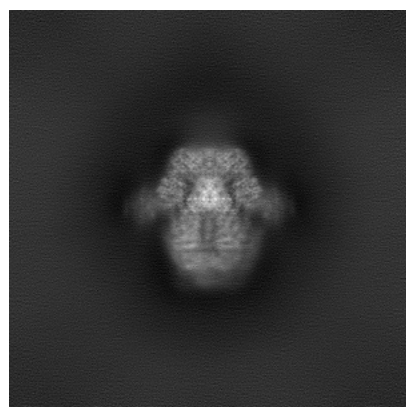


Y

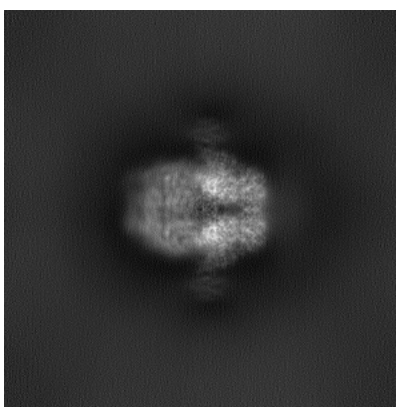


Z

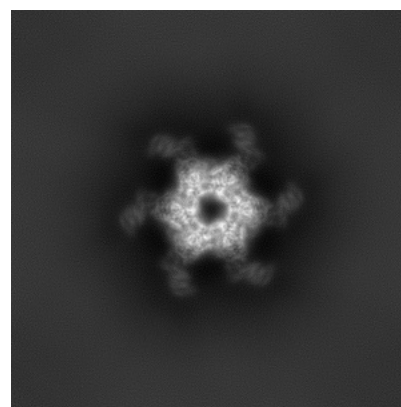
#### 6.1.2 Raw map



X



Y

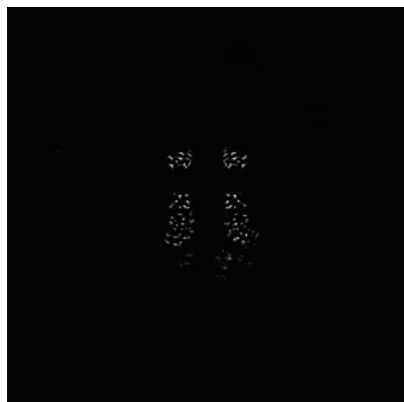


Z

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

## 6.2 Central slices [i](#)

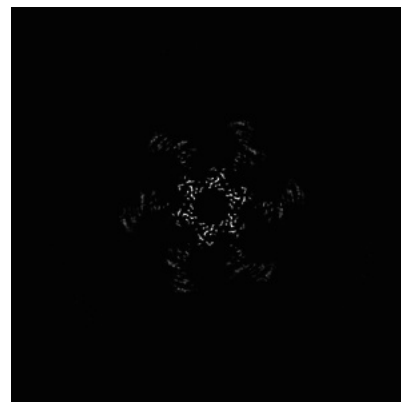
### 6.2.1 Primary map



X Index: 220

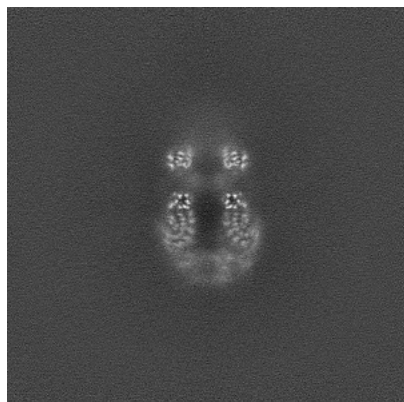


Y Index: 220

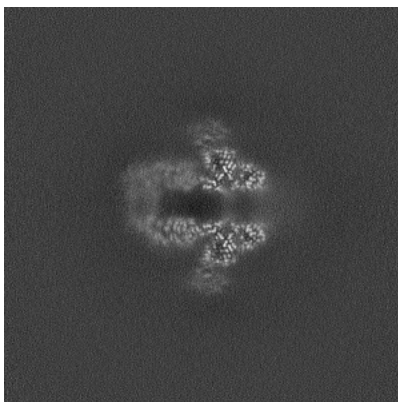


Z Index: 220

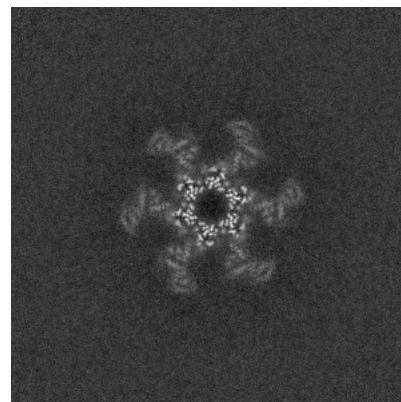
### 6.2.2 Raw map



X Index: 220



Y Index: 220

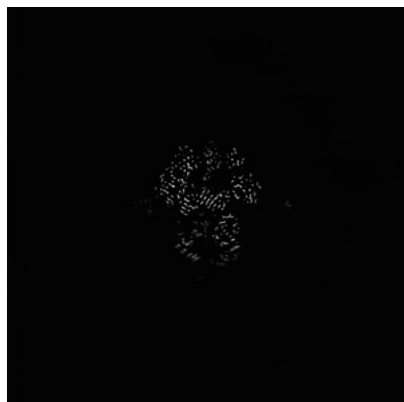


Z Index: 220

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

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

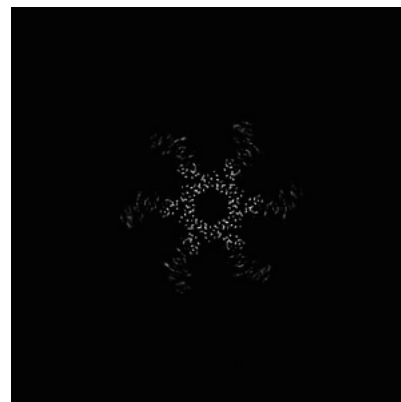
### 6.3.1 Primary map



X Index: 241

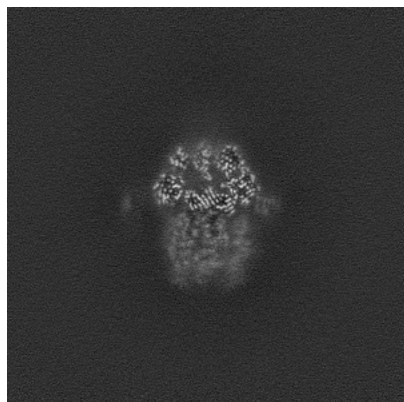


Y Index: 250

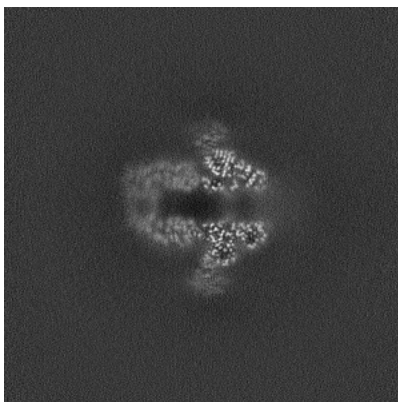


Z Index: 231

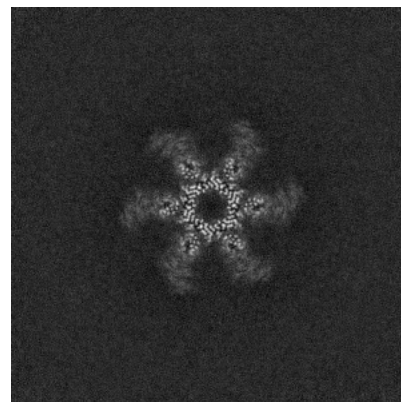
### 6.3.2 Raw map



X Index: 199



Y Index: 218

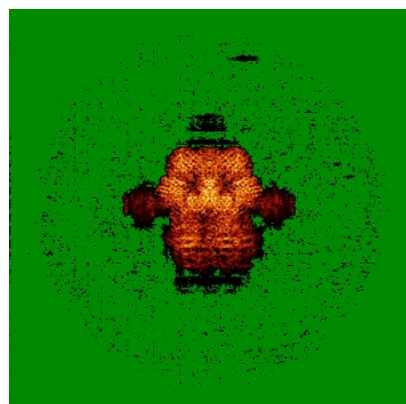


Z Index: 232

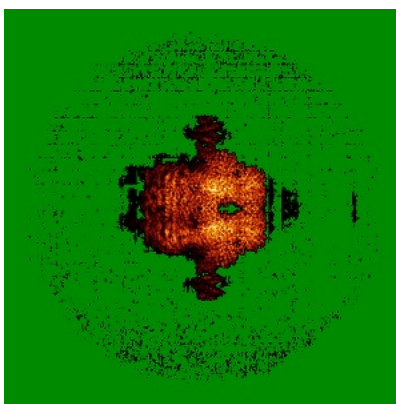
The images above show the largest variance slices of the map in three orthogonal directions.

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

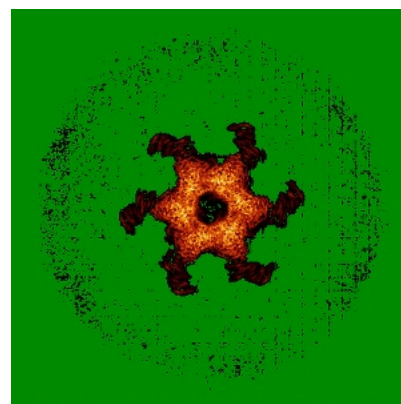
### 6.4.1 Primary map



X

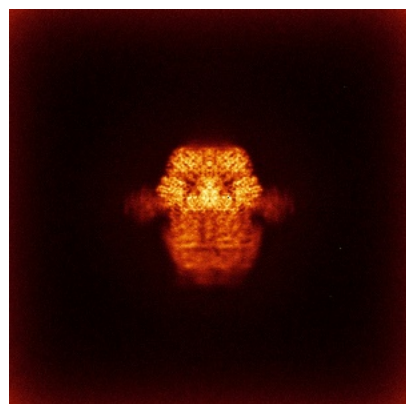


Y

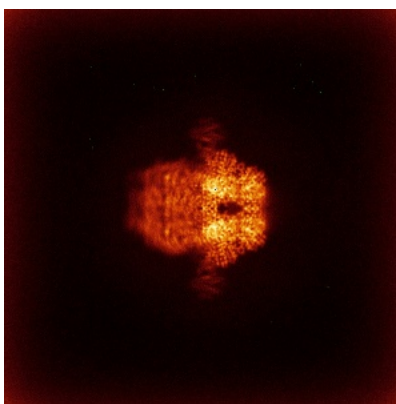


Z

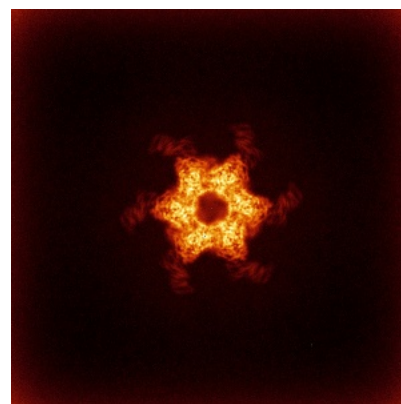
### 6.4.2 Raw map



X



Y

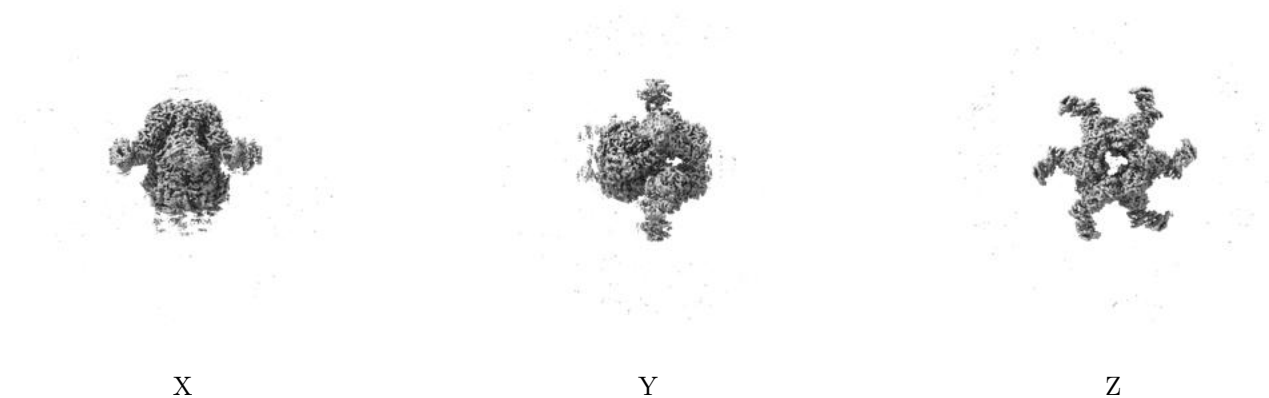


Z

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.

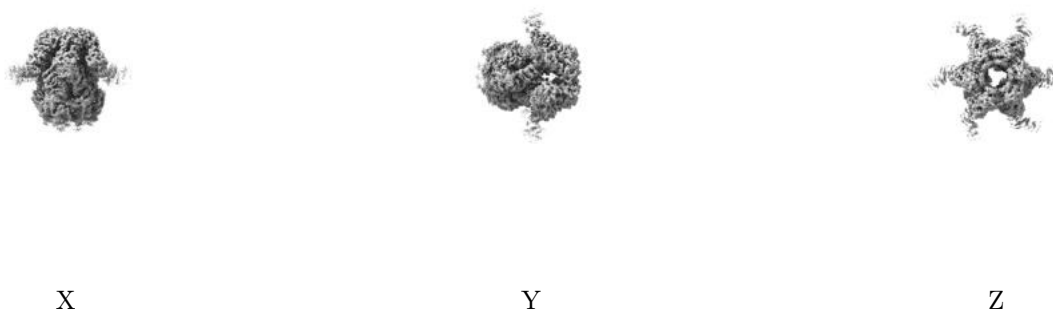
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

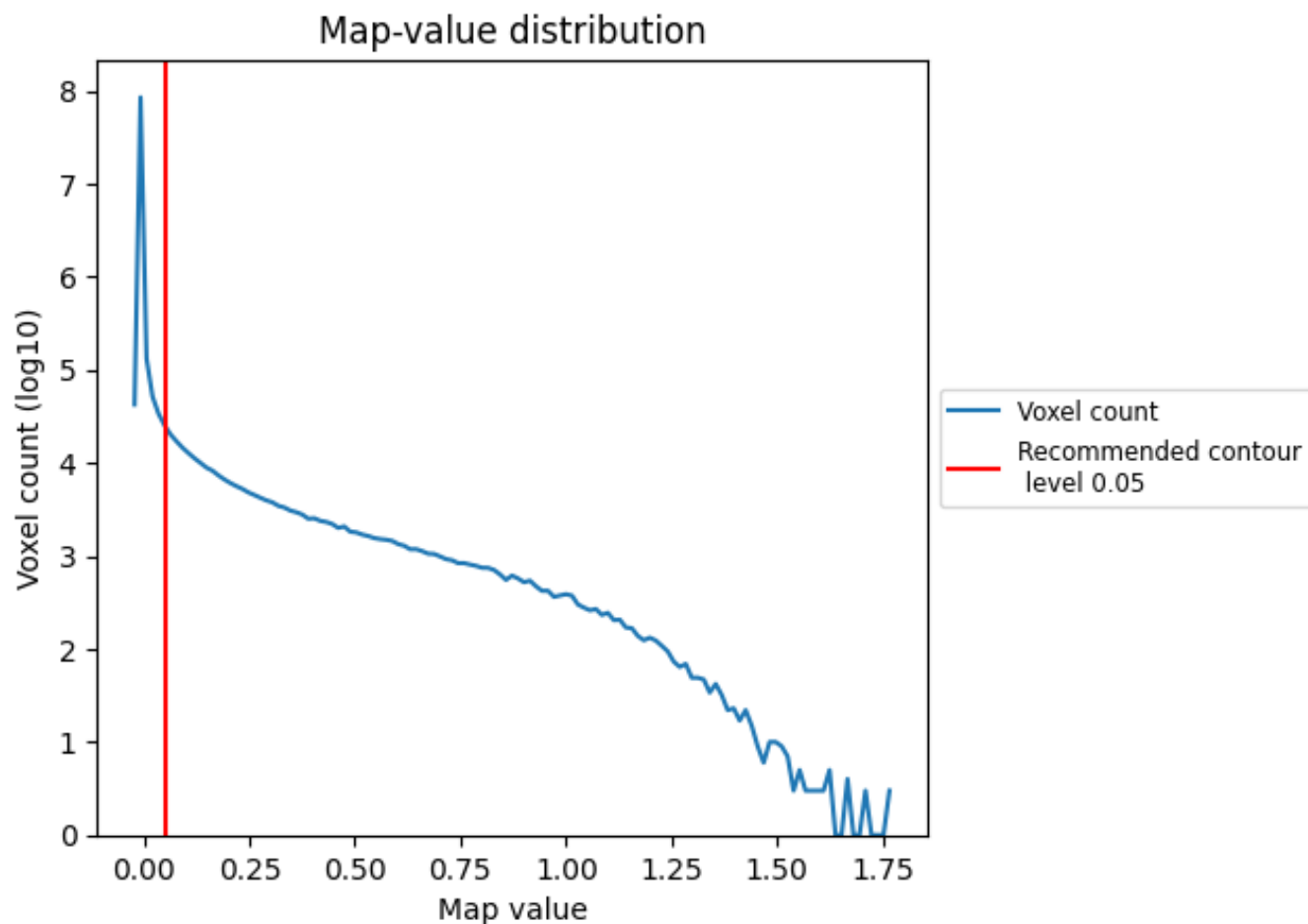
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

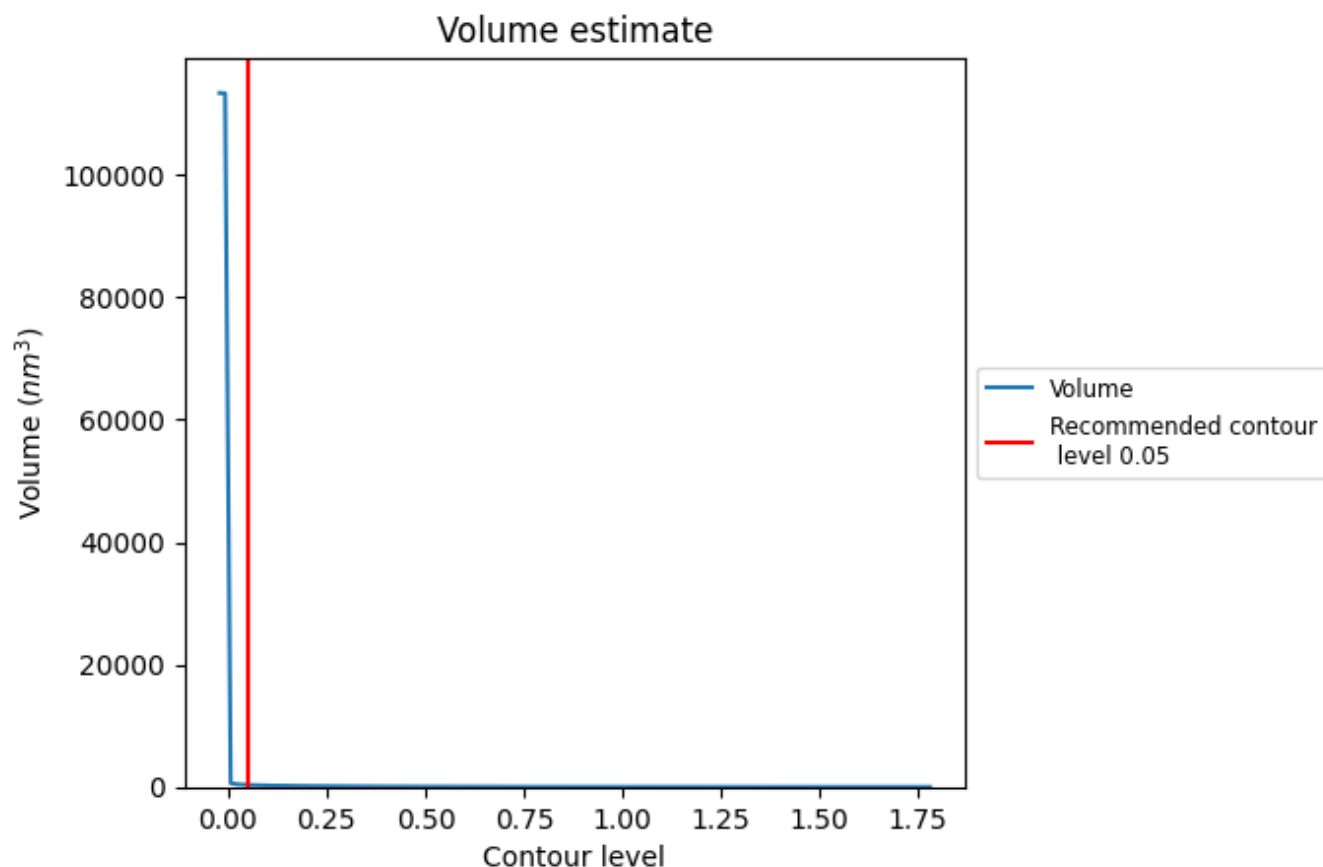
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

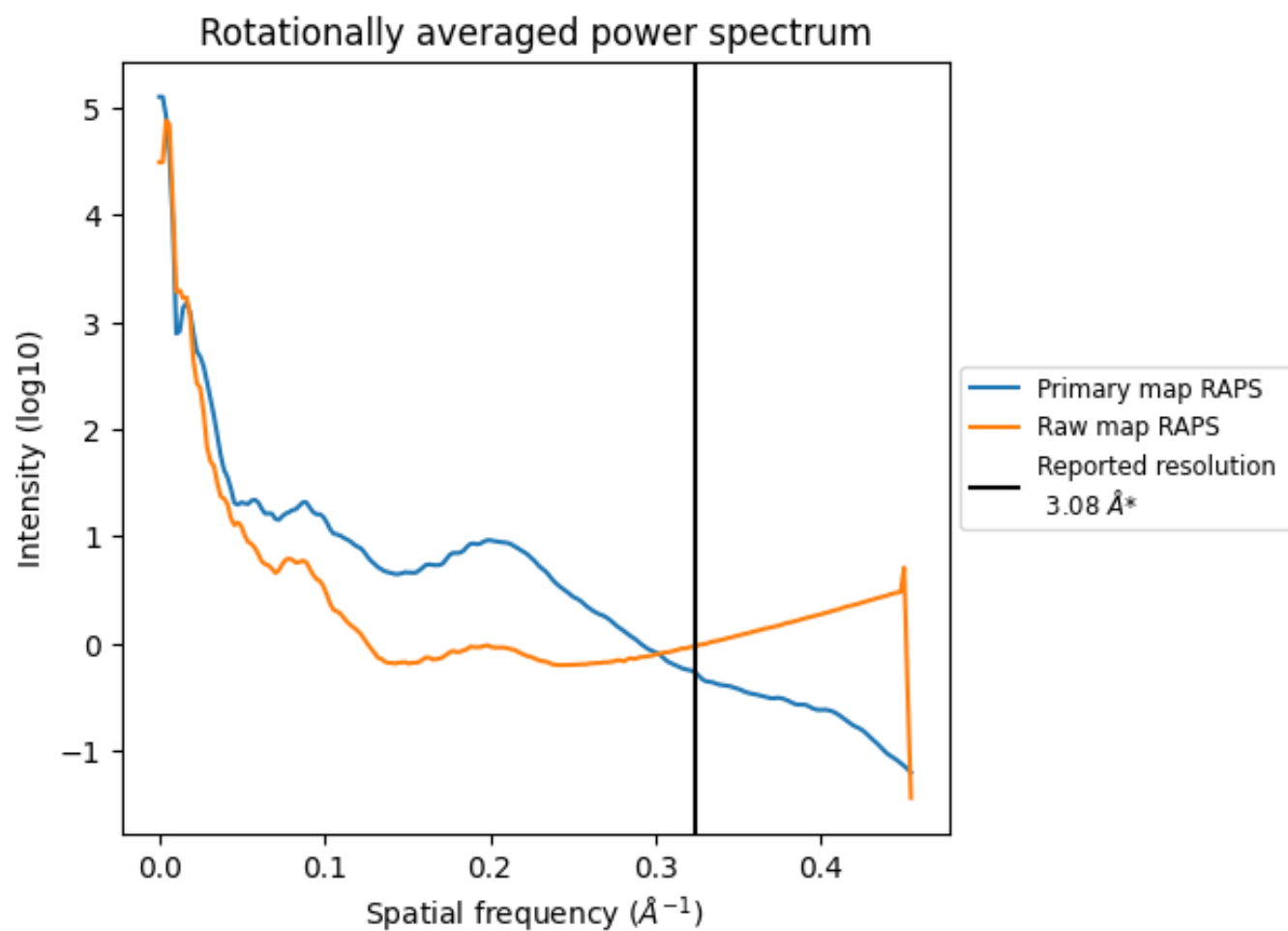
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332  $\text{nm}^3$ ; this corresponds to an approximate mass of 300 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 ⓘ

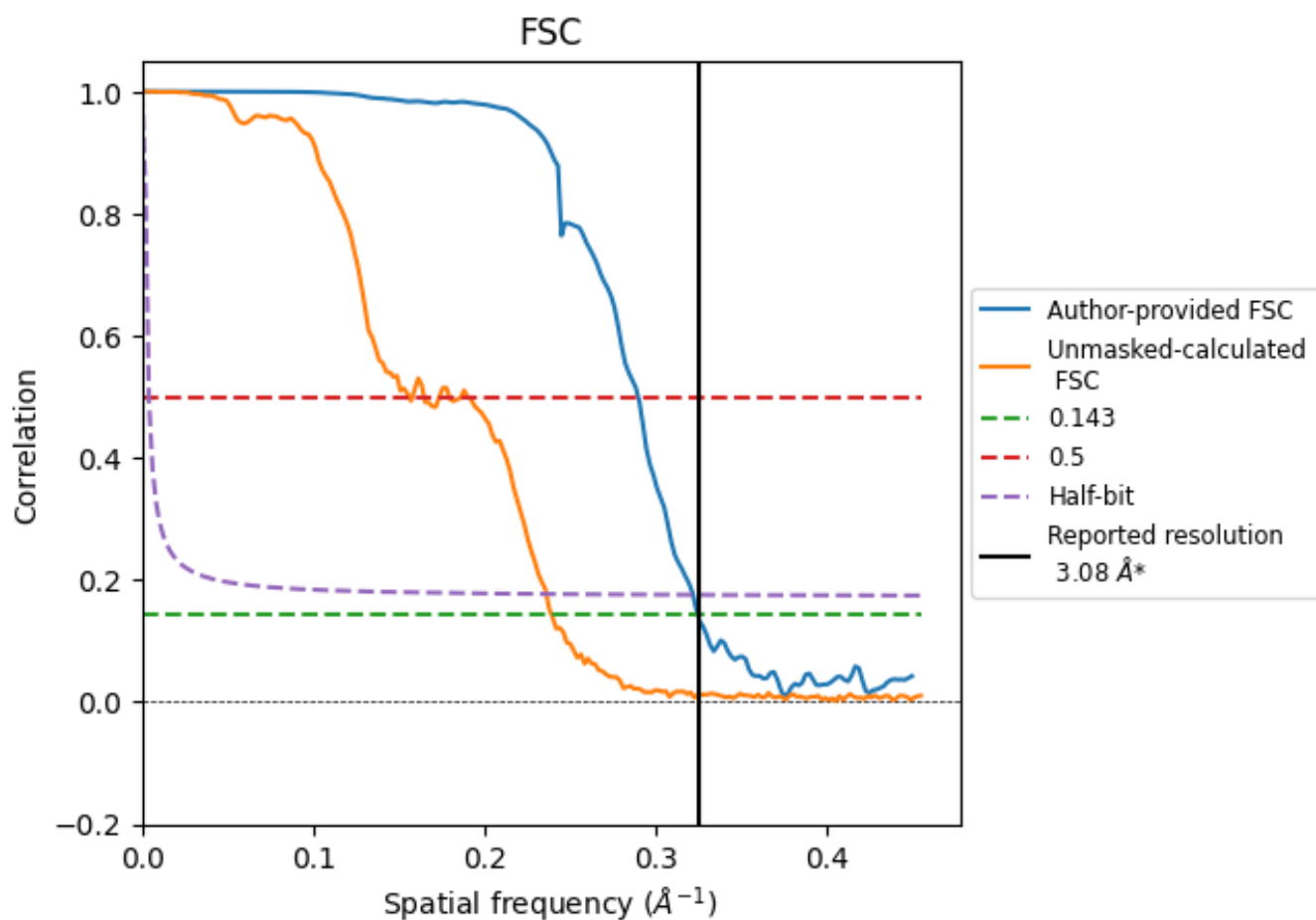


\*Reported resolution corresponds to spatial frequency of  $0.325 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

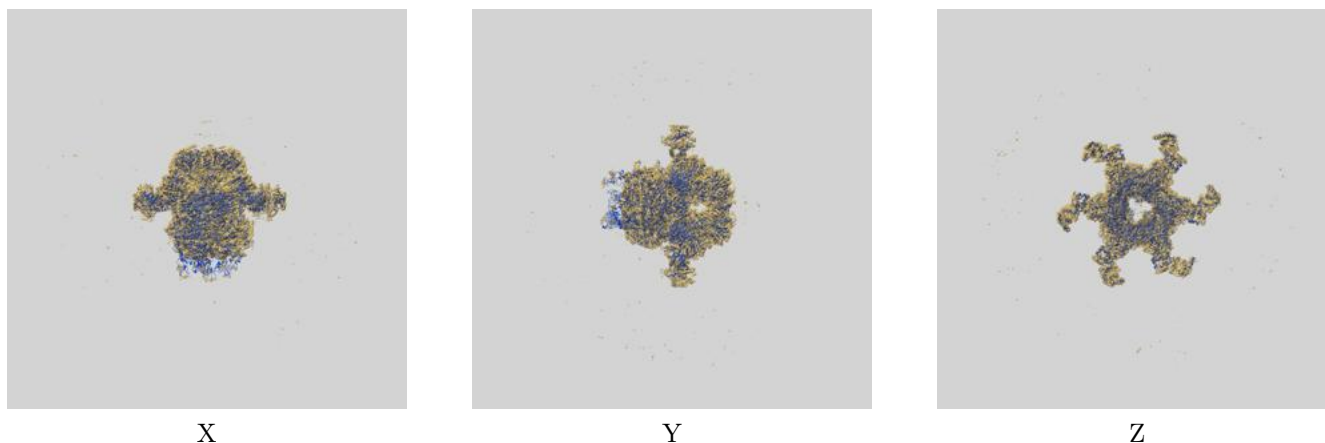
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.08                               | -    | -        |
| Author-provided FSC curve | 3.08                               | 3.45 | 3.11     |
| Unmasked-calculated*      | 4.18                               | 6.42 | 4.24     |

\*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 4.18 differs from the reported value 3.08 by more than 10 %

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

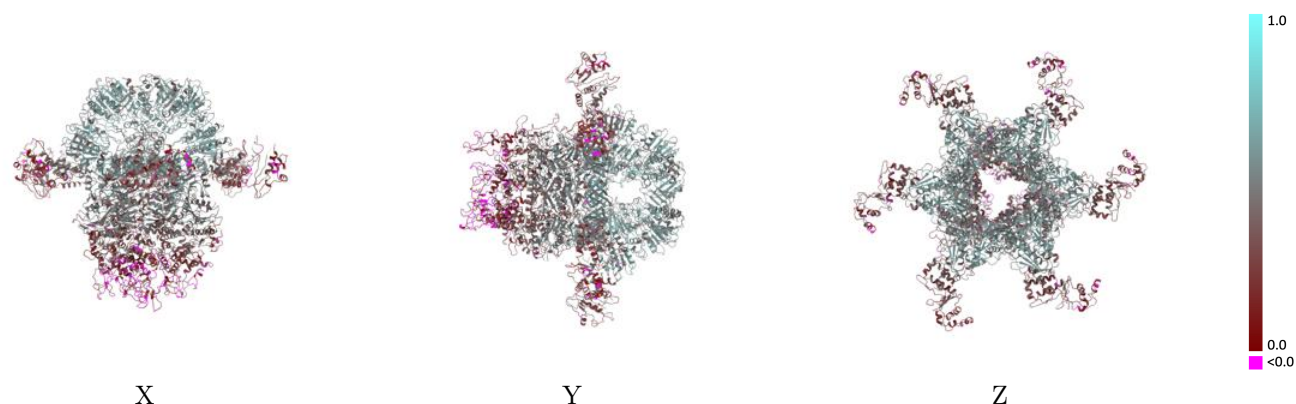
This section contains information regarding the fit between EMDB map EMD-60127 and PDB model 8ZIR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



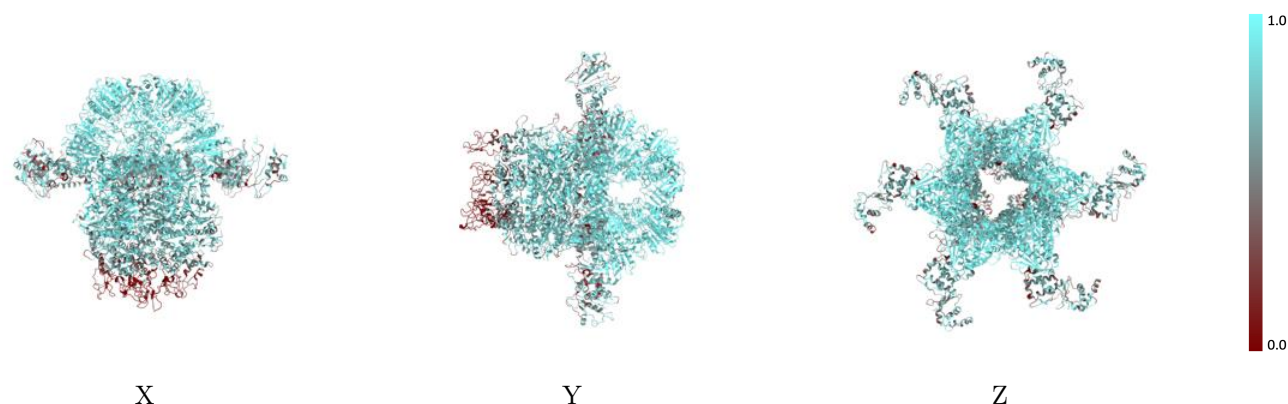
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



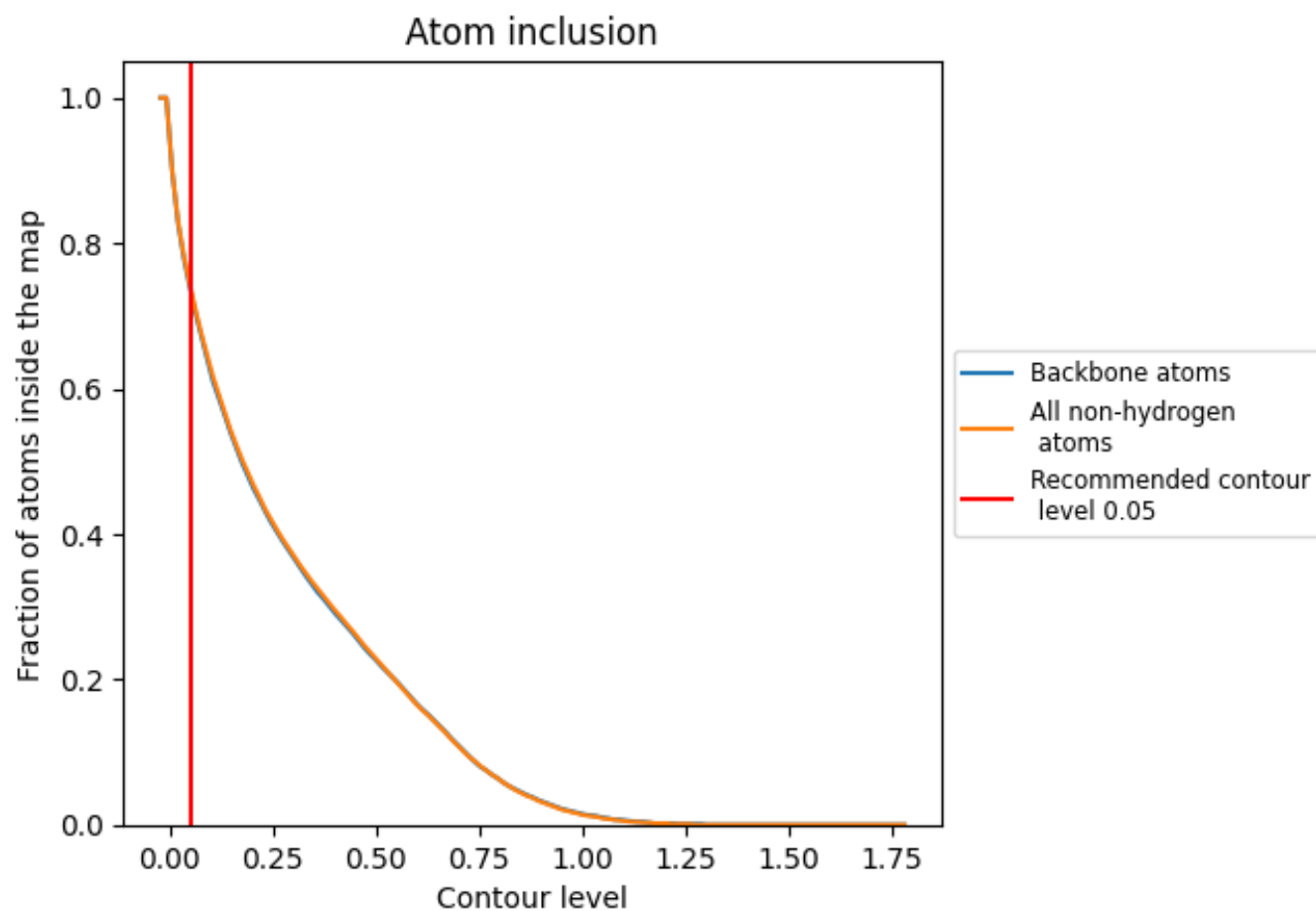
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7410   |  0.4110   |
| A     |  0.7450   |  0.4090   |
| B     |  0.8950   |  0.5380   |
| C     |  0.7570   |  0.4100   |
| D     |  0.8940   |  0.5360   |
| E     |  0.7430   |  0.4090   |
| F     |  0.8890   |  0.5340   |
| G     |  0.7530   |  0.4150   |
| H     |  0.9010   |  0.5390   |
| I     |  0.7450   |  0.4040   |
| J     |  0.8850   |  0.5250   |
| K     |  0.7340   |  0.4060   |
| L     |  0.8920   |  0.5290   |
| M     |  0.7590   |  0.3960   |
| N     |  0.6770  |  0.3560  |
| O     |  0.7590 |  0.3930 |
| P     |  0.6490 |  0.3480 |
| Q     |  0.7470 |  0.3850 |
| R     |  0.6710 |  0.3530 |

