



## Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:25 AM UTC

PDB ID : 8XBU / pdb\_00008xbu  
EMDB ID : EMD-38229  
Title : The cryo-EM structure of the decameric RAD51 ring bound to the nucleosome with the linker DNA binding  
Authors : Shioi, T.; Hatazawa, S.; Ogasawara, M.; Takizawa, Y.; Kurumizaka, H.  
Deposited on : 2023-12-07  
Resolution : 4.24 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
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) : 2.49

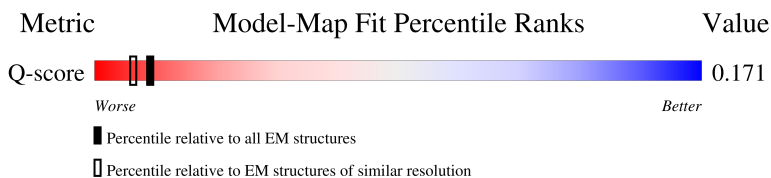
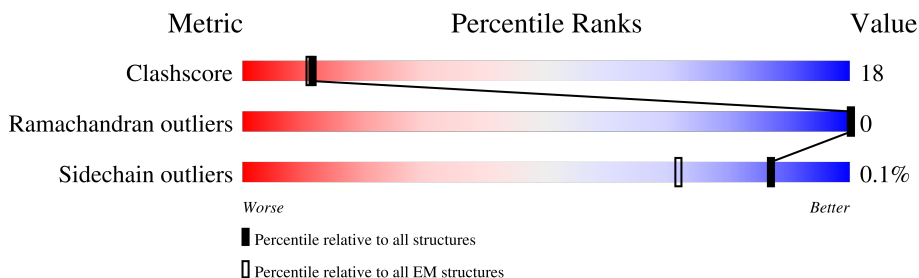
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.24 Å.

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



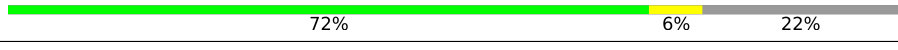
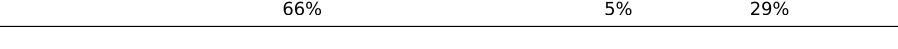
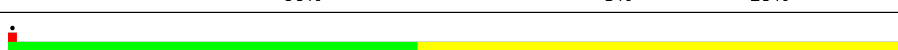
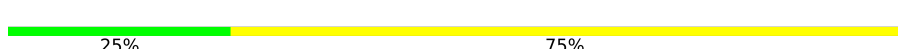
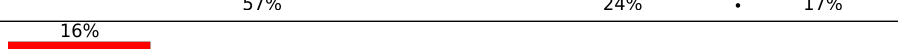
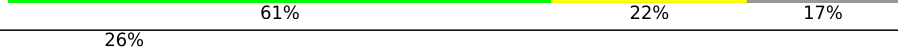
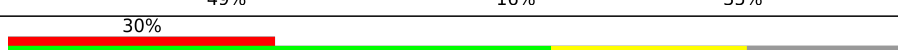
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 4688 ( 3.74 - 4.74 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 139    |                  |
| 1   | E     | 139    |                  |
| 2   | B     | 106    |                  |
| 2   | F     | 106    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | C     | 133    |    |
| 3   | G     | 133    |    |
| 4   | D     | 129    |    |
| 4   | H     | 129    |    |
| 5   | I     | 156    |    |
| 6   | J     | 153    |    |
| 7   | K     | 342    |    |
| 7   | L     | 342    |    |
| 7   | M     | 342    |    |
| 7   | N     | 342    |   |
| 7   | O     | 342    |  |
| 7   | P     | 342    |  |
| 7   | Q     | 342    |  |
| 7   | R     | 342    |  |
| 7   | S     | 342    |  |
| 7   | T     | 342    |  |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32567 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 499 | 151 | 136 | 4 |         |       |
| 1   | E     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 517 | 159 | 139 | 4 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -3      | GLY      | -      | expression tag | UNP P68431 |
| A     | -2      | SER      | -      | expression tag | UNP P68431 |
| A     | -1      | HIS      | -      | expression tag | UNP P68431 |
| E     | -3      | GLY      | -      | expression tag | UNP P68431 |
| E     | -2      | SER      | -      | expression tag | UNP P68431 |
| E     | -1      | HIS      | -      | expression tag | UNP P68431 |

- Molecule 2 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 614   | 389 | 119 | 105 | 1 |         |       |
| 2   | F     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 442 | 142 | 118 | 1 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -3      | GLY      | -      | expression tag | UNP P62805 |
| B     | -2      | SER      | -      | expression tag | UNP P62805 |
| B     | -1      | HIS      | -      | expression tag | UNP P62805 |
| F     | -3      | GLY      | -      | expression tag | UNP P62805 |
| F     | -2      | SER      | -      | expression tag | UNP P62805 |
| F     | -1      | HIS      | -      | expression tag | UNP P62805 |

- Molecule 3 is a protein called Histone H2A type 1-B/E.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | C     | 108      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 526 | 165 | 144 |         |       |
| 3   | G     | 104      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 508 | 157 | 140 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -3      | GLY      | -      | expression tag | UNP P04908 |
| C     | -2      | SER      | -      | expression tag | UNP P04908 |
| C     | -1      | HIS      | -      | expression tag | UNP P04908 |
| G     | -3      | GLY      | -      | expression tag | UNP P04908 |
| G     | -2      | SER      | -      | expression tag | UNP P04908 |
| G     | -1      | HIS      | -      | expression tag | UNP P04908 |

- Molecule 4 is a protein called Histone H2B type 1-J.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 720   | 453 | 129 | 136 | 2 |         |       |
| 4   | H     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 450 | 128 | 134 | 2 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -3      | GLY      | -      | expression tag | UNP P06899 |
| D     | -2      | SER      | -      | expression tag | UNP P06899 |
| D     | -1      | HIS      | -      | expression tag | UNP P06899 |
| H     | -3      | GLY      | -      | expression tag | UNP P06899 |
| H     | -2      | SER      | -      | expression tag | UNP P06899 |
| H     | -1      | HIS      | -      | expression tag | UNP P06899 |

- Molecule 5 is a DNA chain called DNA (156-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | I     | 156      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 3189  | 1509 | 615 | 909 | 156 |         |       |

- Molecule 6 is a DNA chain called DNA (153-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 6   | J     | 153      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 3143  | 1494 | 552 | 944 | 153 |         |       |

- Molecule 7 is a protein called DNA repair protein RAD51 homolog 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | K     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |
| 7   | L     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |
| 7   | M     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |
| 7   | N     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |
| 7   | O     | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1698  | 1058 | 301 | 328 | 11 |         |       |
| 7   | P     | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1698  | 1058 | 301 | 328 | 11 |         |       |
| 7   | Q     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |
| 7   | R     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |
| 7   | S     | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1698  | 1058 | 301 | 328 | 11 |         |       |
| 7   | T     | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1353 | 381 | 417 | 12 |         |       |

There are 30 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| K     | -1      | SER      | -      | expression tag | UNP Q06609 |
| K     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| L     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| L     | -1      | SER      | -      | expression tag | UNP Q06609 |
| L     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| M     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| M     | -1      | SER      | -      | expression tag | UNP Q06609 |
| M     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| N     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| N     | -1      | SER      | -      | expression tag | UNP Q06609 |
| N     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| O     | -2      | GLY      | -      | expression tag | UNP Q06609 |

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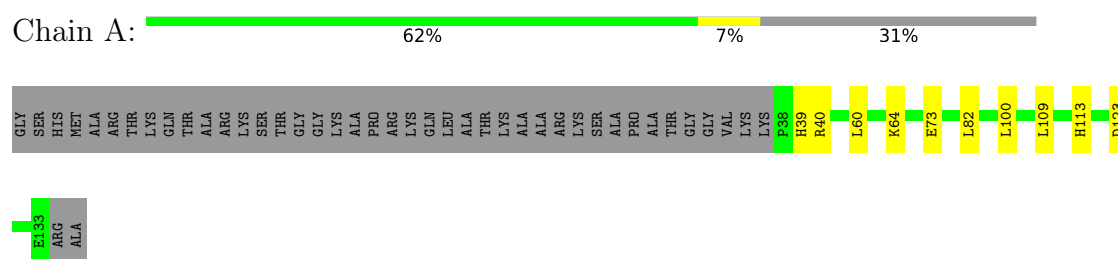
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| O     | -1      | SER      | -      | expression tag | UNP Q06609 |
| O     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| P     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| P     | -1      | SER      | -      | expression tag | UNP Q06609 |
| P     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| Q     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| Q     | -1      | SER      | -      | expression tag | UNP Q06609 |
| Q     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| R     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| R     | -1      | SER      | -      | expression tag | UNP Q06609 |
| R     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| S     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| S     | -1      | SER      | -      | expression tag | UNP Q06609 |
| S     | 0       | HIS      | -      | expression tag | UNP Q06609 |
| T     | -2      | GLY      | -      | expression tag | UNP Q06609 |
| T     | -1      | SER      | -      | expression tag | UNP Q06609 |
| T     | 0       | HIS      | -      | expression tag | UNP Q06609 |

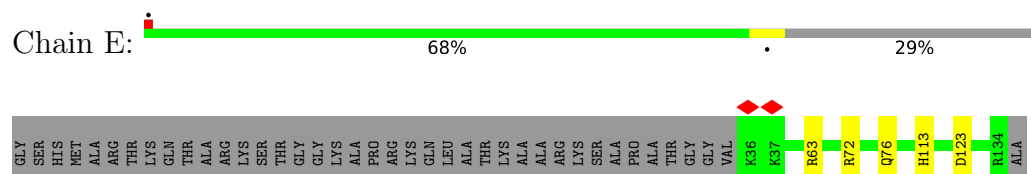
### 3 Residue-property plots [i](#)

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.

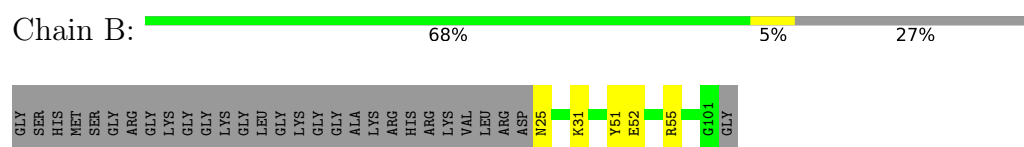
#### • Molecule 1: Histone H3.1



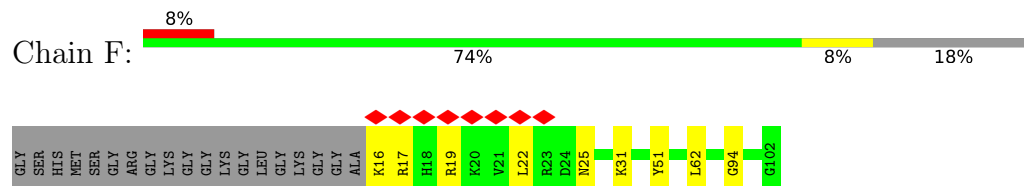
#### • Molecule 1: Histone H3.1



#### • Molecule 2: Histone H4

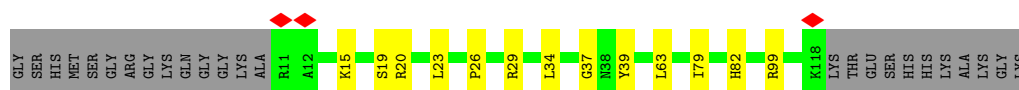


#### • Molecule 2: Histone H4



#### • Molecule 3: Histone H2A type 1-B/E

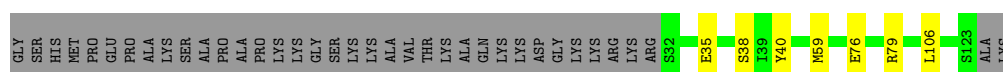




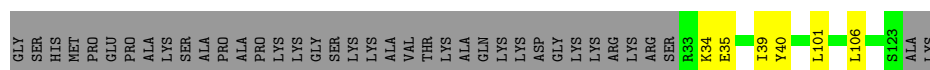
• Molecule 3: Histone H2A type 1-B/E



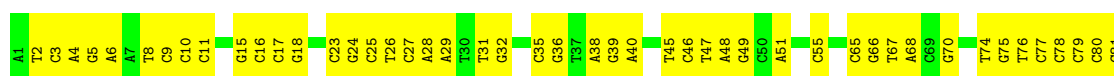
• Molecule 4: Histone H2B type 1-J



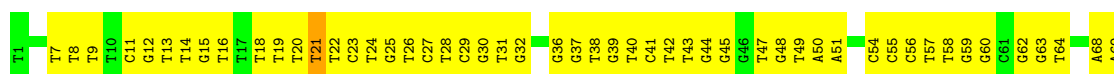
• Molecule 4: Histone H2B type 1-J



• Molecule 5: DNA (156-MER)



• Molecule 6: DNA (153-MER)

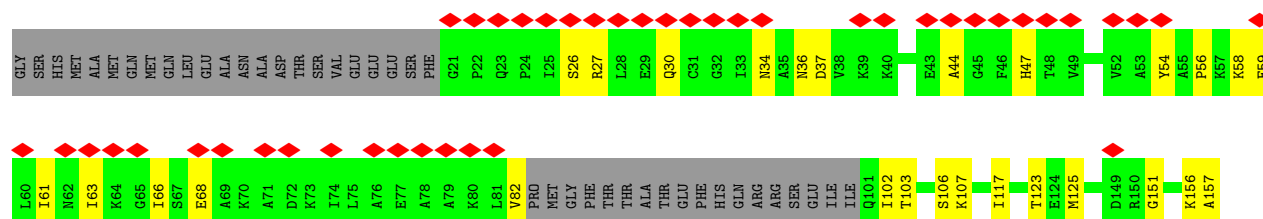


• Molecule 7: DNA repair protein RAD51 homolog 1

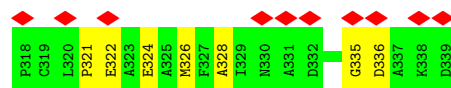
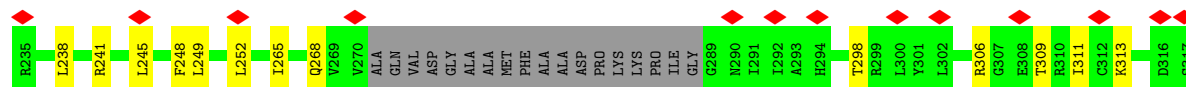
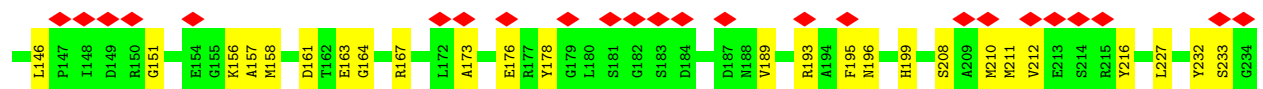
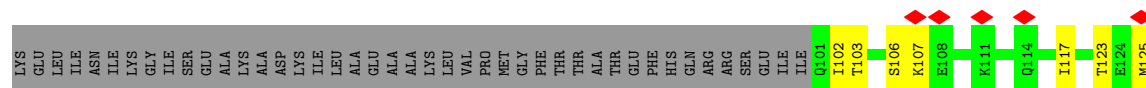




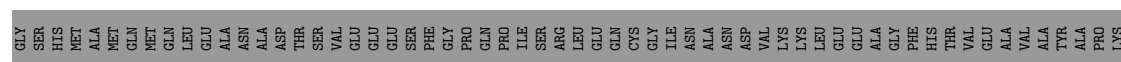
• Molecule 7: DNA repair protein RAD51 homolog 1



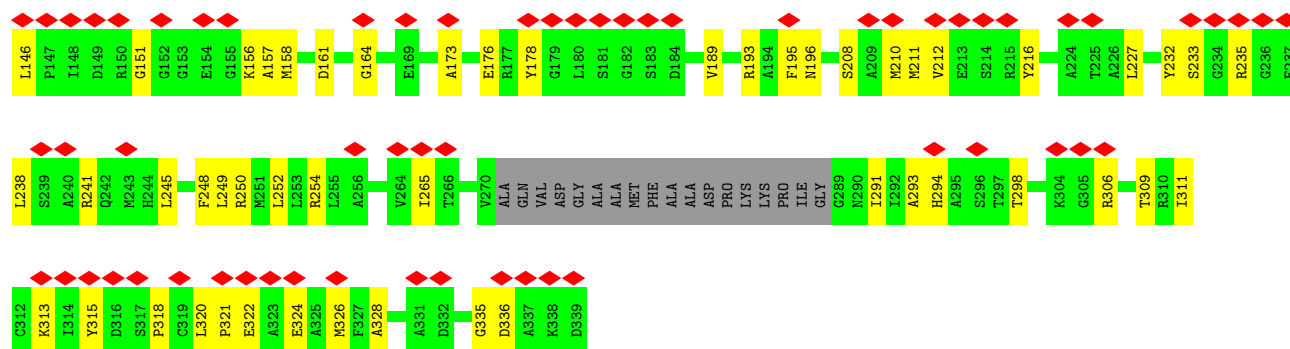
• Molecule 7: DNA repair protein RAD51 homolog 1



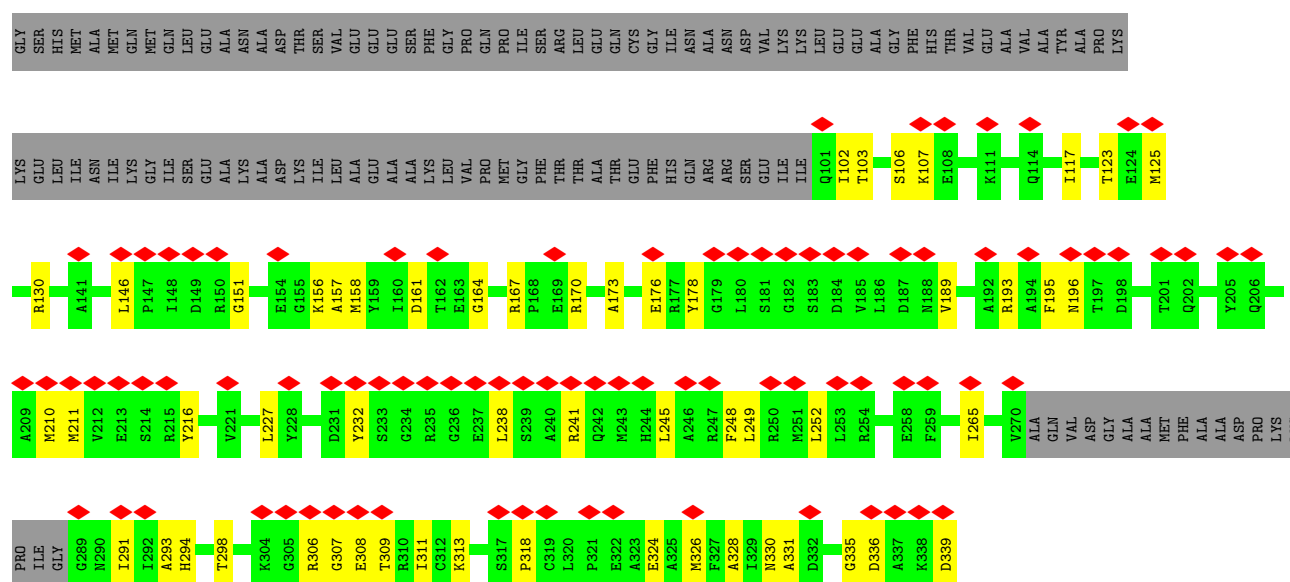
• Molecule 7: DNA repair protein RAD51 homolog 1



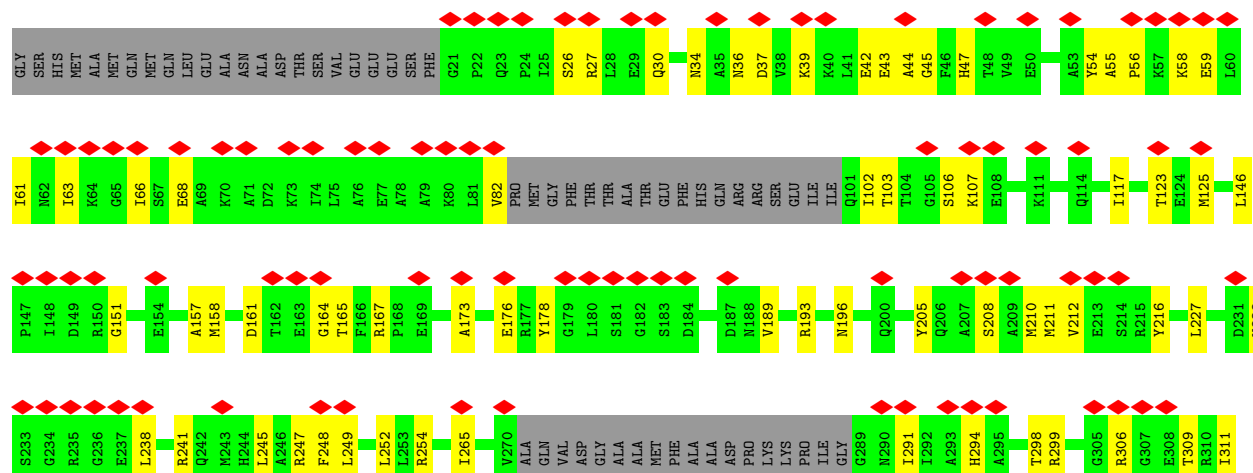


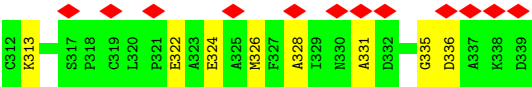


• Molecule 7: DNA repair protein RAD51 homolog 1



• Molecule 7: DNA repair protein RAD51 homolog 1





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 30612                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 58.8                                    | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.025                                   | Depositor |
| Minimum map value                    | -0.010                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.0042                                  | Depositor |
| Map size (Å)                         | 296.8, 296.8, 296.8                     | wwPDB     |
| Map dimensions                       | 280, 280, 280                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.35         | 0/802           | 0.70        | 0/1076          |
| 1   | E     | 0.36         | 0/831           | 0.70        | 0/1113          |
| 2   | B     | 0.42         | 0/621           | 0.70        | 0/832           |
| 2   | F     | 0.39         | 0/711           | 0.71        | 0/948           |
| 3   | C     | 0.34         | 0/845           | 0.65        | 0/1139          |
| 3   | G     | 0.32         | 0/815           | 0.60        | 0/1100          |
| 4   | D     | 0.35         | 0/731           | 0.60        | 0/983           |
| 4   | H     | 0.35         | 0/725           | 0.63        | 0/975           |
| 5   | I     | 0.43         | 0/3584          | 0.60        | 0/5522          |
| 6   | J     | 0.43         | 0/3518          | 0.58        | 1/5434 (0.0%)   |
| 7   | K     | 0.29         | 0/2190          | 0.53        | 0/2949          |
| 7   | L     | 0.92         | 9/2190 (0.4%)   | 1.09        | 30/2949 (1.0%)  |
| 7   | M     | 0.93         | 8/2190 (0.4%)   | 1.11        | 35/2949 (1.2%)  |
| 7   | N     | 0.28         | 0/2190          | 0.52        | 0/2949          |
| 7   | O     | 0.16         | 0/1720          | 0.47        | 0/2317          |
| 7   | P     | 0.36         | 2/1720 (0.1%)   | 0.63        | 2/2317 (0.1%)   |
| 7   | Q     | 0.42         | 2/2190 (0.1%)   | 0.58        | 2/2949 (0.1%)   |
| 7   | R     | 0.29         | 0/2190          | 0.52        | 0/2949          |
| 7   | S     | 0.16         | 0/1720          | 0.47        | 0/2317          |
| 7   | T     | 0.28         | 0/2190          | 0.53        | 0/2949          |
| All | All   | 0.46         | 21/33673 (0.1%) | 0.67        | 70/46716 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 7   | L     | 0                   | 4                   |
| 7   | M     | 0                   | 4                   |
| 7   | Q     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 7   | Q     | 167 | ARG  | CA-CB   | -13.17 | 1.36        | 1.53     |
| 7   | P     | 318 | PRO  | C-O     | -10.95 | 1.10        | 1.24     |
| 7   | L     | 47  | HIS  | CE1-NE2 | -8.81  | 1.23        | 1.32     |
| 7   | M     | 47  | HIS  | CE1-NE2 | -8.75  | 1.23        | 1.32     |
| 7   | L     | 47  | HIS  | CD2-NE2 | -7.92  | 1.29        | 1.37     |
| 7   | M     | 47  | HIS  | CD2-NE2 | -7.89  | 1.29        | 1.37     |
| 7   | L     | 217 | ALA  | CA-CB   | -7.08  | 1.43        | 1.54     |
| 7   | P     | 318 | PRO  | CA-CB   | 7.06   | 1.63        | 1.53     |
| 7   | L     | 207 | ALA  | CA-CB   | -6.88  | 1.42        | 1.53     |
| 7   | L     | 256 | ALA  | CA-CB   | -6.66  | 1.43        | 1.53     |
| 7   | M     | 246 | ALA  | CA-CB   | -6.62  | 1.43        | 1.53     |
| 7   | M     | 256 | ALA  | CA-CB   | -6.53  | 1.43        | 1.53     |
| 7   | L     | 53  | ALA  | CA-CB   | -6.47  | 1.43        | 1.53     |
| 7   | L     | 209 | ALA  | CA-CB   | -6.46  | 1.43        | 1.53     |
| 7   | M     | 53  | ALA  | CA-CB   | -6.38  | 1.43        | 1.53     |
| 7   | M     | 295 | ALA  | CA-CB   | -6.28  | 1.43        | 1.53     |
| 7   | Q     | 166 | PHE  | CA-C    | 6.02   | 1.60        | 1.52     |
| 7   | M     | 51  | ALA  | CA-CB   | -5.99  | 1.43        | 1.53     |
| 7   | L     | 51  | ALA  | CA-CB   | -5.99  | 1.43        | 1.53     |
| 7   | L     | 254 | ARG  | C-O     | -5.57  | 1.17        | 1.24     |
| 7   | M     | 247 | ARG  | C-O     | -5.04  | 1.18        | 1.24     |

All (70) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 7   | P     | 318 | PRO  | O-C-N    | 14.14  | 140.46      | 122.22   |
| 7   | P     | 318 | PRO  | CA-C-O   | -12.75 | 100.16      | 119.55   |
| 7   | Q     | 167 | ARG  | CA-CB-CG | 6.93   | 127.96      | 114.10   |
| 7   | L     | 52  | VAL  | CA-C-N   | 6.84   | 129.68      | 120.65   |
| 7   | L     | 52  | VAL  | C-N-CA   | 6.84   | 129.68      | 120.65   |
| 7   | M     | 52  | VAL  | CA-C-N   | 6.82   | 129.65      | 120.65   |
| 7   | M     | 52  | VAL  | C-N-CA   | 6.82   | 129.65      | 120.65   |
| 7   | M     | 248 | PHE  | CA-CB-CG | 6.58   | 120.38      | 113.80   |
| 7   | L     | 47  | HIS  | CA-CB-CG | 6.48   | 120.28      | 113.80   |
| 7   | M     | 47  | HIS  | CA-CB-CG | 6.42   | 120.22      | 113.80   |
| 7   | L     | 257 | ASP  | CA-CB-CG | 6.32   | 118.92      | 112.60   |
| 7   | M     | 257 | ASP  | CA-CB-CG | 6.25   | 118.85      | 112.60   |
| 7   | L     | 259 | PHE  | CA-CB-CG | 6.25   | 120.05      | 113.80   |
| 7   | L     | 215 | ARG  | O-C-N    | 6.21   | 130.57      | 122.93   |
| 7   | M     | 247 | ARG  | CA-C-N   | 6.20   | 128.50      | 120.44   |
| 7   | M     | 247 | ARG  | C-N-CA   | 6.20   | 128.50      | 120.44   |
| 7   | M     | 294 | HIS  | CA-C-N   | 6.16   | 131.00      | 120.71   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 7   | M     | 294 | HIS  | C-N-CA    | 6.16  | 131.00      | 120.71   |
| 7   | M     | 259 | PHE  | CA-CB-CG  | 6.16  | 119.96      | 113.80   |
| 7   | M     | 248 | PHE  | CA-C-N    | 6.16  | 128.44      | 120.44   |
| 7   | M     | 248 | PHE  | C-N-CA    | 6.16  | 128.44      | 120.44   |
| 7   | L     | 254 | ARG  | CA-C-N    | 6.11  | 128.75      | 120.38   |
| 7   | L     | 254 | ARG  | C-N-CA    | 6.11  | 128.75      | 120.38   |
| 7   | M     | 121 | SER  | CA-C-N    | 6.05  | 129.93      | 122.37   |
| 7   | M     | 121 | SER  | C-N-CA    | 6.05  | 129.93      | 122.37   |
| 7   | M     | 257 | ASP  | CA-C-N    | 6.01  | 128.61      | 120.44   |
| 7   | M     | 257 | ASP  | C-N-CA    | 6.01  | 128.61      | 120.44   |
| 7   | L     | 206 | GLN  | CA-C-N    | 6.00  | 128.25      | 120.44   |
| 7   | L     | 206 | GLN  | C-N-CA    | 6.00  | 128.25      | 120.44   |
| 7   | L     | 257 | ASP  | CA-C-N    | 6.00  | 128.60      | 120.44   |
| 7   | L     | 257 | ASP  | C-N-CA    | 6.00  | 128.60      | 120.44   |
| 7   | Q     | 167 | ARG  | CB-CA-C   | -5.92 | 101.84      | 110.13   |
| 7   | L     | 50  | GLU  | CA-CB-CG  | 5.87  | 125.84      | 114.10   |
| 7   | L     | 50  | GLU  | CA-C-N    | 5.85  | 128.40      | 120.44   |
| 7   | L     | 50  | GLU  | C-N-CA    | 5.85  | 128.40      | 120.44   |
| 6   | J     | 21  | DT   | O5'-P-OP1 | -5.84 | 91.49       | 109.00   |
| 7   | L     | 209 | ALA  | CA-C-N    | 5.65  | 128.32      | 120.29   |
| 7   | L     | 209 | ALA  | C-N-CA    | 5.65  | 128.32      | 120.29   |
| 7   | M     | 29  | GLU  | CA-C-N    | 5.50  | 128.20      | 120.28   |
| 7   | M     | 29  | GLU  | C-N-CA    | 5.50  | 128.20      | 120.28   |
| 7   | M     | 255 | LEU  | CA-C-N    | 5.49  | 127.57      | 120.44   |
| 7   | M     | 255 | LEU  | C-N-CA    | 5.49  | 127.57      | 120.44   |
| 7   | M     | 247 | ARG  | CA-C-O    | -5.44 | 114.78      | 120.55   |
| 7   | L     | 29  | GLU  | CA-C-N    | 5.43  | 128.10      | 120.28   |
| 7   | L     | 29  | GLU  | C-N-CA    | 5.43  | 128.10      | 120.28   |
| 7   | M     | 251 | MET  | CA-C-N    | 5.41  | 127.47      | 120.44   |
| 7   | M     | 251 | MET  | C-N-CA    | 5.41  | 127.47      | 120.44   |
| 7   | L     | 255 | LEU  | CA-C-N    | 5.38  | 127.43      | 120.44   |
| 7   | L     | 255 | LEU  | C-N-CA    | 5.38  | 127.43      | 120.44   |
| 7   | L     | 51  | ALA  | CA-C-N    | 5.36  | 127.81      | 120.46   |
| 7   | L     | 51  | ALA  | C-N-CA    | 5.36  | 127.81      | 120.46   |
| 7   | L     | 80  | LYS  | CA-C-N    | 5.35  | 127.71      | 120.44   |
| 7   | L     | 80  | LYS  | C-N-CA    | 5.35  | 127.71      | 120.44   |
| 7   | M     | 51  | ALA  | CA-C-N    | 5.30  | 127.72      | 120.46   |
| 7   | M     | 51  | ALA  | C-N-CA    | 5.30  | 127.72      | 120.46   |
| 7   | M     | 80  | LYS  | CA-C-N    | 5.29  | 127.63      | 120.44   |
| 7   | M     | 80  | LYS  | C-N-CA    | 5.29  | 127.63      | 120.44   |
| 7   | M     | 254 | ARG  | CA-C-N    | 5.28  | 127.36      | 120.28   |
| 7   | M     | 254 | ARG  | C-N-CA    | 5.28  | 127.36      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | M     | 47  | HIS  | CA-C-N | 5.22  | 130.79      | 122.59   |
| 7   | M     | 47  | HIS  | C-N-CA | 5.22  | 130.79      | 122.59   |
| 7   | L     | 47  | HIS  | CA-C-N | 5.22  | 130.78      | 122.59   |
| 7   | L     | 47  | HIS  | C-N-CA | 5.22  | 130.78      | 122.59   |
| 7   | M     | 250 | ARG  | CA-C-N | 5.21  | 127.21      | 120.44   |
| 7   | M     | 250 | ARG  | C-N-CA | 5.21  | 127.21      | 120.44   |
| 7   | L     | 215 | ARG  | CA-C-O | -5.17 | 114.86      | 120.81   |
| 7   | M     | 252 | LEU  | CA-C-N | 5.15  | 127.14      | 120.44   |
| 7   | M     | 252 | LEU  | C-N-CA | 5.15  | 127.14      | 120.44   |
| 7   | L     | 49  | VAL  | CA-C-N | 5.03  | 127.27      | 120.38   |
| 7   | L     | 49  | VAL  | C-N-CA | 5.03  | 127.27      | 120.38   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | L     | 215 | ARG  | Sidechain |
| 7   | L     | 236 | GLY  | Mainchain |
| 7   | L     | 254 | ARG  | Sidechain |
| 7   | L     | 27  | ARG  | Sidechain |
| 7   | M     | 247 | ARG  | Sidechain |
| 7   | M     | 250 | ARG  | Sidechain |
| 7   | M     | 254 | ARG  | Sidechain |
| 7   | M     | 27  | ARG  | Sidechain |
| 7   | Q     | 166 | PHE  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 790   | 0        | 826      | 10      | 0            |
| 1   | E     | 819   | 0        | 864      | 4       | 0            |
| 2   | B     | 614   | 0        | 656      | 3       | 0            |
| 2   | F     | 703   | 0        | 755      | 8       | 0            |
| 3   | C     | 835   | 0        | 897      | 10      | 0            |
| 3   | G     | 805   | 0        | 861      | 6       | 0            |
| 4   | D     | 720   | 0        | 740      | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | H     | 714   | 0        | 735      | 4       | 0            |
| 5   | I     | 3189  | 0        | 1738     | 83      | 0            |
| 6   | J     | 3143  | 0        | 1731     | 100     | 0            |
| 7   | K     | 2163  | 0        | 2179     | 140     | 0            |
| 7   | L     | 2163  | 0        | 2180     | 95      | 0            |
| 7   | M     | 2163  | 0        | 2180     | 110     | 0            |
| 7   | N     | 2163  | 0        | 2181     | 107     | 0            |
| 7   | O     | 1698  | 0        | 1694     | 54      | 0            |
| 7   | P     | 1698  | 0        | 1693     | 99      | 0            |
| 7   | Q     | 2163  | 0        | 2181     | 173     | 0            |
| 7   | R     | 2163  | 0        | 2176     | 155     | 0            |
| 7   | S     | 1698  | 0        | 1694     | 113     | 0            |
| 7   | T     | 2163  | 0        | 2181     | 147     | 0            |
| All | All   | 32567 | 0        | 30142    | 1108    | 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 18.

All (1108) 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) |
|------------------|------------------|--------------------------|-------------------|
| 7:K:199:HIS:CB   | 7:T:56:PRO:HG3   | 1.26                     | 1.57              |
| 7:K:199:HIS:HB2  | 7:T:56:PRO:CG    | 1.34                     | 1.55              |
| 7:M:318:PRO:CB   | 7:N:193:ARG:HH12 | 1.20                     | 1.54              |
| 7:R:58:LYS:N     | 7:S:195:PHE:CZ   | 1.71                     | 1.52              |
| 7:L:50:GLU:CD    | 7:L:258:GLU:HA   | 1.34                     | 1.49              |
| 7:R:58:LYS:HE2   | 7:S:195:PHE:CE2  | 1.45                     | 1.49              |
| 7:K:54:TYR:HB2   | 7:K:254:ARG:NH1  | 1.27                     | 1.46              |
| 7:K:195:PHE:HD2  | 7:T:55:ALA:CB    | 1.27                     | 1.45              |
| 7:L:50:GLU:OE1   | 7:L:258:GLU:CA   | 1.65                     | 1.43              |
| 7:P:294:HIS:O    | 7:Q:193:ARG:CB   | 1.65                     | 1.43              |
| 7:K:195:PHE:CD2  | 7:T:55:ALA:HB2   | 1.53                     | 1.42              |
| 7:P:297:THR:HG22 | 7:Q:193:ARG:NH2  | 1.34                     | 1.40              |
| 7:R:58:LYS:HB2   | 7:S:195:PHE:CE1  | 1.53                     | 1.40              |
| 7:M:318:PRO:CB   | 7:N:193:ARG:NH1  | 1.85                     | 1.39              |
| 7:T:44:ALA:O     | 7:T:247:ARG:CD   | 1.67                     | 1.39              |
| 7:S:294:HIS:CD2  | 7:T:164:GLY:O    | 1.73                     | 1.38              |
| 7:P:319:CYS:CA   | 7:Q:167:ARG:HG3  | 0.93                     | 1.38              |
| 7:T:47:HIS:CB    | 7:T:254:ARG:NH2  | 1.86                     | 1.38              |
| 7:T:47:HIS:HB2   | 7:T:254:ARG:NH2  | 1.05                     | 1.37              |
| 7:M:318:PRO:HB3  | 7:N:193:ARG:NH1  | 1.35                     | 1.37              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:Q:47:HIS:HB2  | 7:Q:254:ARG:NH1  | 1.39                     | 1.36              |
| 7:R:58:LYS:N    | 7:S:195:PHE:HZ   | 0.92                     | 1.35              |
| 7:S:294:HIS:CG  | 7:T:164:GLY:O    | 1.79                     | 1.34              |
| 7:P:319:CYS:HB2 | 7:Q:168:PRO:CD   | 1.55                     | 1.32              |
| 7:N:59:GLU:CD   | 7:N:254:ARG:HH12 | 1.34                     | 1.31              |
| 7:M:54:TYR:HB3  | 7:N:195:PHE:CD2  | 1.67                     | 1.29              |
| 7:R:58:LYS:CE   | 7:S:195:PHE:CD2  | 2.15                     | 1.28              |
| 5:I:55:DC:OP1   | 7:M:70:LYS:HE3   | 1.21                     | 1.27              |
| 7:K:46:PHE:CE1  | 7:K:247:ARG:HD2  | 1.70                     | 1.26              |
| 7:R:58:LYS:HE2  | 7:S:195:PHE:CD2  | 1.69                     | 1.26              |
| 7:R:58:LYS:CA   | 7:S:195:PHE:CZ   | 2.18                     | 1.25              |
| 7:Q:47:HIS:CB   | 7:Q:254:ARG:HH11 | 1.49                     | 1.25              |
| 7:P:319:CYS:HA  | 7:Q:167:ARG:CG   | 0.91                     | 1.25              |
| 7:P:319:CYS:SG  | 7:Q:169:GLU:N    | 2.02                     | 1.24              |
| 7:Q:293:ALA:HB3 | 7:R:195:PHE:CZ   | 1.72                     | 1.23              |
| 7:K:56:PRO:HG3  | 7:L:196:ASN:CG   | 1.64                     | 1.23              |
| 7:K:56:PRO:HG3  | 7:L:196:ASN:CB   | 1.69                     | 1.22              |
| 7:Q:191:TYR:OH  | 7:Q:193:ARG:CZ   | 1.88                     | 1.22              |
| 7:R:45:GLY:O    | 7:R:254:ARG:CZ   | 1.88                     | 1.22              |
| 7:K:46:PHE:HE1  | 7:K:247:ARG:CD   | 1.51                     | 1.21              |
| 7:K:54:TYR:CB   | 7:K:254:ARG:NH1  | 2.04                     | 1.20              |
| 7:P:319:CYS:CB  | 7:Q:168:PRO:HD2  | 1.69                     | 1.20              |
| 7:Q:191:TYR:OH  | 7:Q:193:ARG:NE   | 1.72                     | 1.20              |
| 7:P:319:CYS:C   | 7:Q:167:ARG:HG3  | 1.65                     | 1.19              |
| 7:S:294:HIS:CE1 | 7:T:164:GLY:O    | 1.96                     | 1.19              |
| 7:M:201:THR:CG2 | 7:M:251:MET:HE1  | 1.74                     | 1.18              |
| 7:P:318:PRO:HG3 | 7:Q:166:PHE:N    | 1.48                     | 1.17              |
| 7:O:322:GLU:OE1 | 7:P:167:ARG:NH1  | 1.74                     | 1.17              |
| 7:L:50:GLU:OE1  | 7:L:258:GLU:HA   | 0.99                     | 1.17              |
| 7:Q:291:ILE:HA  | 7:R:195:PHE:CD2  | 1.78                     | 1.17              |
| 7:K:46:PHE:CE1  | 7:K:247:ARG:CD   | 2.27                     | 1.16              |
| 7:M:54:TYR:CG   | 7:N:195:PHE:HE2  | 1.61                     | 1.16              |
| 7:K:195:PHE:HD2 | 7:T:55:ALA:CA    | 1.59                     | 1.16              |
| 7:K:195:PHE:CD2 | 7:T:55:ALA:CB    | 2.16                     | 1.16              |
| 7:N:59:GLU:CD   | 7:N:254:ARG:NH1  | 2.03                     | 1.15              |
| 7:R:291:ILE:O   | 7:R:294:HIS:CE1  | 2.00                     | 1.14              |
| 7:P:291:ILE:O   | 7:P:294:HIS:CE1  | 2.00                     | 1.14              |
| 7:T:291:ILE:O   | 7:T:294:HIS:CE1  | 2.00                     | 1.13              |
| 7:L:50:GLU:OE1  | 7:L:258:GLU:CB   | 1.96                     | 1.12              |
| 7:M:319:CYS:HA  | 7:N:163:GLU:O    | 1.50                     | 1.12              |
| 7:K:54:TYR:HB3  | 7:L:195:PHE:CD2  | 1.86                     | 1.11              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:R:318:PRO:HA  | 7:S:170:ARG:HH21 | 0.98                     | 1.11              |
| 7:K:54:TYR:HD2  | 7:K:254:ARG:CZ   | 1.62                     | 1.11              |
| 7:N:56:PRO:HG2  | 7:O:199:HIS:HB2  | 1.26                     | 1.11              |
| 7:P:319:CYS:HA  | 7:Q:167:ARG:HG2  | 1.19                     | 1.11              |
| 5:I:129:DC:P    | 7:K:67:SER:HB3   | 1.91                     | 1.10              |
| 7:K:54:TYR:CD2  | 7:K:254:ARG:NH1  | 2.20                     | 1.10              |
| 7:Q:48:THR:HG23 | 7:Q:254:ARG:HH12 | 1.10                     | 1.10              |
| 7:Q:167:ARG:HD3 | 7:Q:170:ARG:HG2  | 1.11                     | 1.10              |
| 7:K:195:PHE:CD2 | 7:T:55:ALA:CA    | 2.35                     | 1.09              |
| 7:R:322:GLU:OE1 | 7:S:330:ASN:HA   | 1.51                     | 1.09              |
| 7:R:58:LYS:HB2  | 7:S:195:PHE:CZ   | 1.87                     | 1.08              |
| 7:P:294:HIS:O   | 7:Q:193:ARG:CD   | 2.01                     | 1.08              |
| 7:S:294:HIS:HA  | 7:T:167:ARG:HE   | 0.92                     | 1.08              |
| 7:T:44:ALA:O    | 7:T:247:ARG:HD3  | 0.92                     | 1.08              |
| 7:K:195:PHE:HB2 | 7:T:56:PRO:HD3   | 1.30                     | 1.08              |
| 7:M:56:PRO:HG3  | 7:N:196:ASN:CB   | 1.84                     | 1.08              |
| 7:S:294:HIS:NE2 | 7:T:164:GLY:O    | 1.85                     | 1.08              |
| 7:Q:47:HIS:HB2  | 7:Q:254:ARG:CZ   | 1.84                     | 1.07              |
| 7:P:294:HIS:O   | 7:Q:193:ARG:HB3  | 1.32                     | 1.07              |
| 7:S:294:HIS:CD2 | 7:T:164:GLY:C    | 2.31                     | 1.07              |
| 7:P:318:PRO:CG  | 7:Q:166:PHE:N    | 1.85                     | 1.07              |
| 7:T:43:GLU:O    | 7:T:247:ARG:NH2  | 1.87                     | 1.07              |
| 7:S:294:HIS:HA  | 7:T:167:ARG:NE   | 1.70                     | 1.06              |
| 7:K:46:PHE:HE1  | 7:K:247:ARG:HD2  | 0.95                     | 1.06              |
| 7:K:50:GLU:HG2  | 7:K:254:ARG:HH21 | 1.20                     | 1.05              |
| 7:M:54:TYR:CG   | 7:N:195:PHE:CE2  | 2.44                     | 1.05              |
| 7:R:45:GLY:O    | 7:R:254:ARG:NH1  | 1.78                     | 1.05              |
| 7:T:44:ALA:HA   | 7:T:247:ARG:HH21 | 1.19                     | 1.04              |
| 7:N:44:ALA:O    | 7:N:205:TYR:CD1  | 2.10                     | 1.04              |
| 7:K:54:TYR:CB   | 7:K:254:ARG:HH11 | 1.65                     | 1.04              |
| 7:R:58:LYS:CB   | 7:S:195:PHE:CE1  | 2.41                     | 1.04              |
| 7:R:58:LYS:CB   | 7:S:195:PHE:CZ   | 2.41                     | 1.03              |
| 7:R:58:LYS:HE3  | 7:S:195:PHE:CD2  | 1.92                     | 1.03              |
| 7:R:318:PRO:HA  | 7:S:170:ARG:NH2  | 1.72                     | 1.03              |
| 7:R:58:LYS:CE   | 7:S:195:PHE:CE2  | 2.37                     | 1.02              |
| 7:L:50:GLU:CD   | 7:L:258:GLU:CA   | 2.21                     | 1.02              |
| 7:Q:290:ASN:O   | 7:R:195:PHE:CZ   | 2.12                     | 1.02              |
| 7:S:294:HIS:ND1 | 7:T:164:GLY:O    | 1.91                     | 1.02              |
| 7:R:315:TYR:CD1 | 7:S:308:GLU:OE2  | 2.14                     | 1.01              |
| 7:T:47:HIS:CB   | 7:T:254:ARG:HH22 | 1.61                     | 1.01              |
| 7:K:163:GLU:O   | 7:T:294:HIS:CG   | 2.13                     | 1.01              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:T:47:HIS:CB   | 7:T:254:ARG:HH21 | 1.63                     | 1.00              |
| 7:Q:47:HIS:HB2  | 7:Q:254:ARG:HH11 | 0.88                     | 1.00              |
| 7:L:294:HIS:NE2 | 7:M:223:SER:OG   | 1.92                     | 0.99              |
| 7:R:57:LYS:C    | 7:S:195:PHE:HZ   | 1.69                     | 0.99              |
| 7:M:318:PRO:HB2 | 7:N:193:ARG:HH12 | 1.24                     | 0.99              |
| 7:T:44:ALA:CA   | 7:T:247:ARG:HH21 | 1.74                     | 0.99              |
| 7:R:315:TYR:O   | 7:S:308:GLU:OE2  | 1.80                     | 0.98              |
| 7:Q:290:ASN:O   | 7:R:195:PHE:CE2  | 2.15                     | 0.98              |
| 7:M:318:PRO:CA  | 7:N:193:ARG:HH12 | 1.75                     | 0.98              |
| 7:R:315:TYR:CG  | 7:S:308:GLU:OE2  | 2.16                     | 0.98              |
| 7:P:318:PRO:CB  | 7:Q:165:THR:C    | 2.30                     | 0.98              |
| 7:Q:167:ARG:HD3 | 7:Q:170:ARG:CG   | 1.93                     | 0.98              |
| 7:Q:293:ALA:HB3 | 7:R:195:PHE:CE1  | 1.99                     | 0.98              |
| 7:P:294:HIS:O   | 7:Q:193:ARG:CG   | 2.12                     | 0.97              |
| 7:Q:47:HIS:CB   | 7:Q:254:ARG:NH1  | 2.18                     | 0.97              |
| 7:P:319:CYS:HB2 | 7:Q:168:PRO:HD2  | 0.97                     | 0.97              |
| 7:R:320:LEU:O   | 7:S:331:ALA:HB2  | 1.65                     | 0.97              |
| 7:K:167:ARG:NH1 | 7:T:294:HIS:O    | 1.97                     | 0.96              |
| 7:Q:191:TYR:HE2 | 7:Q:193:ARG:NH2  | 1.64                     | 0.96              |
| 7:L:50:GLU:OE1  | 7:L:258:GLU:CG   | 2.13                     | 0.96              |
| 7:P:294:HIS:CD2 | 7:Q:194:ALA:C    | 2.41                     | 0.96              |
| 7:P:318:PRO:HB3 | 7:Q:165:THR:C    | 1.61                     | 0.96              |
| 7:S:294:HIS:CA  | 7:T:167:ARG:HE   | 1.78                     | 0.95              |
| 7:R:322:GLU:CD  | 7:S:330:ASN:HA   | 1.91                     | 0.95              |
| 7:T:44:ALA:C    | 7:T:247:ARG:CD   | 2.37                     | 0.95              |
| 7:Q:167:ARG:CD  | 7:Q:170:ARG:HG2  | 1.95                     | 0.95              |
| 7:P:319:CYS:O   | 7:Q:167:ARG:NE   | 2.00                     | 0.95              |
| 7:N:44:ALA:O    | 7:N:205:TYR:CE1  | 2.19                     | 0.95              |
| 7:Q:47:HIS:HD2  | 7:Q:254:ARG:HG2  | 1.32                     | 0.94              |
| 7:K:54:TYR:CD2  | 7:K:254:ARG:CZ   | 2.49                     | 0.94              |
| 7:P:294:HIS:O   | 7:Q:193:ARG:HB2  | 1.66                     | 0.94              |
| 7:P:318:PRO:HG3 | 7:Q:165:THR:C    | 1.93                     | 0.94              |
| 7:K:195:PHE:CD2 | 7:T:55:ALA:HA    | 2.01                     | 0.93              |
| 7:L:50:GLU:OE2  | 7:L:258:GLU:HA   | 1.66                     | 0.93              |
| 7:T:44:ALA:HA   | 7:T:247:ARG:NH2  | 1.82                     | 0.93              |
| 7:P:318:PRO:HG3 | 7:Q:166:PHE:H    | 1.31                     | 0.93              |
| 7:Q:293:ALA:HB3 | 7:R:195:PHE:HZ   | 1.32                     | 0.93              |
| 7:L:50:GLU:OE1  | 7:L:258:GLU:HG3  | 1.67                     | 0.93              |
| 5:I:129:DC:OP2  | 7:K:67:SER:CB    | 2.16                     | 0.92              |
| 7:M:54:TYR:HB3  | 7:N:195:PHE:CE2  | 2.03                     | 0.92              |
| 7:M:54:TYR:HB3  | 7:N:195:PHE:HD2  | 1.30                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:K:57:LYS:CE    | 7:L:198:ASP:OD1  | 2.18                     | 0.92              |
| 5:I:55:DC:OP1    | 7:M:70:LYS:CE    | 2.16                     | 0.92              |
| 7:K:54:TYR:HB3   | 7:L:195:PHE:HD2  | 1.19                     | 0.91              |
| 7:N:309:THR:HG22 | 7:N:326:MET:HE3  | 1.53                     | 0.91              |
| 7:N:59:GLU:OE1   | 7:N:254:ARG:NH1  | 1.95                     | 0.91              |
| 7:P:291:ILE:O    | 7:Q:195:PHE:HD1  | 1.51                     | 0.91              |
| 7:Q:48:THR:HG23  | 7:Q:254:ARG:NH1  | 1.84                     | 0.91              |
| 7:T:44:ALA:C     | 7:T:247:ARG:HD2  | 1.96                     | 0.91              |
| 7:K:54:TYR:HB2   | 7:K:254:ARG:HH11 | 0.86                     | 0.91              |
| 7:Q:294:HIS:N    | 7:R:195:PHE:CZ   | 2.39                     | 0.91              |
| 7:T:309:THR:HG22 | 7:T:326:MET:HE3  | 1.53                     | 0.91              |
| 7:T:44:ALA:C     | 7:T:247:ARG:HD3  | 1.96                     | 0.91              |
| 7:O:309:THR:HG22 | 7:O:326:MET:HE3  | 1.53                     | 0.90              |
| 7:K:309:THR:HG22 | 7:K:326:MET:HE3  | 1.53                     | 0.90              |
| 7:P:318:PRO:HD3  | 7:Q:164:GLY:O    | 1.71                     | 0.90              |
| 7:R:309:THR:HG22 | 7:R:326:MET:HE3  | 1.53                     | 0.90              |
| 7:R:45:GLY:C     | 7:R:254:ARG:CZ   | 2.39                     | 0.90              |
| 7:Q:47:HIS:CD2   | 7:Q:254:ARG:HG2  | 2.06                     | 0.90              |
| 7:R:47:HIS:N     | 7:R:254:ARG:CZ   | 2.27                     | 0.90              |
| 7:N:56:PRO:CG    | 7:O:199:HIS:HB2  | 2.02                     | 0.90              |
| 7:M:309:THR:HG22 | 7:M:326:MET:HE3  | 1.53                     | 0.90              |
| 7:K:54:TYR:CG    | 7:K:254:ARG:NH1  | 2.39                     | 0.90              |
| 7:M:201:THR:HG23 | 7:M:251:MET:HE1  | 1.50                     | 0.90              |
| 7:P:297:THR:CG2  | 7:Q:193:ARG:NH2  | 2.31                     | 0.90              |
| 5:I:129:DC:OP1   | 7:K:67:SER:HB3   | 1.70                     | 0.89              |
| 7:K:50:GLU:HG2   | 7:K:254:ARG:NH2  | 1.87                     | 0.89              |
| 7:K:199:HIS:CB   | 7:T:56:PRO:CG    | 2.12                     | 0.89              |
| 7:L:309:THR:HG22 | 7:L:326:MET:HE3  | 1.53                     | 0.89              |
| 7:M:56:PRO:HG3   | 7:N:196:ASN:CG   | 1.96                     | 0.89              |
| 7:M:54:TYR:CD1   | 7:N:195:PHE:HE2  | 1.89                     | 0.88              |
| 7:R:58:LYS:HB2   | 7:S:195:PHE:CD1  | 2.09                     | 0.88              |
| 7:K:195:PHE:HB2  | 7:T:56:PRO:CD    | 2.02                     | 0.88              |
| 7:R:318:PRO:CA   | 7:S:170:ARG:HH21 | 1.86                     | 0.88              |
| 7:S:309:THR:HG22 | 7:S:326:MET:HE3  | 1.53                     | 0.88              |
| 7:P:294:HIS:O    | 7:Q:193:ARG:HD3  | 1.73                     | 0.88              |
| 7:Q:309:THR:HG22 | 7:Q:326:MET:HE3  | 1.53                     | 0.88              |
| 7:P:309:THR:HG22 | 7:P:326:MET:HE3  | 1.53                     | 0.87              |
| 7:K:165:THR:CG2  | 7:T:294:HIS:HB3  | 2.05                     | 0.87              |
| 7:K:54:TYR:HD2   | 7:K:254:ARG:NH1  | 1.62                     | 0.87              |
| 7:K:164:GLY:C    | 7:T:294:HIS:HB2  | 2.00                     | 0.86              |
| 7:Q:294:HIS:N    | 7:R:195:PHE:HZ   | 1.72                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:M:318:PRO:HB2  | 7:N:193:ARG:NH1  | 1.83                     | 0.86              |
| 7:N:47:HIS:CD2   | 7:N:209:ALA:HB2  | 2.10                     | 0.86              |
| 7:M:47:HIS:HE1   | 7:M:243:MET:SD   | 1.98                     | 0.86              |
| 7:Q:291:ILE:O    | 7:R:195:PHE:HE2  | 1.57                     | 0.86              |
| 7:P:318:PRO:CG   | 7:Q:166:PHE:H    | 1.80                     | 0.86              |
| 7:Q:294:HIS:H    | 7:R:195:PHE:HZ   | 1.22                     | 0.86              |
| 7:Q:47:HIS:HB2   | 7:Q:254:ARG:NE   | 1.90                     | 0.85              |
| 7:Q:191:TYR:CE2  | 7:Q:193:ARG:NH2  | 2.43                     | 0.85              |
| 7:P:319:CYS:CA   | 7:Q:167:ARG:CG   | 1.78                     | 0.85              |
| 7:T:47:HIS:HB2   | 7:T:254:ARG:HH22 | 1.22                     | 0.85              |
| 7:K:54:TYR:HB2   | 7:K:254:ARG:HH12 | 1.38                     | 0.85              |
| 7:N:319:CYS:HB2  | 7:O:167:ARG:HE   | 1.42                     | 0.85              |
| 7:R:315:TYR:CD1  | 7:S:308:GLU:CD   | 2.54                     | 0.84              |
| 7:S:294:HIS:HB3  | 7:T:165:THR:HA   | 1.59                     | 0.84              |
| 7:Q:54:TYR:OH    | 7:Q:82:VAL:CG1   | 2.26                     | 0.84              |
| 7:Q:191:TYR:CZ   | 7:Q:193:ARG:CZ   | 2.59                     | 0.84              |
| 7:Q:290:ASN:O    | 7:R:195:PHE:CE1  | 2.30                     | 0.84              |
| 7:R:54:TYR:OH    | 7:R:82:VAL:CG1   | 2.26                     | 0.84              |
| 7:T:47:HIS:CA    | 7:T:254:ARG:HH22 | 1.90                     | 0.84              |
| 7:T:54:TYR:OH    | 7:T:82:VAL:CG1   | 2.26                     | 0.84              |
| 7:P:297:THR:CG2  | 7:Q:193:ARG:HH22 | 1.90                     | 0.84              |
| 7:R:47:HIS:HB3   | 7:R:254:ARG:HD3  | 1.59                     | 0.83              |
| 7:Q:291:ILE:HA   | 7:R:195:PHE:HD2  | 1.38                     | 0.83              |
| 7:R:54:TYR:OH    | 7:R:82:VAL:HG12  | 1.78                     | 0.83              |
| 7:K:54:TYR:OH    | 7:K:82:VAL:HG12  | 1.79                     | 0.83              |
| 7:N:54:TYR:OH    | 7:N:82:VAL:HG12  | 1.78                     | 0.83              |
| 5:I:152:DC:H5''  | 7:R:235:ARG:HG2  | 1.60                     | 0.83              |
| 7:Q:47:HIS:CD2   | 7:Q:254:ARG:HE   | 1.96                     | 0.83              |
| 7:T:54:TYR:OH    | 7:T:82:VAL:HG12  | 1.79                     | 0.83              |
| 7:K:54:TYR:OH    | 7:K:82:VAL:CG1   | 2.26                     | 0.83              |
| 7:K:195:PHE:CE2  | 7:T:55:ALA:HB2   | 2.13                     | 0.83              |
| 7:R:320:LEU:O    | 7:S:331:ALA:CB   | 2.25                     | 0.83              |
| 7:P:318:PRO:HB3  | 7:Q:165:THR:O    | 1.79                     | 0.83              |
| 7:Q:54:TYR:OH    | 7:Q:82:VAL:HG12  | 1.79                     | 0.83              |
| 7:N:54:TYR:OH    | 7:N:82:VAL:CG1   | 2.26                     | 0.83              |
| 7:O:322:GLU:H    | 7:P:167:ARG:NH1  | 1.76                     | 0.83              |
| 7:Q:191:TYR:CE2  | 7:Q:193:ARG:CZ   | 2.62                     | 0.82              |
| 7:K:56:PRO:CG    | 7:L:196:ASN:CB   | 2.56                     | 0.82              |
| 7:M:201:THR:HG23 | 7:M:251:MET:CE   | 2.08                     | 0.82              |
| 7:P:297:THR:HG22 | 7:Q:193:ARG:HH22 | 1.05                     | 0.82              |
| 7:R:46:PHE:HE1   | 7:R:250:ARG:HD2  | 1.45                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:P:319:CYS:HB2  | 7:Q:168:PRO:N    | 1.93                     | 0.82              |
| 7:P:318:PRO:HG3  | 7:Q:164:GLY:O    | 1.79                     | 0.82              |
| 7:M:54:TYR:CB    | 7:N:195:PHE:CD2  | 2.58                     | 0.81              |
| 7:T:47:HIS:CG    | 7:T:254:ARG:NH2  | 2.48                     | 0.81              |
| 7:T:47:HIS:N     | 7:T:254:ARG:HH22 | 1.78                     | 0.81              |
| 7:Q:293:ALA:CB   | 7:R:195:PHE:CZ   | 2.59                     | 0.81              |
| 7:M:54:TYR:CD1   | 7:N:195:PHE:CE2  | 2.69                     | 0.80              |
| 7:M:56:PRO:HG3   | 7:N:196:ASN:HB3  | 1.61                     | 0.80              |
| 7:Q:291:ILE:CA   | 7:R:195:PHE:CD2  | 2.62                     | 0.80              |
| 7:R:315:TYR:CE1  | 7:S:308:GLU:CD   | 2.61                     | 0.79              |
| 7:M:54:TYR:CB    | 7:N:195:PHE:CE2  | 2.64                     | 0.79              |
| 7:R:322:GLU:OE1  | 7:S:330:ASN:CA   | 2.30                     | 0.79              |
| 7:O:321:PRO:HA   | 7:P:167:ARG:CZ   | 2.13                     | 0.79              |
| 5:I:129:DC:OP2   | 7:K:67:SER:HB3   | 1.77                     | 0.78              |
| 7:M:318:PRO:O    | 7:N:163:GLU:C    | 2.26                     | 0.78              |
| 7:S:294:HIS:CB   | 7:T:165:THR:HA   | 2.13                     | 0.78              |
| 7:M:47:HIS:CE1   | 7:M:243:MET:SD   | 2.77                     | 0.78              |
| 7:K:57:LYS:HE3   | 7:L:198:ASP:OD1  | 1.83                     | 0.78              |
| 7:P:294:HIS:C    | 7:Q:193:ARG:HB3  | 2.08                     | 0.78              |
| 7:N:257:ASP:OD2  | 7:O:195:PHE:CE1  | 2.37                     | 0.78              |
| 7:Q:291:ILE:O    | 7:R:195:PHE:CE2  | 2.37                     | 0.77              |
| 7:Q:290:ASN:O    | 7:R:195:PHE:CD2  | 2.36                     | 0.77              |
| 7:M:247:ARG:HE   | 7:M:251:MET:HE2  | 1.50                     | 0.76              |
| 7:R:57:LYS:C     | 7:S:195:PHE:CZ   | 2.53                     | 0.76              |
| 7:K:165:THR:HG23 | 7:T:294:HIS:HB3  | 1.67                     | 0.76              |
| 7:K:308:GLU:OE2  | 7:T:322:GLU:HG2  | 1.85                     | 0.76              |
| 7:K:57:LYS:HE2   | 7:L:198:ASP:OD1  | 1.85                     | 0.76              |
| 7:K:106:SER:OG   | 7:K:336:ASP:OD1  | 2.04                     | 0.76              |
| 7:K:199:HIS:HB3  | 7:T:56:PRO:CG    | 2.16                     | 0.76              |
| 7:Q:106:SER:OG   | 7:Q:336:ASP:OD1  | 2.04                     | 0.75              |
| 7:L:294:HIS:HE2  | 7:M:223:SER:HG   | 1.05                     | 0.75              |
| 7:L:54:TYR:CD2   | 7:M:195:PHE:CE2  | 2.74                     | 0.75              |
| 7:M:106:SER:OG   | 7:M:336:ASP:OD1  | 2.04                     | 0.75              |
| 7:R:58:LYS:CA    | 7:S:195:PHE:CE2  | 2.70                     | 0.75              |
| 7:R:58:LYS:HA    | 7:S:195:PHE:CE2  | 2.22                     | 0.75              |
| 7:O:106:SER:OG   | 7:O:336:ASP:OD1  | 2.04                     | 0.75              |
| 7:M:201:THR:HG21 | 7:M:251:MET:HE1  | 1.67                     | 0.75              |
| 7:L:50:GLU:CG    | 7:L:54:TYR:HE2   | 2.00                     | 0.75              |
| 7:K:46:PHE:HA    | 7:K:205:TYR:OH   | 1.87                     | 0.74              |
| 7:K:56:PRO:HG3   | 7:L:196:ASN:HB2  | 1.68                     | 0.74              |
| 7:O:321:PRO:HA   | 7:P:167:ARG:NH1  | 2.01                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:L:294:HIS:CE1  | 7:M:163:GLU:HB3  | 2.21                     | 0.74              |
| 7:Q:291:ILE:C    | 7:R:195:PHE:CE2  | 2.65                     | 0.74              |
| 7:K:163:GLU:O    | 7:T:294:HIS:CD2  | 2.41                     | 0.74              |
| 7:P:106:SER:OG   | 7:P:336:ASP:OD1  | 2.04                     | 0.74              |
| 7:Q:47:HIS:HD2   | 7:Q:254:ARG:CG   | 2.00                     | 0.73              |
| 7:P:318:PRO:CD   | 7:Q:164:GLY:O    | 2.34                     | 0.73              |
| 7:S:106:SER:OG   | 7:S:336:ASP:OD1  | 2.04                     | 0.73              |
| 6:J:111:DC:H2'   | 6:J:112:DT:H71   | 1.70                     | 0.73              |
| 7:L:106:SER:OG   | 7:L:336:ASP:OD1  | 2.04                     | 0.73              |
| 7:T:106:SER:OG   | 7:T:336:ASP:OD1  | 2.04                     | 0.73              |
| 7:N:106:SER:OG   | 7:N:336:ASP:OD1  | 2.04                     | 0.72              |
| 7:R:58:LYS:HA    | 7:S:195:PHE:CZ   | 2.24                     | 0.72              |
| 7:R:61:ILE:HD12  | 7:S:195:PHE:HE2  | 1.55                     | 0.72              |
| 5:I:141:DA:H2''  | 5:I:142:DC:C6    | 2.24                     | 0.72              |
| 7:P:318:PRO:CG   | 7:Q:164:GLY:O    | 2.37                     | 0.72              |
| 7:P:114:GLN:HG3  | 7:Q:169:GLU:OE2  | 1.89                     | 0.72              |
| 7:Q:47:HIS:HB2   | 7:Q:254:ARG:HE   | 1.53                     | 0.72              |
| 7:L:50:GLU:OE2   | 7:L:257:ASP:C    | 2.32                     | 0.72              |
| 7:Q:293:ALA:CB   | 7:R:195:PHE:HZ   | 1.97                     | 0.71              |
| 7:R:46:PHE:CE1   | 7:R:250:ARG:HD2  | 2.26                     | 0.71              |
| 7:R:47:HIS:HB2   | 7:R:254:ARG:NH2  | 2.05                     | 0.71              |
| 7:K:164:GLY:HA3  | 7:T:294:HIS:CD2  | 2.26                     | 0.71              |
| 7:L:294:HIS:HE1  | 7:M:163:GLU:HB3  | 1.56                     | 0.71              |
| 7:Q:48:THR:CG2   | 7:Q:254:ARG:HH12 | 1.96                     | 0.71              |
| 7:M:318:PRO:O    | 7:N:163:GLU:O    | 2.09                     | 0.71              |
| 7:R:106:SER:OG   | 7:R:336:ASP:OD1  | 2.04                     | 0.71              |
| 7:T:45:GLY:CA    | 7:T:247:ARG:HD2  | 2.21                     | 0.70              |
| 7:P:291:ILE:O    | 7:Q:195:PHE:CD1  | 2.41                     | 0.70              |
| 5:I:129:DC:OP2   | 7:K:67:SER:HB2   | 1.91                     | 0.70              |
| 7:N:294:HIS:HD2  | 7:O:268:GLN:HE22 | 1.40                     | 0.70              |
| 7:K:50:GLU:O     | 7:K:254:ARG:NH2  | 2.23                     | 0.70              |
| 7:Q:47:HIS:CG    | 7:Q:254:ARG:HE   | 2.10                     | 0.70              |
| 7:K:165:THR:HG22 | 7:T:294:HIS:HB3  | 1.74                     | 0.69              |
| 1:E:63:ARG:HD3   | 6:J:98:DA:H4'    | 1.75                     | 0.69              |
| 7:S:294:HIS:O    | 7:T:167:ARG:HG2  | 1.92                     | 0.69              |
| 7:T:44:ALA:C     | 7:T:247:ARG:HH21 | 2.00                     | 0.69              |
| 7:R:58:LYS:HE3   | 7:S:195:PHE:CG   | 2.28                     | 0.69              |
| 7:R:322:GLU:OE1  | 7:S:331:ALA:N    | 2.24                     | 0.69              |
| 7:L:50:GLU:OE2   | 7:L:257:ASP:O    | 2.10                     | 0.69              |
| 7:R:34:ASN:OD1   | 7:R:37:ASP:HB2   | 1.94                     | 0.68              |
| 7:L:34:ASN:OD1   | 7:L:37:ASP:HB2   | 1.94                     | 0.68              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:R:291:ILE:O   | 7:R:294:HIS:ND1  | 2.27                     | 0.68              |
| 7:K:56:PRO:CG   | 7:L:196:ASN:CG   | 2.56                     | 0.68              |
| 7:N:34:ASN:OD1  | 7:N:37:ASP:HB2   | 1.94                     | 0.68              |
| 7:Q:34:ASN:OD1  | 7:Q:37:ASP:HB2   | 1.94                     | 0.68              |
| 7:T:34:ASN:OD1  | 7:T:37:ASP:HB2   | 1.94                     | 0.68              |
| 7:T:291:ILE:O   | 7:T:294:HIS:ND1  | 2.27                     | 0.68              |
| 5:I:55:DC:P     | 7:M:70:LYS:HE3   | 2.33                     | 0.67              |
| 7:K:34:ASN:OD1  | 7:K:37:ASP:HB2   | 1.94                     | 0.67              |
| 1:A:73:GLU:OE1  | 2:B:25:ASN:ND2   | 2.24                     | 0.67              |
| 7:K:46:PHE:CZ   | 7:K:247:ARG:CD   | 2.77                     | 0.67              |
| 7:P:291:ILE:O   | 7:P:294:HIS:ND1  | 2.27                     | 0.67              |
| 4:D:76:GLU:OE1  | 4:D:79:ARG:NH2   | 2.27                     | 0.67              |
| 7:M:34:ASN:OD1  | 7:M:37:ASP:HB2   | 1.94                     | 0.67              |
| 7:K:57:LYS:HE2  | 7:L:198:ASP:CG   | 2.19                     | 0.66              |
| 7:N:27:ARG:HA   | 7:N:30:GLN:OE1   | 1.96                     | 0.66              |
| 7:N:58:LYS:HE2  | 7:N:58:LYS:HA    | 1.78                     | 0.66              |
| 7:O:321:PRO:HA  | 7:P:167:ARG:NE   | 2.09                     | 0.66              |
| 7:M:58:LYS:HE2  | 7:M:58:LYS:HA    | 1.78                     | 0.66              |
| 7:Q:58:LYS:HE2  | 7:Q:58:LYS:HA    | 1.78                     | 0.66              |
| 7:L:50:GLU:HG3  | 7:L:54:TYR:HE2   | 1.60                     | 0.66              |
| 7:M:318:PRO:CB  | 7:N:193:ARG:CZ   | 2.71                     | 0.66              |
| 7:K:196:ASN:OD1 | 7:T:56:PRO:CB    | 2.37                     | 0.66              |
| 7:T:58:LYS:HA   | 7:T:58:LYS:HE2   | 1.78                     | 0.66              |
| 7:K:56:PRO:HG3  | 7:L:196:ASN:HB3  | 1.73                     | 0.66              |
| 7:M:318:PRO:HB2 | 7:N:193:ARG:CZ   | 2.25                     | 0.66              |
| 7:K:27:ARG:HA   | 7:K:30:GLN:OE1   | 1.95                     | 0.66              |
| 7:K:58:LYS:HE2  | 7:K:58:LYS:HA    | 1.78                     | 0.66              |
| 7:R:27:ARG:HA   | 7:R:30:GLN:OE1   | 1.95                     | 0.66              |
| 7:L:58:LYS:HE2  | 7:L:58:LYS:HA    | 1.77                     | 0.66              |
| 7:Q:27:ARG:HA   | 7:Q:30:GLN:OE1   | 1.95                     | 0.66              |
| 7:S:294:HIS:NE2 | 7:T:164:GLY:C    | 2.48                     | 0.65              |
| 7:R:58:LYS:HE2  | 7:R:58:LYS:HA    | 1.78                     | 0.65              |
| 7:R:313:LYS:NZ  | 7:S:307:GLY:HA2  | 2.10                     | 0.65              |
| 7:L:36:ASN:OD1  | 7:L:37:ASP:N     | 2.30                     | 0.65              |
| 7:T:27:ARG:HA   | 7:T:30:GLN:OE1   | 1.95                     | 0.65              |
| 7:T:45:GLY:HA3  | 7:T:247:ARG:HD2  | 1.79                     | 0.65              |
| 7:Q:36:ASN:OD1  | 7:Q:37:ASP:N     | 2.30                     | 0.65              |
| 7:R:322:GLU:OE2 | 7:S:330:ASN:HA   | 1.96                     | 0.65              |
| 7:M:36:ASN:OD1  | 7:M:37:ASP:N     | 2.30                     | 0.65              |
| 7:Q:47:HIS:HB3  | 7:Q:254:ARG:HH11 | 1.59                     | 0.65              |
| 7:K:46:PHE:CZ   | 7:K:247:ARG:HD3  | 2.32                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:Q:191:TYR:OH   | 7:Q:193:ARG:NH1  | 2.30                     | 0.65              |
| 7:Q:290:ASN:O    | 7:R:195:PHE:CD1  | 2.50                     | 0.65              |
| 7:M:201:THR:CG2  | 7:M:251:MET:CE   | 2.60                     | 0.64              |
| 7:K:45:GLY:O     | 7:K:205:TYR:CE2  | 2.51                     | 0.64              |
| 7:K:294:HIS:CD2  | 7:L:226:ALA:HB1  | 2.32                     | 0.64              |
| 7:P:318:PRO:CG   | 7:Q:165:THR:C    | 2.50                     | 0.64              |
| 7:Q:47:HIS:C     | 7:Q:254:ARG:NH1  | 2.55                     | 0.64              |
| 7:K:36:ASN:OD1   | 7:K:37:ASP:N     | 2.30                     | 0.64              |
| 7:T:36:ASN:OD1   | 7:T:37:ASP:N     | 2.30                     | 0.64              |
| 7:Q:47:HIS:CB    | 7:Q:254:ARG:HE   | 2.11                     | 0.64              |
| 7:M:318:PRO:HB2  | 7:N:193:ARG:NH2  | 2.13                     | 0.64              |
| 7:R:36:ASN:OD1   | 7:R:37:ASP:N     | 2.30                     | 0.64              |
| 7:N:36:ASN:OD1   | 7:N:37:ASP:N     | 2.30                     | 0.64              |
| 7:K:50:GLU:C     | 7:K:254:ARG:HH22 | 2.05                     | 0.64              |
| 7:N:257:ASP:OD2  | 7:O:195:PHE:CZ   | 2.51                     | 0.64              |
| 7:L:50:GLU:CD    | 7:L:258:GLU:CB   | 2.64                     | 0.63              |
| 7:P:294:HIS:HD2  | 7:Q:194:ALA:C    | 2.04                     | 0.63              |
| 7:K:54:TYR:CB    | 7:K:254:ARG:HH12 | 1.95                     | 0.63              |
| 7:P:291:ILE:HG13 | 7:Q:195:PHE:HB3  | 1.78                     | 0.63              |
| 5:I:81:DC:H2''   | 5:I:82:DG:C8     | 2.34                     | 0.63              |
| 7:P:318:PRO:HG3  | 7:Q:164:GLY:C    | 2.23                     | 0.63              |
| 7:K:46:PHE:CE1   | 7:K:247:ARG:HD3  | 2.33                     | 0.63              |
| 7:Q:191:TYR:HE2  | 7:Q:193:ARG:HH22 | 1.47                     | 0.62              |
| 7:O:321:PRO:HB3  | 7:P:167:ARG:HE   | 1.63                     | 0.62              |
| 7:R:318:PRO:HB3  | 7:S:170:ARG:HD2  | 1.81                     | 0.62              |
| 5:I:97:DA:H2''   | 5:I:98:DG:C8     | 2.35                     | 0.62              |
| 7:M:318:PRO:C    | 7:N:193:ARG:HH12 | 2.06                     | 0.62              |
| 7:P:318:PRO:HG2  | 7:Q:166:PHE:N    | 2.08                     | 0.62              |
| 6:J:37:DG:C2'    | 6:J:38:DT:H71    | 2.30                     | 0.62              |
| 7:N:257:ASP:CB   | 7:O:195:PHE:HZ   | 2.13                     | 0.62              |
| 7:T:47:HIS:HB2   | 7:T:254:ARG:HH21 | 0.80                     | 0.62              |
| 5:I:129:DC:P     | 7:K:67:SER:CB    | 2.77                     | 0.62              |
| 6:J:31:DT:H2''   | 6:J:32:DG:C8     | 2.35                     | 0.62              |
| 7:S:291:ILE:HD12 | 7:T:193:ARG:HH22 | 1.65                     | 0.62              |
| 5:I:28:DA:H1'    | 5:I:29:DA:C8     | 2.35                     | 0.62              |
| 1:A:39:HIS:HD2   | 1:A:40:ARG:N     | 1.98                     | 0.61              |
| 7:T:45:GLY:HA3   | 7:T:247:ARG:CG   | 2.30                     | 0.61              |
| 7:M:56:PRO:CG    | 7:N:196:ASN:CB   | 2.72                     | 0.61              |
| 7:M:318:PRO:O    | 7:N:163:GLU:HA   | 1.99                     | 0.61              |
| 7:T:43:GLU:O     | 7:T:247:ARG:CZ   | 2.48                     | 0.61              |
| 7:P:294:HIS:CD2  | 7:Q:194:ALA:O    | 2.53                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:59:GLU:CG    | 7:N:254:ARG:HH12 | 2.12                     | 0.61              |
| 6:J:37:DG:H2"    | 6:J:38:DT:H71    | 1.81                     | 0.61              |
| 7:K:50:GLU:CG    | 7:K:254:ARG:NH2  | 2.64                     | 0.61              |
| 7:L:50:GLU:OE1   | 7:L:258:GLU:C    | 2.41                     | 0.61              |
| 7:R:291:ILE:HG13 | 7:R:294:HIS:HE1  | 1.66                     | 0.61              |
| 7:S:291:ILE:CD1  | 7:T:193:ARG:HH22 | 2.13                     | 0.61              |
| 5:I:118:DC:H2"   | 5:I:119:DA:N7    | 2.16                     | 0.61              |
| 7:T:45:GLY:HA3   | 7:T:247:ARG:CD   | 2.30                     | 0.61              |
| 7:M:247:ARG:HE   | 7:M:251:MET:CE   | 2.14                     | 0.60              |
| 7:M:318:PRO:HB2  | 7:N:193:ARG:HH22 | 1.65                     | 0.60              |
| 7:R:321:PRO:HA   | 7:S:331:ALA:CB   | 2.31                     | 0.60              |
| 7:Q:290:ASN:O    | 7:R:195:PHE:CG   | 2.55                     | 0.60              |
| 7:K:196:ASN:HB3  | 7:T:59:GLU:OE2   | 2.02                     | 0.60              |
| 7:P:291:ILE:HG13 | 7:P:294:HIS:HE1  | 1.66                     | 0.60              |
| 7:K:199:HIS:CB   | 7:T:56:PRO:HG2   | 2.27                     | 0.60              |
| 7:Q:103:THR:N    | 7:Q:151:GLY:O    | 2.30                     | 0.60              |
| 7:R:47:HIS:H     | 7:R:254:ARG:CZ   | 2.13                     | 0.60              |
| 7:R:322:GLU:OE2  | 7:S:330:ASN:CA   | 2.49                     | 0.60              |
| 7:T:45:GLY:N     | 7:T:247:ARG:HD2  | 2.15                     | 0.60              |
| 7:L:211:MET:HE2  | 7:L:216:TYR:CG   | 2.36                     | 0.60              |
| 7:T:47:HIS:CD2   | 7:T:254:ARG:NH2  | 2.70                     | 0.60              |
| 7:Q:293:ALA:CA   | 7:R:195:PHE:HZ   | 2.15                     | 0.60              |
| 5:I:126:DA:H2"   | 5:I:127:DG:C8    | 2.37                     | 0.59              |
| 7:L:50:GLU:HG2   | 7:L:54:TYR:HE2   | 1.67                     | 0.59              |
| 7:T:291:ILE:HG13 | 7:T:294:HIS:HE1  | 1.66                     | 0.59              |
| 5:I:137:DA:H2"   | 5:I:138:DA:C8    | 2.38                     | 0.59              |
| 7:T:45:GLY:HA3   | 7:T:247:ARG:HG3  | 1.83                     | 0.59              |
| 7:L:50:GLU:OE2   | 7:L:258:GLU:CA   | 2.43                     | 0.59              |
| 7:L:158:MET:HG3  | 7:L:211:MET:HE1  | 1.85                     | 0.59              |
| 7:K:54:TYR:CB    | 7:L:195:PHE:CD2  | 2.76                     | 0.59              |
| 7:L:103:THR:N    | 7:L:151:GLY:O    | 2.30                     | 0.59              |
| 7:K:199:HIS:CG   | 7:T:56:PRO:HG3   | 2.26                     | 0.58              |
| 7:P:107:LYS:N    | 7:P:336:ASP:OD2  | 2.37                     | 0.58              |
| 7:T:107:LYS:N    | 7:T:336:ASP:OD2  | 2.37                     | 0.58              |
| 7:K:58:LYS:HZ3   | 7:K:61:ILE:CD1   | 2.16                     | 0.58              |
| 7:M:107:LYS:N    | 7:M:336:ASP:OD2  | 2.37                     | 0.58              |
| 7:R:107:LYS:N    | 7:R:336:ASP:OD2  | 2.37                     | 0.58              |
| 7:L:107:LYS:N    | 7:L:336:ASP:OD2  | 2.37                     | 0.58              |
| 7:N:107:LYS:N    | 7:N:336:ASP:OD2  | 2.37                     | 0.58              |
| 7:T:44:ALA:CA    | 7:T:247:ARG:NH2  | 2.51                     | 0.58              |
| 7:P:294:HIS:CG   | 7:Q:194:ALA:O    | 2.57                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:123:ASP:OD1 | 1:E:113:HIS:NE2  | 2.37                     | 0.57              |
| 7:L:322:GLU:OE1 | 7:M:308:GLU:OE2  | 2.21                     | 0.57              |
| 7:R:318:PRO:HG3 | 7:S:170:ARG:HD3  | 1.85                     | 0.57              |
| 7:L:50:GLU:HG2  | 7:L:54:TYR:CE2   | 2.40                     | 0.57              |
| 7:M:244:HIS:CE1 | 7:M:247:ARG:HH12 | 2.22                     | 0.57              |
| 7:K:107:LYS:N   | 7:K:336:ASP:OD2  | 2.37                     | 0.57              |
| 7:S:103:THR:N   | 7:S:151:GLY:O    | 2.30                     | 0.57              |
| 7:S:107:LYS:N   | 7:S:336:ASP:OD2  | 2.37                     | 0.57              |
| 7:K:103:THR:N   | 7:K:151:GLY:O    | 2.30                     | 0.57              |
| 7:S:294:HIS:CG  | 7:T:165:THR:HA   | 2.40                     | 0.57              |
| 7:T:47:HIS:H    | 7:T:254:ARG:HH22 | 1.52                     | 0.57              |
| 7:O:107:LYS:N   | 7:O:336:ASP:OD2  | 2.37                     | 0.57              |
| 7:P:318:PRO:HG3 | 7:Q:165:THR:CA   | 2.35                     | 0.57              |
| 7:R:103:THR:N   | 7:R:151:GLY:O    | 2.30                     | 0.57              |
| 7:L:294:HIS:CE1 | 7:M:163:GLU:CB   | 2.87                     | 0.57              |
| 7:Q:47:HIS:CD2  | 7:Q:254:ARG:NE   | 2.69                     | 0.57              |
| 7:R:322:GLU:CD  | 7:S:330:ASN:CA   | 2.72                     | 0.57              |
| 7:S:293:ALA:C   | 7:T:167:ARG:HH11 | 2.13                     | 0.57              |
| 7:K:58:LYS:HZ3  | 7:K:61:ILE:HD12  | 1.69                     | 0.57              |
| 7:R:315:TYR:OH  | 7:S:130:ARG:NH2  | 2.37                     | 0.57              |
| 7:P:103:THR:N   | 7:P:151:GLY:O    | 2.30                     | 0.57              |
| 7:M:103:THR:N   | 7:M:151:GLY:O    | 2.30                     | 0.57              |
| 7:Q:232:TYR:CG  | 7:Q:241:ARG:HB3  | 2.40                     | 0.57              |
| 5:I:45:DT:H2''  | 5:I:46:DC:C6     | 2.39                     | 0.57              |
| 7:R:58:LYS:HE2  | 7:S:195:PHE:CZ   | 2.28                     | 0.57              |
| 7:R:232:TYR:CG  | 7:R:241:ARG:HB3  | 2.40                     | 0.57              |
| 7:P:232:TYR:CG  | 7:P:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:T:103:THR:N   | 7:T:151:GLY:O    | 2.30                     | 0.56              |
| 7:L:232:TYR:CG  | 7:L:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:M:232:TYR:CG  | 7:M:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:N:103:THR:N   | 7:N:151:GLY:O    | 2.30                     | 0.56              |
| 7:O:103:THR:N   | 7:O:151:GLY:O    | 2.30                     | 0.56              |
| 7:Q:107:LYS:N   | 7:Q:336:ASP:OD2  | 2.37                     | 0.56              |
| 7:T:232:TYR:CG  | 7:T:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:K:232:TYR:CG  | 7:K:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:L:28:LEU:HD13 | 7:L:49:VAL:HG13  | 1.88                     | 0.56              |
| 6:J:57:DT:H2'   | 6:J:58:DT:H71    | 1.86                     | 0.56              |
| 7:N:232:TYR:CG  | 7:N:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:N:59:GLU:CG   | 7:N:254:ARG:NH1  | 2.67                     | 0.56              |
| 7:O:232:TYR:CG  | 7:O:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:P:319:CYS:C   | 7:Q:167:ARG:CG   | 2.53                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:48:DG:H2'    | 6:J:49:DT:H71    | 1.88                     | 0.56              |
| 6:J:130:DC:H2''  | 6:J:131:DG:C8    | 2.41                     | 0.56              |
| 7:Q:47:HIS:CD2   | 7:Q:254:ARG:CG   | 2.81                     | 0.56              |
| 7:S:294:HIS:HA   | 7:T:167:ARG:CZ   | 2.33                     | 0.56              |
| 7:Q:328:ALA:N    | 7:Q:335:GLY:O    | 2.31                     | 0.56              |
| 7:S:232:TYR:CG   | 7:S:241:ARG:HB3  | 2.40                     | 0.56              |
| 7:N:294:HIS:CE1  | 7:O:163:GLU:HB3  | 2.41                     | 0.55              |
| 7:R:318:PRO:CB   | 7:S:170:ARG:HD2  | 2.36                     | 0.55              |
| 2:B:52:GLU:OE2   | 2:B:55:ARG:NH2   | 2.40                     | 0.55              |
| 7:K:45:GLY:O     | 7:K:205:TYR:CZ   | 2.59                     | 0.55              |
| 7:K:328:ALA:N    | 7:K:335:GLY:O    | 2.31                     | 0.55              |
| 6:J:29:DC:H2''   | 6:J:30:DG:H8     | 1.72                     | 0.55              |
| 7:O:328:ALA:N    | 7:O:335:GLY:O    | 2.31                     | 0.55              |
| 1:A:39:HIS:CD2   | 1:A:40:ARG:N     | 2.74                     | 0.55              |
| 7:M:318:PRO:O    | 7:N:163:GLU:CA   | 2.55                     | 0.55              |
| 7:R:45:GLY:C     | 7:R:254:ARG:NH2  | 2.63                     | 0.55              |
| 5:I:152:DC:P     | 7:R:235:ARG:HE   | 2.29                     | 0.55              |
| 7:T:42:GLU:O     | 7:T:205:TYR:OH   | 2.25                     | 0.55              |
| 7:O:322:GLU:N    | 7:P:167:ARG:NH1  | 2.49                     | 0.55              |
| 7:R:328:ALA:N    | 7:R:335:GLY:O    | 2.31                     | 0.55              |
| 1:A:113:HIS:NE2  | 1:E:123:ASP:OD1  | 2.40                     | 0.55              |
| 5:I:89:DA:H1'    | 5:I:90:DA:N7     | 2.22                     | 0.55              |
| 7:K:56:PRO:HG3   | 7:L:196:ASN:ND2  | 2.18                     | 0.55              |
| 6:J:116:DT:H2''  | 6:J:117:DA:C8    | 2.41                     | 0.54              |
| 7:N:328:ALA:N    | 7:N:335:GLY:O    | 2.31                     | 0.54              |
| 2:F:31:LYS:HG3   | 2:F:51:TYR:CZ    | 2.42                     | 0.54              |
| 5:I:16:DC:H2''   | 5:I:17:DC:C5     | 2.42                     | 0.54              |
| 7:K:164:GLY:HA3  | 7:T:294:HIS:HD2  | 1.71                     | 0.54              |
| 7:L:50:GLU:OE2   | 7:L:258:GLU:N    | 2.41                     | 0.54              |
| 7:Q:47:HIS:CB    | 7:Q:254:ARG:NE   | 2.67                     | 0.54              |
| 7:K:54:TYR:HD2   | 7:K:254:ARG:NE   | 2.01                     | 0.54              |
| 7:Q:58:LYS:HZ3   | 7:Q:61:ILE:CD1   | 2.20                     | 0.54              |
| 5:I:128:DA:H2''  | 5:I:129:DC:C5    | 2.42                     | 0.54              |
| 7:P:319:CYS:CA   | 7:Q:167:ARG:CA   | 2.69                     | 0.54              |
| 7:K:54:TYR:HB3   | 7:L:195:PHE:CE2  | 2.36                     | 0.54              |
| 7:R:318:PRO:HG3  | 7:S:170:ARG:CD   | 2.38                     | 0.54              |
| 7:T:47:HIS:CG    | 7:T:254:ARG:HH21 | 2.20                     | 0.54              |
| 3:C:29:ARG:NH2   | 4:D:35:GLU:HB3   | 2.22                     | 0.54              |
| 7:L:123:THR:HG23 | 7:L:298:THR:HB   | 1.90                     | 0.54              |
| 7:Q:123:THR:HG23 | 7:Q:298:THR:HB   | 1.90                     | 0.54              |
| 2:F:16:LYS:HD3   | 2:F:16:LYS:N     | 2.22                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:123:THR:HG23 | 7:N:298:THR:HB   | 1.90                     | 0.54              |
| 7:K:123:THR:HG23 | 7:K:298:THR:HB   | 1.90                     | 0.53              |
| 6:J:96:DT:H2"    | 6:J:97:DA:C8     | 2.44                     | 0.53              |
| 7:S:196:ASN:C    | 7:S:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:L:50:GLU:HB3   | 7:L:258:GLU:HG3  | 1.90                     | 0.53              |
| 7:P:196:ASN:C    | 7:P:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:P:291:ILE:CG1  | 7:Q:195:PHE:HB3  | 2.38                     | 0.53              |
| 7:R:61:ILE:HD12  | 7:S:195:PHE:CE2  | 2.41                     | 0.53              |
| 7:L:196:ASN:C    | 7:L:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:Q:34:ASN:CG    | 7:Q:36:ASN:OD1   | 2.52                     | 0.53              |
| 7:M:58:LYS:HZ3   | 7:M:61:ILE:HD12  | 1.73                     | 0.53              |
| 6:J:54:DC:H2"    | 6:J:55:DC:C5     | 2.43                     | 0.53              |
| 6:J:56:DC:H2"    | 6:J:57:DT:H72    | 1.89                     | 0.53              |
| 7:M:34:ASN:CG    | 7:M:36:ASN:OD1   | 2.52                     | 0.53              |
| 7:N:248:PHE:CE2  | 7:N:252:LEU:HD11 | 2.44                     | 0.53              |
| 7:K:34:ASN:CG    | 7:K:36:ASN:OD1   | 2.52                     | 0.53              |
| 7:K:56:PRO:CG    | 7:L:196:ASN:HB2  | 2.34                     | 0.53              |
| 7:L:328:ALA:N    | 7:L:335:GLY:O    | 2.31                     | 0.53              |
| 7:N:319:CYS:HB2  | 7:O:167:ARG:NE   | 2.20                     | 0.53              |
| 7:O:123:THR:HG23 | 7:O:298:THR:HB   | 1.90                     | 0.53              |
| 7:O:196:ASN:C    | 7:O:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:Q:196:ASN:C    | 7:Q:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:R:123:THR:HG23 | 7:R:298:THR:HB   | 1.90                     | 0.53              |
| 7:R:196:ASN:C    | 7:R:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:T:248:PHE:CE2  | 7:T:252:LEU:HD11 | 2.44                     | 0.53              |
| 5:I:4:DA:H2"     | 5:I:5:DG:C8      | 2.43                     | 0.53              |
| 7:K:46:PHE:HE1   | 7:K:247:ARG:NE   | 1.89                     | 0.53              |
| 7:M:201:THR:HG21 | 7:M:247:ARG:CZ   | 2.39                     | 0.53              |
| 7:P:123:THR:HG23 | 7:P:298:THR:HB   | 1.90                     | 0.53              |
| 7:R:248:PHE:CE2  | 7:R:252:LEU:HD11 | 2.44                     | 0.53              |
| 7:T:196:ASN:C    | 7:T:227:LEU:HD13 | 2.34                     | 0.53              |
| 7:M:123:THR:HG23 | 7:M:298:THR:HB   | 1.90                     | 0.53              |
| 7:P:248:PHE:CE2  | 7:P:252:LEU:HD11 | 2.44                     | 0.53              |
| 7:N:319:CYS:CB   | 7:O:167:ARG:HE   | 2.20                     | 0.53              |
| 7:P:319:CYS:CB   | 7:Q:168:PRO:CD   | 2.47                     | 0.53              |
| 7:R:313:LYS:NZ   | 7:S:307:GLY:CA   | 2.72                     | 0.53              |
| 7:K:196:ASN:C    | 7:K:227:LEU:HD13 | 2.34                     | 0.52              |
| 7:L:34:ASN:CG    | 7:L:36:ASN:OD1   | 2.52                     | 0.52              |
| 7:M:28:LEU:HD13  | 7:M:49:VAL:HG13  | 1.91                     | 0.52              |
| 7:M:196:ASN:C    | 7:M:227:LEU:HD13 | 2.34                     | 0.52              |
| 7:N:34:ASN:CG    | 7:N:36:ASN:OD1   | 2.52                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:248:PHE:CE2  | 7:O:252:LEU:HD11 | 2.44                     | 0.52              |
| 7:R:34:ASN:CG    | 7:R:36:ASN:OD1   | 2.52                     | 0.52              |
| 7:S:248:PHE:CE2  | 7:S:252:LEU:HD11 | 2.44                     | 0.52              |
| 7:T:34:ASN:CG    | 7:T:36:ASN:OD1   | 2.52                     | 0.52              |
| 7:Q:248:PHE:CE2  | 7:Q:252:LEU:HD11 | 2.44                     | 0.52              |
| 7:S:328:ALA:N    | 7:S:335:GLY:O    | 2.31                     | 0.52              |
| 5:I:47:DT:H2''   | 5:I:48:DA:C8     | 2.44                     | 0.52              |
| 5:I:130:DA:H2''  | 5:I:131:DG:C8    | 2.44                     | 0.52              |
| 7:K:248:PHE:CE2  | 7:K:252:LEU:HD11 | 2.44                     | 0.52              |
| 7:Q:291:ILE:CA   | 7:R:195:PHE:CE2  | 2.92                     | 0.52              |
| 7:R:47:HIS:HB2   | 7:R:254:ARG:HH21 | 1.74                     | 0.52              |
| 7:S:123:THR:HG23 | 7:S:298:THR:HB   | 1.90                     | 0.52              |
| 7:Q:293:ALA:C    | 7:R:195:PHE:HZ   | 2.18                     | 0.52              |
| 1:E:72:ARG:HD3   | 2:F:19:ARG:CZ    | 2.39                     | 0.52              |
| 7:L:56:PRO:HG3   | 7:M:196:ASN:HB2  | 1.91                     | 0.52              |
| 7:N:196:ASN:C    | 7:N:227:LEU:HD13 | 2.34                     | 0.52              |
| 5:I:152:DC:C5'   | 7:R:235:ARG:HG2  | 2.36                     | 0.52              |
| 6:J:82:DC:H2''   | 6:J:83:DG:C8     | 2.45                     | 0.52              |
| 7:L:248:PHE:CE2  | 7:L:252:LEU:HD11 | 2.44                     | 0.52              |
| 7:P:328:ALA:N    | 7:P:335:GLY:O    | 2.31                     | 0.52              |
| 7:Q:58:LYS:HZ3   | 7:Q:61:ILE:HD12  | 1.75                     | 0.52              |
| 6:J:143:DG:H2''  | 6:J:144:DG:C8    | 2.45                     | 0.52              |
| 7:L:28:LEU:HD21  | 7:L:74:ILE:HG23  | 1.92                     | 0.52              |
| 7:M:28:LEU:HD21  | 7:M:74:ILE:HG23  | 1.91                     | 0.51              |
| 7:M:58:LYS:HZ3   | 7:M:61:ILE:CD1   | 2.23                     | 0.51              |
| 7:M:54:TYR:CB    | 7:N:195:PHE:HD2  | 2.11                     | 0.51              |
| 7:T:58:LYS:HA    | 7:T:58:LYS:CE    | 2.40                     | 0.51              |
| 7:N:243:MET:HE1  | 7:O:233:SER:HB3  | 1.91                     | 0.51              |
| 7:T:123:THR:HG23 | 7:T:298:THR:HB   | 1.90                     | 0.51              |
| 7:S:294:HIS:NE2  | 7:T:164:GLY:CA   | 2.74                     | 0.51              |
| 5:I:123:DA:OP1   | 5:I:123:DA:H8    | 1.93                     | 0.51              |
| 7:R:321:PRO:HA   | 7:S:331:ALA:HB3  | 1.91                     | 0.51              |
| 5:I:117:DC:H2''  | 5:I:118:DC:C6    | 2.46                     | 0.51              |
| 6:J:95:DT:H2''   | 6:J:96:DT:H72    | 1.93                     | 0.51              |
| 6:J:18:DT:C6     | 6:J:19:DT:H72    | 2.46                     | 0.51              |
| 6:J:101:DG:H1'   | 6:J:102:DG:H5'   | 1.92                     | 0.51              |
| 5:I:17:DC:H1'    | 5:I:18:DG:C8     | 2.46                     | 0.51              |
| 7:S:318:PRO:O    | 7:T:331:ALA:CB   | 2.59                     | 0.51              |
| 5:I:76:DT:H2''   | 5:I:77:DC:C6     | 2.46                     | 0.51              |
| 6:J:62:DG:H2''   | 6:J:63:DG:C8     | 2.46                     | 0.50              |
| 7:L:34:ASN:ND2   | 7:L:36:ASN:OD1   | 2.45                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:T:43:GLU:C     | 7:T:247:ARG:NH2  | 2.68                     | 0.50              |
| 7:O:322:GLU:N    | 7:P:167:ARG:HH11 | 2.08                     | 0.50              |
| 7:S:318:PRO:O    | 7:T:331:ALA:HB2  | 2.12                     | 0.50              |
| 7:M:328:ALA:N    | 7:M:335:GLY:O    | 2.31                     | 0.50              |
| 7:T:34:ASN:ND2   | 7:T:36:ASN:OD1   | 2.44                     | 0.50              |
| 5:I:108:DC:H2''  | 5:I:109:DC:C5    | 2.46                     | 0.50              |
| 7:R:315:TYR:C    | 7:S:308:GLU:OE2  | 2.52                     | 0.50              |
| 5:I:25:DC:H2''   | 5:I:26:DT:H72    | 1.94                     | 0.50              |
| 5:I:152:DC:H5''  | 7:R:235:ARG:CG   | 2.39                     | 0.50              |
| 7:K:50:GLU:OE2   | 7:K:254:ARG:HD3  | 2.11                     | 0.50              |
| 7:N:27:ARG:CA    | 7:N:30:GLN:OE1   | 2.60                     | 0.50              |
| 7:N:34:ASN:ND2   | 7:N:36:ASN:OD1   | 2.44                     | 0.50              |
| 7:T:27:ARG:CA    | 7:T:30:GLN:OE1   | 2.60                     | 0.50              |
| 7:M:34:ASN:ND2   | 7:M:36:ASN:OD1   | 2.45                     | 0.50              |
| 7:Q:311:ILE:HG12 | 7:Q:326:MET:SD   | 2.52                     | 0.50              |
| 5:I:65:DC:H2''   | 5:I:66:DG:C8     | 2.46                     | 0.50              |
| 6:J:126:DT:H2''  | 6:J:127:DG:N7    | 2.26                     | 0.50              |
| 7:N:294:HIS:CD2  | 7:O:268:GLN:HE22 | 2.26                     | 0.50              |
| 7:R:34:ASN:ND2   | 7:R:36:ASN:OD1   | 2.44                     | 0.50              |
| 3:C:20:ARG:NH1   | 6:J:39:DG:OP1    | 2.34                     | 0.49              |
| 7:K:311:ILE:HG12 | 7:K:326:MET:SD   | 2.52                     | 0.49              |
| 7:Q:34:ASN:ND2   | 7:Q:36:ASN:OD1   | 2.44                     | 0.49              |
| 7:Q:173:ALA:O    | 7:Q:176:GLU:HG3  | 2.12                     | 0.49              |
| 7:K:34:ASN:ND2   | 7:K:36:ASN:OD1   | 2.45                     | 0.49              |
| 6:J:111:DC:C2'   | 6:J:112:DT:H71   | 2.42                     | 0.49              |
| 7:O:173:ALA:O    | 7:O:176:GLU:HG3  | 2.12                     | 0.49              |
| 7:P:311:ILE:HG12 | 7:P:326:MET:SD   | 2.52                     | 0.49              |
| 7:R:320:LEU:C    | 7:S:331:ALA:CB   | 2.85                     | 0.49              |
| 7:R:173:ALA:O    | 7:R:176:GLU:HG3  | 2.12                     | 0.49              |
| 7:R:311:ILE:HG12 | 7:R:326:MET:SD   | 2.52                     | 0.49              |
| 5:I:2:DT:H2''    | 5:I:3:DC:C6      | 2.47                     | 0.49              |
| 6:J:25:DG:H2''   | 6:J:26:DT:C7     | 2.43                     | 0.49              |
| 7:M:125:MET:SD   | 7:M:265:ILE:O    | 2.71                     | 0.49              |
| 7:P:291:ILE:HG13 | 7:P:294:HIS:CE1  | 2.48                     | 0.49              |
| 7:T:125:MET:SD   | 7:T:265:ILE:O    | 2.71                     | 0.49              |
| 3:G:32:ARG:NH1   | 4:H:35:GLU:OE2   | 2.37                     | 0.49              |
| 7:K:57:LYS:HE2   | 7:L:198:ASP:OD2  | 2.12                     | 0.49              |
| 7:L:311:ILE:HG12 | 7:L:326:MET:SD   | 2.52                     | 0.49              |
| 7:S:173:ALA:O    | 7:S:176:GLU:HG3  | 2.12                     | 0.49              |
| 7:T:291:ILE:HG13 | 7:T:294:HIS:CE1  | 2.47                     | 0.49              |
| 5:I:48:DA:H1'    | 5:I:49:DG:C8     | 2.48                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 7:N:311:ILE:HG12 | 7:N:326:MET:SD  | 2.52                     | 0.49              |
| 7:P:125:MET:SD   | 7:P:265:ILE:O   | 2.71                     | 0.49              |
| 7:Q:125:MET:SD   | 7:Q:265:ILE:O   | 2.71                     | 0.49              |
| 7:S:311:ILE:HG12 | 7:S:326:MET:SD  | 2.52                     | 0.49              |
| 7:T:311:ILE:HG12 | 7:T:326:MET:SD  | 2.52                     | 0.49              |
| 7:K:173:ALA:O    | 7:K:176:GLU:HG3 | 2.12                     | 0.49              |
| 7:N:26:SER:O     | 7:N:30:GLN:OE1  | 2.31                     | 0.49              |
| 7:S:125:MET:SD   | 7:S:125:MET:N   | 2.86                     | 0.49              |
| 7:S:125:MET:SD   | 7:S:265:ILE:O   | 2.71                     | 0.49              |
| 5:I:55:DC:H5''   | 7:M:70:LYS:HZ2  | 1.78                     | 0.49              |
| 6:J:150:DT:H2''  | 6:J:151:DG:C8   | 2.47                     | 0.49              |
| 7:K:26:SER:O     | 7:K:30:GLN:OE1  | 2.31                     | 0.49              |
| 7:L:125:MET:SD   | 7:L:265:ILE:O   | 2.71                     | 0.49              |
| 7:L:173:ALA:O    | 7:L:176:GLU:HG3 | 2.12                     | 0.49              |
| 7:M:173:ALA:O    | 7:M:176:GLU:HG3 | 2.12                     | 0.49              |
| 7:R:125:MET:SD   | 7:R:265:ILE:O   | 2.71                     | 0.49              |
| 6:J:30:DG:H2'    | 6:J:31:DT:H71   | 1.95                     | 0.49              |
| 7:M:319:CYS:SG   | 7:N:164:GLY:O   | 2.71                     | 0.49              |
| 7:N:125:MET:SD   | 7:N:265:ILE:O   | 2.71                     | 0.49              |
| 7:R:125:MET:SD   | 7:R:125:MET:N   | 2.86                     | 0.49              |
| 7:R:293:ALA:C    | 7:S:167:ARG:NH1 | 2.71                     | 0.49              |
| 6:J:27:DC:H2''   | 6:J:28:DT:H72   | 1.95                     | 0.48              |
| 7:L:56:PRO:HG3   | 7:M:196:ASN:CB  | 2.42                     | 0.48              |
| 7:M:311:ILE:HG12 | 7:M:326:MET:SD  | 2.52                     | 0.48              |
| 7:N:257:ASP:CB   | 7:O:195:PHE:CZ  | 2.95                     | 0.48              |
| 7:O:125:MET:SD   | 7:O:125:MET:N   | 2.86                     | 0.48              |
| 7:Q:26:SER:O     | 7:Q:30:GLN:OE1  | 2.31                     | 0.48              |
| 7:Q:27:ARG:CA    | 7:Q:30:GLN:OE1  | 2.60                     | 0.48              |
| 7:Q:54:TYR:CZ    | 7:Q:82:VAL:CG1  | 2.96                     | 0.48              |
| 7:Q:61:ILE:HD13  | 7:Q:68:GLU:HG2  | 1.96                     | 0.48              |
| 7:N:173:ALA:O    | 7:N:176:GLU:HG3 | 2.12                     | 0.48              |
| 7:P:294:HIS:C    | 7:Q:193:ARG:HD3 | 2.37                     | 0.48              |
| 7:R:54:TYR:CZ    | 7:R:82:VAL:CG1  | 2.96                     | 0.48              |
| 7:T:54:TYR:CZ    | 7:T:82:VAL:CG1  | 2.96                     | 0.48              |
| 7:T:291:ILE:C    | 7:T:294:HIS:CE1 | 2.88                     | 0.48              |
| 6:J:12:DG:C5     | 6:J:13:DT:C4    | 3.01                     | 0.48              |
| 7:L:26:SER:O     | 7:L:30:GLN:OE1  | 2.31                     | 0.48              |
| 7:M:201:THR:HG23 | 7:M:251:MET:HE3 | 1.94                     | 0.48              |
| 7:R:26:SER:O     | 7:R:30:GLN:OE1  | 2.31                     | 0.48              |
| 1:A:39:HIS:HD2   | 1:A:40:ARG:H    | 1.59                     | 0.48              |
| 6:J:92:DC:H2''   | 6:J:93:DG:C8    | 2.48                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 7:K:54:TYR:CZ    | 7:K:82:VAL:CG1  | 2.96                     | 0.48              |
| 7:K:125:MET:SD   | 7:K:125:MET:N   | 2.86                     | 0.48              |
| 7:O:311:ILE:HG12 | 7:O:326:MET:SD  | 2.52                     | 0.48              |
| 7:T:61:ILE:HD13  | 7:T:68:GLU:HG2  | 1.96                     | 0.48              |
| 6:J:59:DG:C2     | 6:J:60:DG:C5    | 3.01                     | 0.48              |
| 7:R:321:PRO:HA   | 7:S:331:ALA:HB2 | 1.94                     | 0.48              |
| 7:T:173:ALA:O    | 7:T:176:GLU:HG3 | 2.12                     | 0.48              |
| 7:K:125:MET:SD   | 7:K:265:ILE:O   | 2.71                     | 0.48              |
| 7:R:27:ARG:CA    | 7:R:30:GLN:OE1  | 2.60                     | 0.48              |
| 6:J:25:DG:H2''   | 6:J:26:DT:C5    | 2.49                     | 0.48              |
| 7:K:61:ILE:HD13  | 7:K:68:GLU:HG2  | 1.96                     | 0.48              |
| 7:M:58:LYS:HA    | 7:M:58:LYS:CE   | 2.40                     | 0.48              |
| 7:M:61:ILE:HD13  | 7:M:68:GLU:HG2  | 1.96                     | 0.48              |
| 7:P:173:ALA:O    | 7:P:176:GLU:HG3 | 2.12                     | 0.48              |
| 7:R:58:LYS:CE    | 7:R:58:LYS:HA   | 2.40                     | 0.48              |
| 7:T:328:ALA:N    | 7:T:335:GLY:O   | 2.31                     | 0.48              |
| 6:J:8:DT:H2''    | 6:J:9:DT:C6     | 2.49                     | 0.48              |
| 7:M:26:SER:O     | 7:M:30:GLN:OE1  | 2.31                     | 0.48              |
| 7:M:125:MET:SD   | 7:M:125:MET:N   | 2.86                     | 0.48              |
| 7:O:321:PRO:CB   | 7:P:167:ARG:HE  | 2.27                     | 0.48              |
| 6:J:38:DT:C2     | 6:J:39:DG:N7    | 2.82                     | 0.48              |
| 7:N:54:TYR:CZ    | 7:N:82:VAL:CG1  | 2.96                     | 0.48              |
| 7:O:125:MET:SD   | 7:O:265:ILE:O   | 2.71                     | 0.48              |
| 7:P:291:ILE:C    | 7:P:294:HIS:CE1 | 2.88                     | 0.48              |
| 6:J:84:DC:H2''   | 6:J:85:DG:C8    | 2.48                     | 0.48              |
| 7:M:63:ILE:HB    | 7:M:66:ILE:HD12 | 1.96                     | 0.48              |
| 7:S:291:ILE:O    | 7:S:294:HIS:NE2 | 2.47                     | 0.48              |
| 5:I:99:DG:H1'    | 5:I:100:DG:C8   | 2.48                     | 0.47              |
| 5:I:120:DG:C5    | 5:I:121:DG:C6   | 3.02                     | 0.47              |
| 6:J:23:DC:H2''   | 6:J:24:DT:C6    | 2.49                     | 0.47              |
| 6:J:128:DA:H2''  | 6:J:129:DG:C8   | 2.49                     | 0.47              |
| 7:N:125:MET:SD   | 7:N:125:MET:N   | 2.86                     | 0.47              |
| 7:Q:63:ILE:HB    | 7:Q:66:ILE:HD12 | 1.96                     | 0.47              |
| 7:T:26:SER:O     | 7:T:30:GLN:OE1  | 2.31                     | 0.47              |
| 7:T:291:ILE:CG1  | 7:T:294:HIS:HE1 | 2.27                     | 0.47              |
| 5:I:15:DG:H2''   | 5:I:16:DC:C6    | 2.50                     | 0.47              |
| 7:Q:47:HIS:CA    | 7:Q:254:ARG:NH1 | 2.74                     | 0.47              |
| 5:I:26:DT:H2''   | 5:I:27:DC:C5    | 2.49                     | 0.47              |
| 5:I:107:DA:H2''  | 5:I:108:DC:C6   | 2.49                     | 0.47              |
| 6:J:30:DG:C2'    | 6:J:31:DT:H71   | 2.45                     | 0.47              |
| 7:K:63:ILE:HB    | 7:K:66:ILE:HD12 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:61:ILE:HD13  | 7:N:68:GLU:HG2   | 1.96                     | 0.47              |
| 6:J:24:DT:H2"    | 6:J:25:DG:N7     | 2.29                     | 0.47              |
| 7:K:27:ARG:CA    | 7:K:30:GLN:OE1   | 2.60                     | 0.47              |
| 7:R:291:ILE:HG13 | 7:R:294:HIS:CE1  | 2.47                     | 0.47              |
| 7:T:63:ILE:HB    | 7:T:66:ILE:HD12  | 1.96                     | 0.47              |
| 7:M:211:MET:HE2  | 7:M:216:TYR:HB2  | 1.97                     | 0.47              |
| 7:P:291:ILE:CG1  | 7:P:294:HIS:HE1  | 2.27                     | 0.47              |
| 2:B:31:LYS:HG3   | 2:B:51:TYR:CZ    | 2.50                     | 0.47              |
| 7:K:58:LYS:HA    | 7:K:58:LYS:CE    | 2.40                     | 0.47              |
| 7:K:211:MET:HE2  | 7:K:216:TYR:HB2  | 1.97                     | 0.47              |
| 7:L:61:ILE:HD13  | 7:L:68:GLU:HG2   | 1.96                     | 0.47              |
| 7:N:211:MET:HE2  | 7:N:216:TYR:HB2  | 1.97                     | 0.47              |
| 7:Q:211:MET:HE2  | 7:Q:216:TYR:HB2  | 1.97                     | 0.47              |
| 7:R:61:ILE:HD13  | 7:R:68:GLU:HG2   | 1.96                     | 0.47              |
| 7:T:211:MET:HE2  | 7:T:216:TYR:HB2  | 1.97                     | 0.47              |
| 5:I:152:DC:C4    | 5:I:153:DA:N6    | 2.83                     | 0.47              |
| 6:J:58:DT:H2"    | 6:J:59:DG:H8     | 1.79                     | 0.47              |
| 7:M:56:PRO:HG3   | 7:N:196:ASN:HB2  | 1.87                     | 0.47              |
| 7:O:211:MET:HE2  | 7:O:216:TYR:HB2  | 1.97                     | 0.47              |
| 7:P:211:MET:HE2  | 7:P:216:TYR:HB2  | 1.97                     | 0.47              |
| 7:R:47:HIS:CB    | 7:R:254:ARG:HD3  | 2.37                     | 0.47              |
| 7:R:63:ILE:HB    | 7:R:66:ILE:HD12  | 1.96                     | 0.47              |
| 3:G:79:ILE:HG12  | 3:G:82:HIS:CE1   | 2.50                     | 0.47              |
| 7:S:291:ILE:O    | 7:S:294:HIS:CD2  | 2.67                     | 0.47              |
| 7:M:248:PHE:CE2  | 7:M:252:LEU:HD11 | 2.50                     | 0.47              |
| 7:M:248:PHE:HA   | 7:M:251:MET:HE3  | 1.96                     | 0.47              |
| 6:J:118:DC:H2"   | 6:J:119:DG:C8    | 2.50                     | 0.46              |
| 6:J:143:DG:H2"   | 6:J:144:DG:H8    | 1.80                     | 0.46              |
| 7:K:50:GLU:C     | 7:K:254:ARG:NH2  | 2.71                     | 0.46              |
| 7:S:294:HIS:NE2  | 7:T:164:GLY:HA3  | 2.30                     | 0.46              |
| 3:C:99:ARG:NH1   | 2:F:94:GLY:HA3   | 2.30                     | 0.46              |
| 6:J:44:DG:H2"    | 6:J:45:DG:C8     | 2.49                     | 0.46              |
| 7:K:163:GLU:O    | 7:T:294:HIS:ND1  | 2.47                     | 0.46              |
| 7:N:63:ILE:HB    | 7:N:66:ILE:HD12  | 1.96                     | 0.46              |
| 7:T:27:ARG:C     | 7:T:30:GLN:OE1   | 2.59                     | 0.46              |
| 6:J:139:DC:H2"   | 6:J:140:DA:C8    | 2.51                     | 0.46              |
| 7:K:27:ARG:C     | 7:K:30:GLN:OE1   | 2.59                     | 0.46              |
| 7:L:63:ILE:HB    | 7:L:66:ILE:HD12  | 1.96                     | 0.46              |
| 7:Q:191:TYR:HE2  | 7:Q:193:ARG:CZ   | 2.09                     | 0.46              |
| 7:R:211:MET:HE2  | 7:R:216:TYR:HB2  | 1.97                     | 0.46              |
| 7:R:291:ILE:C    | 7:R:294:HIS:CE1  | 2.88                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:S:211:MET:HE2 | 7:S:216:TYR:HB2  | 1.97                     | 0.46              |
| 6:J:63:DG:H2''  | 6:J:64:DT:C6     | 2.50                     | 0.46              |
| 7:M:50:GLU:HA   | 7:M:82:VAL:HG21  | 1.98                     | 0.46              |
| 7:P:297:THR:HA  | 7:Q:193:ARG:CZ   | 2.46                     | 0.46              |
| 7:Q:191:TYR:OH  | 7:Q:193:ARG:CG   | 2.64                     | 0.46              |
| 7:R:102:ILE:HA  | 7:R:151:GLY:O    | 2.16                     | 0.46              |
| 7:R:291:ILE:CG1 | 7:R:294:HIS:HE1  | 2.27                     | 0.46              |
| 6:J:100:DC:C2   | 6:J:101:DG:N7    | 2.84                     | 0.46              |
| 7:L:208:SER:O   | 7:L:212:VAL:HG23 | 2.16                     | 0.46              |
| 7:R:315:TYR:CA  | 7:S:308:GLU:OE2  | 2.64                     | 0.46              |
| 7:L:58:LYS:HA   | 7:L:58:LYS:CE    | 2.40                     | 0.46              |
| 7:R:30:GLN:OE1  | 7:R:30:GLN:N     | 2.47                     | 0.46              |
| 5:I:17:DC:H1'   | 5:I:18:DG:C5     | 2.51                     | 0.46              |
| 6:J:48:DG:C2'   | 6:J:49:DT:H71    | 2.46                     | 0.46              |
| 6:J:126:DT:H2'' | 6:J:127:DG:C8    | 2.51                     | 0.46              |
| 7:M:102:ILE:HA  | 7:M:151:GLY:O    | 2.16                     | 0.46              |
| 7:N:58:LYS:HA   | 7:N:58:LYS:CE    | 2.40                     | 0.46              |
| 7:Q:30:GLN:OE1  | 7:Q:30:GLN:N     | 2.46                     | 0.46              |
| 7:Q:191:TYR:CZ  | 7:Q:193:ARG:NH1  | 2.84                     | 0.46              |
| 7:R:27:ARG:C    | 7:R:30:GLN:OE1   | 2.59                     | 0.46              |
| 7:S:102:ILE:HA  | 7:S:151:GLY:O    | 2.16                     | 0.46              |
| 5:I:10:DC:H2''  | 5:I:11:DC:C6     | 2.51                     | 0.45              |
| 7:K:54:TYR:CB   | 7:L:195:PHE:HD2  | 2.08                     | 0.45              |
| 7:M:56:PRO:CG   | 7:N:196:ASN:HB3  | 2.41                     | 0.45              |
| 6:J:59:DG:C4    | 6:J:60:DG:N7     | 2.84                     | 0.45              |
| 7:P:125:MET:SD  | 7:P:125:MET:N    | 2.86                     | 0.45              |
| 7:P:294:HIS:O   | 7:Q:193:ARG:HD2  | 2.06                     | 0.45              |
| 7:Q:27:ARG:C    | 7:Q:30:GLN:OE1   | 2.59                     | 0.45              |
| 5:I:122:DC:H1'  | 5:I:123:DA:OP2   | 2.16                     | 0.45              |
| 6:J:29:DC:H2''  | 6:J:30:DG:C8     | 2.52                     | 0.45              |
| 7:N:30:GLN:OE1  | 7:N:30:GLN:N     | 2.47                     | 0.45              |
| 7:O:102:ILE:HA  | 7:O:151:GLY:O    | 2.16                     | 0.45              |
| 7:Q:48:THR:HG23 | 7:Q:254:ARG:CZ   | 2.42                     | 0.45              |
| 7:R:158:MET:SD  | 7:R:210:MET:HE1  | 2.57                     | 0.45              |
| 7:L:250:ARG:HD3 | 7:M:230:THR:HB   | 1.99                     | 0.45              |
| 7:O:158:MET:SD  | 7:O:210:MET:HE1  | 2.57                     | 0.45              |
| 7:Q:191:TYR:CE2 | 7:Q:193:ARG:NH1  | 2.84                     | 0.45              |
| 7:R:47:HIS:CG   | 7:R:47:HIS:O     | 2.70                     | 0.45              |
| 7:R:58:LYS:HZ3  | 7:R:61:ILE:HB    | 1.82                     | 0.45              |
| 3:C:79:ILE:HG12 | 3:C:82:HIS:CE1   | 2.52                     | 0.45              |
| 6:J:84:DC:H2''  | 6:J:85:DG:N7     | 2.31                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 7:L:102:ILE:HA  | 7:L:151:GLY:O   | 2.16                     | 0.45              |
| 7:M:158:MET:SD  | 7:M:210:MET:HE1 | 2.57                     | 0.45              |
| 7:N:27:ARG:C    | 7:N:30:GLN:OE1  | 2.59                     | 0.45              |
| 5:I:81:DC:H2''  | 5:I:82:DG:H8    | 1.80                     | 0.45              |
| 7:Q:125:MET:SD  | 7:Q:125:MET:N   | 2.86                     | 0.45              |
| 7:R:58:LYS:N    | 7:S:195:PHE:CE1 | 2.64                     | 0.45              |
| 3:G:93:LEU:HD23 | 3:G:93:LEU:HA   | 1.81                     | 0.45              |
| 6:J:58:DT:C2    | 6:J:59:DG:N7    | 2.85                     | 0.45              |
| 6:J:131:DG:H2'' | 6:J:132:DG:H8   | 1.82                     | 0.45              |
| 7:K:158:MET:SD  | 7:K:210:MET:HE1 | 2.57                     | 0.45              |
| 7:N:158:MET:SD  | 7:N:210:MET:HE1 | 2.57                     | 0.45              |
| 6:J:41:DC:H2'   | 6:J:42:DT:H71   | 1.98                     | 0.45              |
| 6:J:148:DT:H2'' | 6:J:149:DC:C6   | 2.51                     | 0.45              |
| 7:K:46:PHE:HA   | 7:K:205:TYR:HH  | 1.80                     | 0.45              |
| 7:Q:58:LYS:HA   | 7:Q:58:LYS:CE   | 2.40                     | 0.45              |
| 7:T:47:HIS:CA   | 7:T:254:ARG:NH2 | 2.58                     | 0.45              |
| 6:J:47:DT:H2''  | 6:J:48:DG:H8    | 1.82                     | 0.45              |
| 5:I:35:DC:H2''  | 5:I:36:DG:C8    | 2.52                     | 0.45              |
| 5:I:38:DA:H2''  | 5:I:39:DG:C8    | 2.52                     | 0.45              |
| 5:I:88:DT:H2''  | 5:I:89:DA:N7    | 2.31                     | 0.45              |
| 5:I:100:DG:H1'  | 5:I:101:DG:C8   | 2.52                     | 0.45              |
| 6:J:39:DG:H2'   | 6:J:40:DT:H71   | 1.98                     | 0.45              |
| 6:J:88:DC:H2''  | 6:J:89:DG:C8    | 2.52                     | 0.45              |
| 7:K:54:TYR:CB   | 7:L:195:PHE:CE2 | 3.00                     | 0.45              |
| 7:K:102:ILE:HA  | 7:K:151:GLY:O   | 2.16                     | 0.45              |
| 7:N:58:LYS:HZ3  | 7:N:61:ILE:HB   | 1.82                     | 0.45              |
| 7:N:102:ILE:HA  | 7:N:151:GLY:O   | 2.16                     | 0.45              |
| 7:T:102:ILE:HA  | 7:T:151:GLY:O   | 2.16                     | 0.45              |
| 7:T:158:MET:SD  | 7:T:210:MET:HE1 | 2.57                     | 0.45              |
| 2:F:62:LEU:HD23 | 2:F:62:LEU:HA   | 1.81                     | 0.44              |
| 6:J:50:DA:H2''  | 6:J:51:DA:C8    | 2.52                     | 0.44              |
| 7:P:158:MET:SD  | 7:P:210:MET:HE1 | 2.57                     | 0.44              |
| 7:Q:102:ILE:HA  | 7:Q:151:GLY:O   | 2.16                     | 0.44              |
| 7:T:58:LYS:HZ3  | 7:T:61:ILE:HB   | 1.82                     | 0.44              |
| 5:I:144:DA:C6   | 5:I:145:DA:C6   | 3.06                     | 0.44              |
| 7:O:306:ARG:HD2 | 7:O:306:ARG:N   | 2.33                     | 0.44              |
| 7:T:125:MET:SD  | 7:T:125:MET:N   | 2.86                     | 0.44              |
| 5:I:31:DT:H2''  | 5:I:32:DG:C8    | 2.53                     | 0.44              |
| 6:J:110:DG:C4   | 6:J:111:DC:C5   | 3.05                     | 0.44              |
| 6:J:119:DG:C2   | 6:J:120:DA:C6   | 3.06                     | 0.44              |
| 7:L:58:LYS:HZ3  | 7:L:61:ILE:HB   | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:R:322:GLU:OE1  | 7:S:330:ASN:C    | 2.60                     | 0.44              |
| 7:S:158:MET:SD   | 7:S:210:MET:HE1  | 2.57                     | 0.44              |
| 6:J:47:DT:H2''   | 6:J:48:DG:C8     | 2.51                     | 0.44              |
| 7:N:306:ARG:N    | 7:N:306:ARG:HD2  | 2.33                     | 0.44              |
| 5:I:141:DA:H2''  | 5:I:142:DC:H6    | 1.80                     | 0.44              |
| 7:M:306:ARG:HD2  | 7:M:306:ARG:N    | 2.33                     | 0.44              |
| 7:Q:48:THR:HG23  | 7:Q:254:ARG:HH22 | 1.82                     | 0.44              |
| 7:Q:158:MET:SD   | 7:Q:210:MET:HE1  | 2.57                     | 0.44              |
| 4:H:106:LEU:HD23 | 4:H:106:LEU:HA   | 1.81                     | 0.44              |
| 7:K:306:ARG:HD2  | 7:K:306:ARG:N    | 2.32                     | 0.44              |
| 7:P:102:ILE:HA   | 7:P:151:GLY:O    | 2.16                     | 0.44              |
| 7:Q:54:TYR:CZ    | 7:Q:82:VAL:HG12  | 2.53                     | 0.44              |
| 7:T:158:MET:HG2  | 7:T:216:TYR:CD2  | 2.53                     | 0.44              |
| 7:K:158:MET:HG2  | 7:K:216:TYR:CD2  | 2.53                     | 0.44              |
| 7:P:158:MET:HG2  | 7:P:216:TYR:CD2  | 2.53                     | 0.44              |
| 7:Q:306:ARG:HD2  | 7:Q:306:ARG:N    | 2.33                     | 0.44              |
| 3:C:34:LEU:HD23  | 3:C:34:LEU:HA    | 1.89                     | 0.44              |
| 5:I:79:DC:H1'    | 5:I:80:DC:C5     | 2.53                     | 0.44              |
| 6:J:7:DT:H2''    | 6:J:8:DT:C6      | 2.53                     | 0.44              |
| 7:Q:158:MET:HG2  | 7:Q:216:TYR:CD2  | 2.53                     | 0.44              |
| 5:I:140:DA:H2''  | 5:I:141:DA:C8    | 2.53                     | 0.44              |
| 6:J:57:DT:C2'    | 6:J:58:DT:H71    | 2.47                     | 0.44              |
| 6:J:120:DA:C4    | 6:J:121:DC:C5    | 3.06                     | 0.44              |
| 7:K:54:TYR:CZ    | 7:K:82:VAL:HG12  | 2.53                     | 0.44              |
| 7:M:318:PRO:CA   | 7:N:193:ARG:NH1  | 2.53                     | 0.44              |
| 7:R:158:MET:HG2  | 7:R:216:TYR:CD2  | 2.53                     | 0.44              |
| 3:G:23:LEU:HA    | 3:G:23:LEU:HD23  | 1.79                     | 0.43              |
| 5:I:23:DC:H2''   | 5:I:24:DG:C8     | 2.53                     | 0.43              |
| 7:M:56:PRO:HG3   | 7:N:196:ASN:ND2  | 2.30                     | 0.43              |
| 7:M:318:PRO:HB3  | 7:N:193:ARG:HH11 | 1.60                     | 0.43              |
| 7:N:257:ASP:HB2  | 7:O:195:PHE:CZ   | 2.53                     | 0.43              |
| 7:S:158:MET:HG2  | 7:S:216:TYR:CD2  | 2.53                     | 0.43              |
| 7:S:306:ARG:N    | 7:S:306:ARG:HD2  | 2.33                     | 0.43              |
| 5:I:109:DC:H2''  | 5:I:110:DC:C5    | 2.53                     | 0.43              |
| 5:I:145:DA:C2    | 5:I:146:DA:C2    | 3.06                     | 0.43              |
| 7:Q:47:HIS:HD2   | 7:Q:254:ARG:NE   | 2.12                     | 0.43              |
| 7:R:210:MET:SD   | 7:R:216:TYR:CE1  | 3.12                     | 0.43              |
| 3:C:26:PRO:HG3   | 4:D:40:TYR:CE2   | 2.53                     | 0.43              |
| 5:I:39:DG:H1'    | 5:I:40:DA:C8     | 2.53                     | 0.43              |
| 6:J:99:DG:C4     | 6:J:100:DC:C5    | 3.06                     | 0.43              |
| 7:M:158:MET:HG2  | 7:M:216:TYR:CD2  | 2.53                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:K:199:HIS:HB3 | 7:T:56:PRO:HG2   | 1.96                     | 0.43              |
| 7:L:39:LYS:HD3  | 7:L:39:LYS:HA    | 1.79                     | 0.43              |
| 7:L:125:MET:SD  | 7:L:125:MET:N    | 2.86                     | 0.43              |
| 7:M:318:PRO:C   | 7:N:193:ARG:NH1  | 2.72                     | 0.43              |
| 7:P:210:MET:SD  | 7:P:216:TYR:CE1  | 3.12                     | 0.43              |
| 7:Q:47:HIS:HD2  | 7:Q:254:ARG:CD   | 2.30                     | 0.43              |
| 7:R:54:TYR:CZ   | 7:R:82:VAL:HG12  | 2.53                     | 0.43              |
| 7:R:320:LEU:O   | 7:S:331:ALA:HB1  | 2.14                     | 0.43              |
| 7:T:306:ARG:HD2 | 7:T:306:ARG:N    | 2.33                     | 0.43              |
| 6:J:20:DT:H2'   | 6:J:21:DT:H71    | 2.00                     | 0.43              |
| 7:N:210:MET:SD  | 7:N:216:TYR:CE1  | 3.12                     | 0.43              |
| 7:O:158:MET:HG2 | 7:O:216:TYR:CD2  | 2.53                     | 0.43              |
| 7:Q:210:MET:SD  | 7:Q:216:TYR:CE1  | 3.12                     | 0.43              |
| 7:S:293:ALA:O   | 7:T:167:ARG:NH1  | 2.52                     | 0.43              |
| 7:S:294:HIS:HA  | 7:T:167:ARG:NH1  | 2.33                     | 0.43              |
| 7:T:54:TYR:CZ   | 7:T:82:VAL:HG12  | 2.53                     | 0.43              |
| 6:J:22:DT:H2''  | 6:J:23:DC:C6     | 2.54                     | 0.43              |
| 6:J:139:DC:H2'' | 6:J:140:DA:H8    | 1.83                     | 0.43              |
| 7:P:306:ARG:N   | 7:P:306:ARG:HD2  | 2.32                     | 0.43              |
| 3:C:63:LEU:HD23 | 3:C:63:LEU:HA    | 1.85                     | 0.43              |
| 6:J:59:DG:H2''  | 6:J:60:DG:H8     | 1.84                     | 0.43              |
| 6:J:116:DT:H2'' | 6:J:117:DA:N7    | 2.34                     | 0.43              |
| 7:K:210:MET:SD  | 7:K:216:TYR:CE1  | 3.12                     | 0.43              |
| 7:N:56:PRO:CG   | 7:O:199:HIS:CB   | 2.86                     | 0.43              |
| 7:S:161:ASP:OD2 | 7:S:164:GLY:N    | 2.43                     | 0.43              |
| 7:S:210:MET:SD  | 7:S:216:TYR:CE1  | 3.12                     | 0.43              |
| 7:T:210:MET:SD  | 7:T:216:TYR:CE1  | 3.12                     | 0.43              |
| 5:I:136:DA:C6   | 5:I:137:DA:C6    | 3.07                     | 0.43              |
| 6:J:140:DA:H2'' | 6:J:141:DC:C6    | 2.54                     | 0.43              |
| 7:K:30:GLN:OE1  | 7:K:30:GLN:N     | 2.46                     | 0.43              |
| 7:N:158:MET:HG2 | 7:N:216:TYR:CD2  | 2.53                     | 0.43              |
| 3:C:23:LEU:HD23 | 3:C:23:LEU:HA    | 1.81                     | 0.43              |
| 5:I:80:DC:H2''  | 5:I:81:DC:C5     | 2.54                     | 0.43              |
| 6:J:135:DT:H2'' | 6:J:136:DC:C5    | 2.54                     | 0.43              |
| 7:L:306:ARG:HD2 | 7:L:306:ARG:N    | 2.33                     | 0.43              |
| 7:O:210:MET:SD  | 7:O:216:TYR:CE1  | 3.12                     | 0.43              |
| 2:F:17:ARG:O    | 5:I:51:DA:H5''   | 2.19                     | 0.43              |
| 6:J:98:DA:H2''  | 6:J:99:DG:H8     | 1.84                     | 0.43              |
| 7:L:27:ARG:HA   | 7:L:30:GLN:OE1   | 2.18                     | 0.43              |
| 7:L:211:MET:HE2 | 7:L:216:TYR:CD1  | 2.54                     | 0.43              |
| 7:T:157:ALA:HB3 | 7:T:189:VAL:HG22 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:72:DC:H2''   | 6:J:73:DG:C8     | 2.54                     | 0.42              |
| 7:M:157:ALA:HB3  | 7:M:189:VAL:HG22 | 2.01                     | 0.42              |
| 7:O:117:ILE:CD1  | 7:O:123:THR:HG21 | 2.49                     | 0.42              |
| 7:O:313:LYS:HG3  | 7:O:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:P:313:LYS:HG3  | 7:P:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:R:157:ALA:HB3  | 7:R:189:VAL:HG22 | 2.01                     | 0.42              |
| 7:R:161:ASP:OD2  | 7:R:164:GLY:N    | 2.43                     | 0.42              |
| 7:T:313:LYS:HG3  | 7:T:324:GLU:HG2  | 2.01                     | 0.42              |
| 5:I:88:DT:H2''   | 5:I:89:DA:C8     | 2.54                     | 0.42              |
| 5:I:127:DG:H2''  | 5:I:128:DA:C8    | 2.54                     | 0.42              |
| 7:M:210:MET:SD   | 7:M:216:TYR:CE1  | 3.12                     | 0.42              |
| 7:P:117:ILE:CD1  | 7:P:123:THR:HG21 | 2.49                     | 0.42              |
| 7:R:306:ARG:HD2  | 7:R:306:ARG:N    | 2.33                     | 0.42              |
| 3:G:37:GLY:HA3   | 3:G:39:TYR:CE2   | 2.54                     | 0.42              |
| 5:I:129:DC:H2''  | 5:I:130:DA:N7    | 2.34                     | 0.42              |
| 7:K:157:ALA:HB3  | 7:K:189:VAL:HG22 | 2.01                     | 0.42              |
| 7:M:313:LYS:HG3  | 7:M:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:N:157:ALA:HB3  | 7:N:189:VAL:HG22 | 2.01                     | 0.42              |
| 7:R:117:ILE:CD1  | 7:R:123:THR:HG21 | 2.49                     | 0.42              |
| 1:A:100:LEU:HD23 | 1:A:100:LEU:HA   | 1.86                     | 0.42              |
| 5:I:67:DT:H2''   | 5:I:68:DA:N7     | 2.34                     | 0.42              |
| 6:J:36:DG:H2''   | 6:J:37:DG:C8     | 2.54                     | 0.42              |
| 7:K:117:ILE:CD1  | 7:K:123:THR:HG21 | 2.49                     | 0.42              |
| 7:L:158:MET:HG2  | 7:L:216:TYR:CD2  | 2.53                     | 0.42              |
| 7:O:157:ALA:HB3  | 7:O:189:VAL:HG22 | 2.01                     | 0.42              |
| 7:T:117:ILE:CD1  | 7:T:123:THR:HG21 | 2.49                     | 0.42              |
| 5:I:8:DT:H2''    | 5:I:9:DC:C6      | 2.54                     | 0.42              |
| 6:J:104:DG:H5'   | 6:J:104:DG:C8    | 2.54                     | 0.42              |
| 7:K:199:HIS:HB2  | 7:T:56:PRO:CB    | 2.32                     | 0.42              |
| 7:K:294:HIS:HE1  | 7:L:162:THR:O    | 2.03                     | 0.42              |
| 7:L:313:LYS:HG3  | 7:L:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:N:313:LYS:HG3  | 7:N:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:Q:117:ILE:CD1  | 7:Q:123:THR:HG21 | 2.49                     | 0.42              |
| 7:R:318:PRO:O    | 7:S:173:ALA:HB2  | 2.19                     | 0.42              |
| 7:S:157:ALA:HB3  | 7:S:189:VAL:HG22 | 2.01                     | 0.42              |
| 7:T:161:ASP:OD2  | 7:T:164:GLY:N    | 2.43                     | 0.42              |
| 6:J:90:DT:H2''   | 6:J:91:DG:H8     | 1.83                     | 0.42              |
| 6:J:137:DG:H2''  | 6:J:138:DG:N7    | 2.34                     | 0.42              |
| 6:J:147:DT:H2'   | 6:J:148:DT:H71   | 2.02                     | 0.42              |
| 7:R:313:LYS:HG3  | 7:R:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:S:117:ILE:CD1  | 7:S:123:THR:HG21 | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:110:DC:H1'   | 5:I:111:DA:C8    | 2.54                     | 0.42              |
| 5:I:153:DA:OP1   | 7:R:233:SER:HB3  | 2.19                     | 0.42              |
| 7:N:238:LEU:O    | 7:N:241:ARG:HG2  | 2.20                     | 0.42              |
| 7:Q:167:ARG:CG   | 7:Q:170:ARG:HG2  | 2.50                     | 0.42              |
| 7:S:313:LYS:HG3  | 7:S:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:T:58:LYS:HE2   | 7:T:58:LYS:CA    | 2.45                     | 0.42              |
| 4:D:38:SER:HA    | 4:D:59:MET:SD    | 2.60                     | 0.42              |
| 4:D:106:LEU:HA   | 4:D:106:LEU:HD12 | 1.71                     | 0.42              |
| 2:F:22:LEU:HB3   | 2:F:25:ASN:ND2   | 2.35                     | 0.42              |
| 4:H:34:LYS:HD2   | 4:H:34:LYS:HA    | 1.82                     | 0.42              |
| 6:J:75:DG:H2''   | 6:J:76:DG:C8     | 2.55                     | 0.42              |
| 7:K:195:PHE:HB2  | 7:T:55:ALA:HA    | 2.00                     | 0.42              |
| 7:K:313:LYS:HG3  | 7:K:324:GLU:HG2  | 2.01                     | 0.42              |
| 7:N:117:ILE:CD1  | 7:N:123:THR:HG21 | 2.49                     | 0.42              |
| 7:O:238:LEU:O    | 7:O:241:ARG:HG2  | 2.20                     | 0.42              |
| 7:S:294:HIS:HA   | 7:T:167:ARG:HH11 | 1.85                     | 0.42              |
| 7:K:130:ARG:HH11 | 7:T:299:ARG:HH12 | 1.67                     | 0.42              |
| 7:L:117:ILE:CD1  | 7:L:123:THR:HG21 | 2.49                     | 0.42              |
| 7:M:117:ILE:CD1  | 7:M:123:THR:HG21 | 2.49                     | 0.42              |
| 7:P:319:CYS:CB   | 7:Q:169:GLU:H    | 2.25                     | 0.42              |
| 7:Q:157:ALA:HB3  | 7:Q:189:VAL:HG22 | 2.01                     | 0.42              |
| 5:I:27:DC:H1'    | 5:I:28:DA:C5     | 2.55                     | 0.42              |
| 6:J:42:DT:H2'    | 6:J:43:DT:C5     | 2.55                     | 0.42              |
| 6:J:151:DG:H2''  | 6:J:152:DA:C8    | 2.55                     | 0.42              |
| 7:Q:293:ALA:CA   | 7:R:195:PHE:CZ   | 2.98                     | 0.42              |
| 7:T:39:LYS:HD3   | 7:T:39:LYS:HA    | 1.79                     | 0.42              |
| 7:T:238:LEU:O    | 7:T:241:ARG:HG2  | 2.20                     | 0.42              |
| 3:C:15:LYS:HE2   | 3:C:19:SER:HB2   | 2.02                     | 0.41              |
| 5:I:5:DG:H2''    | 5:I:6:DA:C8      | 2.55                     | 0.41              |
| 5:I:78:DC:H2''   | 5:I:79:DC:C5     | 2.55                     | 0.41              |
| 5:I:152:DC:N3    | 5:I:153:DA:N6    | 2.67                     | 0.41              |
| 6:J:134:DC:H2''  | 6:J:135:DT:C6    | 2.55                     | 0.41              |
| 7:K:245:LEU:O    | 7:K:249:LEU:HG   | 2.21                     | 0.41              |
| 7:L:157:ALA:HB3  | 7:L:189:VAL:HG22 | 2.01                     | 0.41              |
| 1:A:82:LEU:HD23  | 1:A:82:LEU:HA    | 1.86                     | 0.41              |
| 6:J:39:DG:C2'    | 6:J:40:DT:H71    | 2.49                     | 0.41              |
| 7:K:195:PHE:CG   | 7:T:55:ALA:HA    | 2.50                     | 0.41              |
| 7:L:161:ASP:OD2  | 7:L:164:GLY:N    | 2.43                     | 0.41              |
| 7:Q:313:LYS:HG3  | 7:Q:324:GLU:HG2  | 2.02                     | 0.41              |
| 7:S:245:LEU:O    | 7:S:249:LEU:HG   | 2.21                     | 0.41              |
| 5:I:46:DC:H2''   | 5:I:47:DT:H71    | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:11:DC:C2     | 6:J:12:DG:C5     | 3.07                     | 0.41              |
| 6:J:38:DT:H2''   | 6:J:39:DG:H8     | 1.86                     | 0.41              |
| 7:K:45:GLY:O     | 7:K:205:TYR:OH   | 2.35                     | 0.41              |
| 7:L:49:VAL:HG11  | 7:L:81:LEU:HB2   | 2.02                     | 0.41              |
| 7:L:54:TYR:HB2   | 7:M:195:PHE:HB3  | 1.70                     | 0.41              |
| 7:N:245:LEU:O    | 7:N:249:LEU:HG   | 2.21                     | 0.41              |
| 7:O:161:ASP:OD2  | 7:O:164:GLY:N    | 2.43                     | 0.41              |
| 7:P:157:ALA:HB3  | 7:P:189:VAL:HG22 | 2.01                     | 0.41              |
| 7:Q:146:LEU:HD21 | 7:Q:178:TYR:HB3  | 2.02                     | 0.41              |
| 7:R:245:LEU:O    | 7:R:249:LEU:HG   | 2.21                     | 0.41              |
| 7:S:238:LEU:O    | 7:S:241:ARG:HG2  | 2.20                     | 0.41              |
| 1:A:60:LEU:HD12  | 1:A:64:LYS:HE2   | 2.02                     | 0.41              |
| 6:J:89:DG:C2'    | 6:J:90:DT:H71    | 2.51                     | 0.41              |
| 7:K:146:LEU:HD21 | 7:K:178:TYR:HB3  | 2.02                     | 0.41              |
| 7:M:146:LEU:HD21 | 7:M:178:TYR:HB3  | 2.02                     | 0.41              |
| 7:O:245:LEU:O    | 7:O:249:LEU:HG   | 2.21                     | 0.41              |
| 7:P:238:LEU:O    | 7:P:241:ARG:HG2  | 2.20                     | 0.41              |
| 7:Q:48:THR:HG23  | 7:Q:254:ARG:NH2  | 2.35                     | 0.41              |
| 7:Q:161:ASP:OD2  | 7:Q:164:GLY:N    | 2.43                     | 0.41              |
| 7:R:238:LEU:O    | 7:R:241:ARG:HG2  | 2.20                     | 0.41              |
| 5:I:140:DA:H2''  | 5:I:141:DA:H8    | 1.85                     | 0.41              |
| 6:J:102:DG:H2'   | 6:J:103:DT:H71   | 2.01                     | 0.41              |
| 7:M:49:VAL:HG11  | 7:M:81:LEU:HB2   | 2.02                     | 0.41              |
| 7:P:318:PRO:HG2  | 7:Q:166:PHE:HB3  | 2.02                     | 0.41              |
| 7:Q:167:ARG:HG2  | 7:Q:170:ARG:H    | 1.85                     | 0.41              |
| 7:R:146:LEU:HD21 | 7:R:178:TYR:HB3  | 2.02                     | 0.41              |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:HA   | 1.88                     | 0.41              |
| 5:I:24:DG:H2''   | 5:I:25:DC:C6     | 2.56                     | 0.41              |
| 5:I:70:DG:C2     | 6:J:85:DG:N2     | 2.89                     | 0.41              |
| 7:L:245:LEU:O    | 7:L:249:LEU:HG   | 2.20                     | 0.41              |
| 7:N:58:LYS:HE2   | 7:N:58:LYS:CA    | 2.45                     | 0.41              |
| 2:F:31:LYS:HG3   | 2:F:51:TYR:CE1   | 2.55                     | 0.41              |
| 5:I:47:DT:C4     | 5:I:48:DA:C6     | 3.09                     | 0.41              |
| 6:J:29:DC:C2     | 6:J:30:DG:N7     | 2.89                     | 0.41              |
| 6:J:107:DA:H2''  | 6:J:108:DG:C8    | 2.56                     | 0.41              |
| 7:O:161:ASP:O    | 7:O:193:ARG:HG3  | 2.21                     | 0.41              |
| 7:R:58:LYS:HE2   | 7:R:58:LYS:CA    | 2.45                     | 0.41              |
| 7:T:30:GLN:OE1   | 7:T:30:GLN:N     | 2.47                     | 0.41              |
| 7:T:146:LEU:HD21 | 7:T:178:TYR:HB3  | 2.02                     | 0.41              |
| 5:I:3:DC:H2''    | 5:I:4:DA:C8      | 2.56                     | 0.41              |
| 7:K:238:LEU:O    | 7:K:241:ARG:HG2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:L:238:LEU:O    | 7:L:241:ARG:HG2  | 2.20                     | 0.41              |
| 7:N:161:ASP:O    | 7:N:193:ARG:HG3  | 2.21                     | 0.41              |
| 7:P:146:LEU:HD21 | 7:P:178:TYR:HB3  | 2.02                     | 0.41              |
| 7:P:319:CYS:CB   | 7:Q:168:PRO:N    | 2.76                     | 0.41              |
| 7:T:196:ASN:CA   | 7:T:227:LEU:HD13 | 2.51                     | 0.41              |
| 4:H:39:ILE:HD11  | 4:H:40:TYR:CZ    | 2.56                     | 0.41              |
| 6:J:49:DT:C2     | 6:J:50:DA:N7     | 2.89                     | 0.41              |
| 6:J:68:DA:C2     | 6:J:69:DA:C4     | 3.09                     | 0.41              |
| 6:J:113:DG:H1'   | 6:J:114:DT:H5'   | 2.03                     | 0.41              |
| 7:K:208:SER:O    | 7:K:212:VAL:HG23 | 2.21                     | 0.41              |
| 7:M:156:LYS:HB2  | 7:M:216:TYR:CD2  | 2.56                     | 0.41              |
| 7:M:161:ASP:O    | 7:M:193:ARG:HG3  | 2.21                     | 0.41              |
| 7:M:238:LEU:O    | 7:M:241:ARG:HG2  | 2.20                     | 0.41              |
| 7:M:244:HIS:CE1  | 7:M:247:ARG:HH22 | 2.39                     | 0.41              |
| 7:Q:245:LEU:O    | 7:Q:249:LEU:HG   | 2.21                     | 0.41              |
| 6:J:38:DT:H2''   | 6:J:39:DG:C8     | 2.56                     | 0.41              |
| 6:J:123:DA:H2''  | 6:J:124:DA:C8    | 2.56                     | 0.41              |
| 7:L:56:PRO:HG3   | 7:M:196:ASN:CG   | 2.46                     | 0.41              |
| 7:L:161:ASP:O    | 7:L:193:ARG:HG3  | 2.21                     | 0.41              |
| 7:R:156:LYS:HB2  | 7:R:216:TYR:CD2  | 2.56                     | 0.41              |
| 7:T:161:ASP:O    | 7:T:193:ARG:HG3  | 2.21                     | 0.41              |
| 3:C:37:GLY:HA3   | 3:C:39:TYR:CE2   | 2.57                     | 0.40              |
| 5:I:74:DT:H2''   | 5:I:75:DG:C8     | 2.56                     | 0.40              |
| 6:J:14:DT:H1'    | 6:J:15:DG:C8     | 2.56                     | 0.40              |
| 6:J:74:DG:H2''   | 6:J:75:DG:C8     | 2.56                     | 0.40              |
| 7:P:196:ASN:CA   | 7:P:227:LEU:HD13 | 2.51                     | 0.40              |
| 7:P:208:SER:O    | 7:P:212:VAL:HG23 | 2.21                     | 0.40              |
| 7:Q:238:LEU:O    | 7:Q:241:ARG:HG2  | 2.20                     | 0.40              |
| 7:R:196:ASN:CA   | 7:R:227:LEU:HD13 | 2.51                     | 0.40              |
| 3:G:76:THR:N     | 6:J:139:DC:OP1   | 2.53                     | 0.40              |
| 6:J:122:DC:H2''  | 6:J:123:DA:C8    | 2.56                     | 0.40              |
| 7:O:208:SER:O    | 7:O:212:VAL:HG23 | 2.21                     | 0.40              |
| 7:Q:208:SER:O    | 7:Q:212:VAL:HG23 | 2.21                     | 0.40              |
| 7:R:161:ASP:O    | 7:R:193:ARG:HG3  | 2.21                     | 0.40              |
| 7:K:54:TYR:CZ    | 7:K:82:VAL:HG11  | 2.56                     | 0.40              |
| 7:K:161:ASP:O    | 7:K:193:ARG:HG3  | 2.21                     | 0.40              |
| 7:K:167:ARG:HH12 | 7:T:294:HIS:C    | 2.11                     | 0.40              |
| 7:N:208:SER:O    | 7:N:212:VAL:HG23 | 2.21                     | 0.40              |
| 7:N:210:MET:SD   | 7:N:210:MET:C    | 3.05                     | 0.40              |
| 7:O:196:ASN:CA   | 7:O:227:LEU:HD13 | 2.51                     | 0.40              |
| 7:P:245:LEU:O    | 7:P:249:LEU:HG   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:R:210:MET:SD   | 7:R:210:MET:C    | 3.05                     | 0.40              |
| 7:S:146:LEU:HD21 | 7:S:178:TYR:HB3  | 2.02                     | 0.40              |
| 7:S:156:LYS:HB2  | 7:S:216:TYR:CD2  | 2.56                     | 0.40              |
| 7:S:339:ASP:N    | 7:S:339:ASP:OD1  | 2.54                     | 0.40              |
| 5:I:99:DG:C2     | 5:I:100:DG:C2    | 3.09                     | 0.40              |
| 5:I:130:DA:H2''  | 5:I:131:DG:H8    | 1.87                     | 0.40              |
| 7:L:158:MET:SD   | 7:L:210:MET:HE1  | 2.62                     | 0.40              |
| 7:M:196:ASN:CA   | 7:M:227:LEU:HD13 | 2.51                     | 0.40              |
| 7:N:156:LYS:HB2  | 7:N:216:TYR:CD2  | 2.56                     | 0.40              |
| 7:N:196:ASN:CA   | 7:N:227:LEU:HD13 | 2.51                     | 0.40              |
| 7:Q:54:TYR:CZ    | 7:Q:82:VAL:HG11  | 2.56                     | 0.40              |
| 7:Q:156:LYS:HB2  | 7:Q:216:TYR:CD2  | 2.56                     | 0.40              |
| 7:Q:210:MET:SD   | 7:Q:210:MET:C    | 3.05                     | 0.40              |
| 7:R:208:SER:O    | 7:R:212:VAL:HG23 | 2.21                     | 0.40              |
| 7:S:161:ASP:O    | 7:S:193:ARG:HG3  | 2.21                     | 0.40              |
| 7:T:208:SER:O    | 7:T:212:VAL:HG23 | 2.21                     | 0.40              |
| 7:T:245:LEU:O    | 7:T:249:LEU:HG   | 2.21                     | 0.40              |
| 6:J:15:DG:C2'    | 6:J:16:DT:H71    | 2.51                     | 0.40              |
| 7:M:210:MET:SD   | 7:M:210:MET:C    | 3.05                     | 0.40              |
| 7:O:146:LEU:HD21 | 7:O:178:TYR:HB3  | 2.02                     | 0.40              |
| 7:O:156:LYS:HB2  | 7:O:216:TYR:CD2  | 2.56                     | 0.40              |
| 7:P:156:LYS:HB2  | 7:P:216:TYR:CD2  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed     | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 94/139 (68%) | 94 (100%) | 0       | 0        | 100         | 100 |
| 1   | E     | 97/139 (70%) | 97 (100%) | 0       | 0        | 100         | 100 |
| 2   | B     | 75/106 (71%) | 73 (97%)  | 2 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 2   | F     | 85/106 (80%)    | 82 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 3   | C     | 106/133 (80%)   | 104 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 3   | G     | 102/133 (77%)   | 100 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 4   | D     | 90/129 (70%)    | 89 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 4   | H     | 89/129 (69%)    | 88 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 7   | K     | 277/342 (81%)   | 275 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | L     | 277/342 (81%)   | 274 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 7   | M     | 277/342 (81%)   | 274 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 7   | N     | 277/342 (81%)   | 275 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | O     | 217/342 (64%)   | 215 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | P     | 217/342 (64%)   | 215 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | Q     | 277/342 (81%)   | 275 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | R     | 277/342 (81%)   | 275 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | S     | 217/342 (64%)   | 215 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 7   | T     | 277/342 (81%)   | 275 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| All | All   | 3328/4434 (75%) | 3295 (99%) | 33 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | A     | 84/113 (74%) | 84 (100%) | 0        | 100         | 100 |
| 1   | E     | 87/113 (77%) | 86 (99%)  | 1 (1%)   | 65          | 73  |
| 2   | B     | 63/81 (78%)  | 63 (100%) | 0        | 100         | 100 |
| 2   | F     | 72/81 (89%)  | 72 (100%) | 0        | 100         | 100 |
| 3   | C     | 85/102 (83%) | 85 (100%) | 0        | 100         | 100 |
| 3   | G     | 83/102 (81%) | 83 (100%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 4   | D     | 79/107 (74%)    | 79 (100%)   | 0        | 100         | 100 |
| 4   | H     | 78/107 (73%)    | 77 (99%)    | 1 (1%)   | 61          | 71  |
| 7   | K     | 225/271 (83%)   | 225 (100%)  | 0        | 100         | 100 |
| 7   | L     | 225/271 (83%)   | 224 (100%)  | 1 (0%)   | 84          | 82  |
| 7   | M     | 225/271 (83%)   | 224 (100%)  | 1 (0%)   | 84          | 82  |
| 7   | N     | 225/271 (83%)   | 225 (100%)  | 0        | 100         | 100 |
| 7   | O     | 177/271 (65%)   | 177 (100%)  | 0        | 100         | 100 |
| 7   | P     | 177/271 (65%)   | 177 (100%)  | 0        | 100         | 100 |
| 7   | Q     | 225/271 (83%)   | 225 (100%)  | 0        | 100         | 100 |
| 7   | R     | 225/271 (83%)   | 225 (100%)  | 0        | 100         | 100 |
| 7   | S     | 177/271 (65%)   | 177 (100%)  | 0        | 100         | 100 |
| 7   | T     | 225/271 (83%)   | 225 (100%)  | 0        | 100         | 100 |
| All | All   | 2737/3516 (78%) | 2733 (100%) | 4 (0%)   | 87          | 88  |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 76  | GLN  |
| 4   | H     | 101 | LEU  |
| 7   | L     | 211 | MET  |
| 7   | M     | 119 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | HIS  |
| 1   | A     | 68  | GLN  |
| 3   | C     | 24  | GLN  |
| 3   | G     | 94  | ASN  |
| 4   | H     | 49  | HIS  |
| 7   | K     | 23  | GLN  |
| 7   | K     | 294 | HIS  |
| 7   | M     | 47  | HIS  |
| 7   | M     | 244 | HIS  |
| 7   | N     | 23  | GLN  |
| 7   | N     | 47  | HIS  |
| 7   | O     | 268 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Q     | 23  | GLN  |
| 7   | Q     | 47  | HIS  |
| 7   | R     | 23  | GLN  |
| 7   | R     | 294 | HIS  |
| 7   | T     | 23  | GLN  |
| 7   | T     | 294 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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.

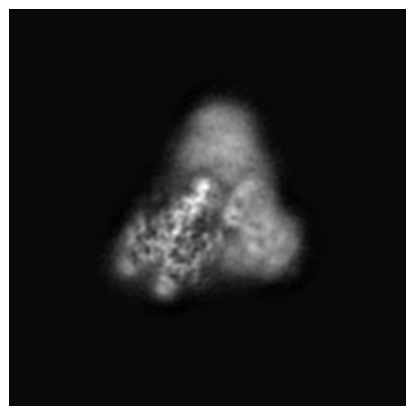
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38229. These allow visual inspection of the internal detail of the map and identification of artifacts.

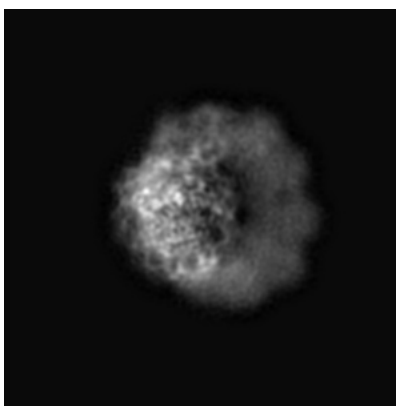
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

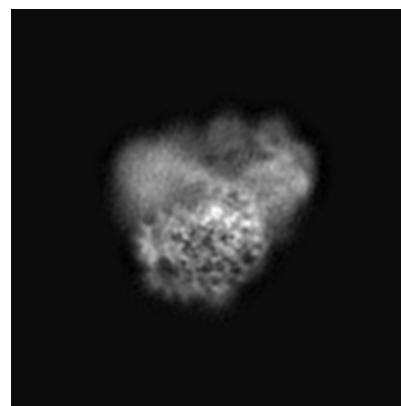
#### 6.1.1 Primary map



X

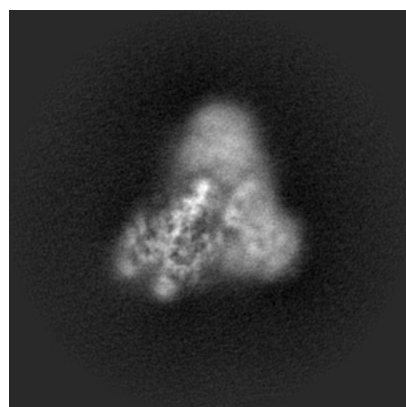


Y

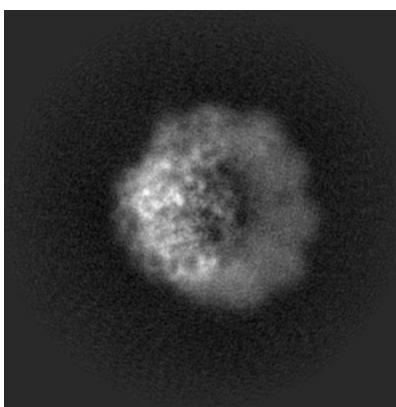


Z

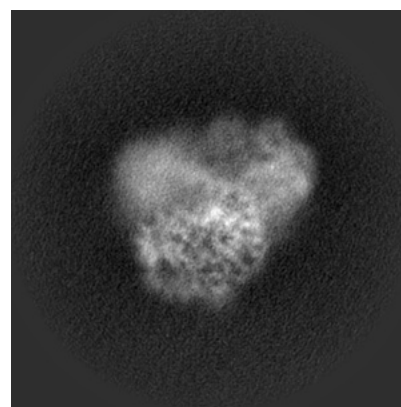
#### 6.1.2 Raw map



X



Y

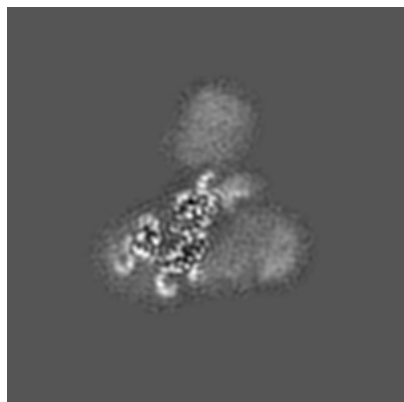


Z

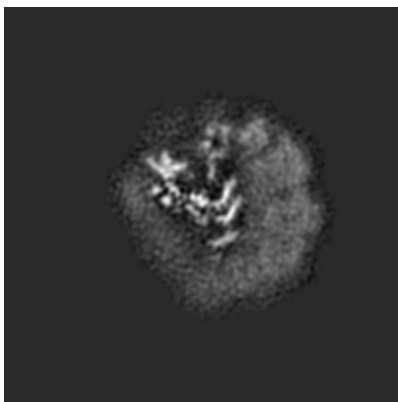
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

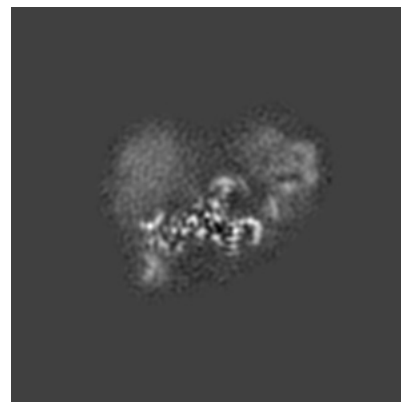
### 6.2.1 Primary map



X Index: 140

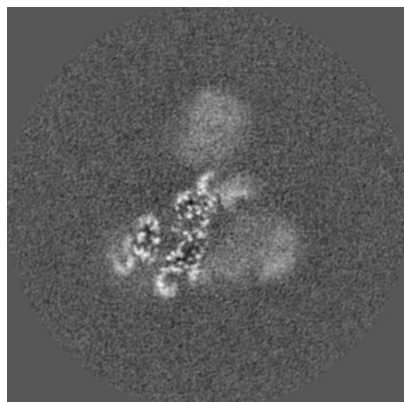


Y Index: 140

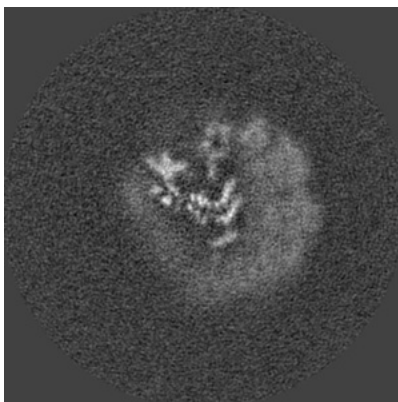


Z Index: 140

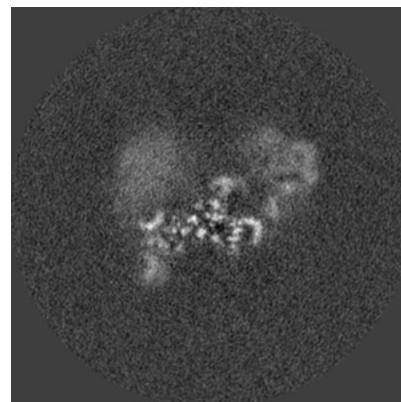
### 6.2.2 Raw map



X Index: 140



Y Index: 140

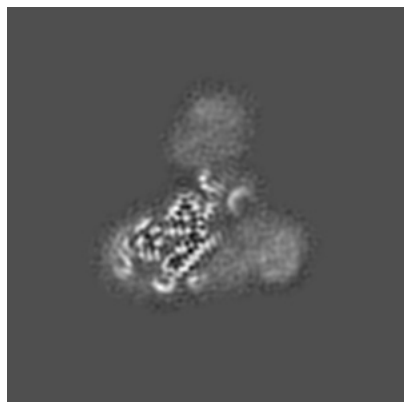


Z Index: 140

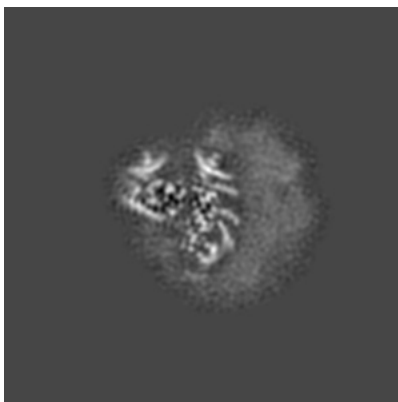
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 144

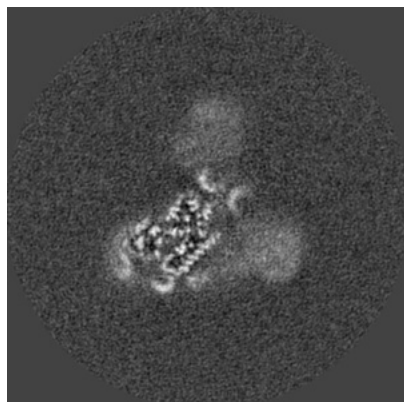


Y Index: 130

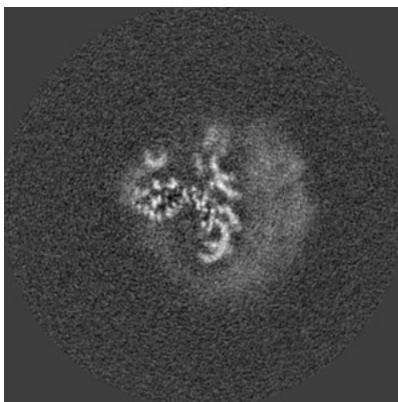


Z Index: 114

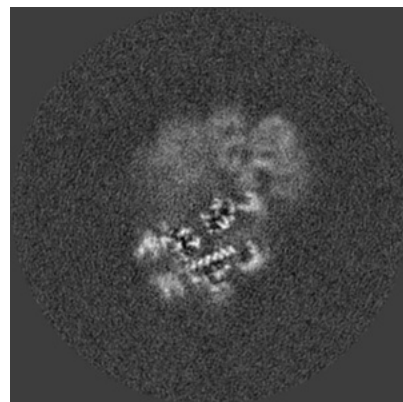
### 6.3.2 Raw map



X Index: 145



Y Index: 133

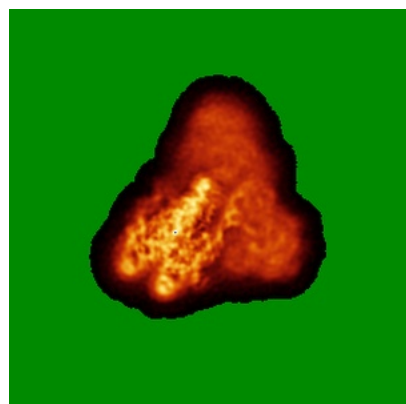


Z Index: 114

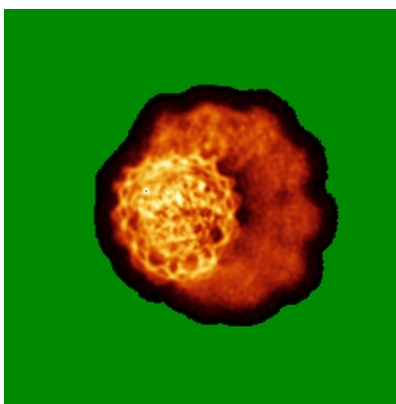
The images above show the largest variance slices of the map in three orthogonal directions.

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

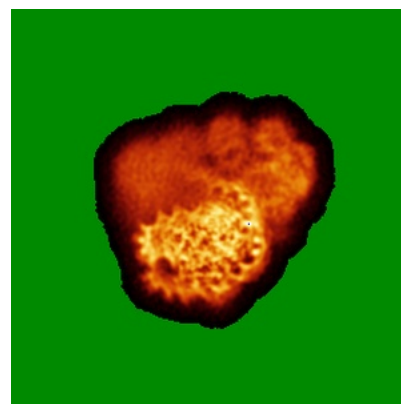
### 6.4.1 Primary map



X

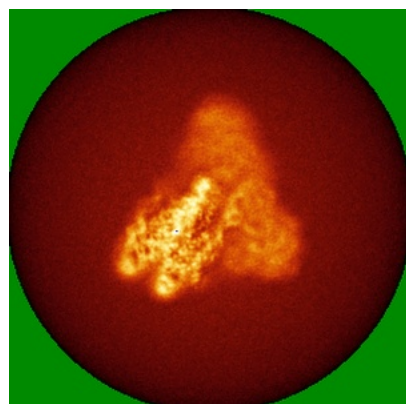


Y

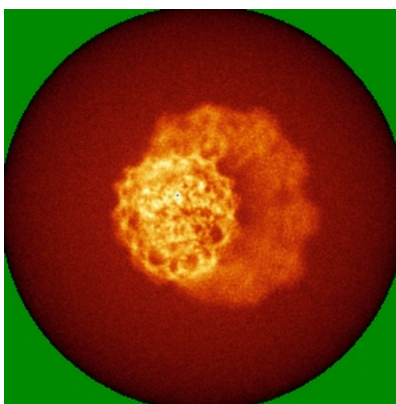


Z

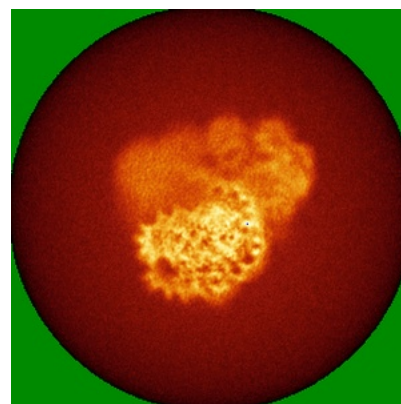
### 6.4.2 Raw map



X



Y

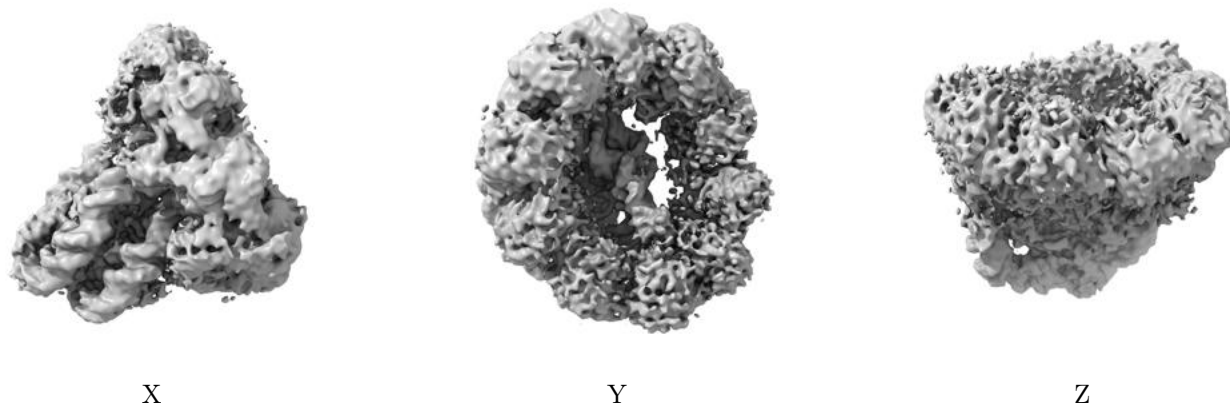


Z

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

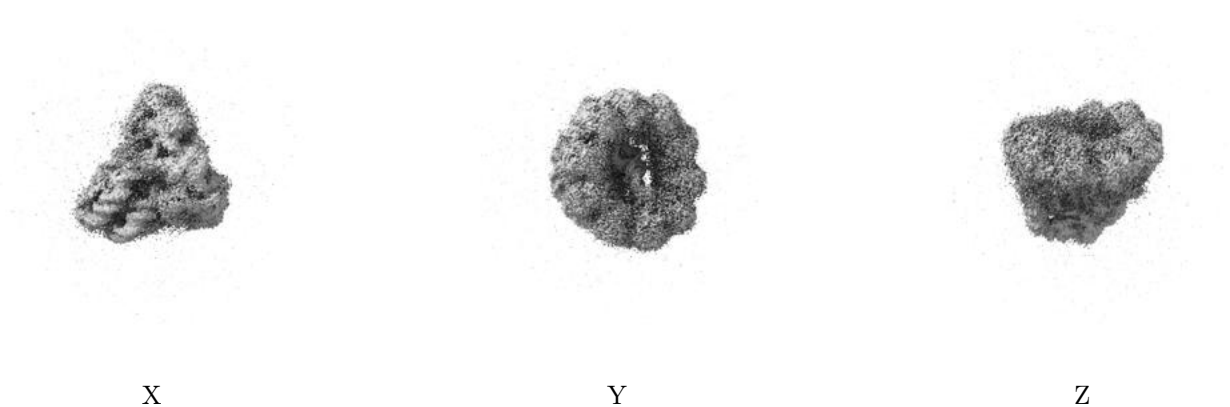
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0042. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

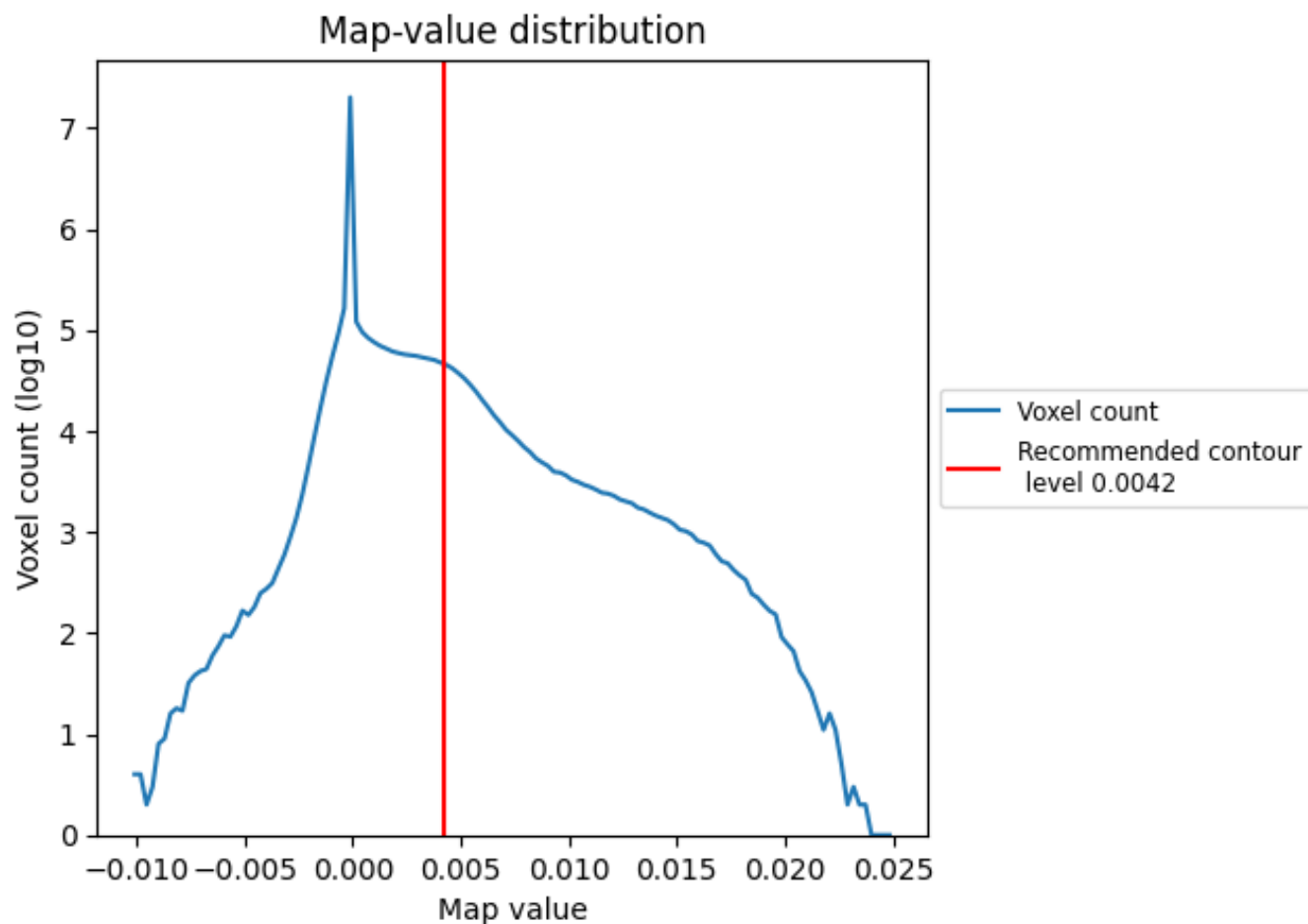
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

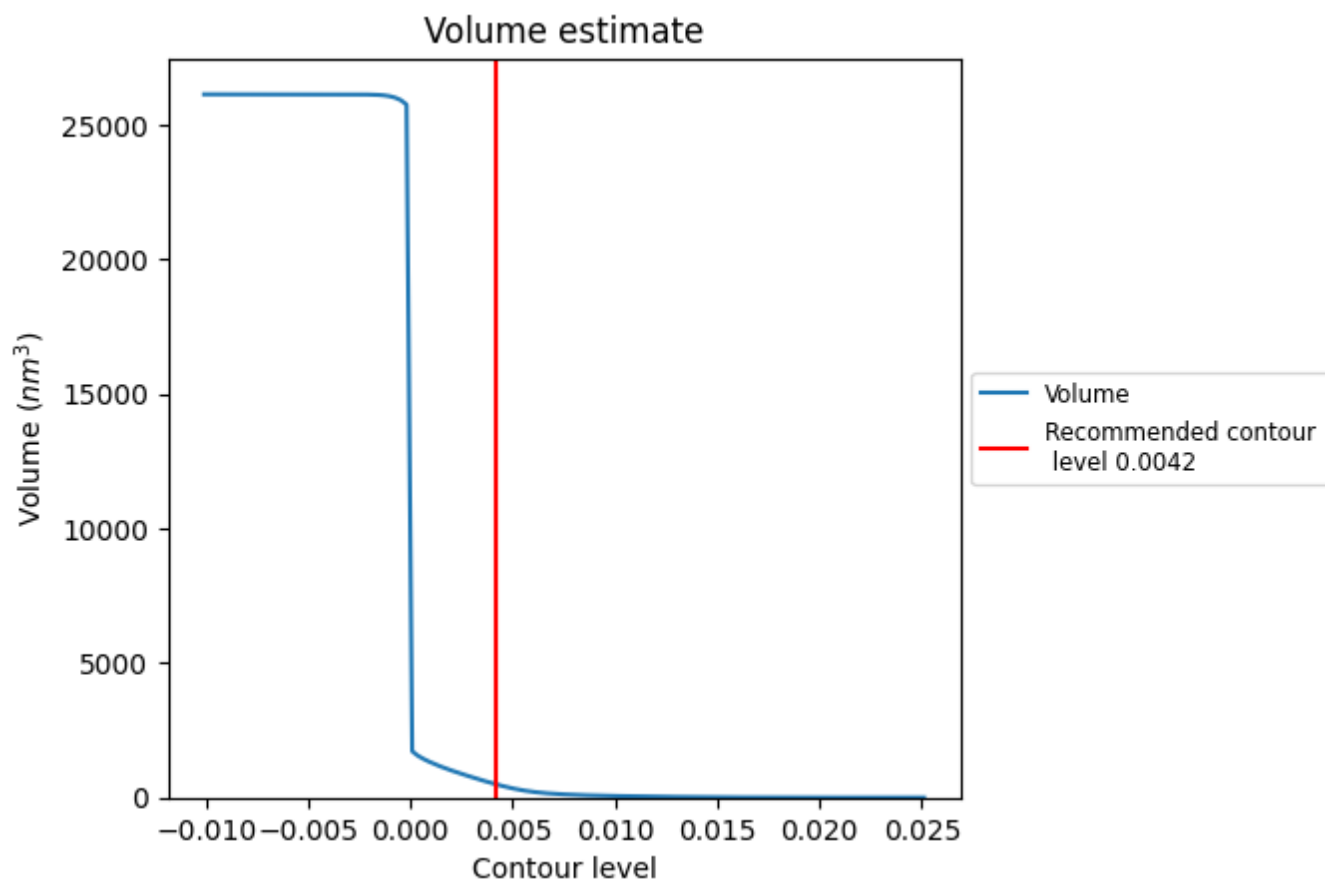
This section contains the results of statistical analysis of the map.

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



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

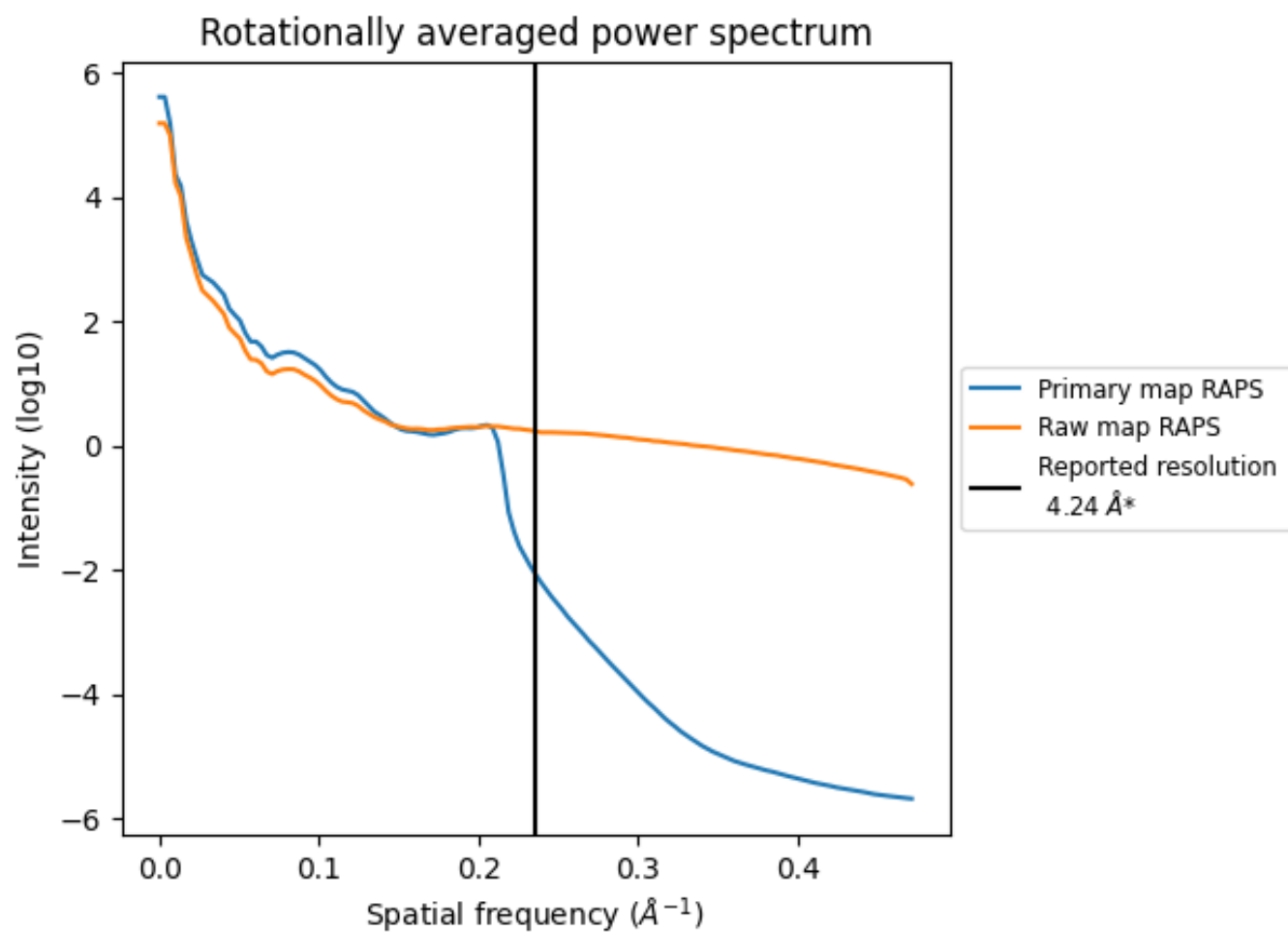
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489  $\text{nm}^3$ ; this corresponds to an approximate mass of 442 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 ⓘ

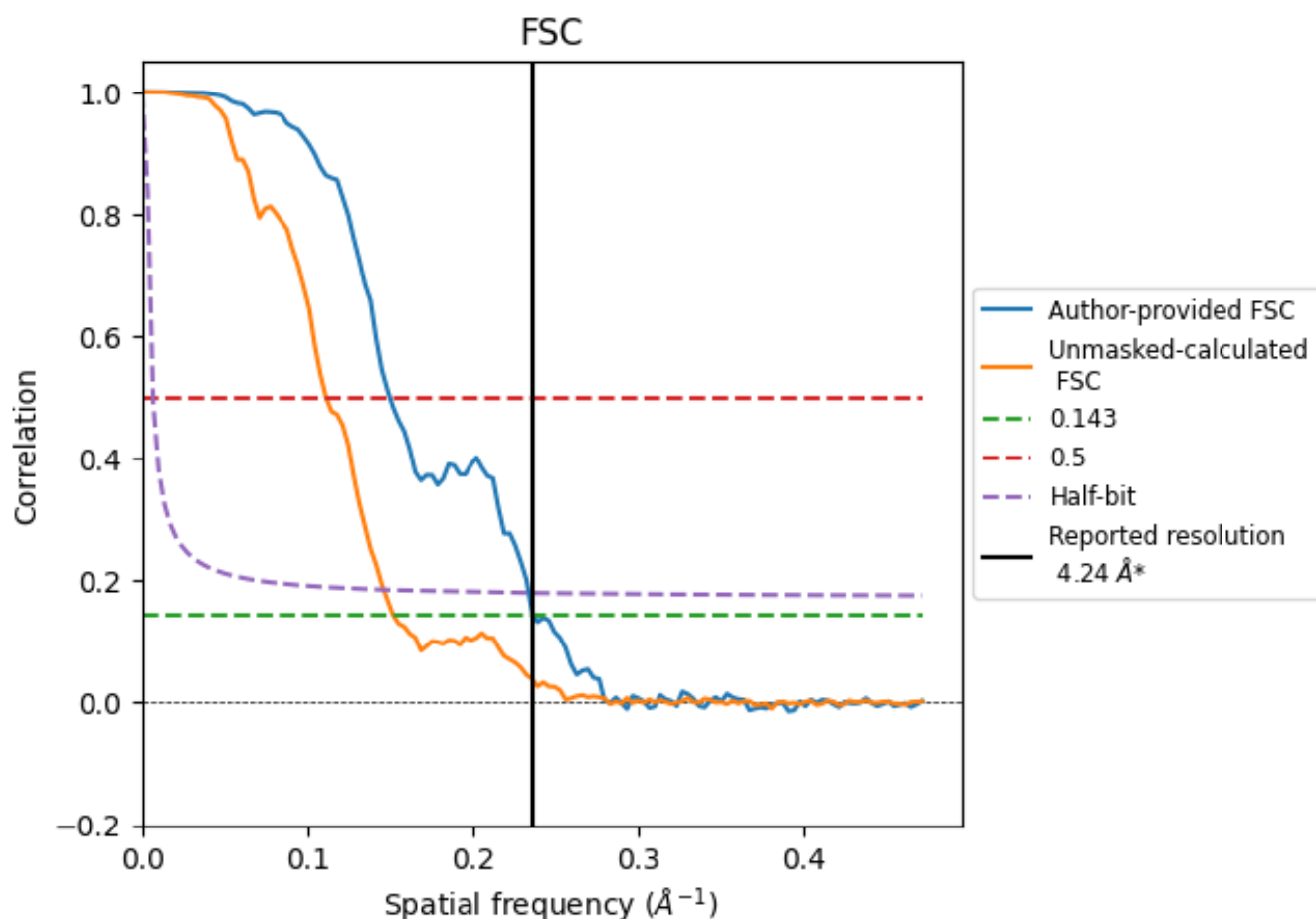


\*Reported resolution corresponds to spatial frequency of 0.236  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.236  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

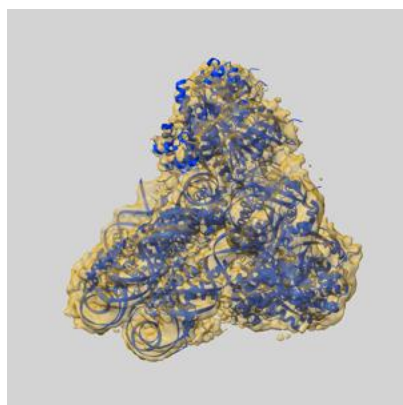
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.24                               | -    | -        |
| Author-provided FSC curve | 4.22                               | 6.68 | 4.28     |
| Unmasked-calculated*      | 6.59                               | 8.99 | 6.85     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.59 differs from the reported value 4.24 by more than 10 %

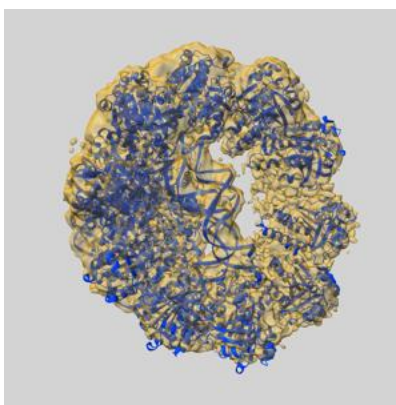
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38229 and PDB model 8XBU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

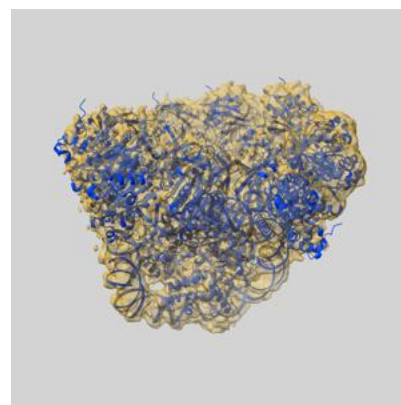
### 9.1 Map-model overlay [i](#)



X



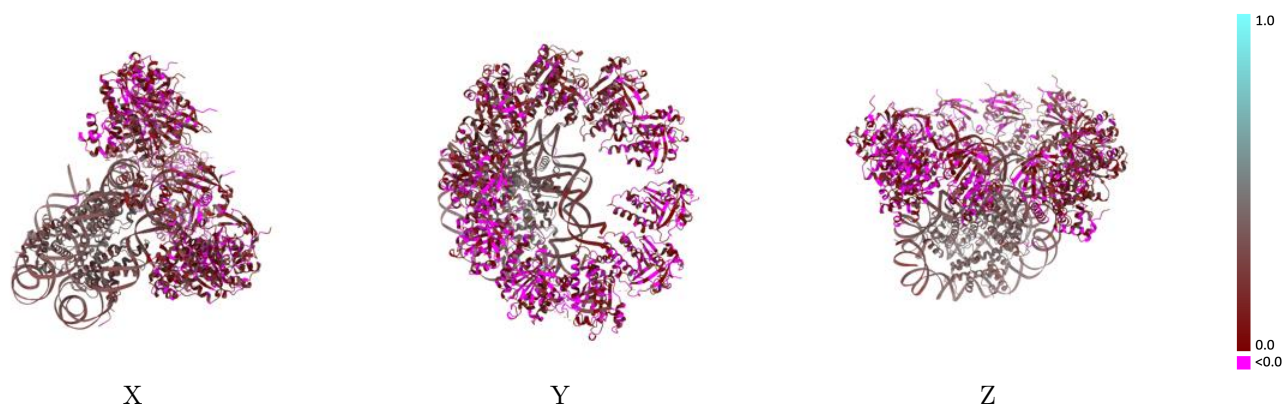
Y



Z

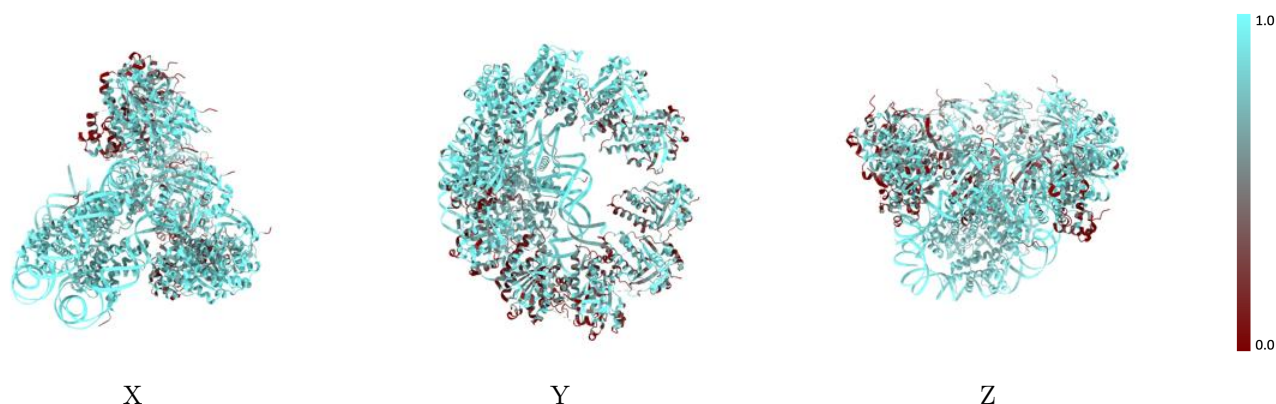
The images above show the 3D surface view of the map at the recommended contour level 0.0042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



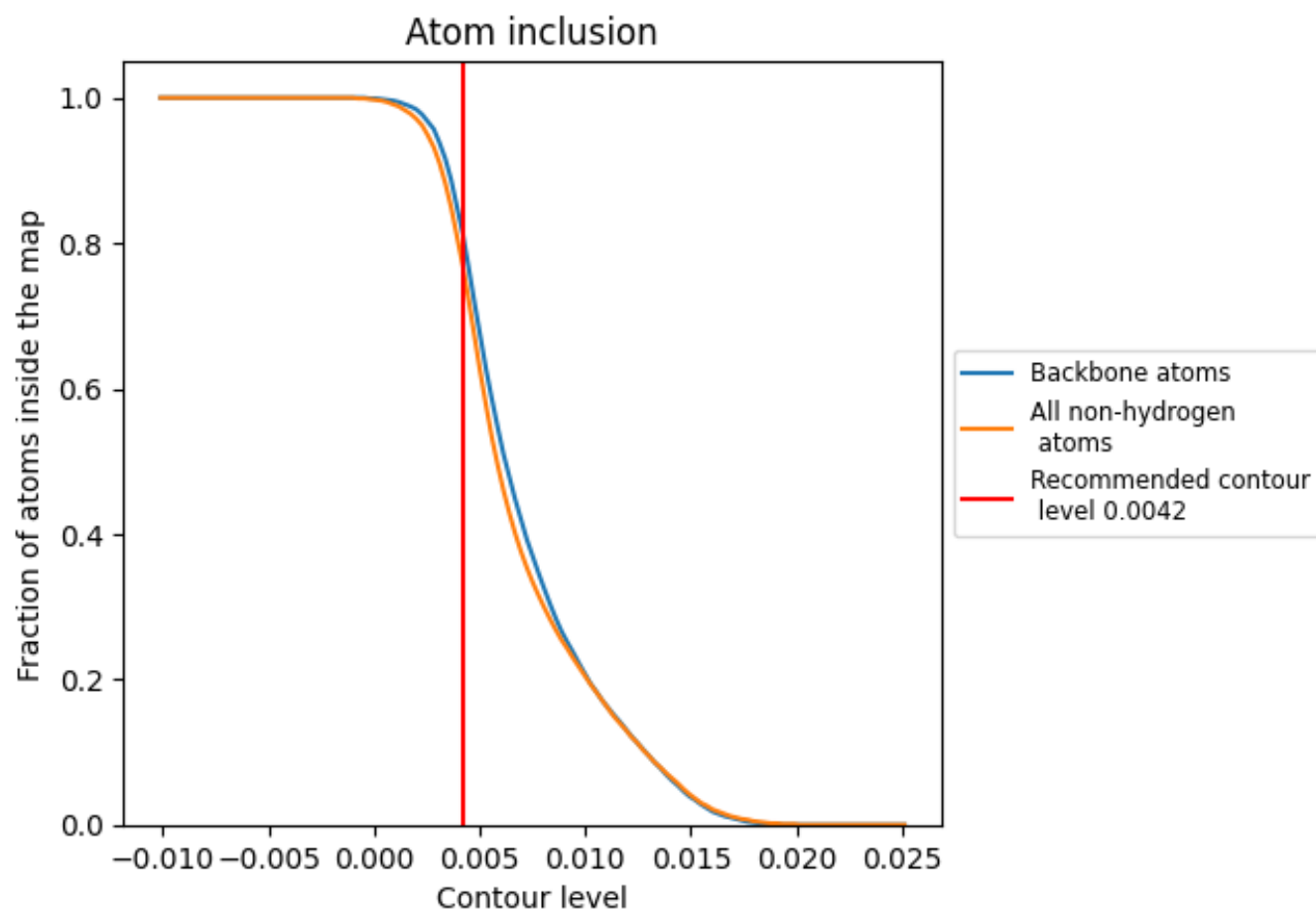
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0042).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.0042) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7700   |  0.1710   |
| A     |  0.8910   |  0.3490   |
| B     |  0.8910   |  0.3630   |
| C     |  0.8340   |  0.3340   |
| D     |  0.8890   |  0.3260   |
| E     |  0.8520   |  0.3520   |
| F     |  0.8070   |  0.3150   |
| G     |  0.8870   |  0.3380   |
| H     |  0.9180   |  0.3300   |
| I     |  0.9630   |  0.3030   |
| J     |  0.9770   |  0.3100   |
| K     |  0.8000   |  0.0990   |
| L     |  0.8170   |  0.1340   |
| M     |  0.8280   |  0.1690   |
| N     |  0.7080  |  0.1310  |
| O     |  0.6770 |  0.0500 |
| P     |  0.6570 |  0.0540 |
| Q     |  0.6080 |  0.0410 |
| R     |  0.5290 |  0.0390 |
| S     |  0.5270 |  0.0280 |
| T     |  0.5820 |  0.0190 |

