



## Full wwPDB EM Validation Report ⓘ

Jul 21, 2026 – 08:22 AM EDT

PDB ID : 9NQ7 / pdb\_00009nq7  
EMDB ID : EMD-49645  
Title : Cryo-EM structure of Csm/AcrIIIA2/enolase 4:3 complex  
Authors : Goswami, H.N.; Li, H.  
Deposited on : 2025-03-11  
Resolution : 2.72 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:

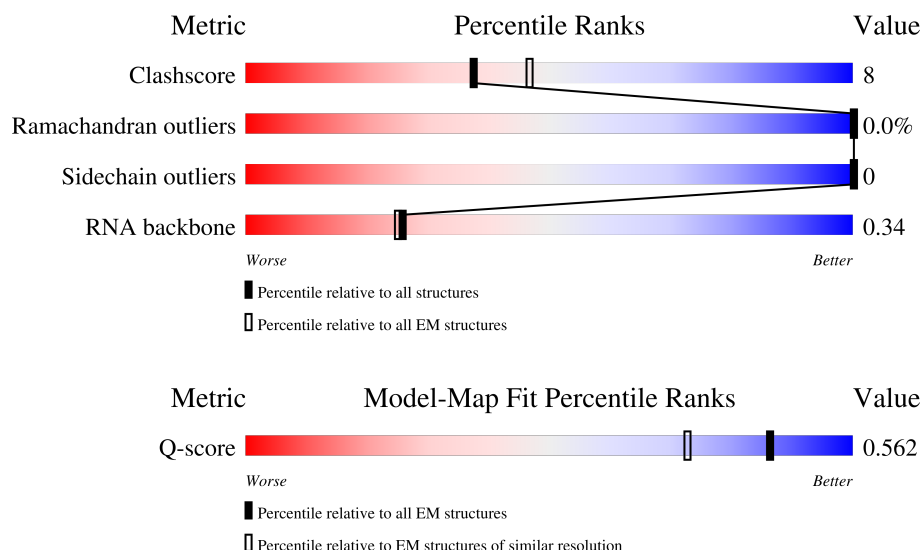
EMDB validation analysis : 0.0.1.dev133  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 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                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 10355 ( 2.22 - 3.22 )                                    |

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   | R     | 41     |                  |
| 2   | H     | 357    |                  |
| 3   | A     | 758    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | B     | 299    |                  |
| 5   | C     | 220    |                  |
| 5   | E     | 220    |                  |
| 5   | F     | 220    |                  |
| 5   | G     | 220    |                  |
| 6   | D     | 136    |                  |
| 6   | I     | 136    |                  |
| 6   | J     | 136    |                  |
| 7   | K     | 434    |                  |
| 7   | L     | 434    |                  |
| 7   | M     | 434    |                  |
| 7   | N     | 434    |                  |
| 7   | O     | 434    |                  |
| 7   | P     | 434    |                  |
| 7   | Q     | 434    |                  |
| 7   | S     | 434    |                  |
| 8   | T     | 105    |                  |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 49556 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA (41-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | R     | 41       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 863   | 389 | 151 | 283 | 40 |         |       |

- Molecule 2 is a protein called CRISPR system Cms protein Csm5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | H     | 352      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2863  | 1843 | 496 | 517 | 7 |         |       |

- Molecule 3 is a protein called CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | A     | 758      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6137  | 3919 | 1026 | 1176 | 16 |         |       |

- Molecule 4 is a protein called CRISPR system Cms protein Csm4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | B     | 297      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2321  | 1485 | 384 | 447 | 5 |         |       |

- Molecule 5 is a protein called CRISPR system Cms endoribonuclease Csm3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | F     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1707  | 1079 | 290 | 336 | 2 |         |       |
| 5   | C     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1711  | 1083 | 292 | 333 | 3 |         |       |
| 5   | E     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1706  | 1079 | 289 | 336 | 2 |         |       |
| 5   | G     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1709  | 1081 | 290 | 336 | 2 |         |       |

- Molecule 6 is a protein called CRISPR system Cms protein Csm2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | D     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 686 | 187 | 203 | 4 |         |       |
| 6   | I     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 686 | 187 | 203 | 4 |         |       |
| 6   | J     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 686 | 187 | 203 | 4 |         |       |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| D     | -5      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| D     | -4      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| D     | -3      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| D     | -2      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| D     | -1      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| D     | 0       | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| I     | -5      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| I     | -4      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| I     | -3      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| I     | -2      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| I     | -1      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| I     | 0       | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| J     | -5      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| J     | -4      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| J     | -3      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| J     | -2      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| J     | -1      | HIS      | -      | expression tag | UNP A0A8D6U6W4 |
| J     | 0       | HIS      | -      | expression tag | UNP A0A8D6U6W4 |

- Molecule 7 is a protein called Enolase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | S     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |
| 7   | L     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |
| 7   | P     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |
| 7   | K     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |
| 7   | M     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | O     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |
| 7   | N     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |
| 7   | Q     | 434      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3305  | 2082 | 557 | 657 | 9 |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| S     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| S     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| L     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| L     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| P     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| P     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| K     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| K     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| M     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| M     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| O     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| O     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| N     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| N     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |
| Q     | 253     | HIS      | ARG    | conflict | UNP Q03LI0 |
| Q     | 257     | GLY      | ASP    | conflict | UNP Q03LI0 |

- Molecule 8 is a protein called AcrIIIA2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | T     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 859   | 543 | 153 | 159 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

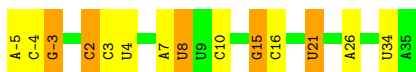
| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| T     | 105     | VAL      | -      | expression tag | UNP A0A3G8FB66 |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

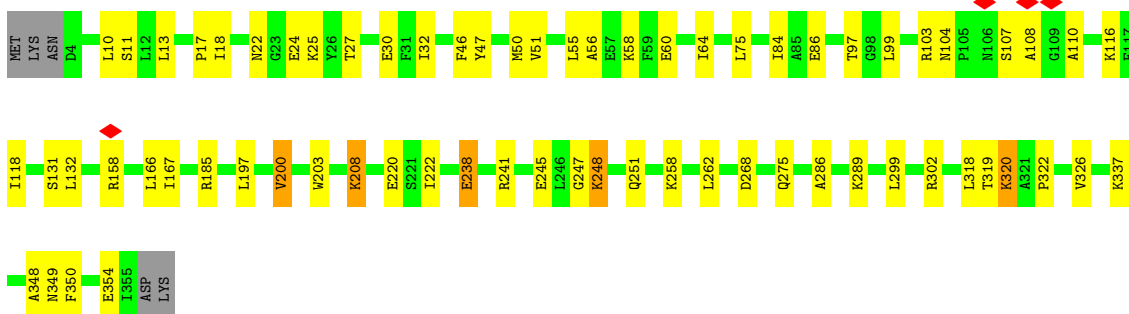
- Molecule 1: RNA (41-MER)

Chain R: 



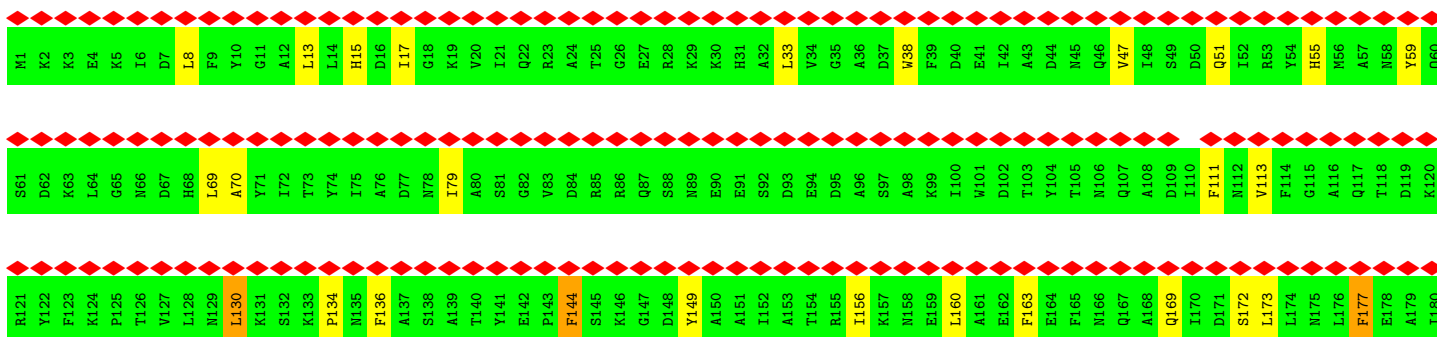
- Molecule 2: CRISPR system Cms protein Csm5

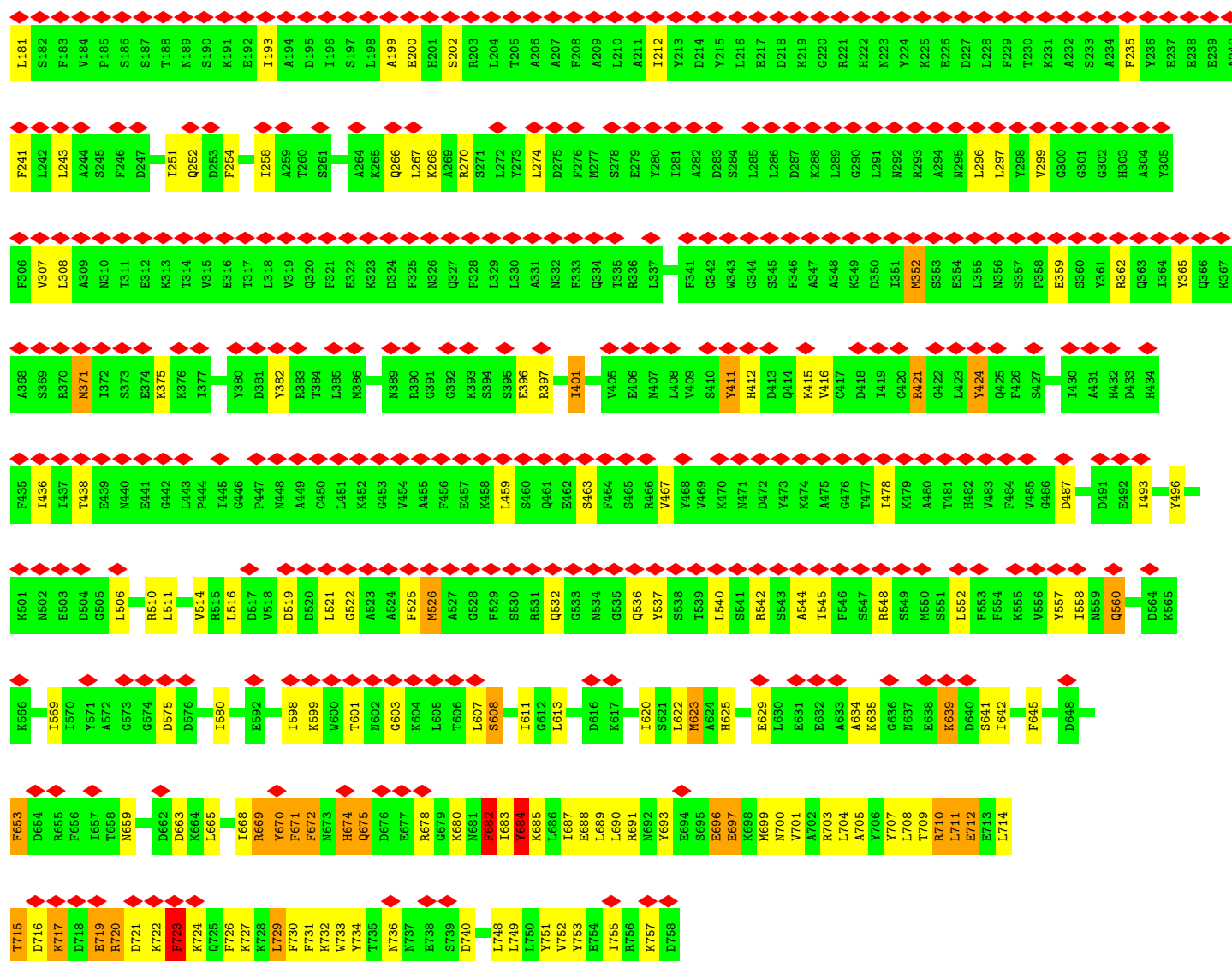
Chain H: 



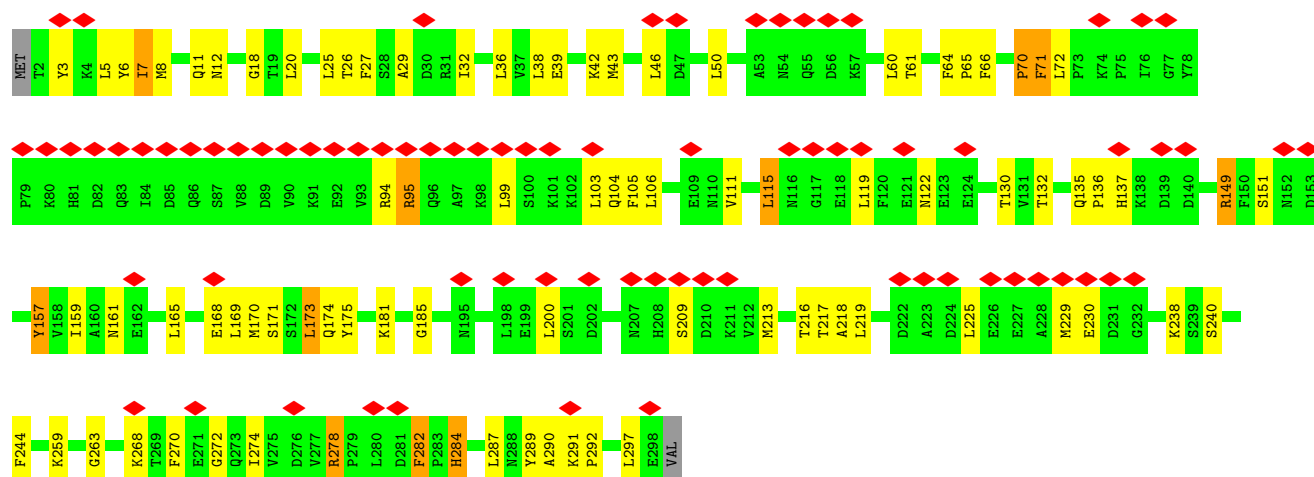
- Molecule 3: CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A)

Chain A: 

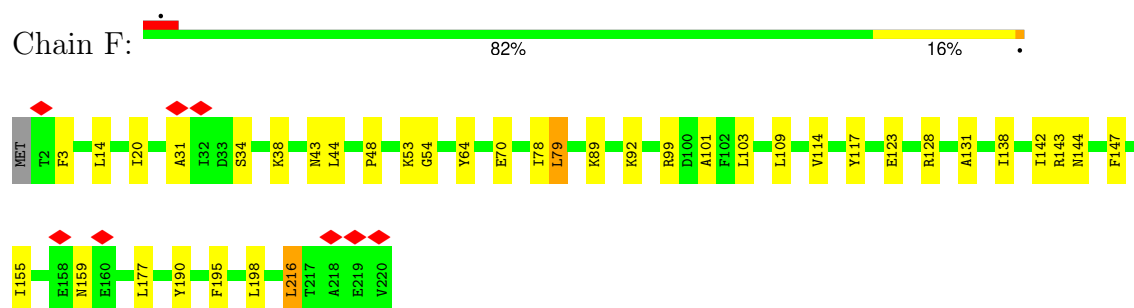




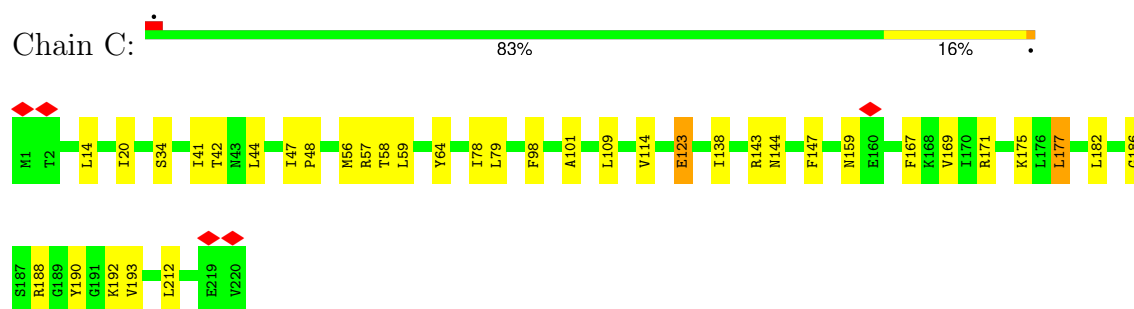
• Molecule 4: CRISPR system Cms protein Csm4



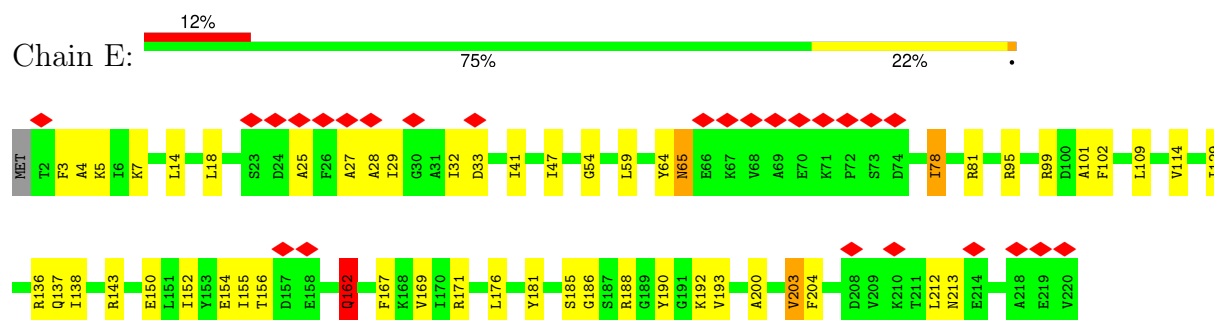
- Molecule 5: CRISPR system Cms endoribonuclease Csm3



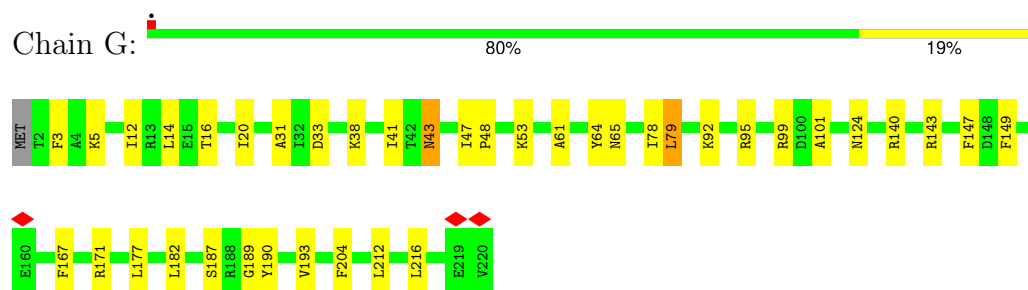
- Molecule 5: CRISPR system Cms endoribonuclease Csm3



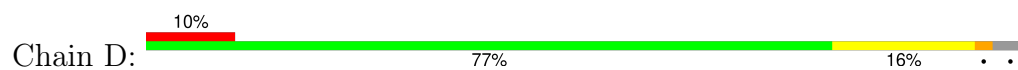
- Molecule 5: CRISPR system Cms endoribonuclease Csm3

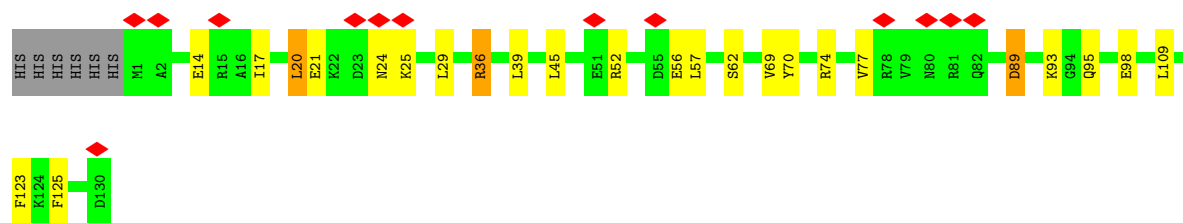


- Molecule 5: CRISPR system Cms endoribonuclease Csm3

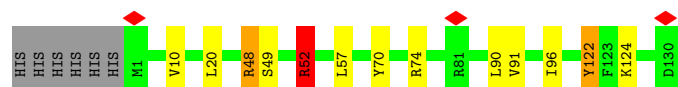
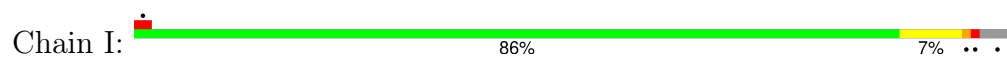


- Molecule 6: CRISPR system Cms protein Csm2

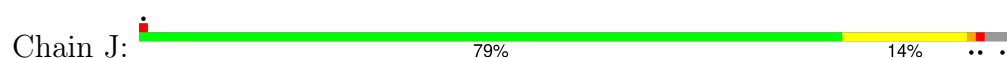




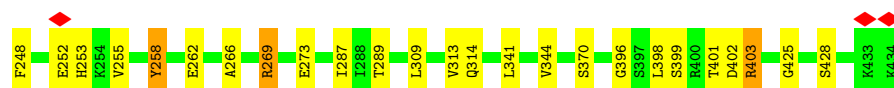
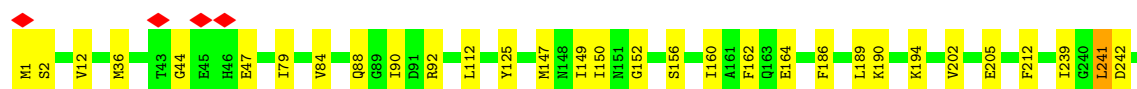
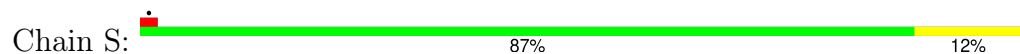
- Molecule 6: CRISPR system Cms protein Csm2



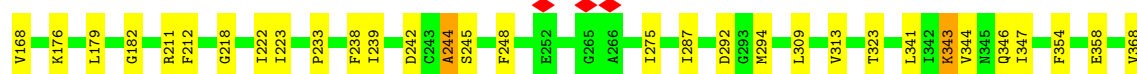
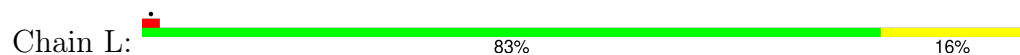
- Molecule 6: CRISPR system Cms protein Csm2



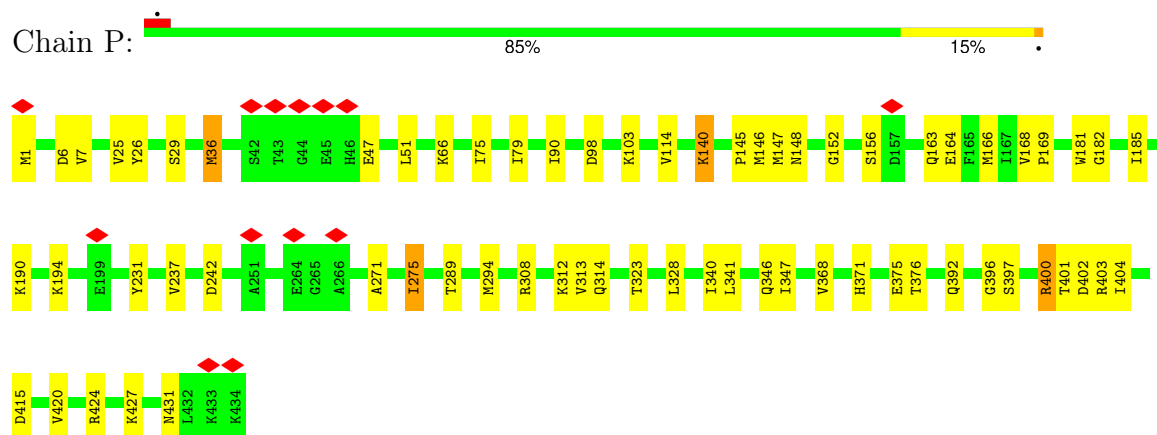
- Molecule 7: Enolase



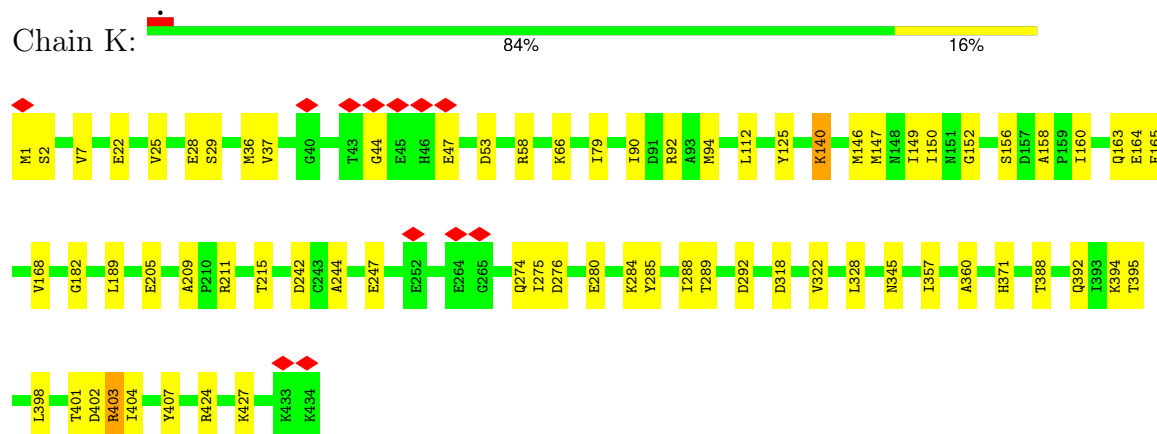
- Molecule 7: Enolase



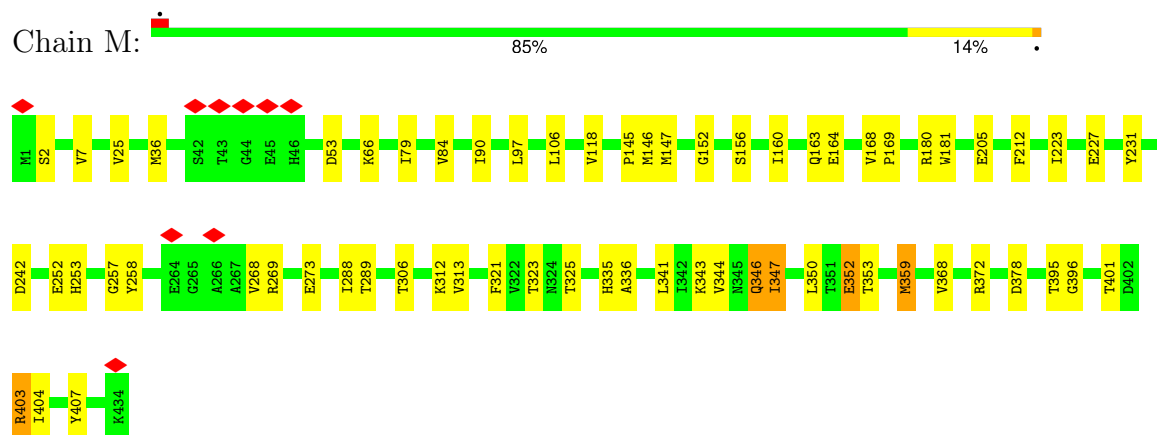
- Molecule 7: Enolase



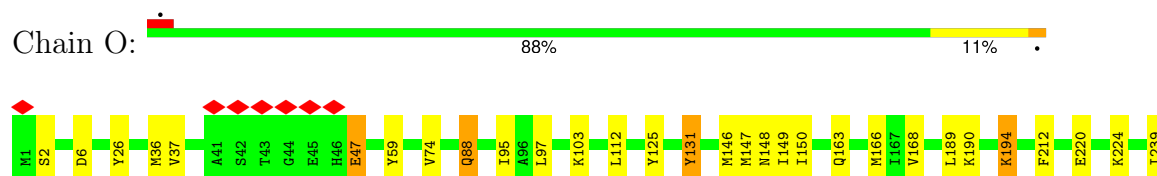
• Molecule 7: Enolase



• Molecule 7: Enolase



• Molecule 7: Enolase

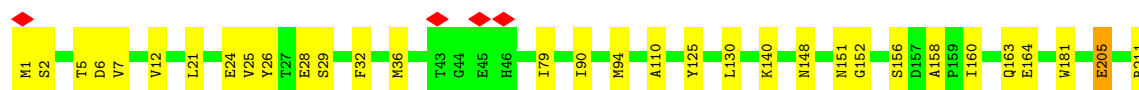
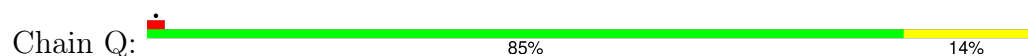




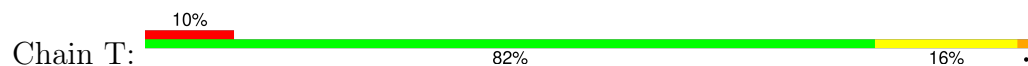
• Molecule 7: Enolase



• Molecule 7: Enolase



• Molecule 8: AcrIIA2



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 325120                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY             | Depositor |
| Microscope                           | TFS KRIOS                       | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                              | Depositor |
| Minimum defocus (nm)                 | 1000                            | Depositor |
| Maximum defocus (nm)                 | 2000                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K3 BIOCONTINUUM (6k x 4k) | Depositor |
| Maximum map value                    | 1.920                           | Depositor |
| Minimum map value                    | -0.716                          | Depositor |
| Average map value                    | 0.009                           | Depositor |
| Map value standard deviation         | 0.033                           | Depositor |
| Recommended contour level            | 0.19                            | Depositor |
| Map size ( $\text{\AA}$ )            | 463.68, 463.68, 463.68          | wwPDB     |
| Map dimensions                       | 560, 560, 560                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.828, 0.828, 0.828             | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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   | R     | 0.36         | 0/964            | 0.52        | 0/1498           |
| 2   | H     | 0.87         | 9/2930 (0.3%)    | 0.87        | 12/3940 (0.3%)   |
| 3   | A     | 0.96         | 50/6264 (0.8%)   | 1.03        | 37/8436 (0.4%)   |
| 4   | B     | 0.87         | 15/2373 (0.6%)   | 0.81        | 8/3215 (0.2%)    |
| 5   | C     | 0.55         | 2/1736 (0.1%)    | 0.62        | 1/2338 (0.0%)    |
| 5   | E     | 0.77         | 4/1731 (0.2%)    | 0.77        | 1/2335 (0.0%)    |
| 5   | F     | 0.54         | 4/1732 (0.2%)    | 0.61        | 1/2335 (0.0%)    |
| 5   | G     | 0.62         | 4/1734 (0.2%)    | 0.69        | 4/2337 (0.2%)    |
| 6   | D     | 0.70         | 3/1095 (0.3%)    | 0.66        | 0/1465           |
| 6   | I     | 0.85         | 4/1095 (0.4%)    | 0.70        | 5/1465 (0.3%)    |
| 6   | J     | 1.01         | 9/1095 (0.8%)    | 1.13        | 15/1465 (1.0%)   |
| 7   | K     | 0.54         | 6/3362 (0.2%)    | 0.59        | 2/4548 (0.0%)    |
| 7   | L     | 0.61         | 7/3362 (0.2%)    | 0.67        | 7/4548 (0.2%)    |
| 7   | M     | 0.54         | 7/3362 (0.2%)    | 0.68        | 8/4548 (0.2%)    |
| 7   | N     | 0.49         | 3/3362 (0.1%)    | 0.60        | 4/4548 (0.1%)    |
| 7   | O     | 0.59         | 9/3362 (0.3%)    | 0.63        | 2/4548 (0.0%)    |
| 7   | P     | 0.53         | 4/3362 (0.1%)    | 0.61        | 4/4548 (0.1%)    |
| 7   | Q     | 0.46         | 3/3362 (0.1%)    | 0.55        | 3/4548 (0.1%)    |
| 7   | S     | 0.46         | 5/3362 (0.1%)    | 0.52        | 1/4548 (0.0%)    |
| 8   | T     | 0.85         | 3/880 (0.3%)     | 0.80        | 2/1184 (0.2%)    |
| All | All   | 0.68         | 151/50525 (0.3%) | 0.73        | 117/68397 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | H     | 0                   | 2                   |
| 3   | A     | 0                   | 8                   |
| 4   | B     | 0                   | 1                   |
| 5   | E     | 0                   | 2                   |
| 6   | D     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | I     | 0                   | 1                   |
| 6   | J     | 0                   | 2                   |
| 7   | L     | 0                   | 1                   |
| 7   | N     | 0                   | 1                   |
| 7   | O     | 0                   | 2                   |
| 7   | P     | 0                   | 1                   |
| 8   | T     | 0                   | 1                   |
| All | All   | 0                   | 23                  |

All (151) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | H     | 167 | ILE  | CA-C    | -28.10 | 1.31        | 1.53     |
| 6   | I     | 48  | ARG  | CB-CG   | -16.55 | 1.02        | 1.52     |
| 3   | A     | 715 | THR  | CB-CG2  | -16.54 | 0.97        | 1.52     |
| 4   | B     | 157 | TYR  | CZ-OH   | -15.29 | 1.05        | 1.38     |
| 3   | A     | 699 | MET  | CB-CG   | -14.36 | 1.09        | 1.52     |
| 5   | E     | 203 | VAL  | CB-CG1  | -13.64 | 1.07        | 1.52     |
| 3   | A     | 130 | LEU  | C-O     | -13.29 | 1.08        | 1.24     |
| 3   | A     | 719 | GLU  | CG-CD   | -13.26 | 1.19        | 1.52     |
| 8   | T     | 98  | MET  | SD-CE   | -13.10 | 1.46        | 1.79     |
| 3   | A     | 719 | GLU  | CD-OE1  | -12.36 | 1.01        | 1.25     |
| 3   | A     | 487 | ASP  | CG-OD1  | -12.18 | 1.02        | 1.25     |
| 6   | I     | 48  | ARG  | CG-CD   | 11.94  | 1.88        | 1.52     |
| 3   | A     | 682 | PHE  | CA-CB   | -11.80 | 1.32        | 1.53     |
| 4   | B     | 95  | ARG  | CZ-NH1  | -11.74 | 1.16        | 1.32     |
| 6   | J     | 17  | ILE  | CG1-CD1 | -11.47 | 1.07        | 1.51     |
| 3   | A     | 696 | GLU  | CD-OE1  | -11.32 | 1.03        | 1.25     |
| 3   | A     | 682 | PHE  | CG-CD1  | 11.02  | 1.61        | 1.38     |
| 6   | J     | 52  | ARG  | NE-CZ   | -10.77 | 1.21        | 1.33     |
| 5   | G     | 216 | LEU  | CG-CD1  | -10.39 | 1.18        | 1.52     |
| 7   | L     | 36  | MET  | SD-CE   | -10.35 | 1.53        | 1.79     |
| 3   | A     | 268 | LYS  | CD-CE   | -10.29 | 1.21        | 1.52     |
| 7   | K     | 244 | ALA  | CA-CB   | -10.10 | 1.36        | 1.53     |
| 6   | I     | 52  | ARG  | CZ-NH1  | -10.04 | 1.18        | 1.32     |
| 2   | H     | 167 | ILE  | N-CA    | 10.02  | 1.53        | 1.46     |
| 8   | T     | 44  | LYS  | CE-NZ   | -9.92  | 1.19        | 1.49     |
| 2   | H     | 167 | ILE  | C-N     | 9.53   | 1.46        | 1.33     |
| 7   | L     | 5   | THR  | CB-CG2  | -9.37  | 1.21        | 1.52     |
| 6   | J     | 52  | ARG  | CD-NE   | -9.35  | 1.33        | 1.46     |
| 3   | A     | 684 | TYR  | CA-C    | -9.21  | 1.41        | 1.52     |
| 6   | J     | 14  | GLU  | CD-OE1  | -9.04  | 1.08        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | J     | 60  | ASP  | CG-OD1  | -9.03 | 1.08        | 1.25     |
| 3   | A     | 723 | PHE  | CD2-CE2 | -8.86 | 1.12        | 1.38     |
| 3   | A     | 684 | TYR  | C-O     | -8.81 | 1.13        | 1.24     |
| 3   | A     | 421 | ARG  | CZ-NH1  | -8.80 | 1.20        | 1.32     |
| 7   | K     | 392 | GLN  | CD-NE2  | -8.78 | 1.14        | 1.33     |
| 7   | O     | 347 | ILE  | CG1-CD1 | -8.37 | 1.19        | 1.51     |
| 3   | A     | 421 | ARG  | CG-CD   | -8.34 | 1.27        | 1.52     |
| 6   | D     | 20  | LEU  | CG-CD1  | -8.22 | 1.25        | 1.52     |
| 3   | A     | 672 | PHE  | CE1-CZ  | -8.13 | 1.14        | 1.38     |
| 6   | J     | 48  | ARG  | CZ-NH1  | -8.04 | 1.21        | 1.32     |
| 7   | N     | 334 | GLU  | CD-OE1  | -8.01 | 1.10        | 1.25     |
| 7   | S     | 252 | GLU  | CD-OE1  | -7.99 | 1.10        | 1.25     |
| 7   | P     | 294 | MET  | SD-CE   | -7.95 | 1.59        | 1.79     |
| 7   | O     | 247 | GLU  | CD-OE1  | -7.80 | 1.10        | 1.25     |
| 3   | A     | 421 | ARG  | NE-CZ   | -7.71 | 1.24        | 1.33     |
| 3   | A     | 401 | ILE  | CG1-CD1 | -7.66 | 1.21        | 1.51     |
| 3   | A     | 560 | GLN  | CD-NE2  | -7.64 | 1.17        | 1.33     |
| 7   | L     | 294 | MET  | SD-CE   | -7.62 | 1.60        | 1.79     |
| 5   | C     | 123 | GLU  | CD-OE1  | -7.60 | 1.10        | 1.25     |
| 3   | A     | 712 | GLU  | CG-CD   | -7.52 | 1.33        | 1.52     |
| 3   | A     | 639 | LYS  | CE-NZ   | -7.48 | 1.26        | 1.49     |
| 2   | H     | 248 | LYS  | CD-CE   | -7.47 | 1.30        | 1.52     |
| 7   | L     | 244 | ALA  | CA-CB   | -7.42 | 1.41        | 1.53     |
| 4   | B     | 282 | PHE  | CE2-CZ  | -7.36 | 1.16        | 1.38     |
| 3   | A     | 688 | GLU  | CD-OE1  | -7.24 | 1.11        | 1.25     |
| 4   | B     | 157 | TYR  | CD1-CE1 | -7.10 | 1.17        | 1.38     |
| 7   | Q     | 398 | LEU  | CG-CD2  | -7.08 | 1.29        | 1.52     |
| 3   | A     | 371 | MET  | SD-CE   | -7.07 | 1.61        | 1.79     |
| 2   | H     | 167 | ILE  | C-O     | 7.06  | 1.33        | 1.24     |
| 3   | A     | 144 | PHE  | CD1-CE1 | -6.86 | 1.18        | 1.38     |
| 6   | J     | 48  | ARG  | CZ-NH2  | -6.84 | 1.24        | 1.33     |
| 5   | C     | 159 | ASN  | CG-OD1  | -6.75 | 1.10        | 1.23     |
| 7   | M     | 223 | ILE  | CG1-CD1 | -6.71 | 1.25        | 1.51     |
| 3   | A     | 674 | HIS  | CA-CB   | -6.69 | 1.43        | 1.53     |
| 7   | M     | 163 | GLN  | CD-NE2  | -6.65 | 1.19        | 1.33     |
| 3   | A     | 560 | GLN  | CD-OE1  | -6.63 | 1.10        | 1.23     |
| 5   | F     | 216 | LEU  | CG-CD1  | -6.60 | 1.30        | 1.52     |
| 5   | G     | 79  | LEU  | CG-CD1  | -6.58 | 1.30        | 1.52     |
| 3   | A     | 552 | LEU  | CG-CD1  | -6.56 | 1.30        | 1.52     |
| 4   | B     | 278 | ARG  | CG-CD   | -6.51 | 1.32        | 1.52     |
| 7   | P     | 36  | MET  | SD-CE   | -6.49 | 1.63        | 1.79     |
| 7   | O     | 241 | LEU  | CG-CD2  | -6.45 | 1.31        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 86  | GLU  | CD-OE2  | -6.43 | 1.13        | 1.25     |
| 7   | S     | 241 | LEU  | CG-CD2  | -6.39 | 1.31        | 1.52     |
| 4   | B     | 70  | PRO  | N-CD    | 6.37  | 1.56        | 1.47     |
| 4   | B     | 157 | TYR  | CE1-CZ  | -6.36 | 1.23        | 1.38     |
| 7   | O     | 291 | GLU  | CD-OE1  | -6.34 | 1.13        | 1.25     |
| 7   | K     | 140 | LYS  | CD-CE   | -6.34 | 1.33        | 1.52     |
| 7   | M     | 227 | GLU  | CD-OE1  | -6.33 | 1.13        | 1.25     |
| 7   | S     | 403 | ARG  | CG-CD   | -6.26 | 1.33        | 1.52     |
| 3   | A     | 682 | PHE  | CB-CG   | 6.23  | 1.65        | 1.50     |
| 3   | A     | 266 | GLN  | CB-CG   | -6.21 | 1.33        | 1.52     |
| 7   | N     | 252 | GLU  | CG-CD   | -6.21 | 1.36        | 1.52     |
| 3   | A     | 177 | PHE  | CD2-CE2 | -6.16 | 1.20        | 1.38     |
| 3   | A     | 675 | GLN  | CB-CG   | -6.12 | 1.34        | 1.52     |
| 7   | L     | 22  | GLU  | CD-OE2  | -6.09 | 1.13        | 1.25     |
| 5   | F     | 159 | ASN  | CG-OD1  | -6.06 | 1.12        | 1.23     |
| 5   | E     | 65  | ASN  | CG-ND2  | -6.06 | 1.20        | 1.33     |
| 6   | J     | 48  | ARG  | CG-CD   | -6.03 | 1.34        | 1.52     |
| 3   | A     | 308 | LEU  | CG-CD1  | -6.01 | 1.32        | 1.52     |
| 7   | M     | 347 | ILE  | CB-CG1  | -6.01 | 1.41        | 1.53     |
| 3   | A     | 177 | PHE  | CE1-CZ  | -6.01 | 1.20        | 1.38     |
| 8   | T     | 73  | LYS  | CD-CE   | -6.00 | 1.34        | 1.52     |
| 2   | H     | 208 | LYS  | CE-NZ   | -6.00 | 1.31        | 1.49     |
| 3   | A     | 723 | PHE  | CE1-CZ  | -6.00 | 1.20        | 1.38     |
| 6   | D     | 89  | ASP  | CG-OD1  | -5.97 | 1.14        | 1.25     |
| 7   | P     | 140 | LYS  | CD-CE   | -5.91 | 1.34        | 1.52     |
| 4   | B     | 7   | ILE  | CG1-CD1 | -5.91 | 1.28        | 1.51     |
| 7   | S     | 269 | ARG  | CZ-NH1  | -5.90 | 1.24        | 1.32     |
| 3   | A     | 599 | LYS  | CD-CE   | -5.89 | 1.34        | 1.52     |
| 2   | H     | 200 | VAL  | CB-CG1  | -5.88 | 1.33        | 1.52     |
| 7   | M     | 252 | GLU  | CB-CG   | -5.86 | 1.34        | 1.52     |
| 3   | A     | 682 | PHE  | CG-CD2  | 5.84  | 1.51        | 1.38     |
| 7   | L     | 403 | ARG  | CZ-NH1  | -5.82 | 1.24        | 1.32     |
| 5   | G     | 65  | ASN  | CG-OD1  | -5.80 | 1.12        | 1.23     |
| 7   | O     | 194 | LYS  | CE-NZ   | -5.79 | 1.31        | 1.49     |
| 4   | B     | 282 | PHE  | CG-CD2  | -5.78 | 1.26        | 1.38     |
| 3   | A     | 711 | LEU  | CG-CD2  | -5.73 | 1.33        | 1.52     |
| 7   | L     | 358 | GLU  | CD-OE1  | -5.69 | 1.14        | 1.25     |
| 3   | A     | 697 | GLU  | CD-OE1  | -5.67 | 1.14        | 1.25     |
| 5   | E     | 65  | ASN  | CB-CG   | -5.61 | 1.38        | 1.52     |
| 3   | A     | 623 | MET  | SD-CE   | -5.58 | 1.65        | 1.79     |
| 7   | O     | 244 | ALA  | CA-CB   | -5.57 | 1.44        | 1.53     |
| 7   | M     | 252 | GLU  | CG-CD   | -5.55 | 1.38        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | K     | 275 | ILE  | CG1-CD1 | -5.54 | 1.30        | 1.51     |
| 3   | A     | 424 | TYR  | CZ-OH   | -5.48 | 1.26        | 1.38     |
| 7   | P     | 415 | ASP  | CG-OD2  | -5.47 | 1.15        | 1.25     |
| 4   | B     | 132 | THR  | CB-CG2  | -5.45 | 1.34        | 1.52     |
| 3   | A     | 729 | LEU  | CB-CG   | -5.44 | 1.42        | 1.53     |
| 7   | Q     | 151 | ASN  | CB-CG   | -5.44 | 1.38        | 1.52     |
| 6   | J     | 122 | TYR  | CB-CG   | -5.42 | 1.39        | 1.51     |
| 4   | B     | 278 | ARG  | CB-CG   | -5.42 | 1.36        | 1.52     |
| 3   | A     | 653 | PHE  | CE1-CZ  | -5.40 | 1.22        | 1.38     |
| 5   | G     | 43  | ASN  | CG-OD1  | -5.40 | 1.13        | 1.23     |
| 3   | A     | 670 | TYR  | CZ-OH   | 5.36  | 1.49        | 1.38     |
| 4   | B     | 70  | PRO  | N-CA    | -5.35 | 1.40        | 1.47     |
| 4   | B     | 157 | TYR  | CE2-CZ  | -5.34 | 1.25        | 1.38     |
| 6   | D     | 14  | GLU  | CD-OE2  | -5.34 | 1.15        | 1.25     |
| 3   | A     | 671 | PHE  | C-O     | -5.34 | 1.17        | 1.24     |
| 4   | B     | 230 | GLU  | CD-OE1  | -5.33 | 1.15        | 1.25     |
| 5   | F     | 43  | ASN  | CG-OD1  | -5.31 | 1.13        | 1.23     |
| 3   | A     | 411 | TYR  | CA-CB   | -5.27 | 1.43        | 1.53     |
| 7   | N     | 88  | GLN  | CD-OE1  | -5.27 | 1.13        | 1.23     |
| 7   | O     | 88  | GLN  | CD-OE1  | -5.25 | 1.13        | 1.23     |
| 3   | A     | 653 | PHE  | CD2-CE2 | -5.24 | 1.23        | 1.38     |
| 3   | A     | 526 | MET  | SD-CE   | -5.22 | 1.66        | 1.79     |
| 3   | A     | 653 | PHE  | CG-CD2  | -5.18 | 1.27        | 1.38     |
| 7   | O     | 131 | TYR  | CD2-CE2 | -5.18 | 1.23        | 1.38     |
| 6   | I     | 122 | TYR  | CE1-CZ  | -5.15 | 1.25        | 1.38     |
| 2   | H     | 354 | GLU  | CD-OE1  | -5.13 | 1.15        | 1.25     |
| 3   | A     | 608 | SER  | CA-CB   | -5.13 | 1.43        | 1.53     |
| 7   | K     | 274 | GLN  | CG-CD   | -5.11 | 1.39        | 1.52     |
| 7   | Q     | 205 | GLU  | CD-OE2  | -5.07 | 1.15        | 1.25     |
| 4   | B     | 200 | LEU  | CG-CD2  | -5.07 | 1.35        | 1.52     |
| 7   | O     | 346 | GLN  | CB-CG   | -5.06 | 1.37        | 1.52     |
| 3   | A     | 200 | GLU  | CG-CD   | -5.06 | 1.39        | 1.52     |
| 7   | S     | 258 | TYR  | CE2-CZ  | -5.05 | 1.26        | 1.38     |
| 7   | K     | 392 | GLN  | CG-CD   | -5.05 | 1.39        | 1.52     |
| 5   | F     | 79  | LEU  | CG-CD1  | -5.03 | 1.35        | 1.52     |
| 7   | M     | 325 | THR  | CB-CG2  | -5.01 | 1.36        | 1.52     |
| 5   | E     | 78  | ILE  | CG1-CD1 | -5.00 | 1.32        | 1.51     |

All (117) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | A     | 699 | MET  | CA-CB-CG | 27.82 | 169.75      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | H     | 167 | ILE  | O-C-N      | -20.70 | 106.85      | 121.55   |
| 2   | H     | 167 | ILE  | CA-C-O     | 20.30  | 130.49      | 119.12   |
| 3   | A     | 723 | PHE  | CZ-CE2-CD2 | 18.59  | 153.46      | 120.00   |
| 3   | A     | 696 | GLU  | OE1-CD-OE2 | -17.49 | 80.92       | 122.90   |
| 3   | A     | 684 | TYR  | CA-C-O     | -17.02 | 102.38      | 120.42   |
| 3   | A     | 699 | MET  | N-CA-CB    | 16.93  | 136.85      | 110.44   |
| 6   | J     | 48  | ARG  | NH1-CZ-NH2 | -15.68 | 98.92       | 119.30   |
| 3   | A     | 723 | PHE  | CG-CD2-CE2 | -15.59 | 94.19       | 120.70   |
| 2   | H     | 326 | VAL  | CG1-CB-CG2 | -15.44 | 76.83       | 110.80   |
| 3   | A     | 711 | LEU  | CB-CG-CD2  | -14.35 | 67.66       | 110.70   |
| 3   | A     | 672 | PHE  | CE1-CZ-CE2 | 13.82  | 144.87      | 120.00   |
| 3   | A     | 723 | PHE  | CE1-CZ-CE2 | -13.56 | 95.58       | 120.00   |
| 3   | A     | 688 | GLU  | CG-CD-OE1  | -12.49 | 89.67       | 118.40   |
| 6   | J     | 48  | ARG  | CD-NE-CZ   | -12.47 | 106.94      | 124.40   |
| 6   | J     | 60  | ASP  | CB-CG-OD2  | 12.14  | 146.33      | 118.40   |
| 6   | J     | 48  | ARG  | CG-CD-NE   | 11.99  | 138.37      | 112.00   |
| 3   | A     | 696 | GLU  | CG-CD-OE2  | 11.47  | 144.78      | 118.40   |
| 3   | A     | 699 | MET  | CB-CA-C    | -10.85 | 87.52       | 109.55   |
| 6   | J     | 52  | ARG  | NE-CZ-NH2  | -10.78 | 109.50      | 119.20   |
| 6   | J     | 60  | ASP  | OD1-CG-OD2 | -10.36 | 98.04       | 122.90   |
| 7   | M     | 252 | GLU  | CG-CD-OE2  | -10.19 | 94.97       | 118.40   |
| 3   | A     | 674 | HIS  | CA-CB-CG   | 10.17  | 123.97      | 113.80   |
| 3   | A     | 421 | ARG  | NE-CZ-NH1  | -9.10  | 112.41      | 121.50   |
| 4   | B     | 278 | ARG  | CG-CD-NE   | 8.82   | 131.41      | 112.00   |
| 2   | H     | 326 | VAL  | CA-CB-CG2  | -8.39  | 96.14       | 110.40   |
| 7   | P     | 275 | ILE  | CA-CB-CG2  | -8.38  | 96.26       | 110.50   |
| 6   | I     | 48  | ARG  | CB-CG-CD   | 8.18   | 130.11      | 111.30   |
| 6   | I     | 52  | ARG  | NE-CZ-NH1  | -8.06  | 113.44      | 121.50   |
| 2   | H     | 167 | ILE  | CA-C-N     | 7.95   | 127.94      | 119.76   |
| 2   | H     | 167 | ILE  | C-N-CA     | 7.95   | 127.94      | 119.76   |
| 3   | A     | 401 | ILE  | CB-CG1-CD1 | -7.82  | 97.38       | 113.80   |
| 3   | A     | 688 | GLU  | OE1-CD-OE2 | 7.78   | 141.56      | 122.90   |
| 6   | J     | 52  | ARG  | CB-CG-CD   | -7.55  | 93.93       | 111.30   |
| 8   | T     | 98  | MET  | CG-SD-CE   | 7.50   | 117.40      | 100.90   |
| 6   | J     | 17  | ILE  | CB-CG1-CD1 | -7.38  | 98.30       | 113.80   |
| 7   | P     | 415 | ASP  | CB-CG-OD2  | -7.27  | 101.68      | 118.40   |
| 8   | T     | 73  | LYS  | CD-CE-NZ   | 7.10   | 134.61      | 111.90   |
| 3   | A     | 545 | THR  | CA-CB-CG2  | 7.00   | 122.40      | 110.50   |
| 3   | A     | 672 | PHE  | CD1-CE1-CZ | -6.99  | 107.41      | 120.00   |
| 3   | A     | 352 | MET  | CG-SD-CE   | -6.90  | 85.72       | 100.90   |
| 7   | K     | 403 | ARG  | CB-CG-CD   | 6.86   | 127.07      | 111.30   |
| 3   | A     | 421 | ARG  | CD-NE-CZ   | -6.85  | 114.81      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | A     | 371 | MET  | CG-SD-CE   | -6.81 | 85.91       | 100.90   |
| 7   | L     | 403 | ARG  | CB-CG-CD   | 6.79  | 126.92      | 111.30   |
| 3   | A     | 699 | MET  | CB-CG-SD   | -6.79 | 92.33       | 112.70   |
| 5   | E     | 162 | GLN  | CG-CD-NE2  | -6.57 | 106.54      | 116.40   |
| 7   | M     | 403 | ARG  | CB-CG-CD   | 6.56  | 126.38      | 111.30   |
| 6   | I     | 52  | ARG  | NH1-CZ-NH2 | -6.54 | 110.80      | 119.30   |
| 6   | J     | 52  | ARG  | CD-NE-CZ   | 6.50  | 133.51      | 124.40   |
| 6   | I     | 48  | ARG  | N-CA-CB    | -6.50 | 99.81       | 110.40   |
| 6   | J     | 57  | LEU  | CB-CG-CD2  | -6.47 | 91.28       | 110.70   |
| 4   | B     | 149 | ARG  | CG-CD-NE   | 6.44  | 126.16      | 112.00   |
| 3   | A     | 684 | TYR  | CA-C-N     | 6.40  | 128.86      | 120.28   |
| 3   | A     | 684 | TYR  | C-N-CA     | 6.40  | 128.86      | 120.28   |
| 7   | N     | 296 | GLU  | OE1-CD-OE2 | -6.37 | 107.61      | 122.90   |
| 7   | M     | 359 | MET  | CG-SD-CE   | -6.36 | 86.91       | 100.90   |
| 6   | J     | 52  | ARG  | NE-CZ-NH1  | -6.34 | 115.16      | 121.50   |
| 2   | H     | 166 | LEU  | CA-C-N     | -6.28 | 118.33      | 122.60   |
| 2   | H     | 166 | LEU  | C-N-CA     | -6.28 | 118.33      | 122.60   |
| 7   | M     | 253 | HIS  | N-CA-CB    | 6.24  | 119.99      | 110.44   |
| 7   | P     | 294 | MET  | CG-SD-CE   | -6.18 | 87.31       | 100.90   |
| 3   | A     | 712 | GLU  | O-C-N      | -6.13 | 113.85      | 122.06   |
| 3   | A     | 130 | LEU  | O-C-N      | -6.11 | 115.64      | 122.12   |
| 3   | A     | 675 | GLN  | CB-CG-CD   | 6.11  | 122.98      | 112.60   |
| 3   | A     | 699 | MET  | CG-SD-CE   | -6.07 | 87.55       | 100.90   |
| 3   | A     | 712 | GLU  | CA-C-O     | 6.05  | 127.90      | 119.80   |
| 7   | L     | 358 | GLU  | CG-CD-OE1  | -6.04 | 104.52      | 118.40   |
| 6   | I     | 52  | ARG  | NE-CZ-NH2  | 6.03  | 124.63      | 119.20   |
| 7   | L     | 343 | LYS  | CG-CD-CE   | 5.93  | 124.94      | 111.30   |
| 4   | B     | 284 | HIS  | O-C-N      | -5.92 | 114.74      | 122.97   |
| 3   | A     | 672 | PHE  | CZ-CE2-CD2 | -5.89 | 109.40      | 120.00   |
| 3   | A     | 70  | ALA  | N-CA-CB    | 5.84  | 119.33      | 110.28   |
| 4   | B     | 71  | PHE  | O-C-N      | -5.84 | 115.81      | 123.16   |
| 7   | O     | 346 | GLN  | CG-CD-NE2  | -5.76 | 107.75      | 116.40   |
| 6   | J     | 52  | ARG  | NH1-CZ-NH2 | 5.66  | 126.66      | 119.30   |
| 2   | H     | 320 | LYS  | CG-CD-CE   | 5.65  | 124.29      | 111.30   |
| 6   | J     | 48  | ARG  | CB-CG-CD   | -5.63 | 98.35       | 111.30   |
| 6   | J     | 48  | ARG  | NE-CZ-NH2  | 5.61  | 124.25      | 119.20   |
| 7   | L     | 403 | ARG  | CG-CD-NE   | 5.57  | 124.24      | 112.00   |
| 7   | N     | 296 | GLU  | CG-CD-OE2  | 5.54  | 131.15      | 118.40   |
| 2   | H     | 302 | ARG  | CG-CD-NE   | -5.53 | 99.83       | 112.00   |
| 5   | F     | 38  | LYS  | CG-CD-CE   | 5.53  | 124.02      | 111.30   |
| 7   | Q     | 401 | THR  | OG1-CB-CG2 | 5.53  | 120.36      | 109.30   |
| 2   | H     | 238 | GLU  | CB-CG-CD   | 5.53  | 122.00      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | B     | 157 | TYR  | CE1-CZ-CE2 | 5.51  | 131.32      | 120.30   |
| 5   | G     | 61  | ALA  | CA-C-N     | -5.47 | 113.51      | 122.54   |
| 5   | G     | 61  | ALA  | C-N-CA     | -5.47 | 113.51      | 122.54   |
| 7   | M     | 346 | GLN  | N-CA-C     | -5.46 | 106.29      | 113.17   |
| 4   | B     | 115 | LEU  | CB-CG-CD1  | -5.38 | 94.56       | 110.70   |
| 3   | A     | 684 | TYR  | O-C-N      | 5.35  | 128.25      | 122.15   |
| 7   | N     | 334 | GLU  | CG-CD-OE2  | 5.34  | 130.68      | 118.40   |
| 7   | L     | 36  | MET  | CG-SD-CE   | 5.33  | 112.62      | 100.90   |
| 5   | C     | 177 | LEU  | CB-CG-CD1  | -5.30 | 94.79       | 110.70   |
| 4   | B     | 173 | LEU  | CD1-CG-CD2 | -5.29 | 99.16       | 110.80   |
| 4   | B     | 278 | ARG  | CD-NE-CZ   | -5.27 | 117.02      | 124.40   |
| 7   | O     | 47  | GLU  | OE1-CD-OE2 | -5.27 | 110.25      | 122.90   |
| 7   | M     | 321 | PHE  | CB-CA-C    | -5.26 | 102.38      | 111.23   |
| 7   | M     | 352 | GLU  | CB-CA-C    | 5.26  | 120.97      | 109.99   |
| 7   | N     | 319 | ASP  | CA-CB-CG   | 5.26  | 117.86      | 112.60   |
| 7   | P     | 415 | ASP  | CB-CG-OD1  | 5.24  | 130.46      | 118.40   |
| 3   | A     | 719 | GLU  | CG-CD-OE2  | -5.22 | 106.40      | 118.40   |
| 3   | A     | 696 | GLU  | CG-CD-OE1  | 5.15  | 130.25      | 118.40   |
| 7   | L     | 358 | GLU  | CG-CD-OE2  | 5.14  | 130.23      | 118.40   |
| 7   | L     | 354 | PHE  | CA-C-O     | -5.12 | 115.45      | 120.82   |
| 6   | J     | 52  | ARG  | CG-CD-NE   | 5.12  | 123.26      | 112.00   |
| 5   | G     | 216 | LEU  | CD1-CG-CD2 | -5.11 | 99.56       | 110.80   |
| 7   | S     | 252 | GLU  | CG-CD-OE2  | 5.11  | 130.14      | 118.40   |
| 5   | G     | 177 | LEU  | CB-CG-CD1  | -5.10 | 95.39       | 110.70   |
| 3   | A     | 688 | GLU  | CB-CG-CD   | 5.10  | 121.27      | 112.60   |
| 2   | H     | 326 | VAL  | CA-CB-CG1  | 5.05  | 118.98      | 110.40   |
| 3   | A     | 623 | MET  | CG-SD-CE   | -5.05 | 89.80       | 100.90   |
| 7   | M     | 347 | ILE  | CB-CG1-CD1 | 5.03  | 124.37      | 113.80   |
| 3   | A     | 682 | PHE  | CA-CB-CG   | -5.03 | 108.77      | 113.80   |
| 7   | Q     | 205 | GLU  | CG-CD-OE1  | 5.03  | 129.96      | 118.40   |
| 7   | K     | 392 | GLN  | CG-CD-NE2  | -5.03 | 108.86      | 116.40   |
| 7   | Q     | 399 | SER  | CA-C-O     | -5.01 | 113.92      | 119.08   |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | A     | 669 | ARG  | Sidechain |
| 3   | A     | 678 | ARG  | Sidechain |
| 3   | A     | 682 | PHE  | Sidechain |
| 3   | A     | 684 | TYR  | Mainchain |
| 3   | A     | 691 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | A     | 710 | ARG  | Sidechain |
| 3   | A     | 720 | ARG  | Sidechain |
| 3   | A     | 723 | PHE  | Sidechain |
| 4   | B     | 278 | ARG  | Sidechain |
| 6   | D     | 36  | ARG  | Sidechain |
| 5   | E     | 162 | GLN  | Sidechain |
| 5   | E     | 65  | ASN  | Sidechain |
| 2   | H     | 158 | ARG  | Sidechain |
| 2   | H     | 30  | GLU  | Sidechain |
| 6   | I     | 52  | ARG  | Sidechain |
| 6   | J     | 48  | ARG  | Sidechain |
| 6   | J     | 52  | ARG  | Sidechain |
| 7   | L     | 403 | ARG  | Sidechain |
| 7   | N     | 330 | LYS  | Mainchain |
| 7   | O     | 416 | GLN  | Sidechain |
| 7   | O     | 47  | GLU  | Sidechain |
| 7   | P     | 400 | ARG  | Sidechain |
| 8   | T     | 86  | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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   | R     | 863   | 0        | 441      | 12      | 0            |
| 2   | H     | 2863  | 0        | 2898     | 44      | 0            |
| 3   | A     | 6137  | 0        | 5989     | 168     | 0            |
| 4   | B     | 2321  | 0        | 2224     | 75      | 0            |
| 5   | C     | 1711  | 0        | 1697     | 26      | 0            |
| 5   | E     | 1706  | 0        | 1686     | 45      | 0            |
| 5   | F     | 1707  | 0        | 1688     | 30      | 0            |
| 5   | G     | 1709  | 0        | 1695     | 28      | 0            |
| 6   | D     | 1080  | 0        | 1099     | 22      | 0            |
| 6   | I     | 1080  | 0        | 1099     | 13      | 0            |
| 6   | J     | 1080  | 0        | 1099     | 15      | 0            |
| 7   | K     | 3305  | 0        | 3241     | 46      | 0            |
| 7   | L     | 3305  | 0        | 3241     | 48      | 0            |
| 7   | M     | 3305  | 0        | 3241     | 40      | 0            |
| 7   | N     | 3305  | 0        | 3241     | 25      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | O     | 3305  | 0        | 3241     | 34      | 0            |
| 7   | P     | 3305  | 0        | 3241     | 47      | 0            |
| 7   | Q     | 3305  | 0        | 3241     | 40      | 0            |
| 7   | S     | 3305  | 0        | 3241     | 39      | 0            |
| 8   | T     | 859   | 0        | 854      | 19      | 0            |
| All | All   | 49556 | 0        | 48397    | 738     | 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 8.

All (738) 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) |
|------------------|------------------|--------------------------|-------------------|
| 6:I:48:ARG:CD    | 6:I:48:ARG:CG    | 1.88                     | 1.51              |
| 3:A:715:THR:HB   | 3:A:720:ARG:HG2  | 1.23                     | 1.08              |
| 3:A:680:LYS:HD3  | 3:A:755:ILE:HD12 | 1.38                     | 1.06              |
| 3:A:675:GLN:HG2  | 3:A:723:PHE:CZ   | 1.94                     | 1.03              |
| 6:D:52:ARG:HB3   | 6:D:56:GLU:OE2   | 1.68                     | 0.94              |
| 6:J:80:ASN:HB3   | 8:T:46:LEU:HD22  | 1.49                     | 0.93              |
| 7:M:347:ILE:HG13 | 7:M:352:GLU:HG3  | 1.53                     | 0.90              |
| 3:A:79:ILE:HA    | 3:A:352:MET:HE1  | 1.54                     | 0.90              |
| 3:A:715:THR:HG22 | 3:A:716:ASP:H    | 1.36                     | 0.88              |
| 4:B:115:LEU:HD11 | 4:B:297:LEU:HD12 | 1.56                     | 0.87              |
| 3:A:397:ARG:HD3  | 3:A:415:LYS:HG3  | 1.60                     | 0.84              |
| 4:B:238:LYS:HE2  | 4:B:240:SER:CB   | 2.07                     | 0.83              |
| 7:L:78:HIS:HE1   | 7:L:93:ALA:HB1   | 1.44                     | 0.83              |
| 3:A:674:HIS:HB3  | 3:A:719:GLU:OE2  | 1.78                     | 0.83              |
| 5:E:25:ALA:HA    | 5:E:29:ILE:HD13  | 1.62                     | 0.82              |
| 6:D:21:GLU:HG2   | 6:D:89:ASP:OD2   | 1.80                     | 0.81              |
| 3:A:212:ILE:HD12 | 3:A:235:PHE:HZ   | 1.45                     | 0.81              |
| 3:A:113:VAL:HA   | 3:A:532:GLN:HE22 | 1.46                     | 0.80              |
| 7:P:400:ARG:HE   | 7:Q:400:ARG:HG2  | 1.46                     | 0.80              |
| 6:J:17:ILE:HD11  | 6:J:122:TYR:HB3  | 1.62                     | 0.79              |
| 3:A:212:ILE:HD12 | 3:A:235:PHE:CZ   | 2.18                     | 0.79              |
| 6:D:21:GLU:OE1   | 6:D:93:LYS:HE2   | 1.83                     | 0.78              |
| 4:B:238:LYS:HE2  | 4:B:240:SER:HB3  | 1.62                     | 0.78              |
| 7:K:1:MET:HB2    | 7:K:29:SER:HB3   | 1.65                     | 0.78              |
| 3:A:8:LEU:HB2    | 3:A:69:LEU:HD23  | 1.66                     | 0.77              |
| 3:A:371:MET:HE2  | 3:A:375:LYS:HE3  | 1.66                     | 0.77              |
| 3:A:753:TYR:OH   | 5:E:29:ILE:HG23  | 1.85                     | 0.77              |
| 3:A:511:LEU:HD11 | 3:A:623:MET:HE1  | 1.67                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:715:THR:HG22 | 3:A:716:ASP:N    | 1.96                     | 0.77              |
| 7:M:347:ILE:CG1  | 7:M:352:GLU:HG3  | 2.15                     | 0.76              |
| 7:P:275:ILE:HG21 | 7:P:308:ARG:HH11 | 1.50                     | 0.76              |
| 5:E:4:ALA:HA     | 5:E:204:PHE:O    | 1.85                     | 0.76              |
| 4:B:219:LEU:H    | 4:B:290:ALA:HB1  | 1.51                     | 0.76              |
| 3:A:382:TYR:HA   | 4:B:229:MET:HE3  | 1.68                     | 0.75              |
| 6:D:17:ILE:HA    | 6:D:20:LEU:HD13  | 1.68                     | 0.75              |
| 7:S:205:GLU:HA   | 7:S:403:ARG:HE   | 1.51                     | 0.74              |
| 7:Q:90:ILE:HG22  | 7:Q:94:MET:HE2   | 1.68                     | 0.74              |
| 4:B:238:LYS:HE2  | 4:B:240:SER:OG   | 1.88                     | 0.73              |
| 7:M:269:ARG:HD2  | 7:M:273:GLU:HB3  | 1.68                     | 0.73              |
| 7:Q:148:ASN:HD22 | 7:Q:205:GLU:HG3  | 1.52                     | 0.73              |
| 3:A:715:THR:HB   | 3:A:720:ARG:CG   | 2.11                     | 0.73              |
| 7:O:401:THR:HA   | 7:O:404:ILE:HB   | 1.69                     | 0.72              |
| 3:A:371:MET:CE   | 3:A:375:LYS:HE3  | 2.21                     | 0.71              |
| 5:F:31:ALA:H     | 6:D:36:ARG:NH1   | 1.86                     | 0.71              |
| 7:K:395:THR:O    | 7:K:403:ARG:HG3  | 1.91                     | 0.70              |
| 3:A:639:LYS:NZ   | 4:B:95:ARG:HH12  | 1.89                     | 0.70              |
| 7:L:395:THR:O    | 7:L:403:ARG:HG3  | 1.91                     | 0.70              |
| 7:P:400:ARG:NE   | 7:Q:400:ARG:HG2  | 2.04                     | 0.70              |
| 7:L:78:HIS:CE1   | 7:L:93:ALA:HB1   | 2.26                     | 0.70              |
| 5:F:31:ALA:H     | 6:D:36:ARG:HH12  | 1.39                     | 0.70              |
| 7:N:296:GLU:OE2  | 7:N:319:ASP:HB3  | 1.91                     | 0.69              |
| 3:A:749:LEU:HD21 | 5:E:29:ILE:HG21  | 1.74                     | 0.69              |
| 6:D:69:VAL:HG21  | 6:I:122:TYR:CE1  | 2.26                     | 0.69              |
| 5:C:182:LEU:HD12 | 5:C:193:VAL:HG11 | 1.74                     | 0.69              |
| 7:M:343:LYS:HD3  | 7:M:346:GLN:NE2  | 2.06                     | 0.69              |
| 7:K:284:LYS:HD2  | 7:K:285:TYR:CZ   | 2.28                     | 0.69              |
| 4:B:66:PHE:HB2   | 4:B:157:TYR:HD1  | 1.58                     | 0.68              |
| 5:C:192:LYS:HD2  | 5:G:99:ARG:HD2   | 1.74                     | 0.68              |
| 4:B:42:LYS:HG2   | 5:E:156:THR:HG21 | 1.75                     | 0.68              |
| 7:P:275:ILE:HG21 | 7:P:308:ARG:NH1  | 2.09                     | 0.68              |
| 3:A:749:LEU:HD11 | 3:A:753:TYR:CZ   | 2.28                     | 0.68              |
| 4:B:103:LEU:HD21 | 4:B:106:LEU:HD21 | 1.77                     | 0.67              |
| 7:M:344:VAL:HG12 | 7:M:353:THR:HG21 | 1.78                     | 0.66              |
| 3:A:639:LYS:NZ   | 4:B:95:ARG:NH1   | 2.43                     | 0.66              |
| 5:G:182:LEU:HD12 | 5:G:193:VAL:HG11 | 1.76                     | 0.66              |
| 7:O:190:LYS:HG2  | 7:O:194:LYS:NZ   | 2.10                     | 0.66              |
| 7:K:164:GLU:HB2  | 7:K:242:ASP:HB3  | 1.78                     | 0.66              |
| 3:A:675:GLN:HG2  | 3:A:723:PHE:CE1  | 2.30                     | 0.66              |
| 3:A:729:LEU:HA   | 3:A:732:LYS:HZ3  | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:M:395:THR:O    | 7:M:403:ARG:HG3  | 1.96                     | 0.66              |
| 3:A:177:PHE:CE2  | 3:A:199:ALA:HA   | 2.31                     | 0.66              |
| 7:L:22:GLU:OE2   | 7:L:34:ARG:HD3   | 1.95                     | 0.65              |
| 5:F:138:ILE:HD11 | 5:F:190:TYR:HE2  | 1.61                     | 0.65              |
| 7:L:176:LYS:HE2  | 7:K:58:ARG:HH22  | 1.62                     | 0.65              |
| 8:T:98:MET:SD    | 8:T:101:LEU:HD13 | 2.36                     | 0.65              |
| 7:S:396:GLY:HA3  | 7:S:403:ARG:HG2  | 1.77                     | 0.65              |
| 7:M:164:GLU:HB2  | 7:M:242:ASP:HB3  | 1.78                     | 0.65              |
| 7:L:147:MET:SD   | 7:L:398:LEU:HD21 | 2.37                     | 0.65              |
| 3:A:683:ILE:HD12 | 3:A:752:VAL:HG22 | 1.78                     | 0.65              |
| 7:M:401:THR:HA   | 7:M:404:ILE:HB   | 1.78                     | 0.65              |
| 7:Q:341:LEU:HD11 | 7:Q:370:SER:HB2  | 1.79                     | 0.65              |
| 3:A:675:GLN:NE2  | 3:A:723:PHE:CE2  | 2.65                     | 0.64              |
| 5:E:14:LEU:HD23  | 5:E:193:VAL:HG12 | 1.78                     | 0.64              |
| 7:L:150:ILE:HD12 | 7:L:222:ILE:HD11 | 1.78                     | 0.64              |
| 2:H:25:LYS:HB2   | 6:J:74:ARG:HH22  | 1.62                     | 0.64              |
| 7:M:323:THR:HG21 | 7:M:343:LYS:H    | 1.63                     | 0.64              |
| 7:S:79:ILE:HD12  | 7:S:90:ILE:HG23  | 1.79                     | 0.64              |
| 3:A:671:PHE:O    | 3:A:723:PHE:HE1  | 1.81                     | 0.64              |
| 7:N:341:LEU:HD11 | 7:N:370:SER:HB2  | 1.80                     | 0.64              |
| 2:H:13:LEU:CD1   | 8:T:98:MET:HE1   | 2.27                     | 0.63              |
| 3:A:672:PHE:HZ   | 3:A:726:PHE:CE2  | 2.17                     | 0.63              |
| 7:K:163:GLN:NE2  | 7:K:247:GLU:HG3  | 2.14                     | 0.63              |
| 7:Q:289:THR:HG22 | 7:Q:314:GLN:HE21 | 1.64                     | 0.63              |
| 7:L:1:MET:HB2    | 7:L:29:SER:HB3   | 1.80                     | 0.63              |
| 2:H:238:GLU:HA   | 2:H:241:ARG:HE   | 1.63                     | 0.63              |
| 2:H:18:ILE:HD11  | 2:H:348:ALA:HB2  | 1.81                     | 0.62              |
| 7:K:90:ILE:HG22  | 7:K:94:MET:HE2   | 1.81                     | 0.62              |
| 7:O:190:LYS:HG2  | 7:O:194:LYS:HZ2  | 1.62                     | 0.62              |
| 3:A:521:LEU:HD13 | 3:A:575:ASP:HB3  | 1.80                     | 0.62              |
| 4:B:185:GLY:HA2  | 5:E:99:ARG:HA    | 1.82                     | 0.62              |
| 6:D:89:ASP:OD1   | 6:D:93:LYS:HD2   | 1.99                     | 0.62              |
| 7:S:341:LEU:HD11 | 7:S:370:SER:HB2  | 1.80                     | 0.62              |
| 7:M:205:GLU:HG2  | 7:M:403:ARG:HH21 | 1.65                     | 0.62              |
| 7:O:314:GLN:HG3  | 7:O:431:ASN:HD21 | 1.65                     | 0.62              |
| 7:Q:36:MET:HB2   | 7:Q:378:ASP:HB2  | 1.82                     | 0.62              |
| 6:D:69:VAL:HG21  | 6:I:122:TYR:HE1  | 1.65                     | 0.61              |
| 7:N:158:ALA:HA   | 7:N:211:ARG:HH11 | 1.66                     | 0.61              |
| 4:B:5:LEU:HD21   | 4:B:70:PRO:HG3   | 1.82                     | 0.61              |
| 3:A:693:TYR:CZ   | 3:A:697:GLU:HG2  | 2.35                     | 0.61              |
| 7:K:160:ILE:HG23 | 7:K:215:THR:HG22 | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:I:48:ARG:HG3   | 6:I:52:ARG:NH1   | 2.16                     | 0.61              |
| 7:P:146:MET:HE1  | 7:P:289:THR:HG21 | 1.83                     | 0.61              |
| 7:K:288:ILE:HG23 | 7:K:289:THR:HG23 | 1.83                     | 0.61              |
| 7:M:2:SER:HB2    | 7:M:84:VAL:HG12  | 1.83                     | 0.60              |
| 6:I:48:ARG:HE    | 6:I:52:ARG:CZ    | 2.14                     | 0.60              |
| 3:A:130:LEU:O    | 3:A:560:GLN:NE2  | 2.34                     | 0.60              |
| 5:C:64:TYR:HB2   | 5:C:79:LEU:HD11  | 1.82                     | 0.60              |
| 5:G:38:LYS:HD3   | 5:G:43:ASN:OD1   | 2.02                     | 0.60              |
| 7:O:371:HIS:HD2  | 7:O:403:ARG:HH21 | 1.47                     | 0.60              |
| 1:R:2:C:H5'      | 5:E:54:GLY:HA3   | 1.83                     | 0.60              |
| 6:I:70:TYR:CZ    | 6:I:74:ARG:HD3   | 2.36                     | 0.60              |
| 3:A:459:LEU:HD22 | 3:A:478:ILE:HD13 | 1.84                     | 0.60              |
| 2:H:13:LEU:HD11  | 8:T:98:MET:HE1   | 1.84                     | 0.59              |
| 5:F:131:ALA:HB3  | 5:G:92:LYS:HD2   | 1.84                     | 0.59              |
| 7:S:164:GLU:HG2  | 7:S:242:ASP:HB3  | 1.84                     | 0.59              |
| 1:R:2:C:H2'      | 4:B:136:PRO:HD3  | 1.83                     | 0.59              |
| 3:A:709:THR:HG22 | 3:A:727:LYS:HD2  | 1.83                     | 0.59              |
| 7:Q:164:GLU:HB2  | 7:Q:242:ASP:HB3  | 1.85                     | 0.59              |
| 7:M:79:ILE:HD12  | 7:M:90:ILE:HG23  | 1.85                     | 0.59              |
| 2:H:247:GLY:O    | 2:H:248:LYS:HG3  | 2.01                     | 0.59              |
| 2:H:103:ARG:HD2  | 2:H:110:ALA:HA   | 1.85                     | 0.58              |
| 7:O:37:VAL:HG13  | 7:O:112:LEU:HD23 | 1.84                     | 0.58              |
| 3:A:212:ILE:HD11 | 3:A:241:PHE:CZ   | 2.38                     | 0.58              |
| 3:A:522:GLY:HA3  | 4:B:94:ARG:HH12  | 1.69                     | 0.58              |
| 7:K:149:ILE:HG23 | 7:K:150:ILE:HG12 | 1.84                     | 0.58              |
| 2:H:208:LYS:HD3  | 8:T:61:TYR:CD2   | 2.38                     | 0.58              |
| 3:A:557:TYR:HA   | 3:A:560:GLN:OE1  | 2.04                     | 0.58              |
| 7:L:146:MET:HG2  | 7:L:168:VAL:HG22 | 1.84                     | 0.58              |
| 3:A:177:PHE:CZ   | 3:A:199:ALA:HA   | 2.39                     | 0.58              |
| 7:Q:401:THR:HA   | 7:Q:404:ILE:HB   | 1.85                     | 0.58              |
| 5:F:20:ILE:HD13  | 5:F:48:PRO:HD2   | 1.86                     | 0.58              |
| 7:K:401:THR:HA   | 7:K:404:ILE:HB   | 1.83                     | 0.58              |
| 7:Q:148:ASN:ND2  | 7:Q:205:GLU:HG3  | 2.18                     | 0.58              |
| 7:M:347:ILE:HG13 | 7:M:352:GLU:CG   | 2.31                     | 0.58              |
| 3:A:712:GLU:O    | 3:A:712:GLU:HG2  | 2.03                     | 0.58              |
| 5:E:25:ALA:HA    | 5:E:29:ILE:CD1   | 2.34                     | 0.57              |
| 3:A:163:PHE:HZ   | 3:A:173:LEU:HB2  | 1.69                     | 0.57              |
| 7:M:312:LYS:HG3  | 7:M:313:VAL:HG23 | 1.86                     | 0.57              |
| 3:A:436:ILE:HG22 | 3:A:467:VAL:HG12 | 1.85                     | 0.57              |
| 5:F:99:ARG:NE    | 5:E:192:LYS:HD2  | 2.18                     | 0.57              |
| 7:M:97:LEU:HD22  | 7:M:106:LEU:HD11 | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:47:VAL:HG12  | 3:A:51:GLN:HE21  | 1.68                     | 0.57              |
| 5:F:198:LEU:HG   | 5:F:216:LEU:HD23 | 1.85                     | 0.57              |
| 7:P:181:TRP:CD1  | 7:P:231:TYR:HH   | 2.22                     | 0.57              |
| 5:C:144:ASN:HB2  | 5:G:41:ILE:HD12  | 1.85                     | 0.57              |
| 2:H:25:LYS:HB2   | 6:J:74:ARG:NH2   | 2.18                     | 0.57              |
| 3:A:684:TYR:O    | 3:A:687:ILE:HB   | 2.03                     | 0.57              |
| 7:S:262:GLU:HB2  | 7:S:266:ALA:HB2  | 1.87                     | 0.57              |
| 7:L:164:GLU:HB2  | 7:L:242:ASP:HB3  | 1.86                     | 0.57              |
| 5:G:3:PHE:HZ     | 5:G:5:LYS:HE3    | 1.70                     | 0.57              |
| 7:P:402:ASP:CG   | 7:P:403:ARG:HH11 | 2.13                     | 0.57              |
| 5:E:7:LYS:HD2    | 5:E:150:GLU:OE2  | 2.03                     | 0.57              |
| 7:Q:288:ILE:HG23 | 7:Q:289:THR:HG23 | 1.86                     | 0.57              |
| 3:A:674:HIS:HB2  | 3:A:723:PHE:CZ   | 2.40                     | 0.56              |
| 7:P:314:GLN:HG3  | 7:P:431:ASN:HD21 | 1.69                     | 0.56              |
| 3:A:516:LEU:HD21 | 3:A:607:LEU:HD13 | 1.87                     | 0.56              |
| 3:A:613:LEU:HG   | 3:A:645:PHE:CD1  | 2.39                     | 0.56              |
| 3:A:721:ASP:HA   | 3:A:724:LYS:HE2  | 1.87                     | 0.56              |
| 7:P:140:LYS:HE3  | 7:O:88:GLN:OE1   | 2.05                     | 0.56              |
| 5:E:14:LEU:HD21  | 5:E:18:LEU:HD22  | 1.86                     | 0.56              |
| 3:A:506:LEU:HD11 | 3:A:757:LYS:HE3  | 1.86                     | 0.56              |
| 5:F:78:ILE:HG23  | 5:F:79:LEU:HD12  | 1.86                     | 0.56              |
| 5:E:185:SER:O    | 5:E:190:TYR:HD2  | 1.89                     | 0.56              |
| 7:M:146:MET:HG2  | 7:M:168:VAL:HG22 | 1.86                     | 0.56              |
| 5:F:128:ARG:HH12 | 5:C:58:THR:HA    | 1.71                     | 0.56              |
| 7:N:371:HIS:HD1  | 7:N:371:HIS:H    | 1.54                     | 0.56              |
| 3:A:134:PRO:HB2  | 3:A:136:PHE:CE2  | 2.39                     | 0.56              |
| 7:L:79:ILE:HD12  | 7:L:90:ILE:HG23  | 1.87                     | 0.56              |
| 3:A:675:GLN:CG   | 3:A:723:PHE:CZ   | 2.80                     | 0.56              |
| 5:G:78:ILE:HG23  | 5:G:79:LEU:HD12  | 1.87                     | 0.56              |
| 7:S:190:LYS:HG2  | 7:S:194:LYS:HE2  | 1.88                     | 0.56              |
| 7:O:347:ILE:HD12 | 7:O:352:GLU:HB2  | 1.88                     | 0.56              |
| 7:K:152:GLY:HA2  | 7:K:156:SER:HB3  | 1.87                     | 0.56              |
| 7:Q:181:TRP:CD1  | 7:Q:231:TYR:HH   | 2.23                     | 0.56              |
| 4:B:72:LEU:HD12  | 4:B:111:VAL:HG21 | 1.86                     | 0.55              |
| 7:O:150:ILE:HD13 | 7:O:212:PHE:HE2  | 1.71                     | 0.55              |
| 7:Q:344:VAL:HG12 | 7:Q:353:THR:HG21 | 1.89                     | 0.55              |
| 2:H:27:THR:HB    | 6:J:74:ARG:HE    | 1.71                     | 0.55              |
| 3:A:177:PHE:CE1  | 3:A:181:LEU:HD12 | 2.41                     | 0.55              |
| 4:B:66:PHE:HB2   | 4:B:157:TYR:CD1  | 2.39                     | 0.55              |
| 7:P:36:MET:SD    | 7:P:376:THR:HB   | 2.46                     | 0.55              |
| 7:O:36:MET:HB2   | 7:O:378:ASP:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:L:379:SER:HA   | 7:L:406:LYS:HE3  | 1.88                     | 0.55              |
| 7:P:328:LEU:HD13 | 7:P:340:ILE:HD12 | 1.88                     | 0.55              |
| 7:K:147:MET:SD   | 7:K:398:LEU:HD21 | 2.46                     | 0.55              |
| 7:Q:396:GLY:HA3  | 7:Q:403:ARG:HD2  | 1.89                     | 0.55              |
| 3:A:721:ASP:OD1  | 3:A:724:LYS:HE2  | 2.05                     | 0.55              |
| 4:B:8:MET:HE1    | 4:B:27:PHE:HZ    | 1.71                     | 0.55              |
| 7:S:147:MET:SD   | 7:S:398:LEU:HD21 | 2.46                     | 0.55              |
| 3:A:720:ARG:HH21 | 3:A:720:ARG:HB3  | 1.71                     | 0.55              |
| 7:O:74:VAL:HG12  | 7:O:97:LEU:HD21  | 1.87                     | 0.55              |
| 3:A:715:THR:HG21 | 3:A:723:PHE:CD2  | 2.42                     | 0.55              |
| 7:S:2:SER:HB2    | 7:S:84:VAL:HG12  | 1.89                     | 0.55              |
| 7:P:164:GLU:CD   | 7:P:242:ASP:HB3  | 2.32                     | 0.55              |
| 3:A:411:TYR:CE2  | 3:A:412:HIS:CD2  | 2.96                     | 0.55              |
| 3:A:680:LYS:HD3  | 3:A:755:ILE:CD1  | 2.26                     | 0.54              |
| 3:A:690:LEU:HD11 | 3:A:730:PHE:CZ   | 2.43                     | 0.54              |
| 2:H:97:THR:HG23  | 2:H:322:PRO:HG3  | 1.88                     | 0.54              |
| 4:B:64:PHE:HB2   | 4:B:157:TYR:CZ   | 2.42                     | 0.54              |
| 4:B:99:LEU:HB3   | 4:B:119:LEU:HD11 | 1.90                     | 0.54              |
| 7:S:205:GLU:HA   | 7:S:403:ARG:HH21 | 1.73                     | 0.54              |
| 7:M:341:LEU:HD12 | 7:M:368:VAL:HB   | 1.89                     | 0.54              |
| 7:Q:323:THR:HA   | 7:Q:340:ILE:HD11 | 1.89                     | 0.54              |
| 3:A:729:LEU:HA   | 3:A:732:LYS:NZ   | 2.22                     | 0.54              |
| 7:Q:160:ILE:HD11 | 7:Q:212:PHE:HB2  | 1.88                     | 0.54              |
| 5:F:34:SER:HB2   | 5:F:138:ILE:HB   | 1.90                     | 0.54              |
| 5:E:95:ARG:HH12  | 5:E:162:GLN:CD   | 2.16                     | 0.54              |
| 7:K:163:GLN:HE21 | 7:K:247:GLU:HG3  | 1.72                     | 0.54              |
| 8:T:98:MET:SD    | 8:T:101:LEU:HD22 | 2.48                     | 0.54              |
| 4:B:32:ILE:HG23  | 4:B:60:LEU:HD21  | 1.90                     | 0.54              |
| 7:P:1:MET:HB3    | 7:P:29:SER:HB3   | 1.90                     | 0.54              |
| 2:H:203:TRP:HB2  | 2:H:318:LEU:O    | 2.07                     | 0.54              |
| 5:E:32:ILE:HA    | 5:E:137:GLN:NE2  | 2.23                     | 0.54              |
| 7:P:400:ARG:HH21 | 7:Q:400:ARG:HA   | 1.73                     | 0.54              |
| 4:B:39:GLU:HG3   | 4:B:173:LEU:HD22 | 1.90                     | 0.54              |
| 7:S:205:GLU:HA   | 7:S:403:ARG:NE   | 2.22                     | 0.54              |
| 3:A:753:TYR:OH   | 5:E:29:ILE:CG2   | 2.54                     | 0.54              |
| 7:K:205:GLU:HG3  | 7:K:403:ARG:NH2  | 2.23                     | 0.54              |
| 1:R:21:U:H5"     | 5:C:123:GLU:HA   | 1.89                     | 0.54              |
| 3:A:705:ALA:O    | 3:A:709:THR:HG23 | 2.08                     | 0.54              |
| 4:B:104:GLN:HG3  | 4:B:105:PHE:CD2  | 2.43                     | 0.54              |
| 7:M:181:TRP:CD1  | 7:M:231:TYR:HH   | 2.25                     | 0.54              |
| 7:O:424:ARG:HB3  | 7:O:427:LYS:HB2  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:104:ASN:HB3  | 2:H:107:SER:HB2  | 1.89                     | 0.53              |
| 3:A:639:LYS:HZ1  | 4:B:95:ARG:NH1   | 2.04                     | 0.53              |
| 5:C:78:ILE:HG21  | 5:C:169:VAL:HG21 | 1.90                     | 0.53              |
| 7:K:205:GLU:HG3  | 7:K:403:ARG:HH21 | 1.74                     | 0.53              |
| 6:D:95:GLN:HG3   | 6:D:98:GLU:OE2   | 2.08                     | 0.53              |
| 7:N:357:ILE:HD13 | 7:N:388:THR:HG21 | 1.89                     | 0.53              |
| 7:L:223:ILE:HG23 | 7:L:233:PRO:HG2  | 1.89                     | 0.53              |
| 7:L:402:ASP:CG   | 7:L:403:ARG:HH11 | 2.15                     | 0.53              |
| 7:M:258:TYR:HE2  | 7:M:269:ARG:NH2  | 2.06                     | 0.53              |
| 7:P:375:GLU:HG3  | 7:P:376:THR:N    | 2.24                     | 0.53              |
| 7:P:145:PRO:HB2  | 7:P:147:MET:SD   | 2.49                     | 0.53              |
| 3:A:38:TRP:HH2   | 3:A:160:LEU:HD12 | 1.74                     | 0.53              |
| 7:Q:6:ASP:HB2    | 7:Q:26:TYR:HB2   | 1.91                     | 0.53              |
| 2:H:55:LEU:HD22  | 2:H:58:LYS:HD3   | 1.91                     | 0.53              |
| 3:A:721:ASP:OD1  | 3:A:724:LYS:CE   | 2.56                     | 0.53              |
| 5:G:47:ILE:HB    | 5:G:101:ALA:HB3  | 1.91                     | 0.53              |
| 6:I:52:ARG:HG2   | 6:I:52:ARG:HH11  | 1.74                     | 0.53              |
| 6:J:100:LEU:HD23 | 6:J:103:ILE:HD12 | 1.90                     | 0.53              |
| 7:Q:163:GLN:HG2  | 7:Q:164:GLU:HG3  | 1.91                     | 0.53              |
| 5:C:175:LYS:HE2  | 5:G:204:PHE:HD1  | 1.74                     | 0.52              |
| 3:A:296:LEU:HD21 | 3:A:299:VAL:HG12 | 1.90                     | 0.52              |
| 5:E:5:LYS:HG2    | 5:E:154:GLU:HG2  | 1.91                     | 0.52              |
| 7:K:357:ILE:HD13 | 7:K:388:THR:HG21 | 1.91                     | 0.52              |
| 7:O:148:ASN:HA   | 7:O:166:MET:HG3  | 1.91                     | 0.52              |
| 3:A:536:GLN:HE21 | 3:A:537:TYR:HE1  | 1.57                     | 0.52              |
| 7:O:131:TYR:HE2  | 7:O:416:GLN:NE2  | 2.07                     | 0.52              |
| 4:B:175:TYR:HB3  | 5:E:152:ILE:HD13 | 1.92                     | 0.52              |
| 4:B:175:TYR:CE2  | 5:E:203:VAL:HG11 | 2.45                     | 0.52              |
| 7:K:147:MET:HE1  | 7:K:182:GLY:HA3  | 1.90                     | 0.52              |
| 3:A:267:LEU:HD22 | 3:A:620:ILE:HD13 | 1.90                     | 0.52              |
| 7:S:253:HIS:HB2  | 7:S:255:VAL:HG22 | 1.92                     | 0.52              |
| 5:C:56:MET:SD    | 5:C:98:PHE:HE2   | 2.32                     | 0.52              |
| 7:P:36:MET:HG2   | 7:P:376:THR:HG21 | 1.92                     | 0.52              |
| 7:O:371:HIS:CD2  | 7:O:403:ARG:HH21 | 2.26                     | 0.52              |
| 2:H:185:ARG:HG2  | 5:G:187:SER:HA   | 1.92                     | 0.52              |
| 3:A:659:ASN:O    | 3:A:663:ASP:HB3  | 2.10                     | 0.52              |
| 7:M:257:GLY:HA2  | 7:M:268:VAL:HG22 | 1.91                     | 0.52              |
| 3:A:690:LEU:HD11 | 3:A:730:PHE:HZ   | 1.74                     | 0.51              |
| 5:F:70:GLU:HG3   | 5:E:129:ILE:HD11 | 1.92                     | 0.51              |
| 7:Q:152:GLY:HA2  | 7:Q:156:SER:HB3  | 1.92                     | 0.51              |
| 3:A:709:THR:HG22 | 3:A:727:LYS:CD   | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:274:ILE:HG22 | 4:B:287:LEU:HD22 | 1.93                     | 0.51              |
| 7:P:341:LEU:HD12 | 7:P:368:VAL:HB   | 1.92                     | 0.51              |
| 3:A:113:VAL:HA   | 3:A:532:GLN:NE2  | 2.20                     | 0.51              |
| 3:A:297:LEU:HD13 | 3:A:540:LEU:HD11 | 1.92                     | 0.51              |
| 7:S:112:LEU:HD11 | 7:S:344:VAL:HG22 | 1.92                     | 0.51              |
| 7:K:292:ASP:OD2  | 7:K:318:ASP:HB3  | 2.10                     | 0.51              |
| 5:F:128:ARG:HH22 | 5:C:57:ARG:HG2   | 1.75                     | 0.51              |
| 7:M:145:PRO:HB2  | 7:M:147:MET:SD   | 2.51                     | 0.51              |
| 7:Q:79:ILE:HD12  | 7:Q:90:ILE:HG23  | 1.92                     | 0.51              |
| 2:H:46:PHE:CZ    | 2:H:50:MET:HE3   | 2.46                     | 0.51              |
| 5:C:42:THR:HB    | 5:C:44:LEU:HG    | 1.93                     | 0.51              |
| 7:K:146:MET:HG2  | 7:K:168:VAL:HG22 | 1.93                     | 0.51              |
| 7:M:288:ILE:HG23 | 7:M:289:THR:HG23 | 1.92                     | 0.51              |
| 3:A:258:ILE:HG23 | 3:A:401:ILE:HG23 | 1.92                     | 0.51              |
| 4:B:135:GLN:HG2  | 4:B:137:HIS:CE1  | 2.46                     | 0.51              |
| 7:N:147:MET:SD   | 7:N:182:GLY:HA3  | 2.51                     | 0.51              |
| 7:O:2:SER:HB3    | 7:O:125:TYR:CZ   | 2.45                     | 0.51              |
| 7:O:289:THR:HG23 | 7:O:314:GLN:HE21 | 1.76                     | 0.51              |
| 1:R:15:G:H5''    | 5:F:123:GLU:HA   | 1.92                     | 0.51              |
| 4:B:270:PHE:CE2  | 4:B:292:PRO:HG3  | 2.46                     | 0.51              |
| 5:F:138:ILE:HD11 | 5:F:190:TYR:CE2  | 2.45                     | 0.51              |
| 7:P:375:GLU:HG3  | 7:P:376:THR:H    | 1.75                     | 0.51              |
| 7:Q:7:VAL:HG22   | 7:Q:25:VAL:HG22  | 1.93                     | 0.51              |
| 3:A:401:ILE:HD11 | 3:A:424:TYR:OH   | 2.10                     | 0.50              |
| 7:S:149:ILE:HG23 | 7:S:150:ILE:HG12 | 1.93                     | 0.50              |
| 7:N:74:VAL:HG12  | 7:N:97:LEU:HD21  | 1.92                     | 0.50              |
| 2:H:60:GLU:O     | 2:H:64:ILE:HG12  | 2.11                     | 0.50              |
| 6:I:48:ARG:HG3   | 6:I:52:ARG:HH12  | 1.76                     | 0.50              |
| 1:R:-5:A:H5'     | 4:B:244:PHE:HD2  | 1.77                     | 0.50              |
| 6:J:30:LEU:HD21  | 6:J:90:LEU:HD22  | 1.94                     | 0.50              |
| 7:Q:1:MET:HB2    | 7:Q:29:SER:HB3   | 1.92                     | 0.50              |
| 3:A:598:ILE:CD1  | 3:A:603:GLY:HA2  | 2.42                     | 0.50              |
| 5:C:47:ILE:HB    | 5:C:101:ALA:HB3  | 1.92                     | 0.50              |
| 1:R:26:A:H1'     | 2:H:131:SER:HA   | 1.93                     | 0.50              |
| 3:A:537:TYR:HA   | 3:A:542:ARG:HH11 | 1.77                     | 0.50              |
| 3:A:670:TYR:CZ   | 3:A:722:LYS:NZ   | 2.73                     | 0.50              |
| 4:B:12:ASN:HD21  | 5:E:102:PHE:HZ   | 1.60                     | 0.50              |
| 6:D:24:ASN:OD1   | 6:D:25:LYS:HG3   | 2.12                     | 0.50              |
| 7:L:424:ARG:HB3  | 7:L:427:LYS:HB2  | 1.94                     | 0.50              |
| 7:K:156:SER:HB2  | 7:K:209:ALA:HB1  | 1.94                     | 0.50              |
| 7:S:152:GLY:HA2  | 7:S:156:SER:HB3  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:K:7:VAL:HG22   | 7:K:25:VAL:HG22  | 1.93                     | 0.49              |
| 4:B:12:ASN:OD1   | 4:B:149:ARG:HD3  | 2.12                     | 0.49              |
| 3:A:680:LYS:O    | 3:A:683:ILE:HG12 | 2.12                     | 0.49              |
| 3:A:696:GLU:HG3  | 3:A:696:GLU:O    | 2.12                     | 0.49              |
| 4:B:36:LEU:HD21  | 4:B:170:MET:HE2  | 1.94                     | 0.49              |
| 4:B:209:SER:HA   | 4:B:268:LYS:HG3  | 1.93                     | 0.49              |
| 7:S:402:ASP:HB3  | 7:N:401:THR:OG1  | 2.11                     | 0.49              |
| 7:P:146:MET:HE2  | 7:P:166:MET:SD   | 2.52                     | 0.49              |
| 7:M:160:ILE:HD11 | 7:M:212:PHE:HB2  | 1.93                     | 0.49              |
| 2:H:99:LEU:HD23  | 2:H:320:LYS:HE3  | 1.94                     | 0.49              |
| 5:G:20:ILE:HD13  | 5:G:48:PRO:HD2   | 1.95                     | 0.49              |
| 7:P:401:THR:HA   | 7:P:404:ILE:HB   | 1.95                     | 0.49              |
| 7:K:284:LYS:HD2  | 7:K:285:TYR:CE2  | 2.48                     | 0.49              |
| 3:A:668:ILE:O    | 3:A:672:PHE:HB2  | 2.12                     | 0.49              |
| 3:A:715:THR:CB   | 3:A:720:ARG:HG2  | 2.17                     | 0.49              |
| 5:G:95:ARG:NH2   | 5:G:158:GLU:HG3  | 2.27                     | 0.49              |
| 3:A:730:PHE:CE2  | 3:A:748:LEU:HD11 | 2.48                     | 0.49              |
| 3:A:751:TYR:CE2  | 3:A:755:ILE:HD13 | 2.48                     | 0.49              |
| 4:B:259:LYS:HE2  | 4:B:290:ALA:HB2  | 1.94                     | 0.49              |
| 6:D:29:LEU:HD22  | 6:D:77:VAL:HG21  | 1.94                     | 0.49              |
| 7:L:36:MET:SD    | 7:L:376:THR:HB   | 2.52                     | 0.49              |
| 7:P:312:LYS:HG3  | 7:P:313:VAL:HG13 | 1.94                     | 0.49              |
| 7:K:79:ILE:HD12  | 7:K:90:ILE:HG23  | 1.94                     | 0.49              |
| 3:A:696:GLU:HB3  | 3:A:700:ASN:ND2  | 2.28                     | 0.49              |
| 7:M:147:MET:HE1  | 7:M:169:PRO:HG3  | 1.93                     | 0.49              |
| 7:M:343:LYS:HD3  | 7:M:346:GLN:HE22 | 1.74                     | 0.49              |
| 8:T:98:MET:O     | 8:T:98:MET:HG2   | 2.11                     | 0.49              |
| 5:E:95:ARG:HH22  | 5:E:162:GLN:NE2  | 2.10                     | 0.49              |
| 3:A:697:GLU:O    | 3:A:701:VAL:HG23 | 2.13                     | 0.49              |
| 5:E:3:PHE:HA     | 5:E:155:ILE:O    | 2.12                     | 0.49              |
| 5:E:167:PHE:CD2  | 5:E:212:LEU:HD13 | 2.48                     | 0.49              |
| 7:N:147:MET:SD   | 7:N:398:LEU:HD21 | 2.53                     | 0.49              |
| 8:T:33:ILE:HB    | 8:T:37:GLU:HG3   | 1.94                     | 0.49              |
| 2:H:103:ARG:HD3  | 2:H:108:ALA:HB3  | 1.95                     | 0.49              |
| 2:H:275:GLN:HB2  | 2:H:349:ASN:HB3  | 1.95                     | 0.49              |
| 3:A:669:ARG:HA   | 3:A:751:TYR:CE1  | 2.48                     | 0.49              |
| 4:B:65:PRO:O     | 4:B:157:TYR:HE1  | 1.95                     | 0.49              |
| 7:S:269:ARG:HB3  | 7:S:273:GLU:HB2  | 1.94                     | 0.49              |
| 7:L:112:LEU:HD11 | 7:L:344:VAL:HG12 | 1.95                     | 0.49              |
| 3:A:675:GLN:CG   | 3:A:723:PHE:CE1  | 2.96                     | 0.48              |
| 4:B:11:GLN:O     | 4:B:149:ARG:HD2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:147:MET:HB2  | 7:N:167:ILE:HG13 | 1.95                     | 0.48              |
| 7:Q:238:PHE:CE1  | 7:Q:426:LEU:HD21 | 2.48                     | 0.48              |
| 7:S:12:VAL:HG21  | 7:S:36:MET:HE3   | 1.94                     | 0.48              |
| 7:S:44:GLY:HA3   | 7:S:47:GLU:HG2   | 1.95                     | 0.48              |
| 7:L:244:ALA:HA   | 7:L:292:ASP:HB3  | 1.95                     | 0.48              |
| 7:K:402:ASP:CG   | 7:K:403:ARG:HH11 | 2.21                     | 0.48              |
| 3:A:693:TYR:CE2  | 3:A:697:GLU:HG2  | 2.48                     | 0.48              |
| 6:J:48:ARG:HH11  | 6:J:48:ARG:HD2   | 1.42                     | 0.48              |
| 6:J:52:ARG:HG2   | 6:J:56:GLU:HB2   | 1.95                     | 0.48              |
| 6:J:68:PHE:CE1   | 6:J:96:ILE:HG21  | 2.48                     | 0.48              |
| 2:H:251:GLN:NE2  | 8:T:104:VAL:HG11 | 2.28                     | 0.48              |
| 5:F:14:LEU:HB2   | 5:F:143:ARG:O    | 2.14                     | 0.48              |
| 6:I:20:LEU:HD11  | 6:I:90:LEU:HD13  | 1.95                     | 0.48              |
| 4:B:151:SER:HB2  | 5:E:41:ILE:HD13  | 1.96                     | 0.48              |
| 7:K:140:LYS:HE2  | 7:N:88:GLN:OE1   | 2.14                     | 0.48              |
| 3:A:685:LYS:HE2  | 3:A:707:TYR:CE2  | 2.49                     | 0.48              |
| 4:B:289:TYR:CZ   | 4:B:291:LYS:HB2  | 2.49                     | 0.48              |
| 6:D:62:SER:HB3   | 6:I:10:VAL:HG21  | 1.96                     | 0.48              |
| 5:F:144:ASN:HB2  | 5:C:41:ILE:HD12  | 1.95                     | 0.48              |
| 7:P:147:MET:HE1  | 7:P:169:PRO:HG3  | 1.95                     | 0.48              |
| 5:G:167:PHE:CE2  | 5:G:212:LEU:HD22 | 2.49                     | 0.47              |
| 7:S:88:GLN:OE1   | 7:Q:140:LYS:HE2  | 2.14                     | 0.47              |
| 7:P:47:GLU:OE2   | 7:P:346:GLN:HG3  | 2.15                     | 0.47              |
| 3:A:716:ASP:O    | 3:A:717:LYS:C    | 2.57                     | 0.47              |
| 3:A:720:ARG:C    | 3:A:722:LYS:H    | 2.21                     | 0.47              |
| 5:F:53:LYS:HD3   | 5:E:188:ARG:HG2  | 1.97                     | 0.47              |
| 5:C:56:MET:SD    | 5:C:98:PHE:CE2   | 3.07                     | 0.47              |
| 3:A:625:HIS:O    | 3:A:629:GLU:HG2  | 2.14                     | 0.47              |
| 4:B:169:LEU:O    | 4:B:173:LEU:HD23 | 2.14                     | 0.47              |
| 5:G:64:TYR:HB2   | 5:G:79:LEU:HD11  | 1.96                     | 0.47              |
| 7:L:341:LEU:HD12 | 7:L:368:VAL:HB   | 1.96                     | 0.47              |
| 7:L:371:HIS:CD2  | 7:L:403:ARG:HH21 | 2.32                     | 0.47              |
| 3:A:671:PHE:O    | 3:A:723:PHE:CE1  | 2.64                     | 0.47              |
| 3:A:675:GLN:NE2  | 3:A:723:PHE:HE2  | 2.13                     | 0.47              |
| 7:L:218:GLY:O    | 7:L:222:ILE:HG12 | 2.15                     | 0.47              |
| 8:T:84:LYS:HD2   | 8:T:84:LYS:O     | 2.14                     | 0.47              |
| 2:H:22:ASN:HB3   | 2:H:118:ILE:HD12 | 1.95                     | 0.47              |
| 3:A:401:ILE:HG21 | 3:A:401:ILE:HD13 | 1.66                     | 0.47              |
| 3:A:537:TYR:HA   | 3:A:542:ARG:NH1  | 2.29                     | 0.47              |
| 3:A:719:GLU:OE2  | 3:A:723:PHE:CZ   | 2.67                     | 0.47              |
| 4:B:25:LEU:HG    | 4:B:26:THR:HG23  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:103:LEU:HD12 | 4:B:122:ASN:OD1  | 2.14                     | 0.47              |
| 4:B:171:SER:O    | 4:B:174:GLN:HG2  | 2.14                     | 0.47              |
| 5:C:59:LEU:HD12  | 5:C:177:LEU:HD23 | 1.97                     | 0.47              |
| 7:P:314:GLN:HE22 | 7:P:392:GLN:HE22 | 1.62                     | 0.47              |
| 5:G:3:PHE:CZ     | 5:G:5:LYS:HE3    | 2.47                     | 0.47              |
| 7:L:53:ASP:HA    | 7:L:66:LYS:HD2   | 1.97                     | 0.47              |
| 4:B:289:TYR:CE1  | 4:B:291:LYS:HD3  | 2.50                     | 0.47              |
| 5:F:31:ALA:N     | 6:D:36:ARG:HH12  | 2.09                     | 0.47              |
| 5:C:14:LEU:HB2   | 5:C:143:ARG:O    | 2.15                     | 0.47              |
| 5:E:81:ARG:HB2   | 5:E:95:ARG:NH2   | 2.30                     | 0.47              |
| 7:K:2:SER:HB3    | 7:K:125:TYR:CZ   | 2.50                     | 0.47              |
| 2:H:238:GLU:HA   | 2:H:241:ARG:HH21 | 1.79                     | 0.47              |
| 3:A:382:TYR:HE1  | 4:B:225:LEU:HD12 | 1.80                     | 0.47              |
| 7:L:75:ILE:HG21  | 7:L:114:VAL:HG21 | 1.97                     | 0.47              |
| 7:K:424:ARG:HB3  | 7:K:427:LYS:HB2  | 1.97                     | 0.47              |
| 7:O:146:MET:HG2  | 7:O:168:VAL:HG22 | 1.97                     | 0.47              |
| 3:A:715:THR:CG2  | 3:A:719:GLU:OE1  | 2.64                     | 0.46              |
| 5:C:20:ILE:HD13  | 5:C:48:PRO:HD2   | 1.95                     | 0.46              |
| 7:K:37:VAL:HG13  | 7:K:112:LEU:HD23 | 1.96                     | 0.46              |
| 3:A:608:SER:HB2  | 3:A:635:LYS:HE3  | 1.98                     | 0.46              |
| 3:A:685:LYS:HE2  | 3:A:707:TYR:CZ   | 2.51                     | 0.46              |
| 3:A:705:ALA:HB1  | 6:D:125:PHE:CG   | 2.49                     | 0.46              |
| 3:A:729:LEU:HD12 | 3:A:732:LYS:HZ3  | 1.80                     | 0.46              |
| 7:S:258:TYR:CE2  | 7:S:269:ARG:NH1  | 2.83                     | 0.46              |
| 2:H:10:LEU:HD22  | 2:H:132:LEU:HD21 | 1.97                     | 0.46              |
| 4:B:272:GLY:HA3  | 4:B:291:LYS:HA   | 1.97                     | 0.46              |
| 5:E:171:ARG:NH1  | 5:E:212:LEU:HD12 | 2.31                     | 0.46              |
| 3:A:519:ASP:OD2  | 3:A:639:LYS:HB3  | 2.15                     | 0.46              |
| 6:J:91:VAL:HG13  | 6:J:96:ILE:HB    | 1.97                     | 0.46              |
| 7:M:90:ILE:HD13  | 7:M:118:VAL:HG11 | 1.98                     | 0.46              |
| 7:M:205:GLU:HG2  | 7:M:403:ARG:NH2  | 2.27                     | 0.46              |
| 3:A:15:HIS:HD2   | 3:A:55:HIS:CD2   | 2.32                     | 0.46              |
| 4:B:175:TYR:CZ   | 5:E:203:VAL:HG11 | 2.50                     | 0.46              |
| 6:J:45:LEU:HD21  | 6:J:109:LEU:HD11 | 1.98                     | 0.46              |
| 3:A:705:ALA:HB1  | 6:D:125:PHE:HB2  | 1.98                     | 0.46              |
| 7:K:158:ALA:HB2  | 7:K:211:ARG:HA   | 1.96                     | 0.46              |
| 3:A:708:LEU:HD13 | 3:A:727:LYS:HA   | 1.97                     | 0.46              |
| 7:L:309:LEU:HB3  | 7:L:313:VAL:HG12 | 1.98                     | 0.46              |
| 7:P:152:GLY:HA2  | 7:P:156:SER:HB3  | 1.98                     | 0.46              |
| 7:P:323:THR:HG23 | 7:P:347:ILE:HB   | 1.97                     | 0.46              |
| 1:R:26:A:C6      | 2:H:289:LYS:HG2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:359:GLU:HA   | 3:A:362:ARG:HE   | 1.80                     | 0.46              |
| 3:A:717:LYS:O    | 3:A:720:ARG:HD3  | 2.16                     | 0.46              |
| 5:F:177:LEU:HD23 | 5:F:195:PHE:CZ   | 2.51                     | 0.46              |
| 1:R:-3:G:C8      | 4:B:18:GLY:HA2   | 2.51                     | 0.46              |
| 7:N:296:GLU:CD   | 7:N:319:ASP:HB3  | 2.41                     | 0.46              |
| 5:E:181:TYR:CG   | 5:E:186:GLY:HA3  | 2.51                     | 0.46              |
| 7:L:147:MET:SD   | 7:L:182:GLY:HA3  | 2.56                     | 0.46              |
| 7:O:341:LEU:HD12 | 7:O:368:VAL:HB   | 1.98                     | 0.46              |
| 6:J:65:ARG:HH22  | 6:J:101:LYS:NZ   | 2.14                     | 0.45              |
| 7:N:424:ARG:HB3  | 7:N:427:LYS:HB2  | 1.98                     | 0.45              |
| 8:T:19:THR:HB    | 8:T:56:ASP:HB3   | 1.97                     | 0.45              |
| 7:S:341:LEU:HA   | 7:S:341:LEU:HD12 | 1.76                     | 0.45              |
| 7:M:396:GLY:HA3  | 7:M:403:ARG:HG2  | 1.99                     | 0.45              |
| 3:A:33:LEU:HD21  | 3:A:59:TYR:CZ    | 2.51                     | 0.45              |
| 3:A:169:GLN:OE1  | 3:A:172:SER:HB2  | 2.16                     | 0.45              |
| 3:A:704:LEU:HD23 | 3:A:731:PHE:CD1  | 2.51                     | 0.45              |
| 3:A:736:ASN:OD1  | 3:A:740:ASP:HB2  | 2.17                     | 0.45              |
| 5:F:64:TYR:HB2   | 5:F:79:LEU:HD11  | 1.98                     | 0.45              |
| 6:I:124:LYS:HB3  | 6:I:124:LYS:HE3  | 1.74                     | 0.45              |
| 3:A:163:PHE:CZ   | 3:A:169:GLN:HG3  | 2.51                     | 0.45              |
| 7:L:148:ASN:HA   | 7:L:166:MET:HG2  | 1.97                     | 0.45              |
| 7:L:343:LYS:HB2  | 7:L:346:GLN:CD   | 2.41                     | 0.45              |
| 7:K:44:GLY:HA3   | 7:K:47:GLU:HG3   | 1.98                     | 0.45              |
| 4:B:218:ALA:HA   | 4:B:290:ALA:HB1  | 1.99                     | 0.45              |
| 7:K:1:MET:HG3    | 7:K:125:TYR:CE1  | 2.51                     | 0.45              |
| 7:K:92:ARG:HD3   | 7:K:92:ARG:HA    | 1.75                     | 0.45              |
| 8:T:40:ASP:OD1   | 8:T:44:LYS:NZ    | 2.49                     | 0.45              |
| 1:R:4:U:H1'      | 4:B:136:PRO:HB3  | 1.99                     | 0.45              |
| 3:A:544:ALA:O    | 3:A:548:ARG:HG3  | 2.17                     | 0.45              |
| 7:L:150:ILE:HD13 | 7:L:212:PHE:HE2  | 1.81                     | 0.45              |
| 7:P:98:ASP:OD2   | 7:P:103:LYS:HA   | 2.16                     | 0.45              |
| 7:N:37:VAL:HG13  | 7:N:112:LEU:HD23 | 1.99                     | 0.45              |
| 2:H:24:GLU:HB3   | 2:H:116:LYS:HE3  | 1.99                     | 0.45              |
| 2:H:208:LYS:HD3  | 8:T:61:TYR:CE2   | 2.52                     | 0.45              |
| 7:K:53:ASP:HA    | 7:K:66:LYS:HD2   | 1.99                     | 0.45              |
| 3:A:163:PHE:CZ   | 3:A:173:LEU:HB2  | 2.50                     | 0.45              |
| 3:A:682:PHE:CD2  | 3:A:711:LEU:HG   | 2.51                     | 0.45              |
| 5:G:14:LEU:HB2   | 5:G:143:ARG:O    | 2.17                     | 0.45              |
| 7:S:239:ILE:O    | 7:S:287:ILE:HA   | 2.17                     | 0.45              |
| 7:P:371:HIS:CD2  | 7:P:403:ARG:HH21 | 2.34                     | 0.45              |
| 7:K:371:HIS:HD2  | 7:K:394:LYS:O    | 2.00                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:416:VAL:HG11 | 3:A:424:TYR:CE2  | 2.52                     | 0.45              |
| 3:A:522:GLY:HA3  | 4:B:94:ARG:NH1   | 2.32                     | 0.45              |
| 5:G:16:THR:HG21  | 5:G:189:GLY:O    | 2.16                     | 0.45              |
| 7:S:150:ILE:HD11 | 7:S:189:LEU:HD21 | 1.98                     | 0.45              |
| 7:K:47:GLU:HB3   | 7:K:322:VAL:HG11 | 1.99                     | 0.45              |
| 7:Q:158:ALA:HB2  | 7:Q:211:ARG:HA   | 1.99                     | 0.45              |
| 6:D:45:LEU:HD21  | 6:D:109:LEU:HD11 | 1.98                     | 0.44              |
| 7:S:160:ILE:HD11 | 7:S:212:PHE:HB2  | 1.99                     | 0.44              |
| 7:P:420:VAL:HG11 | 7:O:88:GLN:HB3   | 1.98                     | 0.44              |
| 3:A:254:PHE:CD2  | 3:A:274:LEU:HD21 | 2.52                     | 0.44              |
| 5:F:89:LYS:HA    | 5:F:92:LYS:HE2   | 2.00                     | 0.44              |
| 5:G:31:ALA:HB1   | 5:G:33:ASP:OD2   | 2.16                     | 0.44              |
| 7:O:163:GLN:CD   | 7:O:244:ALA:HB3  | 2.42                     | 0.44              |
| 7:N:21:LEU:HD21  | 7:N:109:ASN:HB2  | 1.99                     | 0.44              |
| 3:A:729:LEU:HD11 | 3:A:733:TRP:CZ2  | 2.53                     | 0.44              |
| 6:D:17:ILE:HD12  | 6:D:123:PHE:HB2  | 1.98                     | 0.44              |
| 5:C:188:ARG:HG2  | 5:G:53:LYS:HD3   | 2.00                     | 0.44              |
| 7:P:51:LEU:HD21  | 7:P:66:LYS:HB3   | 1.98                     | 0.44              |
| 3:A:270:ARG:O    | 3:A:274:LEU:HD23 | 2.18                     | 0.44              |
| 3:A:558:ILE:HG12 | 3:A:569:ILE:HD13 | 1.99                     | 0.44              |
| 4:B:3:TYR:HB2    | 4:B:161:ASN:HA   | 2.00                     | 0.44              |
| 5:G:3:PHE:HA     | 5:G:155:ILE:O    | 2.18                     | 0.44              |
| 7:P:79:ILE:HD12  | 7:P:90:ILE:HG23  | 1.99                     | 0.44              |
| 7:M:36:MET:HB2   | 7:M:378:ASP:HB2  | 1.98                     | 0.44              |
| 3:A:13:LEU:HD12  | 3:A:202:SER:OG   | 2.17                     | 0.44              |
| 4:B:225:LEU:O    | 4:B:229:MET:HG2  | 2.17                     | 0.44              |
| 6:D:56:GLU:HG2   | 6:D:57:LEU:HD12  | 1.99                     | 0.44              |
| 8:T:94:GLU:HG3   | 8:T:96:ILE:HD13  | 1.98                     | 0.44              |
| 7:P:6:ASP:HB3    | 7:P:26:TYR:HB2   | 2.00                     | 0.44              |
| 7:P:271:ALA:O    | 7:P:275:ILE:HG12 | 2.17                     | 0.44              |
| 7:P:400:ARG:HG2  | 7:Q:400:ARG:CZ   | 2.48                     | 0.44              |
| 3:A:680:LYS:CD   | 3:A:755:ILE:HD12 | 2.27                     | 0.44              |
| 4:B:5:LEU:HD12   | 4:B:159:ILE:HG12 | 1.99                     | 0.44              |
| 4:B:46:LEU:O     | 4:B:50:LEU:HD23  | 2.18                     | 0.44              |
| 5:E:136:ARG:HE   | 5:E:138:ILE:HD11 | 1.81                     | 0.44              |
| 5:C:167:PHE:O    | 5:C:171:ARG:HG3  | 2.18                     | 0.44              |
| 5:E:3:PHE:CD1    | 5:E:156:THR:HG22 | 2.52                     | 0.44              |
| 5:G:64:TYR:CB    | 5:G:79:LEU:HD11  | 2.48                     | 0.44              |
| 5:G:167:PHE:O    | 5:G:171:ARG:HG3  | 2.17                     | 0.44              |
| 7:P:146:MET:HG2  | 7:P:168:VAL:HG22 | 2.00                     | 0.44              |
| 7:N:150:ILE:HB   | 7:N:165:PHE:HB2  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:13:LEU:HD13  | 8:T:98:MET:HE1   | 1.97                     | 0.43              |
| 3:A:193:ILE:HD12 | 3:A:537:TYR:HE2  | 1.83                     | 0.43              |
| 7:L:152:GLY:HA2  | 7:L:156:SER:HB3  | 2.00                     | 0.43              |
| 7:O:239:ILE:O    | 7:O:287:ILE:HA   | 2.18                     | 0.43              |
| 2:H:11:SER:O     | 2:H:350:PHE:HA   | 2.18                     | 0.43              |
| 3:A:537:TYR:O    | 3:A:542:ARG:HD2  | 2.18                     | 0.43              |
| 3:A:674:HIS:CB   | 3:A:719:GLU:OE2  | 2.59                     | 0.43              |
| 3:A:710:ARG:O    | 3:A:714:LEU:HG   | 2.18                     | 0.43              |
| 5:E:167:PHE:CZ   | 5:E:212:LEU:HD22 | 2.53                     | 0.43              |
| 7:L:21:LEU:HD11  | 7:L:110:ALA:HA   | 2.00                     | 0.43              |
| 7:P:7:VAL:HG22   | 7:P:25:VAL:HG22  | 2.00                     | 0.43              |
| 7:K:276:ASP:O    | 7:K:280:GLU:HG2  | 2.18                     | 0.43              |
| 3:A:416:VAL:HG11 | 3:A:424:TYR:HE2  | 1.83                     | 0.43              |
| 3:A:525:PHE:CD2  | 3:A:526:MET:HE2  | 2.53                     | 0.43              |
| 5:E:171:ARG:HH11 | 5:E:212:LEU:HD12 | 1.83                     | 0.43              |
| 7:P:400:ARG:NH2  | 7:Q:400:ARG:HA   | 2.33                     | 0.43              |
| 7:M:7:VAL:HG22   | 7:M:25:VAL:HG22  | 2.00                     | 0.43              |
| 7:Q:21:LEU:HD11  | 7:Q:110:ALA:HA   | 2.01                     | 0.43              |
| 3:A:521:LEU:CD1  | 3:A:575:ASP:HB3  | 2.48                     | 0.43              |
| 3:A:672:PHE:HZ   | 3:A:726:PHE:CZ   | 2.35                     | 0.43              |
| 4:B:213:MET:SD   | 4:B:263:GLY:HA3  | 2.58                     | 0.43              |
| 7:P:147:MET:HE3  | 7:P:182:GLY:HA3  | 2.00                     | 0.43              |
| 7:K:1:MET:HA     | 7:K:28:GLU:HB3   | 1.99                     | 0.43              |
| 7:O:220:GLU:O    | 7:O:224:LYS:HG2  | 2.19                     | 0.43              |
| 7:N:314:GLN:HG3  | 7:N:431:ASN:HD21 | 1.83                     | 0.43              |
| 3:A:17:ILE:HD11  | 3:A:156:ILE:HD13 | 2.00                     | 0.43              |
| 5:C:64:TYR:CZ    | 5:C:169:VAL:HG22 | 2.54                     | 0.43              |
| 7:S:205:GLU:HA   | 7:S:403:ARG:NH2  | 2.33                     | 0.43              |
| 7:N:75:ILE:HG21  | 7:N:114:VAL:HG21 | 2.01                     | 0.43              |
| 7:Q:417:LEU:HB2  | 7:Q:421:ALA:HB2  | 2.01                     | 0.43              |
| 5:F:117:TYR:C    | 5:F:142:ILE:HG12 | 2.44                     | 0.43              |
| 2:H:197:LEU:HD13 | 2:H:220:GLU:OE2  | 2.17                     | 0.43              |
| 3:A:111:PHE:CZ   | 3:A:601:THR:HG22 | 2.54                     | 0.43              |
| 3:A:243:LEU:HD21 | 3:A:365:TYR:CD1  | 2.54                     | 0.43              |
| 3:A:623:MET:HE2  | 3:A:623:MET:HB3  | 1.84                     | 0.43              |
| 5:F:44:LEU:HD13  | 5:F:103:LEU:HD23 | 2.00                     | 0.43              |
| 7:O:6:ASP:HB3    | 7:O:26:TYR:HB2   | 2.00                     | 0.43              |
| 7:Q:130:LEU:HD21 | 7:Q:380:THR:HG23 | 2.01                     | 0.43              |
| 2:H:32:ILE:HD11  | 2:H:75:LEU:HD23  | 2.01                     | 0.43              |
| 2:H:50:MET:HE1   | 2:H:84:ILE:HG12  | 2.01                     | 0.43              |
| 4:B:216:THR:HB   | 4:B:292:PRO:HA   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:S:162:PHE:CE2  | 7:S:241:LEU:HD13 | 2.54                     | 0.43              |
| 7:O:148:ASN:CA   | 7:O:166:MET:HG3  | 2.48                     | 0.43              |
| 8:T:71:TRP:CH2   | 8:T:77:ARG:HD3   | 2.54                     | 0.43              |
| 7:S:202:VAL:HG11 | 7:S:399:SER:OG   | 2.19                     | 0.43              |
| 7:L:323:THR:O    | 7:L:347:ILE:HD13 | 2.19                     | 0.43              |
| 7:P:163:GLN:HB3  | 7:P:164:GLU:OE1  | 2.19                     | 0.43              |
| 7:O:131:TYR:CE2  | 7:O:416:GLN:NE2  | 2.86                     | 0.43              |
| 7:Q:379:SER:HA   | 7:Q:406:LYS:HE3  | 2.01                     | 0.43              |
| 4:B:217:THR:O    | 4:B:259:LYS:HD3  | 2.19                     | 0.42              |
| 5:C:138:ILE:HD11 | 5:C:190:TYR:CE2  | 2.53                     | 0.42              |
| 5:E:109:LEU:O    | 5:E:114:VAL:HG22 | 2.19                     | 0.42              |
| 7:M:180:ARG:HG3  | 7:O:59:TYR:CE2   | 2.54                     | 0.42              |
| 6:J:17:ILE:HA    | 6:J:20:LEU:HG    | 2.00                     | 0.42              |
| 7:S:205:GLU:CA   | 7:S:403:ARG:HE   | 2.26                     | 0.42              |
| 7:S:309:LEU:HB3  | 7:S:313:VAL:HG12 | 2.01                     | 0.42              |
| 7:L:150:ILE:HD13 | 7:L:212:PHE:CE2  | 2.54                     | 0.42              |
| 7:L:157:ASP:HB2  | 7:L:211:ARG:CZ   | 2.49                     | 0.42              |
| 7:M:323:THR:CG2  | 7:M:343:LYS:H    | 2.30                     | 0.42              |
| 7:Q:342:ILE:HG13 | 7:Q:367:ALA:HB1  | 2.01                     | 0.42              |
| 3:A:634:ALA:O    | 3:A:641:SER:HB2  | 2.19                     | 0.42              |
| 5:E:27:ALA:O     | 5:E:28:ALA:HB3   | 2.18                     | 0.42              |
| 5:E:59:LEU:HD13  | 5:E:176:LEU:HB3  | 2.01                     | 0.42              |
| 7:S:1:MET:HG2    | 7:S:125:TYR:HE1  | 1.85                     | 0.42              |
| 7:L:147:MET:HB2  | 7:L:167:ILE:HG13 | 2.01                     | 0.42              |
| 3:A:719:GLU:O    | 3:A:722:LYS:HB3  | 2.19                     | 0.42              |
| 4:B:165:LEU:HD12 | 4:B:168:GLU:OE2  | 2.19                     | 0.42              |
| 5:C:186:GLY:HA2  | 5:C:190:TYR:H    | 1.85                     | 0.42              |
| 3:A:493:ILE:HA   | 3:A:496:TYR:CD2  | 2.55                     | 0.42              |
| 5:F:3:PHE:HA     | 5:F:155:ILE:O    | 2.18                     | 0.42              |
| 2:H:47:TYR:O     | 2:H:51:VAL:HG13  | 2.19                     | 0.42              |
| 3:A:696:GLU:HG2  | 3:A:703:ARG:HH12 | 1.84                     | 0.42              |
| 5:E:47:ILE:HB    | 5:E:101:ALA:HB3  | 2.02                     | 0.42              |
| 7:P:75:ILE:HG21  | 7:P:114:VAL:HG21 | 2.01                     | 0.42              |
| 7:P:323:THR:CG2  | 7:P:346:GLN:HB3  | 2.49                     | 0.42              |
| 7:O:190:LYS:C    | 7:O:194:LYS:HZ3  | 2.27                     | 0.42              |
| 3:A:514:VAL:HG23 | 3:A:611:ILE:HG12 | 2.00                     | 0.42              |
| 3:A:720:ARG:HB3  | 3:A:720:ARG:NH2  | 2.34                     | 0.42              |
| 3:A:720:ARG:O    | 3:A:724:LYS:HG3  | 2.20                     | 0.42              |
| 5:F:109:LEU:O    | 5:F:114:VAL:HG22 | 2.19                     | 0.42              |
| 5:C:109:LEU:O    | 5:C:114:VAL:HG22 | 2.20                     | 0.42              |
| 7:S:1:MET:HG2    | 7:S:125:TYR:CE1  | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:P:396:GLY:HA3  | 7:P:403:ARG:HG2  | 2.01                     | 0.42              |
| 7:Q:402:ASP:OD1  | 7:Q:403:ARG:HG2  | 2.19                     | 0.42              |
| 3:A:144:PHE:HE1  | 3:A:149:TYR:CZ   | 2.38                     | 0.42              |
| 3:A:411:TYR:CE2  | 3:A:412:HIS:HD2  | 2.37                     | 0.42              |
| 3:A:639:LYS:HZ2  | 4:B:95:ARG:NH1   | 2.17                     | 0.42              |
| 5:E:200:ALA:H    | 5:E:213:ASN:ND2  | 2.18                     | 0.42              |
| 7:L:1:MET:HE2    | 7:L:125:TYR:HE1  | 1.84                     | 0.42              |
| 7:P:148:ASN:O    | 7:P:397:SER:HB2  | 2.20                     | 0.42              |
| 7:K:149:ILE:HG12 | 7:K:189:LEU:HD23 | 2.02                     | 0.42              |
| 7:Q:5:THR:HG21   | 7:Q:28:GLU:OE1   | 2.18                     | 0.42              |
| 2:H:51:VAL:HG12  | 2:H:56:ALA:HB2   | 2.01                     | 0.42              |
| 3:A:682:PHE:CZ   | 3:A:714:LEU:HD12 | 2.54                     | 0.42              |
| 3:A:712:GLU:O    | 3:A:712:GLU:CG   | 2.67                     | 0.42              |
| 3:A:729:LEU:HD12 | 3:A:732:LYS:NZ   | 2.35                     | 0.42              |
| 4:B:282:PHE:CZ   | 4:B:284:HIS:CE1  | 3.08                     | 0.42              |
| 7:L:1:MET:HA     | 7:L:28:GLU:HB3   | 2.01                     | 0.42              |
| 7:L:51:LEU:HD12  | 7:L:51:LEU:HA    | 1.90                     | 0.42              |
| 7:N:258:TYR:HB2  | 7:N:267:ALA:O    | 2.19                     | 0.42              |
| 7:N:289:THR:HG23 | 7:N:314:GLN:HE21 | 1.85                     | 0.42              |
| 3:A:254:PHE:CE2  | 3:A:274:LEU:HD21 | 2.55                     | 0.42              |
| 3:A:525:PHE:HD2  | 3:A:526:MET:HE2  | 1.84                     | 0.42              |
| 3:A:608:SER:HA   | 3:A:653:PHE:HZ   | 1.84                     | 0.42              |
| 6:D:36:ARG:HH21  | 6:D:39:LEU:HB2   | 1.85                     | 0.42              |
| 5:G:12:ILE:HG13  | 5:G:149:PHE:HB2  | 2.02                     | 0.42              |
| 6:J:124:LYS:HB3  | 6:J:124:LYS:HE3  | 1.84                     | 0.42              |
| 7:S:289:THR:HG23 | 7:S:314:GLN:HE21 | 1.85                     | 0.42              |
| 7:L:238:PHE:CE1  | 7:L:426:LEU:HD21 | 2.55                     | 0.42              |
| 7:L:245:SER:HA   | 7:L:248:PHE:CE2  | 2.55                     | 0.42              |
| 7:Q:341:LEU:HA   | 7:Q:341:LEU:HD12 | 1.78                     | 0.42              |
| 3:A:608:SER:HA   | 3:A:653:PHE:CZ   | 2.55                     | 0.41              |
| 3:A:665:LEU:O    | 3:A:669:ARG:HG3  | 2.20                     | 0.41              |
| 4:B:32:ILE:HD11  | 4:B:170:MET:HE1  | 2.02                     | 0.41              |
| 5:C:101:ALA:HB1  | 5:C:147:PHE:HB3  | 2.02                     | 0.41              |
| 7:L:79:ILE:HD13  | 7:L:79:ILE:HA    | 1.88                     | 0.41              |
| 7:L:275:ILE:HD12 | 7:L:275:ILE:HG23 | 1.70                     | 0.41              |
| 7:P:424:ARG:O    | 7:P:427:LYS:HE2  | 2.18                     | 0.41              |
| 7:K:150:ILE:HB   | 7:K:165:PHE:HB2  | 2.02                     | 0.41              |
| 7:M:53:ASP:HA    | 7:M:66:LYS:HE3   | 2.01                     | 0.41              |
| 7:N:36:MET:HB2   | 7:N:378:ASP:HB2  | 2.01                     | 0.41              |
| 7:N:341:LEU:HA   | 7:N:341:LEU:HD12 | 1.79                     | 0.41              |
| 3:A:493:ILE:HD13 | 3:A:580:ILE:HD13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:674:HIS:C    | 3:A:723:PHE:HZ   | 2.28                     | 0.41              |
| 4:B:7:ILE:HG21   | 4:B:7:ILE:HD13   | 1.84                     | 0.41              |
| 5:C:34:SER:H     | 5:C:138:ILE:HA   | 1.86                     | 0.41              |
| 7:K:205:GLU:HA   | 7:K:403:ARG:CZ   | 2.50                     | 0.41              |
| 7:M:306:THR:HG21 | 7:M:336:ALA:HA   | 2.02                     | 0.41              |
| 2:H:200:VAL:HB   | 2:H:319:THR:OG1  | 2.20                     | 0.41              |
| 4:B:39:GLU:O     | 4:B:43:MET:HG3   | 2.20                     | 0.41              |
| 5:F:138:ILE:HG21 | 5:F:138:ILE:HD13 | 1.86                     | 0.41              |
| 5:E:33:ASP:H     | 5:E:137:GLN:HE21 | 1.68                     | 0.41              |
| 6:I:49:SER:HA    | 6:I:57:LEU:HD11  | 2.03                     | 0.41              |
| 7:L:36:MET:HG2   | 7:L:376:THR:HG21 | 2.02                     | 0.41              |
| 7:N:343:LYS:HD3  | 7:N:346:GLN:NE2  | 2.34                     | 0.41              |
| 2:H:258:LYS:HA   | 2:H:262:LEU:HB2  | 2.01                     | 0.41              |
| 4:B:29:ALA:HA    | 4:B:32:ILE:HG22  | 2.03                     | 0.41              |
| 5:F:131:ALA:CB   | 5:G:92:LYS:HD2   | 2.49                     | 0.41              |
| 7:S:401:THR:OG1  | 7:N:402:ASP:HB3  | 2.19                     | 0.41              |
| 7:M:350:LEU:HD23 | 7:M:350:LEU:HA   | 1.89                     | 0.41              |
| 7:O:149:ILE:HD12 | 7:O:189:LEU:HD22 | 2.03                     | 0.41              |
| 7:N:160:ILE:HD11 | 7:N:212:PHE:HB2  | 2.01                     | 0.41              |
| 8:T:94:GLU:HG3   | 8:T:96:ILE:CD1   | 2.49                     | 0.41              |
| 4:B:61:THR:HA    | 4:B:216:THR:OG1  | 2.21                     | 0.41              |
| 5:F:64:TYR:CD1   | 5:F:78:ILE:HD13  | 2.56                     | 0.41              |
| 5:F:101:ALA:HB1  | 5:F:147:PHE:HB3  | 2.01                     | 0.41              |
| 7:S:92:ARG:HA    | 7:S:92:ARG:HD3   | 1.85                     | 0.41              |
| 7:O:163:GLN:HE22 | 7:O:247:GLU:CD   | 2.29                     | 0.41              |
| 7:O:292:ASP:OD2  | 7:O:318:ASP:HB3  | 2.20                     | 0.41              |
| 8:T:33:ILE:HB    | 8:T:37:GLU:CG    | 2.51                     | 0.41              |
| 2:H:99:LEU:HD23  | 2:H:320:LYS:HB3  | 2.03                     | 0.41              |
| 3:A:438:THR:HG22 | 3:A:463:SER:O    | 2.20                     | 0.41              |
| 5:G:140:ARG:HD3  | 5:G:190:TYR:CE2  | 2.56                     | 0.41              |
| 7:S:186:PHE:CZ   | 7:S:399:SER:HB2  | 2.55                     | 0.41              |
| 7:L:74:VAL:HG12  | 7:L:97:LEU:HD21  | 2.02                     | 0.41              |
| 7:O:95:ILE:HG12  | 7:O:103:LYS:HE3  | 2.01                     | 0.41              |
| 4:B:65:PRO:O     | 4:B:71:PHE:HB2   | 2.20                     | 0.41              |
| 5:C:167:PHE:CE2  | 5:C:212:LEU:HD22 | 2.55                     | 0.41              |
| 5:E:64:TYR:CE2   | 5:E:169:VAL:HG22 | 2.55                     | 0.41              |
| 7:P:190:LYS:O    | 7:P:194:LYS:HG3  | 2.20                     | 0.41              |
| 7:Q:312:LYS:HG3  | 7:Q:313:VAL:HG23 | 2.02                     | 0.41              |
| 3:A:510:ARG:HH21 | 5:E:25:ALA:HB2   | 1.86                     | 0.41              |
| 3:A:622:LEU:HD21 | 4:B:130:THR:HG21 | 2.03                     | 0.41              |
| 7:P:185:ILE:HD11 | 7:P:237:VAL:HG21 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:M:147:MET:HG3  | 7:M:407:TYR:OH   | 2.21                     | 0.41              |
| 7:M:359:MET:HE3  | 7:M:359:MET:HB2  | 1.87                     | 0.41              |
| 1:R:8:U:H5'      | 5:F:54:GLY:HA3   | 2.02                     | 0.41              |
| 2:H:17:PRO:HA    | 2:H:222:ILE:O    | 2.21                     | 0.41              |
| 2:H:103:ARG:HD2  | 2:H:110:ALA:CA   | 2.50                     | 0.41              |
| 2:H:245:GLU:HG2  | 2:H:248:LYS:HE3  | 2.02                     | 0.41              |
| 2:H:268:ASP:HA   | 2:H:337:LYS:HB2  | 2.01                     | 0.41              |
| 3:A:297:LEU:HD11 | 3:A:307:VAL:HG23 | 2.01                     | 0.41              |
| 3:A:382:TYR:HB2  | 4:B:229:MET:HG3  | 2.03                     | 0.41              |
| 3:A:642:ILE:HB   | 3:A:653:PHE:CE1  | 2.55                     | 0.41              |
| 3:A:696:GLU:O    | 3:A:700:ASN:HB2  | 2.21                     | 0.41              |
| 4:B:6:TYR:CE2    | 4:B:170:MET:HG3  | 2.56                     | 0.41              |
| 4:B:135:GLN:HE21 | 4:B:137:HIS:HE1  | 1.67                     | 0.41              |
| 6:D:70:TYR:CZ    | 6:D:74:ARG:HD3   | 2.56                     | 0.41              |
| 6:I:91:VAL:HG13  | 6:I:96:ILE:HB    | 2.03                     | 0.41              |
| 7:S:248:PHE:CE2  | 7:S:258:TYR:HE1  | 2.39                     | 0.41              |
| 7:L:1:MET:HE2    | 7:L:125:TYR:CE1  | 2.55                     | 0.41              |
| 7:M:306:THR:HG21 | 7:M:335:HIS:O    | 2.20                     | 0.41              |
| 7:O:371:HIS:H    | 7:O:371:HIS:HD1  | 1.69                     | 0.41              |
| 1:R:-5:A:H3'     | 4:B:38:LEU:HD11  | 2.03                     | 0.41              |
| 2:H:286:ALA:HB1  | 2:H:299:LEU:HD21 | 2.03                     | 0.41              |
| 3:A:411:TYR:CD1  | 3:A:421:ARG:NH1  | 2.89                     | 0.41              |
| 7:L:239:ILE:O    | 7:L:287:ILE:HA   | 2.21                     | 0.41              |
| 7:K:112:LEU:HD22 | 7:K:345:ASN:HA   | 2.03                     | 0.41              |
| 7:M:152:GLY:HA2  | 7:M:156:SER:OG   | 2.21                     | 0.41              |
| 7:O:147:MET:SD   | 7:O:398:LEU:HD21 | 2.61                     | 0.41              |
| 3:A:689:LEU:O    | 3:A:734:TYR:OH   | 2.39                     | 0.40              |
| 5:G:101:ALA:HB1  | 5:G:147:PHE:HB3  | 2.03                     | 0.40              |
| 7:S:248:PHE:CE2  | 7:S:258:TYR:CE1  | 3.09                     | 0.40              |
| 7:L:401:THR:OG1  | 7:K:402:ASP:HB3  | 2.21                     | 0.40              |
| 7:M:346:GLN:HE21 | 7:M:372:ARG:NH1  | 2.19                     | 0.40              |
| 7:Q:2:SER:HB3    | 7:Q:125:TYR:CZ   | 2.57                     | 0.40              |
| 2:H:238:GLU:OE1  | 2:H:241:ARG:NH2  | 2.54                     | 0.40              |
| 3:A:251:ILE:HG13 | 3:A:252:GLN:N    | 2.35                     | 0.40              |
| 3:A:716:ASP:O    | 3:A:719:GLU:N    | 2.48                     | 0.40              |
| 5:E:14:LEU:HB2   | 5:E:143:ARG:O    | 2.21                     | 0.40              |
| 7:K:328:LEU:HD21 | 7:K:360:ALA:HB2  | 2.03                     | 0.40              |
| 7:Q:24:GLU:HG2   | 7:Q:32:PHE:CZ    | 2.56                     | 0.40              |
| 8:T:27:ASN:HB3   | 8:T:33:ILE:HD13  | 2.03                     | 0.40              |
| 1:R:26:A:H5'     | 5:G:124:ASN:O    | 2.21                     | 0.40              |
| 7:L:157:ASP:HB2  | 7:L:211:ARG:NE   | 2.37                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:K:22:GLU:HB3  | 7:K:36:MET:HG2   | 2.03                     | 0.40              |
| 4:B:20:LEU:HD11 | 4:B:181:LYS:HE2  | 2.03                     | 0.40              |
| 4:B:135:GLN:NE2 | 4:B:137:HIS:CE1  | 2.90                     | 0.40              |
| 6:D:45:LEU:CD2  | 6:D:109:LEU:HD11 | 2.52                     | 0.40              |
| 5:E:78:ILE:H    | 5:E:78:ILE:HD12  | 1.87                     | 0.40              |
| 7:S:425:GLY:O   | 7:S:428:SER:HB2  | 2.22                     | 0.40              |
| 7:L:147:MET:HE1 | 7:L:179:LEU:HA   | 2.03                     | 0.40              |
| 3:A:396:GLU:OE1 | 3:A:397:ARG:HB2  | 2.22                     | 0.40              |
| 4:B:71:PHE:O    | 4:B:157:TYR:OH   | 2.38                     | 0.40              |
| 5:E:95:ARG:HH12 | 5:E:162:GLN:NE2  | 2.19                     | 0.40              |
| 5:G:156:THR:H   | 5:G:159:ASN:HD22 | 1.69                     | 0.40              |
| 7:K:147:MET:HG2 | 7:K:407:TYR:OH   | 2.21                     | 0.40              |
| 7:Q:12:VAL:HG21 | 7:Q:36:MET:CE    | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 2   | H     | 350/357 (98%)  | 331 (95%) | 19 (5%) | 0        | 100         | 100 |
| 3   | A     | 756/758 (100%) | 731 (97%) | 24 (3%) | 1 (0%)   | 48          | 72  |
| 4   | B     | 295/299 (99%)  | 279 (95%) | 16 (5%) | 0        | 100         | 100 |
| 5   | C     | 218/220 (99%)  | 216 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 5   | E     | 217/220 (99%)  | 205 (94%) | 12 (6%) | 0        | 100         | 100 |
| 5   | F     | 217/220 (99%)  | 210 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 5   | G     | 217/220 (99%)  | 209 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 6   | D     | 128/136 (94%)  | 126 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 6   | I     | 128/136 (94%)  | 127 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 6   | J     | 128/136 (94%)  | 126 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 7   | K     | 432/434 (100%)  | 418 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 7   | L     | 432/434 (100%)  | 419 (97%)  | 13 (3%)  | 0        | 100         | 100 |
| 7   | M     | 432/434 (100%)  | 420 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 7   | N     | 432/434 (100%)  | 423 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 7   | O     | 432/434 (100%)  | 419 (97%)  | 13 (3%)  | 0        | 100         | 100 |
| 7   | P     | 432/434 (100%)  | 422 (98%)  | 10 (2%)  | 0        | 100         | 100 |
| 7   | Q     | 432/434 (100%)  | 420 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 7   | S     | 432/434 (100%)  | 420 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 8   | T     | 103/105 (98%)   | 95 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| All | All   | 6213/6279 (99%) | 6016 (97%) | 196 (3%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 717 | LYS  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | H     | 306/312 (98%)  | 306 (100%) | 0        | 100         | 100 |
| 3   | A     | 649/649 (100%) | 649 (100%) | 0        | 100         | 100 |
| 4   | B     | 247/263 (94%)  | 247 (100%) | 0        | 100         | 100 |
| 5   | C     | 180/188 (96%)  | 180 (100%) | 0        | 100         | 100 |
| 5   | E     | 181/188 (96%)  | 181 (100%) | 0        | 100         | 100 |
| 5   | F     | 181/188 (96%)  | 181 (100%) | 0        | 100         | 100 |
| 5   | G     | 182/188 (97%)  | 182 (100%) | 0        | 100         | 100 |
| 6   | D     | 119/125 (95%)  | 119 (100%) | 0        | 100         | 100 |
| 6   | I     | 119/125 (95%)  | 119 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 6   | J     | 119/125 (95%)   | 119 (100%)  | 0        | 100         | 100 |
| 7   | K     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | L     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | M     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | N     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | O     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | P     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | Q     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 7   | S     | 338/338 (100%)  | 338 (100%)  | 0        | 100         | 100 |
| 8   | T     | 94/94 (100%)    | 94 (100%)   | 0        | 100         | 100 |
| All | All   | 5081/5149 (99%) | 5081 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 65  | GLN  |
| 2   | H     | 115 | ASN  |
| 2   | H     | 124 | ASN  |
| 2   | H     | 154 | ASN  |
| 3   | A     | 15  | HIS  |
| 3   | A     | 107 | GLN  |
| 3   | A     | 412 | HIS  |
| 3   | A     | 532 | GLN  |
| 3   | A     | 692 | ASN  |
| 3   | A     | 700 | ASN  |
| 4   | B     | 134 | ASN  |
| 4   | B     | 137 | HIS  |
| 5   | F     | 11  | GLN  |
| 5   | F     | 134 | ASN  |
| 5   | F     | 144 | ASN  |
| 6   | D     | 75  | ASN  |
| 5   | C     | 137 | GLN  |
| 5   | E     | 134 | ASN  |
| 5   | E     | 162 | GLN  |
| 5   | E     | 213 | ASN  |
| 5   | G     | 161 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | J     | 67  | GLN  |
| 6   | J     | 75  | ASN  |
| 7   | L     | 65  | GLN  |
| 7   | L     | 78  | HIS  |
| 7   | L     | 346 | GLN  |
| 7   | P     | 65  | GLN  |
| 7   | P     | 314 | GLN  |
| 7   | P     | 371 | HIS  |
| 7   | K     | 65  | GLN  |
| 7   | K     | 148 | ASN  |
| 7   | K     | 163 | GLN  |
| 7   | K     | 371 | HIS  |
| 7   | M     | 18  | ASN  |
| 7   | M     | 46  | HIS  |
| 7   | M     | 65  | GLN  |
| 7   | M     | 213 | ASN  |
| 7   | M     | 346 | GLN  |
| 7   | O     | 65  | GLN  |
| 7   | O     | 163 | GLN  |
| 7   | O     | 416 | GLN  |
| 7   | N     | 65  | GLN  |
| 7   | N     | 346 | GLN  |
| 7   | Q     | 65  | GLN  |
| 7   | Q     | 148 | ASN  |
| 7   | Q     | 274 | GLN  |
| 7   | Q     | 346 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 1   | R     | 40/41 (97%) | 11 (27%)          | 1 (2%)          |

All (11) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | -4  | C    |
| 1   | R     | -3  | G    |
| 1   | R     | 2   | C    |
| 1   | R     | 3   | C    |
| 1   | R     | 7   | A    |
| 1   | R     | 8   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 10  | C    |
| 1   | R     | 15  | G    |
| 1   | R     | 16  | C    |
| 1   | R     | 21  | U    |
| 1   | R     | 34  | U    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 2   | C    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

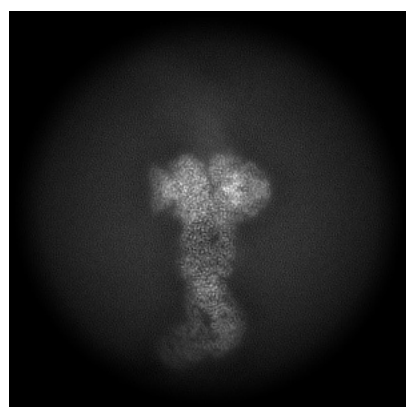
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49645. These allow visual inspection of the internal detail of the map and identification of artifacts.

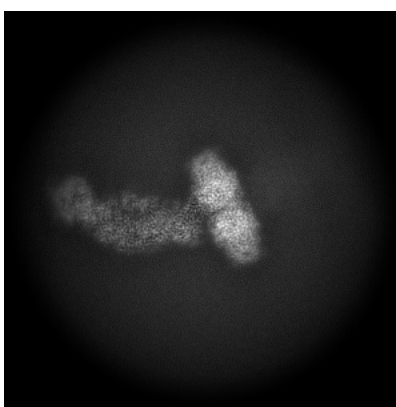
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

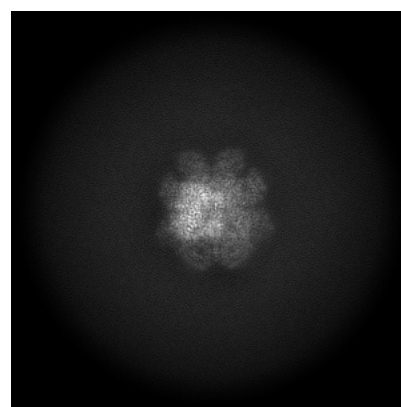
#### 6.1.1 Primary map



X



Y

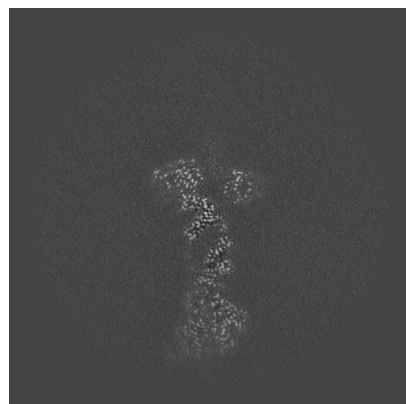


Z

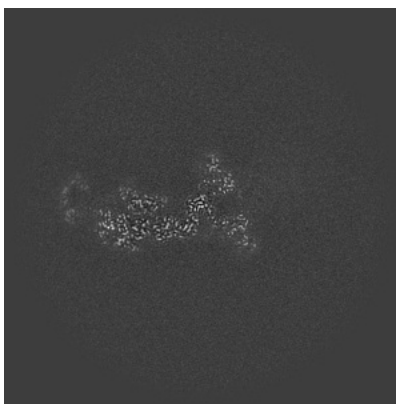
The images above show the map projected in three orthogonal directions.

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

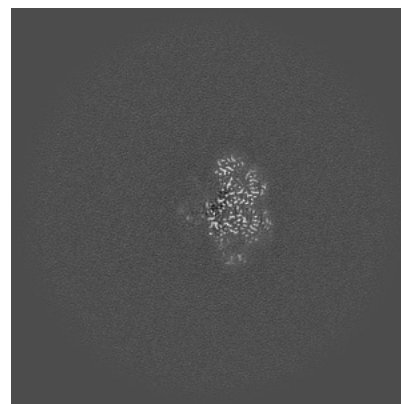
#### 6.2.1 Primary map



X Index: 280



Y Index: 280

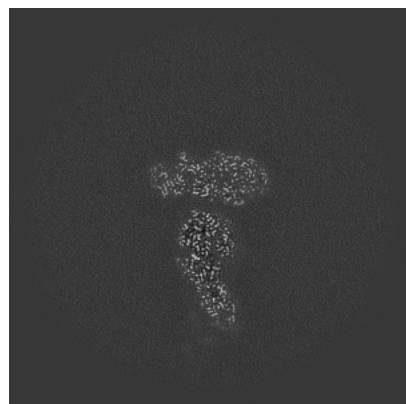


Z Index: 280

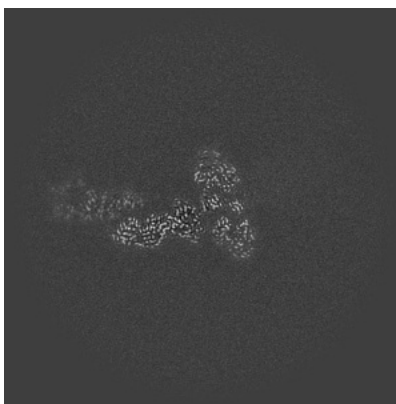
The images above show central slices of the map in three orthogonal directions.

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

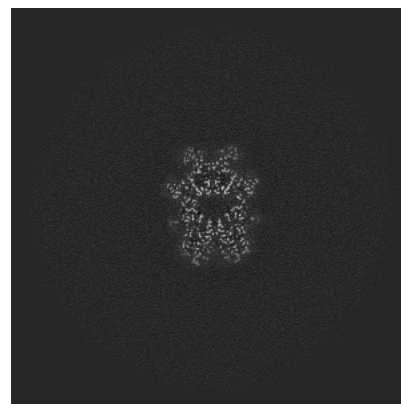
### 6.3.1 Primary map



X Index: 257



Y Index: 264



Z Index: 310

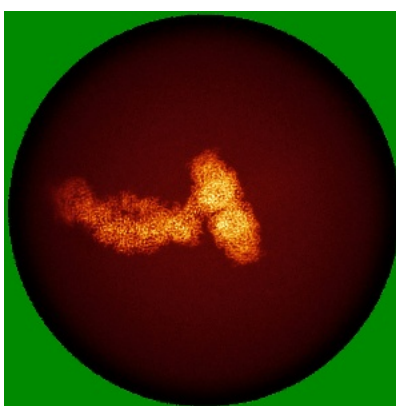
The images above show the largest variance slices of the map in three orthogonal directions.

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

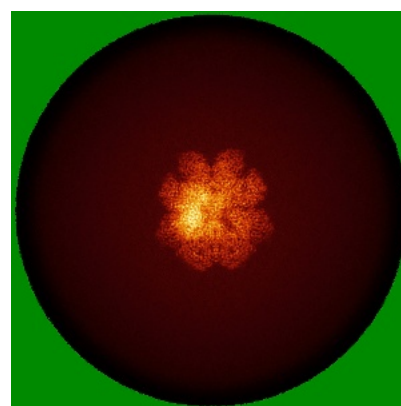
### 6.4.1 Primary map



X



Y

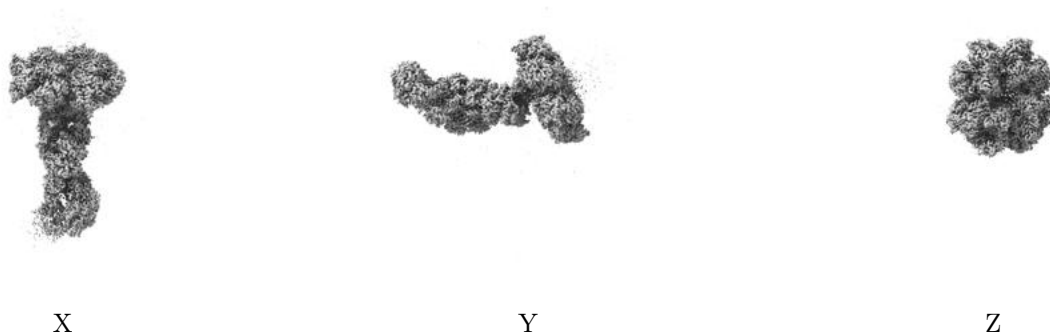


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

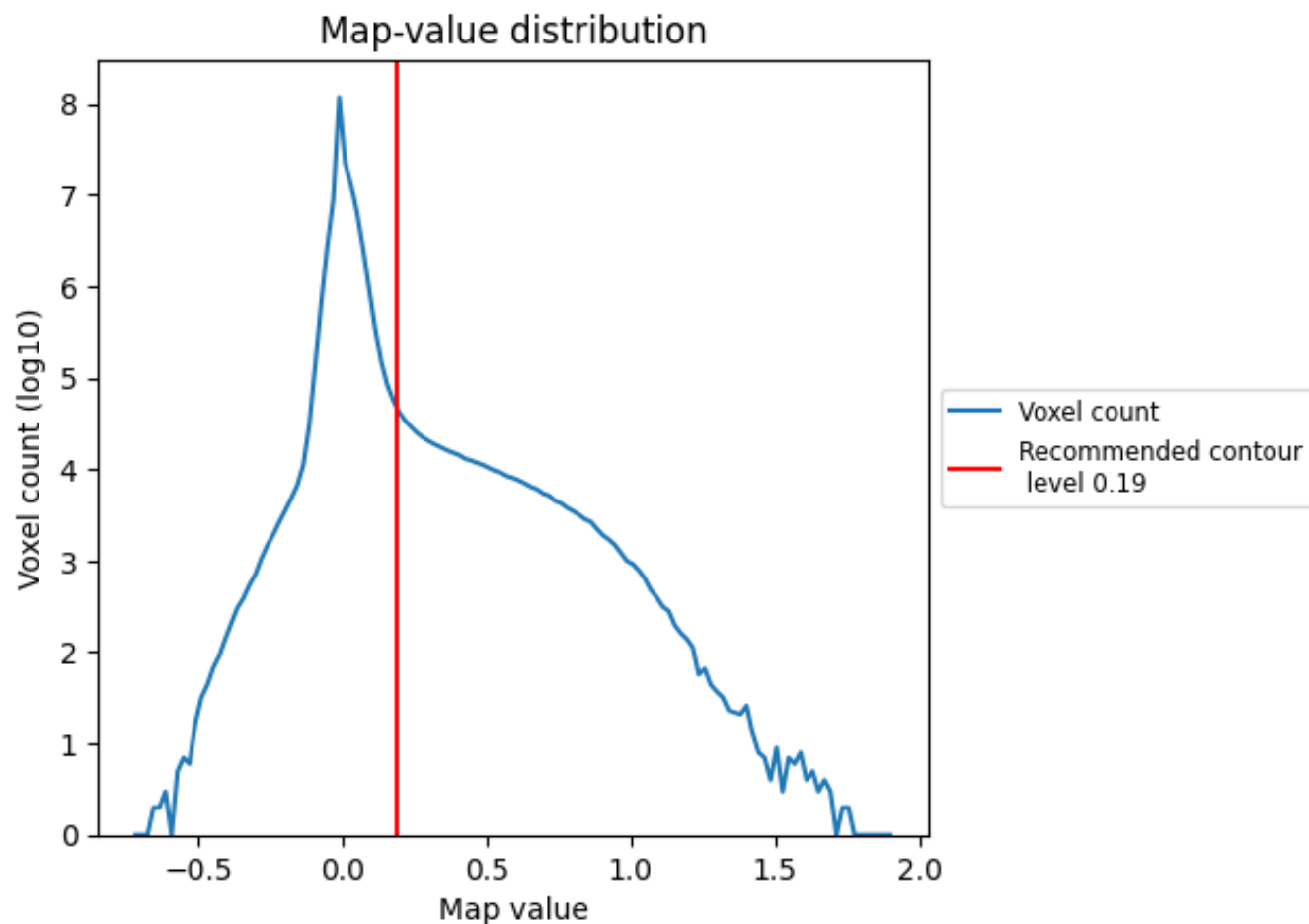
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

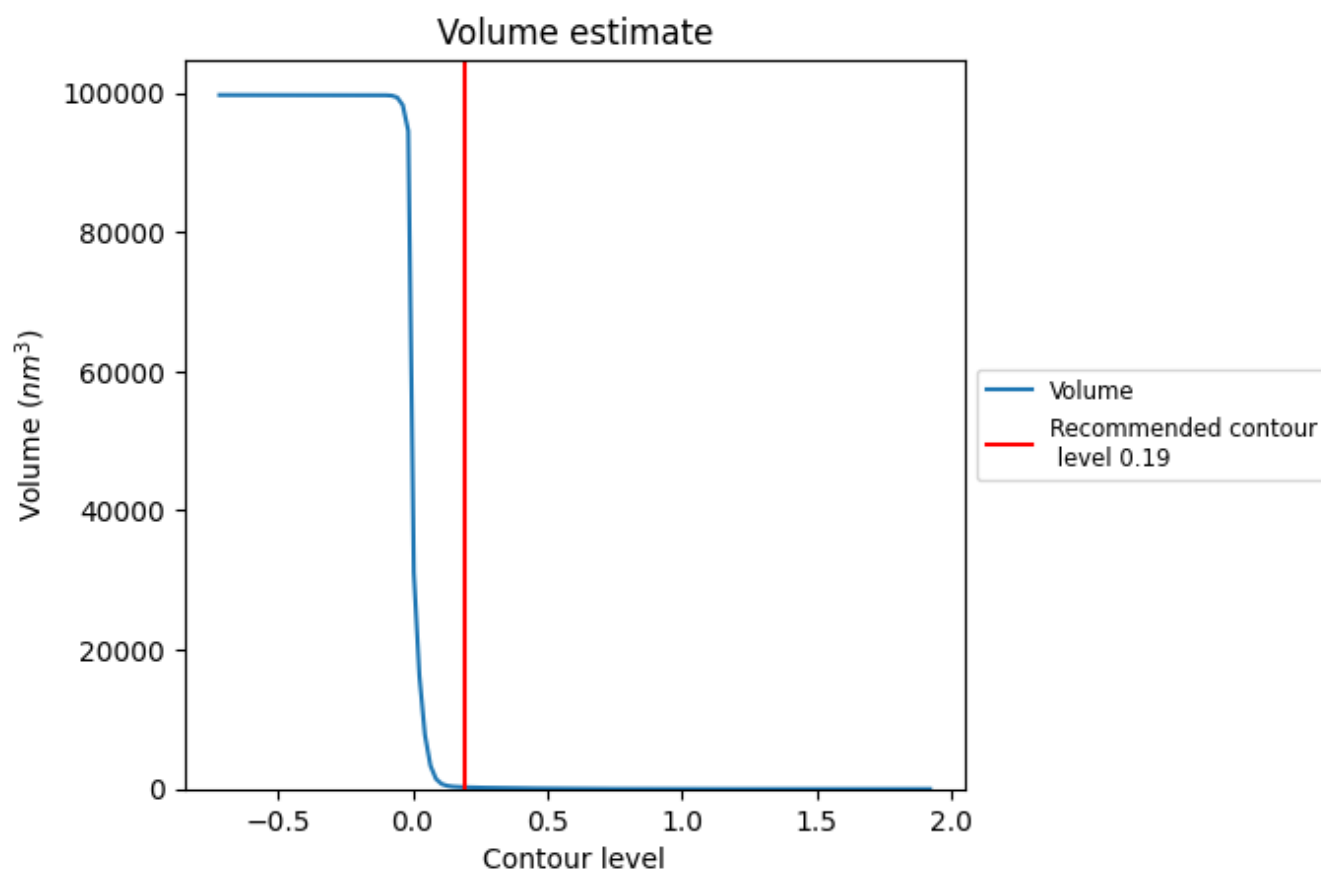
This section contains the results of statistical analysis of the map.

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



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

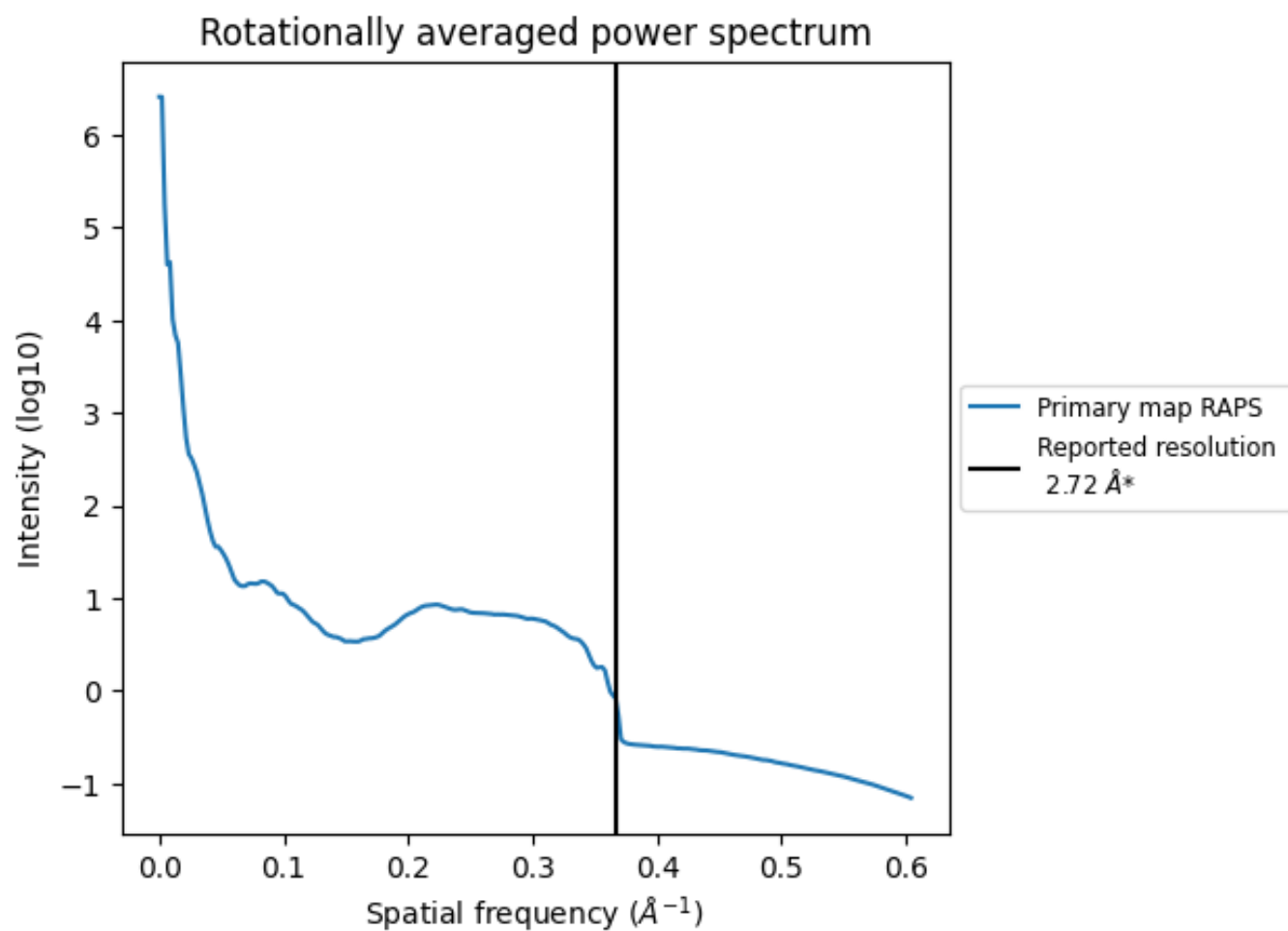
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251  $\text{nm}^3$ ; this corresponds to an approximate mass of 227 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 0.368 Å<sup>-1</sup>

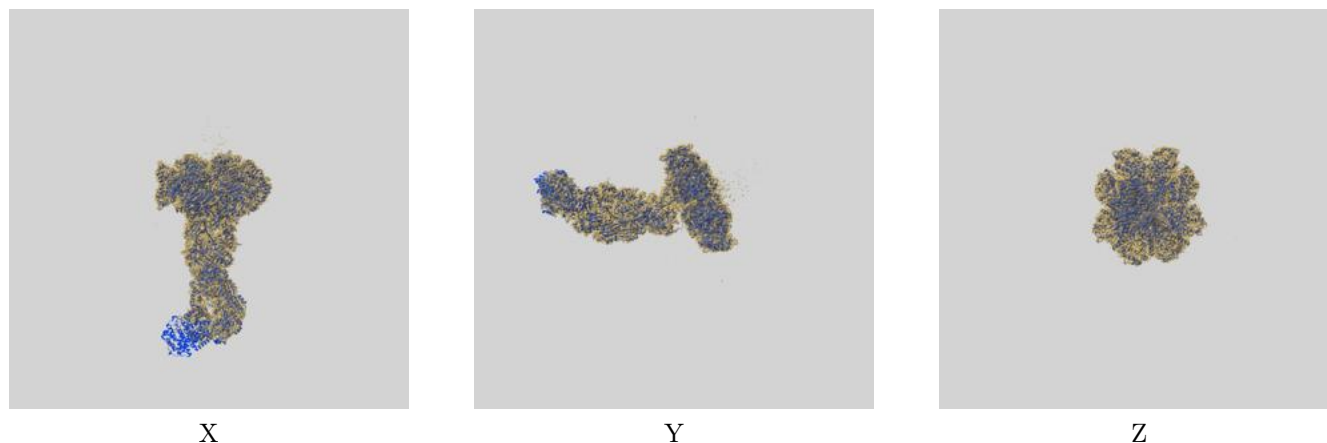
## 8 Fourier-Shell correlation ⓘ

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

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

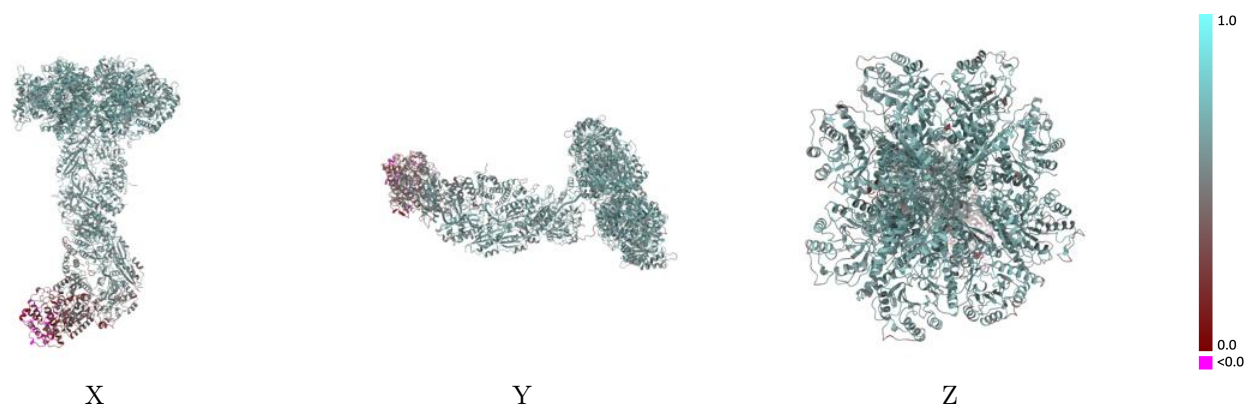
This section contains information regarding the fit between EMDB map EMD-49645 and PDB model 9NQ7. Per-residue inclusion information can be found in section 3 on page 7.

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



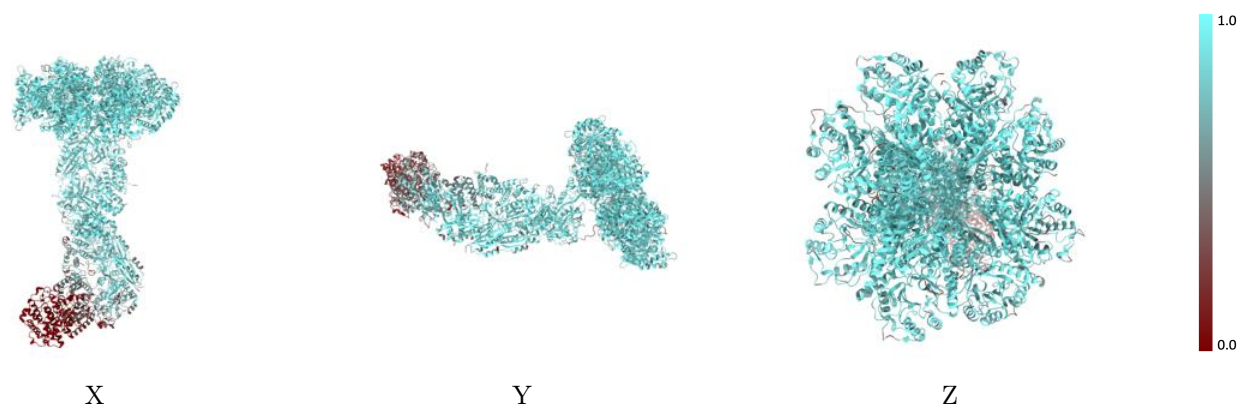
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



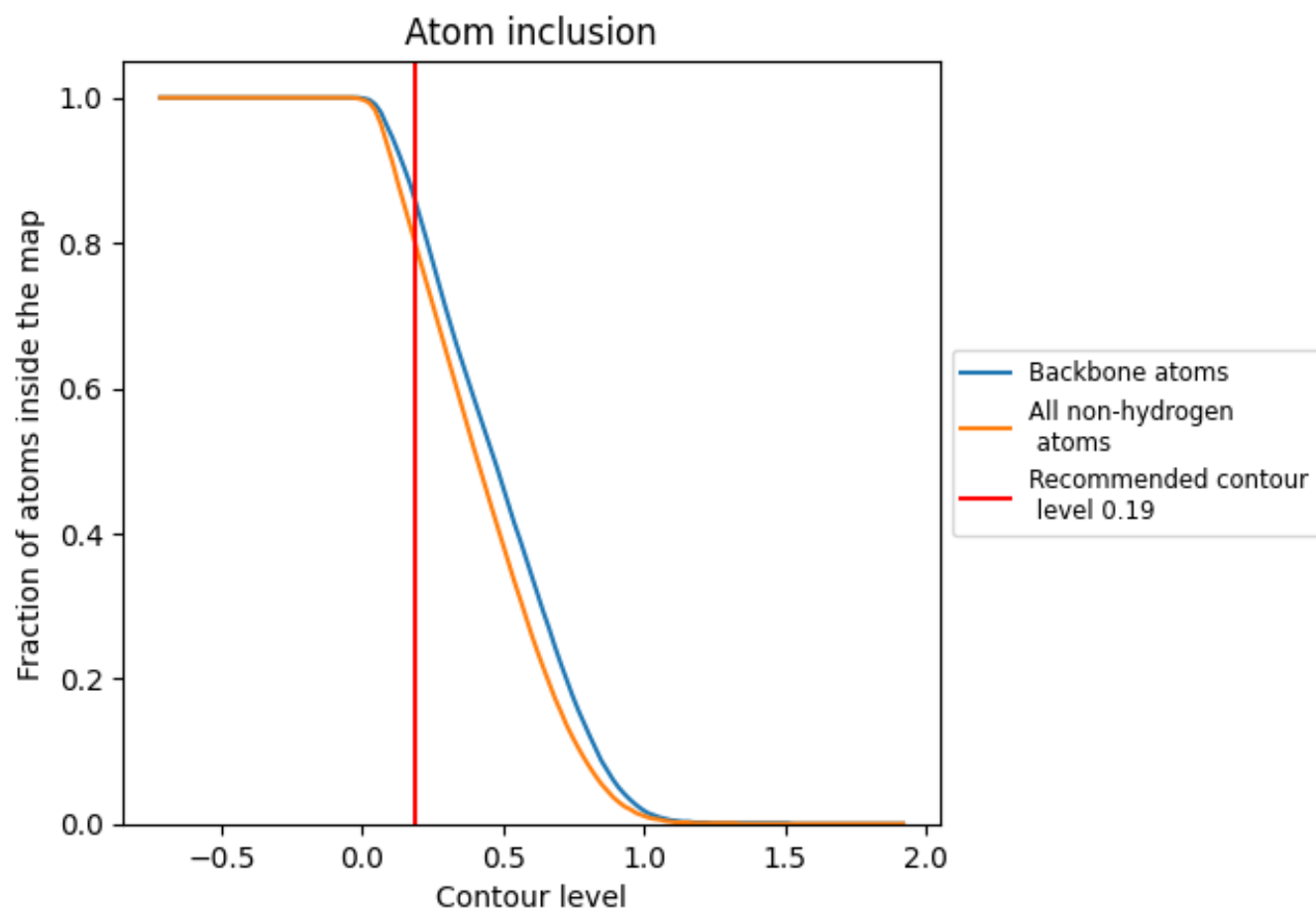
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.19) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7980   |  0.5620   |
| A     |  0.2710   |  0.3300   |
| B     |  0.5930   |  0.4630   |
| C     |  0.8990   |  0.6050   |
| D     |  0.7780   |  0.5510   |
| E     |  0.7570   |  0.5360   |
| F     |  0.8730   |  0.5900   |
| G     |  0.8960   |  0.5960   |
| H     |  0.9090   |  0.6030   |
| I     |  0.8720   |  0.5850   |
| J     |  0.8780   |  0.5820   |
| K     |  0.8970   |  0.6130   |
| L     |  0.9000   |  0.6110   |
| M     |  0.8940   |  0.6150   |
| N     |  0.9100  |  0.6190  |
| O     |  0.8900 |  0.6090 |
| P     |  0.8890 |  0.6060 |
| Q     |  0.8930 |  0.6140 |
| R     |  0.9660 |  0.6020 |
| S     |  0.9120 |  0.6200 |
| T     |  0.8350 |  0.5650 |

