



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:42 PM UTC

PDB ID : 9J1K / pdb\_00009j1k  
EMDB ID : EMD-61074  
Title : Tip region of monocin  
Authors : Wang, J.W.; Gu, Z.W.  
Deposited on : 2024-08-05  
Resolution : 2.88 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>.

---

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

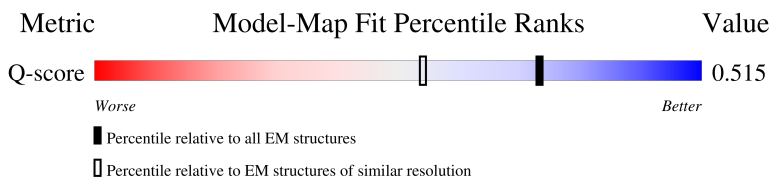
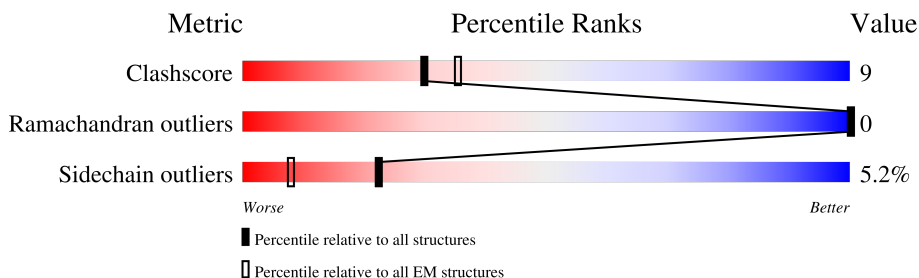
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.88 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.



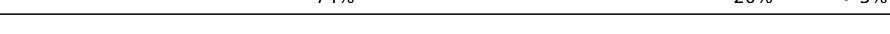
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 12111 ( 2.38 - 3.38 )                                    |

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     | 170    | <br>74% 19% • 5% |
| 1   | B     | 170    | <br>79% 14% • 5% |
| 1   | C     | 170    | <br>71% 22% • 5% |
| 1   | D     | 170    | <br>73% 21% • 5% |

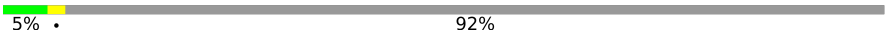
*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 170    |    |
| 1   | F     | 170    |    |
| 1   | G     | 170    |    |
| 1   | H     | 170    |    |
| 1   | I     | 170    |    |
| 1   | N     | 170    |    |
| 1   | S     | 170    |    |
| 1   | T     | 170    |    |
| 1   | U     | 170    |    |
| 1   | V     | 170    |    |
| 1   | W     | 170    |    |
| 1   | Y     | 170    |    |
| 1   | Z     | 170    |  |
| 1   | a     | 170    |  |
| 1   | b     | 170    |  |
| 1   | c     | 170    |  |
| 1   | d     | 170    |  |
| 1   | e     | 170    |  |
| 1   | f     | 170    |  |
| 1   | g     | 170    |  |
| 1   | h     | 170    |  |
| 1   | n     | 170    |  |
| 1   | o     | 170    |  |
| 1   | p     | 170    |  |
| 1   | q     | 170    |  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | r     | 170    |  74%19%6%    |
| 2   | J     | 622    |  6%92%       |
| 2   | O     | 622    |  5%92%       |
| 2   | i     | 622    |  5%92%       |
| 3   | K     | 272    |  77%21%      |
| 3   | P     | 272    |  81%18%      |
| 3   | X     | 272    |  78%21%      |
| 3   | j     | 272    |  78%21%      |
| 3   | k     | 272    |  79%19%      |
| 3   | s     | 272    |  79%19%      |
| 4   | L     | 378    |  76%23%      |
| 4   | Q     | 378    |  81%19%     |
| 4   | l     | 378    |  80%19%    |
| 5   | M     | 99     |  13%14%73% |
| 5   | R     | 99     |  17%10%73% |
| 5   | m     | 99     |  14%13%73% |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60066 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 AA protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | D     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | E     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | F     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | G     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | H     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | a     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | b     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | c     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | d     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | g     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | A     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | B     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | C     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | I     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | N     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | S     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | T     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | U     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | V     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | W     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | Y     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | Z     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | e     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | f     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | h     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | n     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | o     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | p     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 759 | 191 | 242 | 6 |         |       |
| 1   | q     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |
| 1   | r     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 757 | 190 | 241 | 6 |         |       |

- Molecule 2 is a protein called FtbJ.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | J     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 396   | 247 | 70 | 77 | 2 |         |       |
| 2   | O     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 396   | 247 | 70 | 77 | 2 |         |       |
| 2   | i     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 396   | 247 | 70 | 77 | 2 |         |       |

- Molecule 3 is a protein called FtbK.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | K     | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1411 | 370 | 419 | 10 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | k     | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1411 | 370 | 419 | 10 |         |       |
| 3   | P     | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1411 | 370 | 419 | 10 |         |       |
| 3   | X     | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1411 | 370 | 419 | 10 |         |       |
| 3   | j     | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1411 | 370 | 419 | 10 |         |       |
| 3   | s     | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1411 | 370 | 419 | 10 |         |       |

- Molecule 4 is a protein called FtbL.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | L     | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3040  | 1930 | 499 | 600 | 11 |         |       |
| 4   | Q     | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3040  | 1930 | 499 | 600 | 11 |         |       |
| 4   | l     | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3040  | 1930 | 499 | 600 | 11 |         |       |

- Molecule 5 is a protein called CCA-adding enzyme.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | M     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 198   | 124 | 33 | 41 |         |       |
| 5   | R     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 198   | 124 | 33 | 41 |         |       |
| 5   | m     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 198   | 124 | 33 | 41 |         |       |

### 3 Residue-property plots

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

- Molecule 1: AA protein

Chain D: 



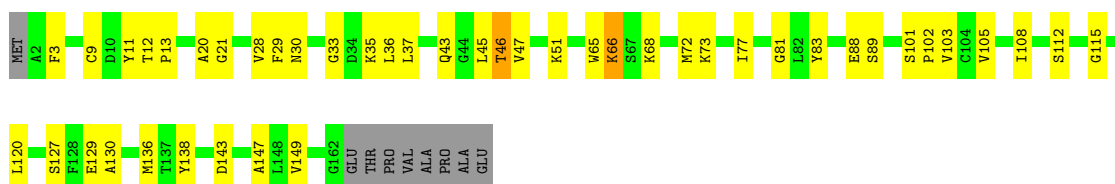
- Molecule 1: AA protein

Chain E: 



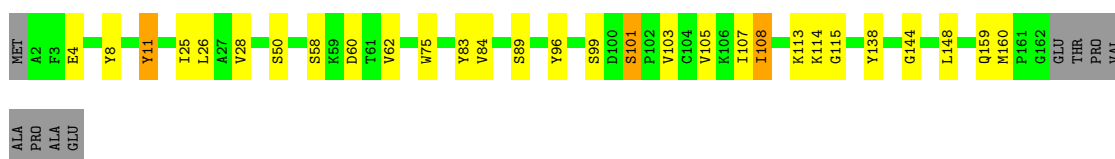
- Molecule 1: AA protein

Chain F: 



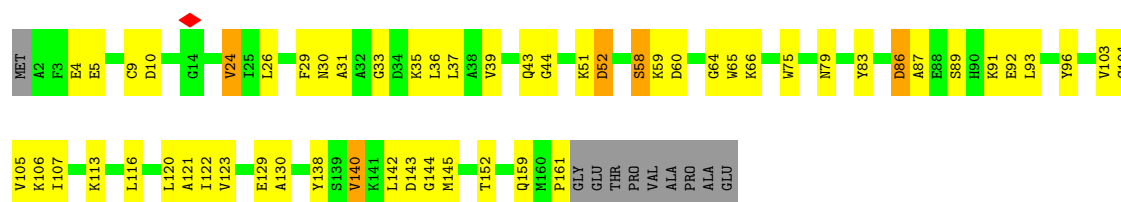
- Molecule 1: AA protein

Chain G: 



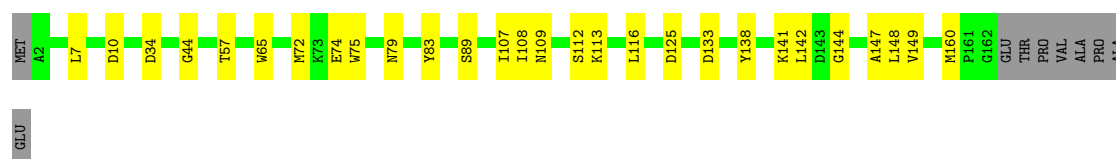
- Molecule 1: AA protein

Chain H:  61% 30% 6%



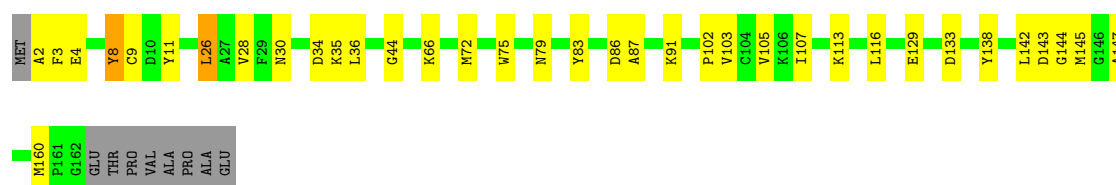
- Molecule 1: AA protein

Chain a:  78% 16% 5%



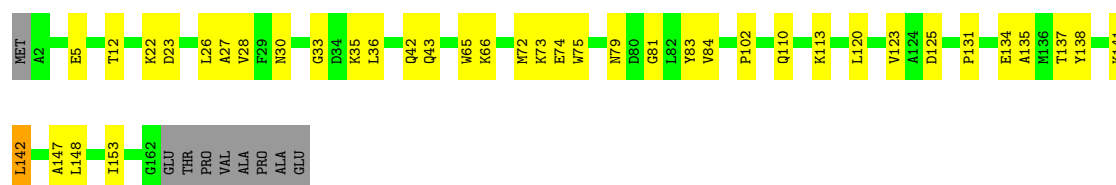
- Molecule 1: AA protein

Chain b:  74% 20% 5%



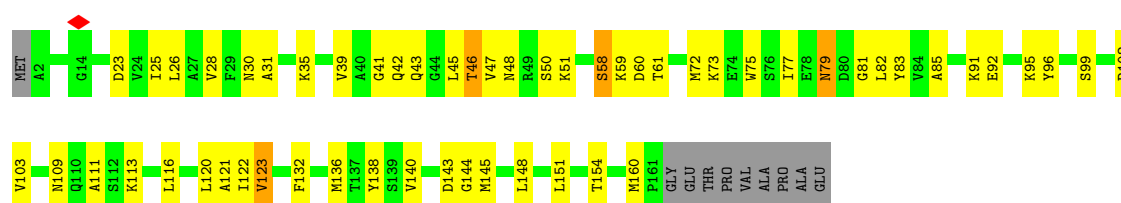
- Molecule 1: AA protein

Chain c:  72% 22% 5%

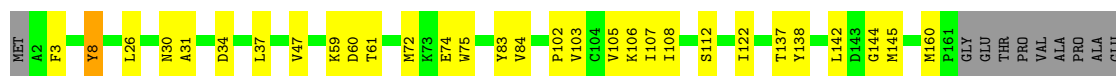


- Molecule 1: AA protein

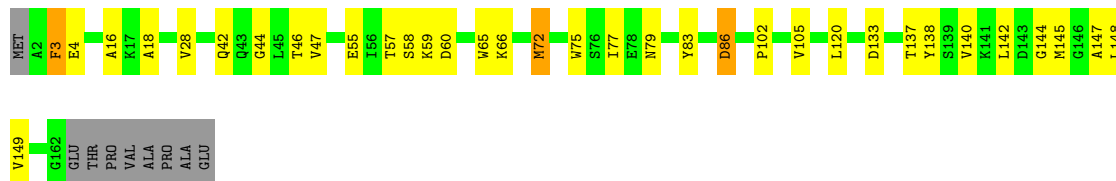
Chain d:  61% 31% 6%



## • Molecule 1: AA protein

Chain g:  76% 17% • 6%

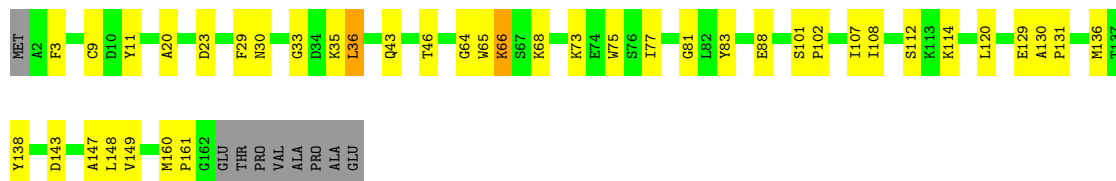
## • Molecule 1: AA protein

Chain A:  74% 19% • 5%

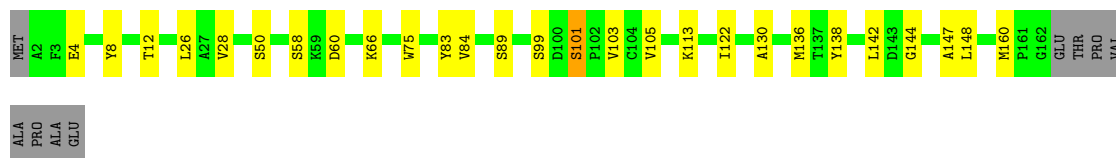
## • Molecule 1: AA protein

Chain B:  79% 14% • 5%

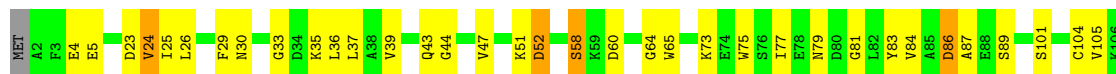
## • Molecule 1: AA protein

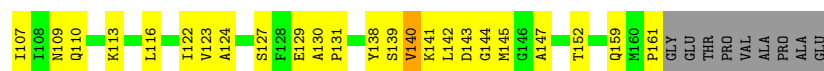
Chain C:  71% 22% • 5%

## • Molecule 1: AA protein

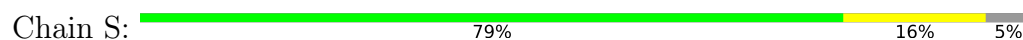
Chain I:  79% 15% • 5%

## • Molecule 1: AA protein

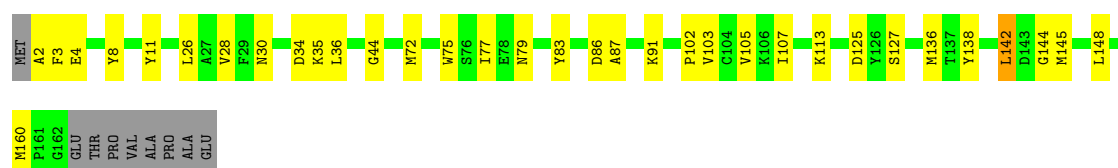
Chain N:  59% 32% • 6%



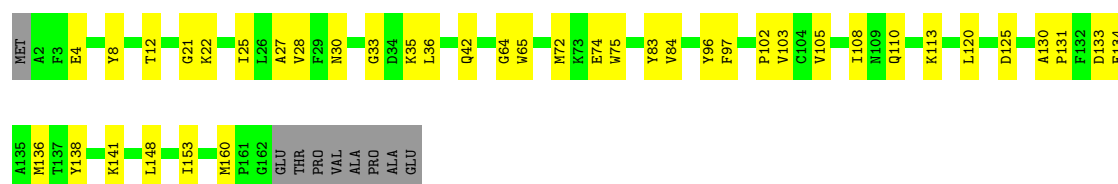
- Molecule 1: AA protein



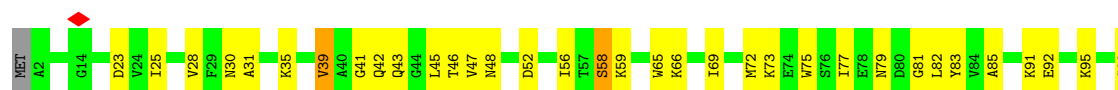
- Molecule 1: AA protein



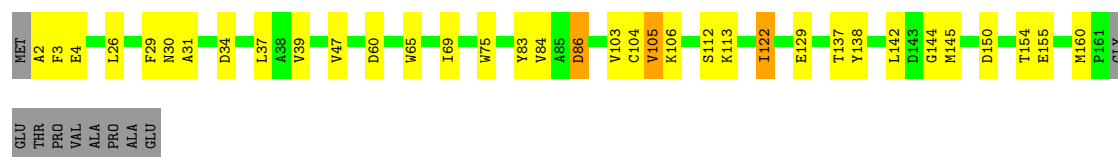
- Molecule 1: AA protein



- Molecule 1: AA protein



- Molecule 1: AA protein



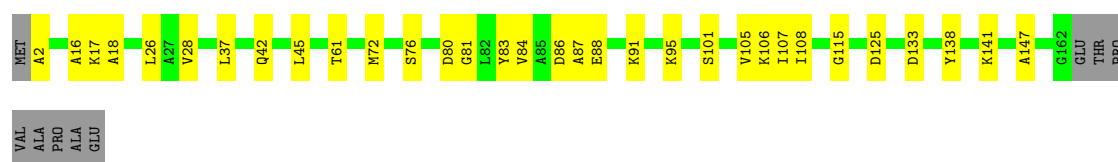
- Molecule 1: AA protein

Chain Y:  70% 25% 5%



- Molecule 1: AA protein

Chain Z:  76% 19% 5%



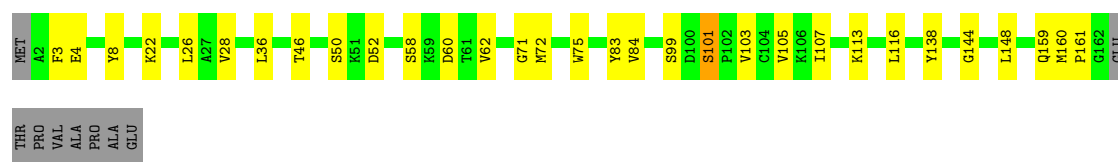
- Molecule 1: AA protein

Chain e:  71% 24% 5%



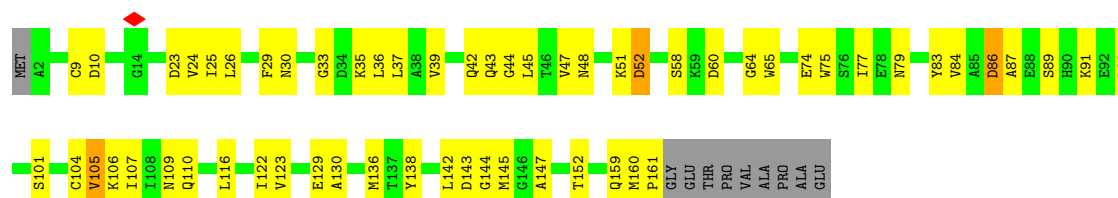
- Molecule 1: AA protein

Chain f:  76% 18% 5%



- Molecule 1: AA protein

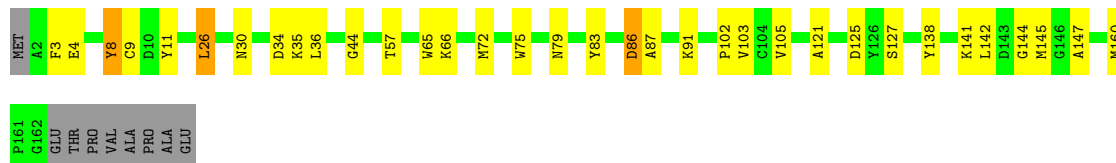
Chain h:  59% 33% 6%



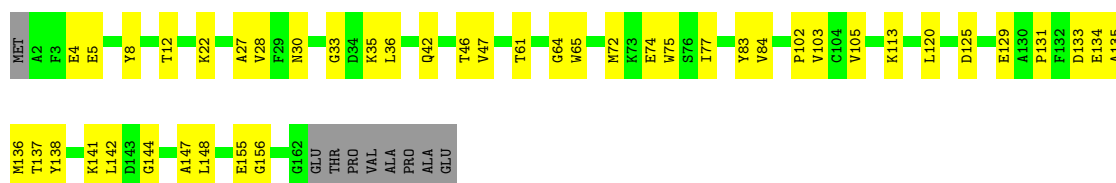
## • Molecule 1: AA protein

Chain n:  75% 19% • 5%

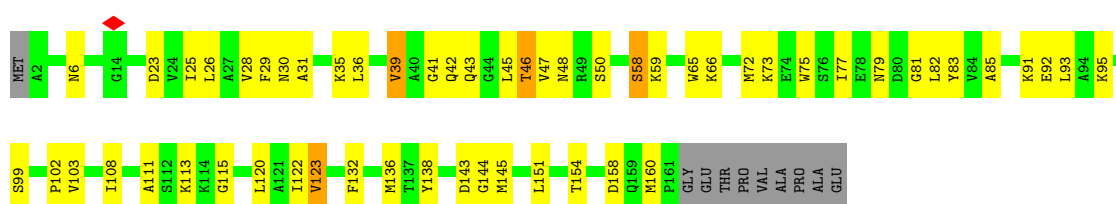
## • Molecule 1: AA protein

Chain o:  75% 18% • 5%

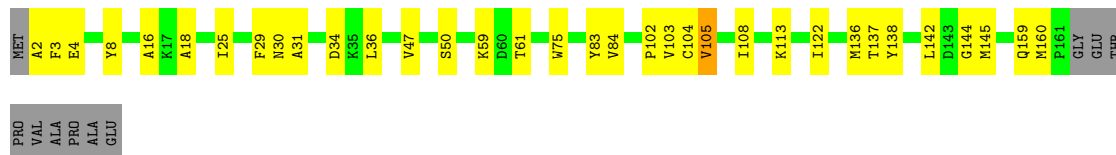
## • Molecule 1: AA protein

Chain p:  69% 26% 5%

## • Molecule 1: AA protein

Chain q:  61% 31% • 6%

## • Molecule 1: AA protein

Chain r:  74% 19% • 6%

Chain J:  6% . 92%

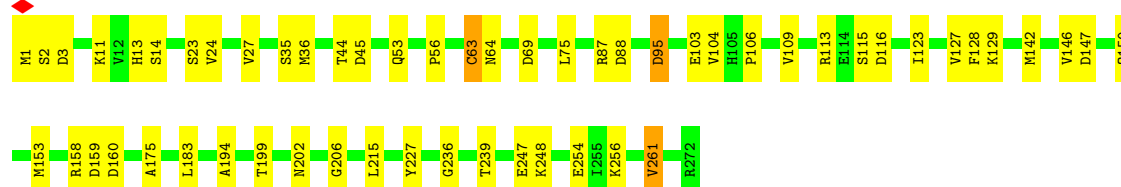
Chain 0:  5% . 92%





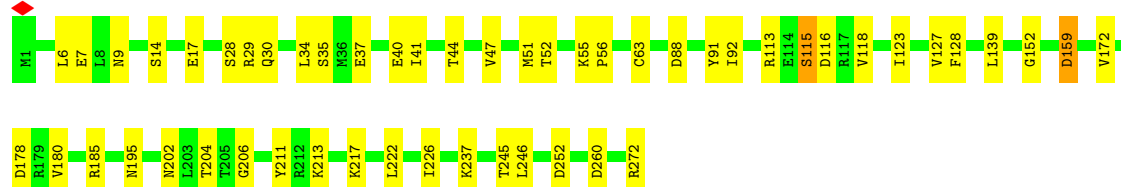
- Molecule 3: FtbK

Chain k:  79% 19%



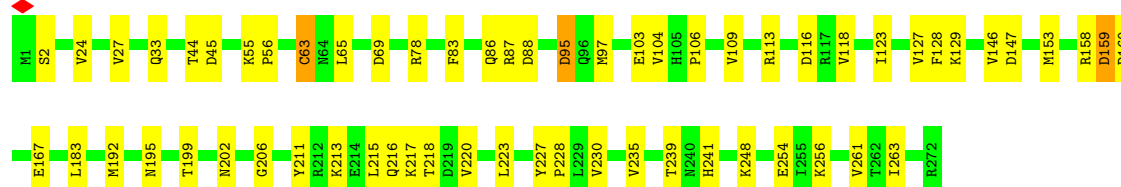
- Molecule 3: FtbK

Chain P:  81% 18%



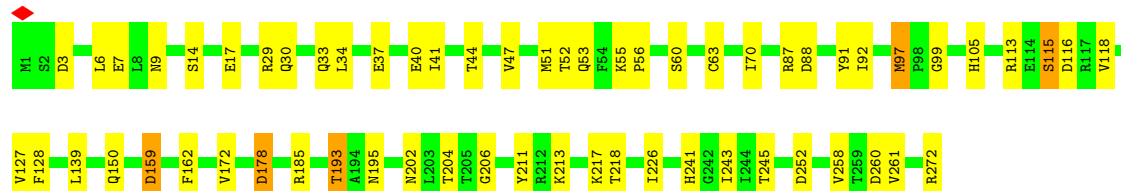
- Molecule 3: FtbK

Chain X:  78% 21%



- Molecule 3: FtbK

Chain j:  78% 21%



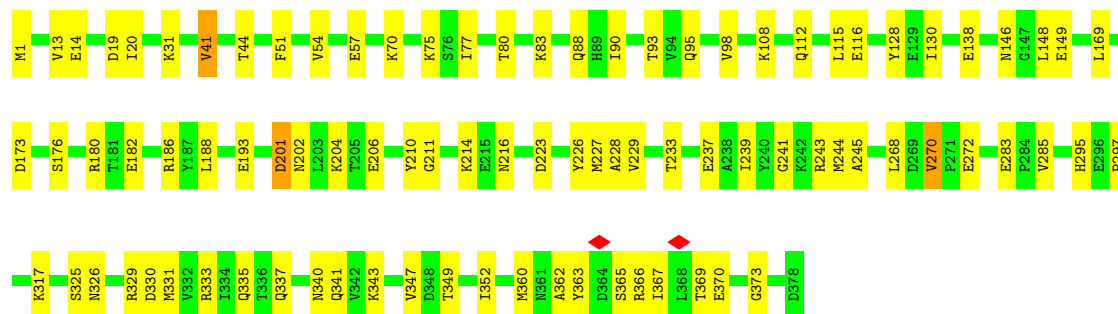
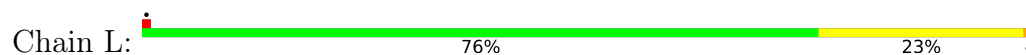
- Molecule 3: FtbK

Chain s:  79% 19%

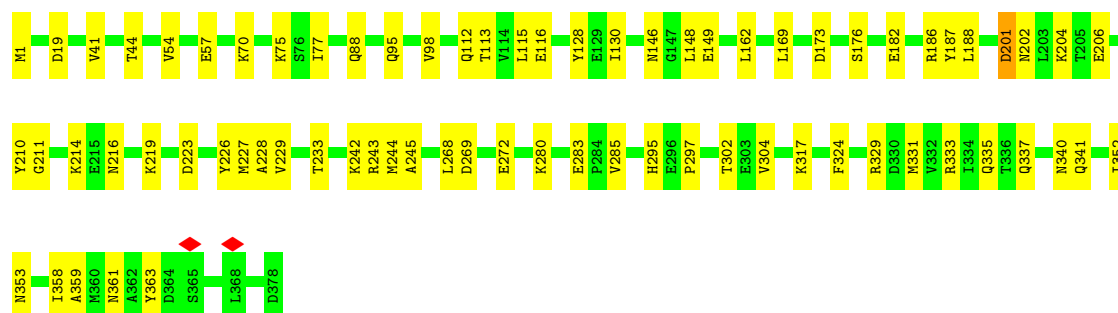
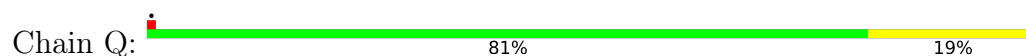




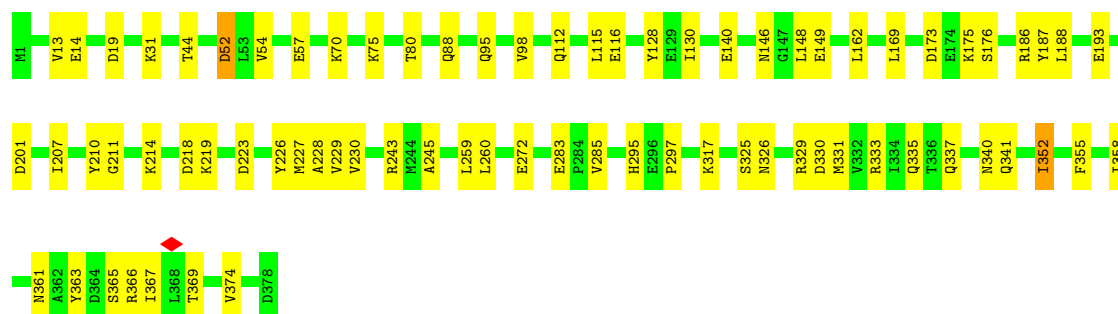
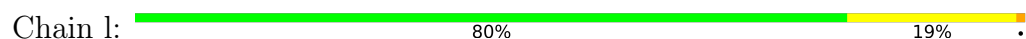
• Molecule 4: FtbL



• Molecule 4: FtbL



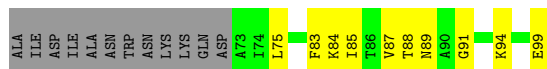
• Molecule 4: FtbL



• Molecule 5: CCA-adding enzyme



- Molecule 5: CCA-adding enzyme



- Molecule 5: CCA-adding enzyme



## 4 Experimental information

| Property                             | Value                        | Source    |
|--------------------------------------|------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE              | Depositor |
| Imposed symmetry                     | POINT, Not provided          |           |
| Number of particles used             | 44283                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF            | Depositor |
| CTF correction method                | NONE                         | Depositor |
| Microscope                           | FEI TITAN KRIOS              | Depositor |
| Voltage (kV)                         | 300                          | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                           | Depositor |
| Minimum defocus (nm)                 | 1000                         | Depositor |
| Maximum defocus (nm)                 | 2000                         | Depositor |
| Magnification                        | Not provided                 |           |
| Image detector                       | GATAN K3 (6k x 4k)           | Depositor |
| Maximum map value                    | 1.763                        | Depositor |
| Minimum map value                    | -0.503                       | Depositor |
| Average map value                    | 0.000                        | Depositor |
| Map value standard deviation         | 0.060                        | Depositor |
| Recommended contour level            | 0.23                         | Depositor |
| Map size ( $\text{\AA}$ )            | 549.9904, 549.9904, 549.9904 | wwPDB     |
| Map dimensions                       | 512, 512, 512                | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0             | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0742, 1.0742, 1.0742       | 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     | 0.11         | 0/1218  | 0.29        | 0/1644  |
| 1   | B     | 0.10         | 0/1218  | 0.28        | 0/1644  |
| 1   | C     | 0.12         | 0/1218  | 0.32        | 0/1644  |
| 1   | D     | 0.11         | 0/1218  | 0.32        | 0/1644  |
| 1   | E     | 0.11         | 0/1218  | 0.32        | 0/1644  |
| 1   | F     | 0.13         | 0/1218  | 0.35        | 0/1644  |
| 1   | G     | 0.11         | 0/1218  | 0.28        | 0/1644  |
| 1   | H     | 0.11         | 0/1214  | 0.38        | 0/1639  |
| 1   | I     | 0.10         | 0/1218  | 0.27        | 0/1644  |
| 1   | N     | 0.13         | 0/1214  | 0.42        | 0/1639  |
| 1   | S     | 0.12         | 0/1218  | 0.34        | 0/1644  |
| 1   | T     | 0.10         | 0/1218  | 0.30        | 0/1644  |
| 1   | U     | 0.12         | 0/1218  | 0.31        | 0/1644  |
| 1   | V     | 0.11         | 0/1214  | 0.35        | 0/1639  |
| 1   | W     | 0.11         | 0/1214  | 0.29        | 0/1639  |
| 1   | Y     | 0.10         | 0/1218  | 0.30        | 0/1644  |
| 1   | Z     | 0.11         | 0/1218  | 0.32        | 0/1644  |
| 1   | a     | 0.12         | 0/1218  | 0.37        | 0/1644  |
| 1   | b     | 0.11         | 0/1218  | 0.32        | 0/1644  |
| 1   | c     | 0.10         | 0/1218  | 0.30        | 0/1644  |
| 1   | d     | 0.11         | 0/1214  | 0.35        | 0/1639  |
| 1   | e     | 0.12         | 0/1218  | 0.34        | 0/1644  |
| 1   | f     | 0.10         | 0/1218  | 0.27        | 0/1644  |
| 1   | g     | 0.11         | 0/1214  | 0.29        | 0/1639  |
| 1   | h     | 0.14         | 0/1214  | 0.44        | 0/1639  |
| 1   | n     | 0.11         | 0/1218  | 0.35        | 0/1644  |
| 1   | o     | 0.11         | 0/1218  | 0.31        | 0/1644  |
| 1   | p     | 0.11         | 0/1218  | 0.32        | 0/1644  |
| 1   | q     | 0.12         | 0/1214  | 0.35        | 0/1639  |
| 1   | r     | 0.12         | 0/1214  | 0.30        | 0/1639  |
| 2   | J     | 0.19         | 0/400   | 0.56        | 0/539   |
| 2   | O     | 0.20         | 0/400   | 0.52        | 0/539   |
| 2   | i     | 0.19         | 0/400   | 0.50        | 0/539   |
| 3   | K     | 0.11         | 0/2264  | 0.29        | 0/3069  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 3   | P     | 0.12         | 0/2264  | 0.29        | 0/3069  |
| 3   | X     | 0.11         | 0/2264  | 0.30        | 0/3069  |
| 3   | j     | 0.11         | 0/2264  | 0.27        | 0/3069  |
| 3   | k     | 0.12         | 0/2264  | 0.32        | 0/3069  |
| 3   | s     | 0.11         | 0/2264  | 0.28        | 0/3069  |
| 4   | L     | 0.09         | 0/3094  | 0.26        | 0/4176  |
| 4   | Q     | 0.09         | 0/3094  | 0.26        | 0/4176  |
| 4   | l     | 0.09         | 0/3094  | 0.27        | 0/4176  |
| 5   | M     | 0.20         | 0/198   | 0.61        | 0/266   |
| 5   | R     | 0.16         | 0/198   | 0.46        | 0/266   |
| 5   | m     | 0.25         | 0/198   | 0.66        | 0/266   |
| All | All   | 0.11         | 0/61164 | 0.32        | 0/82632 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 3   | PHE  | Peptide |
| 1   | D     | 3   | PHE  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1198  | 0        | 1173     | 22      | 0            |
| 1   | B     | 1198  | 0        | 1173     | 13      | 0            |
| 1   | C     | 1198  | 0        | 1173     | 28      | 0            |
| 1   | D     | 1198  | 0        | 1173     | 23      | 0            |
| 1   | E     | 1198  | 0        | 1173     | 16      | 0            |
| 1   | F     | 1198  | 0        | 1173     | 32      | 0            |
| 1   | G     | 1198  | 0        | 1174     | 15      | 0            |
| 1   | H     | 1194  | 0        | 1171     | 43      | 0            |
| 1   | I     | 1198  | 0        | 1174     | 14      | 0            |
| 1   | N     | 1194  | 0        | 1171     | 47      | 0            |
| 1   | S     | 1198  | 0        | 1173     | 19      | 0            |
| 1   | T     | 1198  | 0        | 1173     | 21      | 0            |
| 1   | U     | 1198  | 0        | 1173     | 30      | 0            |
| 1   | V     | 1194  | 0        | 1171     | 41      | 0            |
| 1   | W     | 1194  | 0        | 1171     | 20      | 0            |
| 1   | Y     | 1198  | 0        | 1173     | 24      | 0            |
| 1   | Z     | 1198  | 0        | 1173     | 17      | 0            |
| 1   | a     | 1198  | 0        | 1173     | 18      | 0            |
| 1   | b     | 1198  | 0        | 1173     | 23      | 0            |
| 1   | c     | 1198  | 0        | 1173     | 27      | 0            |
| 1   | d     | 1194  | 0        | 1171     | 41      | 0            |
| 1   | e     | 1198  | 0        | 1173     | 28      | 0            |
| 1   | f     | 1198  | 0        | 1174     | 17      | 0            |
| 1   | g     | 1194  | 0        | 1171     | 17      | 0            |
| 1   | h     | 1194  | 0        | 1171     | 51      | 0            |
| 1   | n     | 1198  | 0        | 1173     | 21      | 0            |
| 1   | o     | 1198  | 0        | 1173     | 20      | 0            |
| 1   | p     | 1198  | 0        | 1173     | 32      | 0            |
| 1   | q     | 1194  | 0        | 1171     | 41      | 0            |
| 1   | r     | 1194  | 0        | 1171     | 23      | 0            |
| 2   | J     | 396   | 0        | 395      | 11      | 0            |
| 2   | O     | 396   | 0        | 395      | 17      | 0            |
| 2   | i     | 396   | 0        | 395      | 20      | 0            |
| 3   | K     | 2210  | 0        | 2142     | 40      | 0            |
| 3   | P     | 2210  | 0        | 2142     | 29      | 0            |
| 3   | X     | 2210  | 0        | 2142     | 40      | 0            |
| 3   | j     | 2210  | 0        | 2142     | 41      | 0            |
| 3   | k     | 2210  | 0        | 2142     | 40      | 0            |
| 3   | s     | 2210  | 0        | 2142     | 40      | 0            |
| 4   | L     | 3040  | 0        | 3009     | 64      | 0            |
| 4   | Q     | 3040  | 0        | 3009     | 50      | 0            |
| 4   | l     | 3040  | 0        | 3009     | 57      | 0            |
| 5   | M     | 198   | 0        | 206      | 17      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | R     | 198   | 0        | 206      | 16      | 0            |
| 5   | m     | 198   | 0        | 206      | 19      | 0            |
| All | All   | 60066 | 0        | 58857    | 1087    | 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 9.

All (1087) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:108:ILE:HD11 | 1:r:160:MET:HE2  | 1.59                     | 0.85              |
| 1:r:83:TYR:HB2   | 1:r:138:TYR:HB3  | 1.58                     | 0.84              |
| 1:d:83:TYR:HB2   | 1:d:138:TYR:HB3  | 1.62                     | 0.81              |
| 3:K:29:ARG:NH1   | 3:K:30:GLN:O     | 2.15                     | 0.80              |
| 1:W:122:ILE:HG22 | 1:W:145:MET:HE2  | 1.64                     | 0.78              |
| 1:U:83:TYR:HB2   | 1:U:138:TYR:HB3  | 1.65                     | 0.78              |
| 1:r:122:ILE:HG23 | 1:r:145:MET:HE2  | 1.64                     | 0.78              |
| 1:G:108:ILE:HG22 | 1:G:115:GLY:HA2  | 1.68                     | 0.76              |
| 1:V:83:TYR:HB2   | 1:V:138:TYR:HB3  | 1.68                     | 0.75              |
| 1:q:83:TYR:HB2   | 1:q:138:TYR:HB3  | 1.68                     | 0.75              |
| 3:P:56:PRO:HB3   | 3:P:128:PHE:HA   | 1.67                     | 0.75              |
| 3:K:56:PRO:HB3   | 3:K:128:PHE:HA   | 1.68                     | 0.75              |
| 3:j:56:PRO:HB3   | 3:j:128:PHE:HA   | 1.67                     | 0.75              |
| 1:p:83:TYR:HB2   | 1:p:138:TYR:HB3  | 1.68                     | 0.74              |
| 3:k:56:PRO:HB3   | 3:k:128:PHE:HA   | 1.69                     | 0.74              |
| 3:s:56:PRO:HB3   | 3:s:128:PHE:HA   | 1.68                     | 0.74              |
| 1:g:83:TYR:HB2   | 1:g:138:TYR:HB3  | 1.70                     | 0.73              |
| 3:X:56:PRO:HB3   | 3:X:128:PHE:HA   | 1.69                     | 0.73              |
| 1:n:109:ASN:O    | 1:n:109:ASN:ND2  | 2.22                     | 0.73              |
| 1:H:83:TYR:HB2   | 1:H:138:TYR:HB3  | 1.72                     | 0.72              |
| 1:W:83:TYR:HB2   | 1:W:138:TYR:HB3  | 1.71                     | 0.72              |
| 1:Z:83:TYR:HB2   | 1:Z:138:TYR:HB3  | 1.72                     | 0.72              |
| 1:q:39:VAL:O     | 1:q:42:GLN:NE2   | 2.22                     | 0.71              |
| 1:F:88:GLU:N     | 1:F:88:GLU:OE2   | 2.21                     | 0.71              |
| 1:I:83:TYR:HB2   | 1:I:138:TYR:HB3  | 1.73                     | 0.70              |
| 1:N:23:ASP:HA    | 1:N:110:GLN:HE21 | 1.55                     | 0.70              |
| 1:f:83:TYR:HB2   | 1:f:138:TYR:HB3  | 1.73                     | 0.70              |
| 1:G:83:TYR:HB2   | 1:G:138:TYR:HB3  | 1.73                     | 0.70              |
| 1:e:88:GLU:OE1   | 1:e:88:GLU:N     | 2.19                     | 0.70              |
| 1:h:23:ASP:HA    | 1:h:110:GLN:HE21 | 1.55                     | 0.70              |
| 1:q:122:ILE:HG12 | 1:q:145:MET:HE1  | 1.73                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:f:113:LYS:HA  | 1:f:160:MET:HE1  | 1.72                     | 0.70              |
| 1:h:83:TYR:HB2  | 1:h:138:TYR:HB3  | 1.74                     | 0.70              |
| 1:C:83:TYR:HB2  | 1:C:138:TYR:HB3  | 1.74                     | 0.70              |
| 1:N:83:TYR:HB2  | 1:N:138:TYR:HB3  | 1.73                     | 0.70              |
| 1:V:83:TYR:HB3  | 1:V:136:MET:HG3  | 1.73                     | 0.70              |
| 1:V:136:MET:HE2 | 1:V:136:MET:HA   | 1.75                     | 0.69              |
| 3:j:29:ARG:NH1  | 3:j:30:GLN:O     | 2.25                     | 0.69              |
| 3:P:37:GLU:HB3  | 4:Q:317:LYS:HD2  | 1.75                     | 0.69              |
| 1:q:136:MET:HE2 | 1:q:136:MET:HA   | 1.73                     | 0.69              |
| 4:L:88:GLN:HE22 | 2:O:611:GLN:HG3  | 1.58                     | 0.69              |
| 1:C:88:GLU:OE1  | 1:C:88:GLU:N     | 2.20                     | 0.68              |
| 1:q:83:TYR:HB3  | 1:q:136:MET:HG3  | 1.76                     | 0.68              |
| 1:H:51:LYS:NZ   | 1:q:123:VAL:O    | 2.25                     | 0.68              |
| 1:b:83:TYR:HB2  | 1:b:138:TYR:HB3  | 1.75                     | 0.68              |
| 1:d:39:VAL:O    | 1:d:42:GLN:NE2   | 2.27                     | 0.67              |
| 3:P:51:MET:HE3  | 3:P:51:MET:HA    | 1.76                     | 0.67              |
| 3:j:37:GLU:HB3  | 4:l:317:LYS:HD2  | 1.75                     | 0.67              |
| 3:s:24:VAL:HA   | 3:s:63:CYS:HB3   | 1.76                     | 0.67              |
| 1:U:28:VAL:HG23 | 1:U:105:VAL:HG12 | 1.77                     | 0.67              |
| 1:B:83:TYR:HB2  | 1:B:138:TYR:HB3  | 1.76                     | 0.67              |
| 1:V:136:MET:HE3 | 1:h:24:VAL:HG21  | 1.77                     | 0.67              |
| 3:s:181:ASN:HB3 | 3:s:184:MET:HG3  | 1.76                     | 0.67              |
| 1:C:102:PRO:HB2 | 1:C:120:LEU:HD22 | 1.76                     | 0.67              |
| 4:Q:88:GLN:HE22 | 2:i:611:GLN:HG3  | 1.60                     | 0.67              |
| 2:J:611:GLN:HG2 | 4:l:88:GLN:HE22  | 1.60                     | 0.67              |
| 2:J:591:LYS:NZ  | 5:M:94:LYS:O     | 2.28                     | 0.66              |
| 1:o:83:TYR:HB2  | 1:o:138:TYR:HB3  | 1.76                     | 0.66              |
| 1:E:83:TYR:HB2  | 1:E:138:TYR:HB3  | 1.76                     | 0.66              |
| 3:s:36:MET:HG3  | 3:s:52:THR:HG22  | 1.77                     | 0.66              |
| 3:j:51:MET:HE3  | 3:j:51:MET:HA    | 1.76                     | 0.66              |
| 1:H:66:LYS:HG2  | 1:q:72:MET:HG3   | 1.74                     | 0.66              |
| 3:K:37:GLU:HB3  | 4:L:317:LYS:HD2  | 1.77                     | 0.66              |
| 1:D:113:LYS:HA  | 1:D:160:MET:HE1  | 1.78                     | 0.66              |
| 3:X:24:VAL:HA   | 3:X:63:CYS:HB3   | 1.78                     | 0.66              |
| 1:Y:113:LYS:HA  | 1:Y:160:MET:HE1  | 1.78                     | 0.66              |
| 1:n:83:TYR:HB2  | 1:n:138:TYR:HB3  | 1.76                     | 0.66              |
| 1:F:102:PRO:HB2 | 1:F:120:LEU:HD22 | 1.77                     | 0.66              |
| 1:T:83:TYR:HB2  | 1:T:138:TYR:HB3  | 1.78                     | 0.66              |
| 3:P:40:GLU:HG3  | 3:P:47:VAL:HG12  | 1.78                     | 0.66              |
| 1:S:83:TYR:HB2  | 1:S:138:TYR:HB3  | 1.78                     | 0.66              |
| 1:a:72:MET:HE3  | 1:a:72:MET:HA    | 1.77                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:29:ARG:NH1   | 3:P:30:GLN:O     | 2.29                     | 0.65              |
| 1:e:9:CYS:HB3    | 1:e:11:TYR:HE2   | 1.60                     | 0.65              |
| 1:F:129:GLU:N    | 1:F:129:GLU:OE2  | 2.30                     | 0.65              |
| 1:C:129:GLU:OE2  | 1:C:129:GLU:N    | 2.29                     | 0.65              |
| 3:k:24:VAL:HA    | 3:k:63:CYS:HB3   | 1.77                     | 0.65              |
| 3:K:216:GLN:N    | 3:K:216:GLN:OE1  | 2.29                     | 0.64              |
| 4:Q:201:ASP:N    | 4:Q:201:ASP:OD1  | 2.30                     | 0.64              |
| 1:a:83:TYR:HB2   | 1:a:138:TYR:HB3  | 1.78                     | 0.64              |
| 1:H:122:ILE:HG23 | 1:H:145:MET:HE1  | 1.78                     | 0.64              |
| 3:k:146:VAL:HG23 | 3:k:147:ASP:H    | 1.63                     | 0.64              |
| 4:Q:173:ASP:OD1  | 4:Q:176:SER:OG   | 2.16                     | 0.64              |
| 1:r:159:GLN:OE1  | 1:r:160:MET:N    | 2.29                     | 0.64              |
| 1:Y:102:PRO:HB2  | 1:Y:120:LEU:HD22 | 1.79                     | 0.64              |
| 1:h:9:CYS:SG     | 1:h:10:ASP:N     | 2.71                     | 0.64              |
| 3:k:45:ASP:OD2   | 3:s:87:ARG:NH2   | 2.30                     | 0.63              |
| 3:X:146:VAL:HG23 | 3:X:147:ASP:H    | 1.63                     | 0.63              |
| 1:e:28:VAL:HG12  | 1:e:105:VAL:HG23 | 1.81                     | 0.63              |
| 1:p:72:MET:HE3   | 1:p:72:MET:HA    | 1.80                     | 0.63              |
| 4:L:98:VAL:H     | 4:Q:244:MET:HE3  | 1.63                     | 0.63              |
| 1:o:72:MET:HE3   | 1:o:72:MET:HA    | 1.79                     | 0.63              |
| 3:K:51:MET:HE3   | 3:K:51:MET:HA    | 1.81                     | 0.63              |
| 3:j:97:MET:HE2   | 3:j:150:GLN:HE22 | 1.63                     | 0.63              |
| 4:L:173:ASP:OD1  | 4:L:176:SER:OG   | 2.15                     | 0.63              |
| 1:h:86:ASP:OD1   | 1:h:86:ASP:N     | 2.32                     | 0.62              |
| 1:c:74:GLU:OE1   | 1:C:68:LYS:NZ    | 2.31                     | 0.62              |
| 3:X:106:PRO:HG2  | 3:j:34:LEU:HD13  | 1.81                     | 0.62              |
| 3:X:87:ARG:NH2   | 3:s:45:ASP:OD2   | 2.32                     | 0.62              |
| 1:V:45:LEU:HD23  | 1:V:79:ASN:HB2   | 1.80                     | 0.62              |
| 1:d:79:ASN:HD21  | 1:d:140:VAL:HB   | 1.65                     | 0.62              |
| 1:F:28:VAL:HG12  | 1:F:105:VAL:HG23 | 1.81                     | 0.62              |
| 3:k:109:VAL:HG11 | 3:k:123:ILE:HA   | 1.82                     | 0.62              |
| 5:R:85:ILE:O     | 5:R:88:THR:OG1   | 2.17                     | 0.62              |
| 3:X:158:ARG:NH2  | 3:X:160:ASP:OD2  | 2.32                     | 0.62              |
| 3:X:167:GLU:N    | 3:X:167:GLU:OE1  | 2.33                     | 0.62              |
| 1:e:83:TYR:HB2   | 1:e:138:TYR:HB3  | 1.81                     | 0.62              |
| 1:e:102:PRO:HB2  | 1:e:120:LEU:HD22 | 1.80                     | 0.62              |
| 1:h:29:PHE:HB2   | 1:h:104:CYS:HB3  | 1.82                     | 0.62              |
| 1:p:28:VAL:HG23  | 1:p:105:VAL:HG12 | 1.81                     | 0.61              |
| 1:U:72:MET:HE2   | 1:U:72:MET:HA    | 1.81                     | 0.61              |
| 1:V:123:VAL:O    | 1:h:51:LYS:NZ    | 2.32                     | 0.61              |
| 3:X:216:GLN:OE1  | 3:X:217:LYS:N    | 2.34                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:122:ILE:HG23 | 1:h:145:MET:HE1  | 1.82                     | 0.61              |
| 3:j:185:ARG:NH2  | 3:s:44:THR:OG1   | 2.33                     | 0.61              |
| 1:D:102:PRO:HB2  | 1:D:120:LEU:HD22 | 1.83                     | 0.61              |
| 1:b:72:MET:HE3   | 1:b:72:MET:HA    | 1.82                     | 0.61              |
| 1:d:31:ALA:N     | 1:d:92:GLU:OE1   | 2.33                     | 0.61              |
| 3:k:87:ARG:NH2   | 3:X:45:ASP:OD2   | 2.33                     | 0.61              |
| 1:Z:2:ALA:HB3    | 1:e:33:GLY:HA3   | 1.83                     | 0.61              |
| 5:m:94:LYS:HE2   | 5:m:94:LYS:HA    | 1.81                     | 0.61              |
| 1:c:30:ASN:OD1   | 1:c:33:GLY:N     | 2.34                     | 0.60              |
| 4:l:173:ASP:OD1  | 4:l:176:SER:OG   | 2.17                     | 0.60              |
| 4:L:272:GLU:OE1  | 4:L:329:ARG:NH1  | 2.35                     | 0.60              |
| 1:Z:37:LEU:HD13  | 1:Z:88:GLU:HG2   | 1.83                     | 0.60              |
| 2:i:590:ILE:H    | 5:m:91:GLY:HA3   | 1.66                     | 0.60              |
| 4:L:366:ARG:O    | 4:L:370:GLU:HG3  | 2.01                     | 0.60              |
| 3:P:7:GLU:HB3    | 3:P:91:TYR:HB2   | 1.82                     | 0.60              |
| 3:k:113:ARG:NH1  | 1:I:60:ASP:OD1   | 2.33                     | 0.60              |
| 3:K:40:GLU:HG3   | 3:K:47:VAL:HG12  | 1.83                     | 0.59              |
| 1:d:25:ILE:HD12  | 1:d:26:LEU:H     | 1.67                     | 0.59              |
| 1:F:47:VAL:HG22  | 1:F:77:ILE:HG12  | 1.82                     | 0.59              |
| 1:T:44:GLY:O     | 1:T:79:ASN:ND2   | 2.36                     | 0.59              |
| 1:c:131:PRO:HG2  | 1:c:134:GLU:HG2  | 1.85                     | 0.59              |
| 1:d:85:ALA:O     | 1:d:91:LYS:NZ    | 2.35                     | 0.59              |
| 1:q:25:ILE:HD12  | 1:q:26:LEU:H     | 1.66                     | 0.59              |
| 1:r:83:TYR:HD2   | 1:r:136:MET:HE3  | 1.68                     | 0.59              |
| 3:P:185:ARG:NH2  | 3:X:44:THR:OG1   | 2.35                     | 0.59              |
| 1:U:102:PRO:HB2  | 1:U:120:LEU:HD22 | 1.85                     | 0.59              |
| 1:h:30:ASN:HD21  | 1:h:35:LYS:H     | 1.50                     | 0.59              |
| 1:d:72:MET:HA    | 1:d:72:MET:HE3   | 1.85                     | 0.59              |
| 1:g:61:THR:HA    | 3:k:1:MET:H2     | 1.67                     | 0.59              |
| 1:V:31:ALA:N     | 1:V:92:GLU:OE1   | 2.34                     | 0.59              |
| 1:d:123:VAL:O    | 1:N:51:LYS:NZ    | 2.25                     | 0.59              |
| 3:k:103:GLU:OE1  | 3:k:129:LYS:NZ   | 2.33                     | 0.59              |
| 1:E:37:LEU:HD13  | 1:E:88:GLU:HG2   | 1.84                     | 0.59              |
| 3:K:7:GLU:HB3    | 3:K:91:TYR:HB2   | 1.85                     | 0.59              |
| 4:l:272:GLU:OE1  | 4:l:329:ARG:NH1  | 2.36                     | 0.59              |
| 1:p:30:ASN:OD1   | 1:p:33:GLY:N     | 2.34                     | 0.59              |
| 1:g:105:VAL:HG11 | 1:g:142:LEU:HD13 | 1.85                     | 0.59              |
| 1:N:29:PHE:HB2   | 1:N:104:CYS:HB3  | 1.85                     | 0.59              |
| 3:k:153:MET:HE3  | 3:k:153:MET:N    | 2.18                     | 0.58              |
| 1:G:60:ASP:OD1   | 3:s:113:ARG:NH1  | 2.36                     | 0.58              |
| 3:K:185:ARG:NH2  | 3:k:44:THR:OG1   | 2.36                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:j:40:GLU:HG3   | 3:j:47:VAL:HG12  | 1.86                     | 0.58              |
| 1:b:11:TYR:OH    | 1:c:102:PRO:O    | 2.22                     | 0.58              |
| 1:r:61:THR:HA    | 3:s:1:MET:H1     | 1.68                     | 0.58              |
| 1:H:29:PHE:HB2   | 1:H:104:CYS:HB3  | 1.84                     | 0.58              |
| 3:K:202:ASN:ND2  | 3:K:245:THR:O    | 2.37                     | 0.58              |
| 1:N:30:ASN:HD21  | 1:N:35:LYS:H     | 1.51                     | 0.58              |
| 1:T:83:TYR:HB3   | 1:T:136:MET:HG2  | 1.86                     | 0.58              |
| 1:W:105:VAL:HG21 | 1:W:142:LEU:HD13 | 1.85                     | 0.58              |
| 1:C:9:CYS:HB3    | 1:C:11:TYR:HE2   | 1.68                     | 0.58              |
| 3:s:69:ASP:OD1   | 3:s:69:ASP:N     | 2.36                     | 0.58              |
| 3:k:69:ASP:OD1   | 3:k:69:ASP:N     | 2.37                     | 0.58              |
| 1:Z:28:VAL:HG12  | 1:Z:105:VAL:HG12 | 1.85                     | 0.58              |
| 3:j:7:GLU:HB3    | 3:j:91:TYR:HB2   | 1.86                     | 0.58              |
| 1:H:24:VAL:HG21  | 1:q:136:MET:HE3  | 1.85                     | 0.58              |
| 1:b:44:GLY:O     | 1:b:79:ASN:ND2   | 2.37                     | 0.58              |
| 3:k:106:PRO:HG2  | 3:P:34:LEU:HD13  | 1.86                     | 0.58              |
| 2:i:590:ILE:HG23 | 5:m:92:GLU:H     | 1.68                     | 0.58              |
| 4:L:98:VAL:HA    | 4:L:146:ASN:HA   | 1.86                     | 0.57              |
| 3:P:159:ASP:N    | 3:P:159:ASP:OD1  | 2.37                     | 0.57              |
| 1:V:75:TRP:CE2   | 1:V:144:GLY:HA3  | 2.39                     | 0.57              |
| 1:E:28:VAL:HG12  | 1:E:105:VAL:HG12 | 1.86                     | 0.57              |
| 1:c:83:TYR:HB2   | 1:c:138:TYR:HB3  | 1.87                     | 0.57              |
| 1:F:30:ASN:HD21  | 1:F:35:LYS:H     | 1.51                     | 0.57              |
| 1:F:66:LYS:HE3   | 1:p:72:MET:HB3   | 1.85                     | 0.57              |
| 1:V:39:VAL:O     | 1:V:42:GLN:NE2   | 2.37                     | 0.57              |
| 1:e:30:ASN:HD21  | 1:e:35:LYS:H     | 1.52                     | 0.57              |
| 4:l:358:ILE:HA   | 4:l:361:ASN:HB2  | 1.85                     | 0.57              |
| 1:r:102:PRO:HB3  | 1:r:145:MET:HE1  | 1.85                     | 0.57              |
| 3:s:159:ASP:OD1  | 3:s:159:ASP:N    | 2.35                     | 0.57              |
| 4:L:201:ASP:OD1  | 4:L:201:ASP:N    | 2.34                     | 0.57              |
| 3:j:6:LEU:HG     | 3:j:92:ILE:HG22  | 1.87                     | 0.57              |
| 3:j:159:ASP:OD1  | 3:j:159:ASP:N    | 2.37                     | 0.57              |
| 4:l:98:VAL:HA    | 4:l:146:ASN:HA   | 1.86                     | 0.57              |
| 1:q:25:ILE:HD11  | 1:q:42:GLN:NE2   | 2.18                     | 0.57              |
| 3:K:6:LEU:HG     | 3:K:92:ILE:HG22  | 1.85                     | 0.57              |
| 3:K:45:ASP:OD2   | 3:j:87:ARG:NH2   | 2.36                     | 0.57              |
| 1:A:58:SER:OG    | 1:A:60:ASP:OD1   | 2.21                     | 0.57              |
| 4:l:230:VAL:HG12 | 4:l:259:LEU:HD23 | 1.86                     | 0.57              |
| 3:s:95:ASP:OD1   | 3:s:95:ASP:N     | 2.37                     | 0.57              |
| 1:U:30:ASN:OD1   | 1:U:33:GLY:N     | 2.36                     | 0.57              |
| 3:X:69:ASP:OD1   | 3:X:69:ASP:N     | 2.38                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:X:109:VAL:HG11 | 3:X:123:ILE:HA   | 1.86                     | 0.57              |
| 1:d:41:GLY:O     | 1:d:82:LEU:N     | 2.38                     | 0.57              |
| 3:K:34:LEU:HD13  | 3:s:106:PRO:HG2  | 1.87                     | 0.57              |
| 1:d:83:TYR:HB3   | 1:d:136:MET:HE1  | 1.86                     | 0.57              |
| 3:k:87:ARG:NH1   | 3:P:52:THR:O     | 2.38                     | 0.57              |
| 1:C:30:ASN:OD1   | 1:C:33:GLY:N     | 2.37                     | 0.57              |
| 3:K:159:ASP:N    | 3:K:159:ASP:OD1  | 2.37                     | 0.56              |
| 1:H:86:ASP:OD1   | 1:H:86:ASP:N     | 2.22                     | 0.56              |
| 3:X:159:ASP:OD1  | 3:X:159:ASP:N    | 2.34                     | 0.56              |
| 3:K:88:ASP:OD1   | 3:K:88:ASP:N     | 2.37                     | 0.56              |
| 1:W:86:ASP:OD1   | 1:W:86:ASP:N     | 2.24                     | 0.56              |
| 3:j:178:ASP:OD1  | 3:j:272:ARG:NH2  | 2.38                     | 0.56              |
| 2:J:593:ASP:OD2  | 2:J:595:LYS:N    | 2.38                     | 0.56              |
| 1:d:75:TRP:CE2   | 1:d:144:GLY:HA3  | 2.40                     | 0.56              |
| 1:B:37:LEU:HD13  | 1:B:88:GLU:HG2   | 1.86                     | 0.56              |
| 1:d:122:ILE:HG12 | 1:d:145:MET:HE1  | 1.87                     | 0.56              |
| 3:P:55:LYS:HE3   | 3:P:55:LYS:HA    | 1.88                     | 0.56              |
| 1:h:130:ALA:HB3  | 1:q:45:LEU:HB3   | 1.87                     | 0.56              |
| 1:D:83:TYR:HB2   | 1:D:138:TYR:HB3  | 1.88                     | 0.56              |
| 1:F:46:THR:HG22  | 1:p:129:GLU:HG3  | 1.88                     | 0.56              |
| 1:c:72:MET:HB3   | 1:C:66:LYS:HE3   | 1.88                     | 0.56              |
| 3:P:6:LEU:HG     | 3:P:92:ILE:HG22  | 1.88                     | 0.56              |
| 1:n:72:MET:HE3   | 1:n:72:MET:HA    | 1.88                     | 0.56              |
| 1:b:4:GLU:OE2    | 1:b:8:TYR:OH     | 2.24                     | 0.55              |
| 1:c:125:ASP:HB3  | 1:c:141:LYS:HB3  | 1.88                     | 0.55              |
| 4:l:146:ASN:ND2  | 4:l:149:GLU:OE1  | 2.39                     | 0.55              |
| 1:o:11:TYR:OH    | 1:p:102:PRO:O    | 2.20                     | 0.55              |
| 3:K:52:THR:O     | 3:s:87:ARG:NH1   | 2.39                     | 0.55              |
| 1:A:102:PRO:HB2  | 1:A:120:LEU:HD22 | 1.87                     | 0.55              |
| 5:m:91:GLY:O     | 5:m:92:GLU:HG2   | 2.06                     | 0.55              |
| 3:X:95:ASP:N     | 3:X:95:ASP:OD1   | 2.39                     | 0.55              |
| 1:F:51:LYS:HE2   | 1:F:73:LYS:HE3   | 1.89                     | 0.55              |
| 1:N:107:ILE:HG22 | 1:N:116:LEU:HB2  | 1.89                     | 0.55              |
| 1:N:127:SER:HG   | 1:N:139:SER:HG   | 1.54                     | 0.55              |
| 4:Q:272:GLU:OE1  | 4:Q:329:ARG:NH1  | 2.40                     | 0.55              |
| 1:h:52:ASP:N     | 1:h:52:ASP:OD1   | 2.39                     | 0.55              |
| 3:K:195:ASN:OD1  | 3:K:217:LYS:N    | 2.39                     | 0.55              |
| 4:L:268:LEU:HD11 | 4:L:270:VAL:HG12 | 1.89                     | 0.55              |
| 1:c:102:PRO:HB2  | 1:c:120:LEU:HD22 | 1.88                     | 0.55              |
| 5:M:94:LYS:HE2   | 2:O:600:VAL:HG11 | 1.89                     | 0.55              |
| 4:Q:98:VAL:HA    | 4:Q:146:ASN:HA   | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:30:ASN:ND2   | 1:T:34:ASP:OD1   | 2.35                     | 0.55              |
| 1:d:25:ILE:HD11  | 1:d:42:GLN:NE2   | 2.22                     | 0.55              |
| 1:D:58:SER:OG    | 1:D:60:ASP:OD1   | 2.21                     | 0.54              |
| 1:b:113:LYS:HA   | 1:b:160:MET:HE1  | 1.90                     | 0.54              |
| 4:L:243:ARG:NH2  | 4:l:57:GLU:OE1   | 2.40                     | 0.54              |
| 3:X:103:GLU:OE1  | 3:X:129:LYS:NZ   | 2.34                     | 0.54              |
| 3:j:99:GLY:HA3   | 3:j:150:GLN:HG2  | 1.89                     | 0.54              |
| 1:o:44:GLY:O     | 1:o:79:ASN:ND2   | 2.40                     | 0.54              |
| 4:Q:211:GLY:N    | 4:Q:228:ALA:O    | 2.39                     | 0.54              |
| 1:V:72:MET:HE3   | 1:V:72:MET:HA    | 1.89                     | 0.54              |
| 3:X:216:GLN:OE1  | 3:X:218:THR:N    | 2.29                     | 0.54              |
| 1:C:160:MET:HG3  | 1:C:161:PRO:HD2  | 1.89                     | 0.54              |
| 1:V:122:ILE:HG23 | 1:V:145:MET:HE1  | 1.89                     | 0.54              |
| 4:L:201:ASP:OD2  | 4:L:329:ARG:NH2  | 2.41                     | 0.54              |
| 3:k:153:MET:HE3  | 3:k:153:MET:H    | 1.73                     | 0.54              |
| 1:H:58:SER:OG    | 1:H:60:ASP:OD1   | 2.26                     | 0.54              |
| 1:H:30:ASN:HD21  | 1:H:35:LYS:H     | 1.55                     | 0.54              |
| 1:a:109:ASN:HD21 | 1:a:112:SER:HB3  | 1.72                     | 0.54              |
| 1:S:109:ASN:HD21 | 1:S:112:SER:HB3  | 1.71                     | 0.54              |
| 1:U:131:PRO:HG2  | 1:U:134:GLU:HG2  | 1.88                     | 0.54              |
| 3:X:104:VAL:HG12 | 3:X:127:VAL:HG22 | 1.89                     | 0.54              |
| 1:Y:28:VAL:HG12  | 1:Y:105:VAL:HG12 | 1.90                     | 0.54              |
| 3:s:199:THR:HB   | 3:s:256:LYS:HG3  | 1.89                     | 0.54              |
| 1:B:84:VAL:HG23  | 1:B:87:ALA:HB2   | 1.89                     | 0.54              |
| 1:h:26:LEU:HD21  | 1:h:105:VAL:HG12 | 1.90                     | 0.54              |
| 1:D:28:VAL:HG12  | 1:D:105:VAL:HG12 | 1.90                     | 0.54              |
| 1:q:41:GLY:O     | 1:q:82:LEU:N     | 2.41                     | 0.54              |
| 3:K:44:THR:HG23  | 4:L:188:LEU:HD22 | 1.90                     | 0.53              |
| 1:c:123:VAL:HA   | 1:c:142:LEU:HD23 | 1.91                     | 0.53              |
| 3:j:88:ASP:OD1   | 3:j:88:ASP:N     | 2.41                     | 0.53              |
| 1:o:86:ASP:N     | 1:o:86:ASP:OD1   | 2.38                     | 0.53              |
| 1:q:75:TRP:CE2   | 1:q:144:GLY:HA3  | 2.43                     | 0.53              |
| 1:e:51:LYS:HE2   | 1:e:73:LYS:HE3   | 1.90                     | 0.53              |
| 1:D:57:THR:HG21  | 1:D:66:LYS:HB2   | 1.90                     | 0.53              |
| 3:K:113:ARG:HG2  | 1:g:59:LYS:HD3   | 1.89                     | 0.53              |
| 5:M:81:SER:HB3   | 2:O:579:LEU:HD21 | 1.89                     | 0.53              |
| 1:N:129:GLU:HG3  | 1:N:131:PRO:HD3  | 1.90                     | 0.53              |
| 1:U:97:PHE:O     | 1:e:73:LYS:NZ    | 2.35                     | 0.53              |
| 1:n:133:ASP:OD1  | 1:n:133:ASP:N    | 2.41                     | 0.53              |
| 1:o:75:TRP:CE2   | 1:o:144:GLY:HA3  | 2.44                     | 0.53              |
| 5:M:79:ASN:O     | 5:M:83:PHE:HB2   | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Q:146:ASN:ND2  | 4:Q:149:GLU:OE1  | 2.42                     | 0.53              |
| 1:S:72:MET:HB3   | 1:Y:66:LYS:HE3   | 1.91                     | 0.53              |
| 1:V:123:VAL:HA   | 1:V:142:LEU:HG   | 1.91                     | 0.53              |
| 3:X:183:LEU:HD21 | 4:l:186:ARG:HD2  | 1.89                     | 0.53              |
| 3:X:223:LEU:HD23 | 3:X:228:PRO:HB3  | 1.90                     | 0.53              |
| 1:N:44:GLY:O     | 1:N:79:ASN:ND2   | 2.41                     | 0.53              |
| 1:Z:72:MET:HE3   | 1:Z:72:MET:HA    | 1.91                     | 0.53              |
| 1:h:36:LEU:HD23  | 1:h:161:PRO:HG2  | 1.90                     | 0.53              |
| 3:s:35:SER:HB3   | 3:s:53:GLN:HG3   | 1.89                     | 0.53              |
| 5:R:94:LYS:HD2   | 2:i:600:VAL:HG11 | 1.91                     | 0.53              |
| 4:l:112:GLN:HG3  | 4:l:130:ILE:HD12 | 1.90                     | 0.53              |
| 1:q:113:LYS:HA   | 1:q:160:MET:HE1  | 1.91                     | 0.53              |
| 1:g:122:ILE:HG22 | 1:g:145:MET:HE2  | 1.91                     | 0.53              |
| 3:k:199:THR:HB   | 3:k:256:LYS:HG3  | 1.90                     | 0.53              |
| 1:N:122:ILE:HG23 | 1:N:145:MET:HE1  | 1.90                     | 0.53              |
| 3:s:88:ASP:OD1   | 3:s:88:ASP:N     | 2.42                     | 0.53              |
| 3:s:167:GLU:OE2  | 3:s:167:GLU:N    | 2.39                     | 0.53              |
| 1:B:72:MET:HA    | 1:B:72:MET:HE3   | 1.89                     | 0.53              |
| 3:P:44:THR:HG23  | 4:Q:188:LEU:HD22 | 1.90                     | 0.53              |
| 1:D:66:LYS:HE3   | 1:n:72:MET:HB3   | 1.89                     | 0.53              |
| 1:H:52:ASP:N     | 1:H:52:ASP:OD1   | 2.40                     | 0.53              |
| 3:K:146:VAL:HG13 | 3:K:148:LEU:HB2  | 1.90                     | 0.53              |
| 3:k:95:ASP:OD1   | 3:k:95:ASP:N     | 2.42                     | 0.53              |
| 1:C:30:ASN:HD21  | 1:C:35:LYS:H     | 1.55                     | 0.53              |
| 1:U:74:GLU:OE1   | 1:e:68:LYS:NZ    | 2.35                     | 0.53              |
| 1:d:92:GLU:O     | 1:d:96:TYR:HD1   | 1.92                     | 0.53              |
| 1:d:122:ILE:HG23 | 1:d:145:MET:HE1  | 1.91                     | 0.53              |
| 1:C:130:ALA:HB2  | 1:C:136:MET:HG3  | 1.91                     | 0.53              |
| 1:p:125:ASP:HB3  | 1:p:141:LYS:HB3  | 1.91                     | 0.53              |
| 1:q:31:ALA:N     | 1:q:92:GLU:OE1   | 2.35                     | 0.53              |
| 1:E:108:ILE:HG22 | 1:E:115:GLY:HA2  | 1.91                     | 0.52              |
| 1:a:74:GLU:HB3   | 1:A:66:LYS:HD2   | 1.90                     | 0.52              |
| 1:b:2:ALA:HB3    | 1:c:33:GLY:HA3   | 1.91                     | 0.52              |
| 1:B:28:VAL:HG12  | 1:B:105:VAL:HG12 | 1.89                     | 0.52              |
| 1:h:44:GLY:O     | 1:h:79:ASN:ND2   | 2.42                     | 0.52              |
| 4:L:193:GLU:OE2  | 4:l:75:LYS:NZ    | 2.39                     | 0.52              |
| 1:V:113:LYS:HA   | 1:V:160:MET:HE1  | 1.92                     | 0.52              |
| 3:P:178:ASP:OD2  | 3:P:272:ARG:NH2  | 2.43                     | 0.52              |
| 1:V:41:GLY:O     | 1:V:82:LEU:N     | 2.43                     | 0.52              |
| 1:F:43:GLN:HB2   | 1:F:81:GLY:HA2   | 1.91                     | 0.52              |
| 1:D:66:LYS:HD2   | 1:n:74:GLU:HB3   | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:45:LEU:HD21  | 1:E:107:ILE:HD13 | 1.91                     | 0.52              |
| 1:F:30:ASN:OD1   | 1:F:33:GLY:N     | 2.40                     | 0.52              |
| 1:H:159:GLN:HB3  | 1:H:161:PRO:HD2  | 1.91                     | 0.52              |
| 2:O:593:ASP:OD1  | 2:O:595:LYS:N    | 2.43                     | 0.52              |
| 3:X:199:THR:HB   | 3:X:256:LYS:HG3  | 1.91                     | 0.52              |
| 3:j:44:THR:HG23  | 4:l:188:LEU:HD22 | 1.92                     | 0.52              |
| 4:L:360:MET:HE1  | 4:Q:359:ALA:HA   | 1.92                     | 0.52              |
| 1:H:130:ALA:N    | 1:d:45:LEU:O     | 2.40                     | 0.52              |
| 1:g:107:ILE:C    | 1:g:108:ILE:HD13 | 2.35                     | 0.52              |
| 1:a:72:MET:HB3   | 1:A:66:LYS:HE3   | 1.92                     | 0.52              |
| 4:Q:75:LYS:NZ    | 4:l:193:GLU:OE2  | 2.41                     | 0.52              |
| 1:q:45:LEU:HD23  | 1:q:79:ASN:HB2   | 1.91                     | 0.52              |
| 1:q:145:MET:SD   | 1:q:145:MET:N    | 2.67                     | 0.52              |
| 1:F:9:CYS:HB3    | 1:F:11:TYR:HE2   | 1.75                     | 0.51              |
| 3:j:195:ASN:OD1  | 3:j:217:LYS:N    | 2.42                     | 0.51              |
| 3:s:254:GLU:OE2  | 3:s:256:LYS:NZ   | 2.38                     | 0.51              |
| 2:J:590:ILE:HG23 | 5:M:92:GLU:H     | 1.75                     | 0.51              |
| 5:R:94:LYS:HG2   | 2:i:600:VAL:HG21 | 1.92                     | 0.51              |
| 1:S:4:GLU:OE1    | 1:S:8:TYR:OH     | 2.23                     | 0.51              |
| 1:T:11:TYR:OH    | 1:U:102:PRO:O    | 2.23                     | 0.51              |
| 1:T:75:TRP:CE2   | 1:T:144:GLY:HA3  | 2.45                     | 0.51              |
| 5:m:95:ALA:HB3   | 5:m:97:LYS:HZ1   | 1.75                     | 0.51              |
| 1:H:26:LEU:HD21  | 1:H:105:VAL:HG13 | 1.92                     | 0.51              |
| 4:L:112:GLN:HG3  | 4:L:130:ILE:HD12 | 1.91                     | 0.51              |
| 1:b:107:ILE:HG22 | 1:b:116:LEU:HB2  | 1.91                     | 0.51              |
| 3:k:142:MET:HA   | 3:k:142:MET:HE2  | 1.92                     | 0.51              |
| 3:s:146:VAL:HG23 | 3:s:147:ASP:H    | 1.75                     | 0.51              |
| 1:h:143:ASP:OD1  | 1:h:143:ASP:N    | 2.44                     | 0.51              |
| 3:j:29:ARG:NH2   | 3:j:272:ARG:O    | 2.44                     | 0.51              |
| 3:j:70:ILE:HG23  | 3:j:113:ARG:HH22 | 1.74                     | 0.51              |
| 4:L:227:MET:SD   | 4:L:227:MET:N    | 2.78                     | 0.51              |
| 4:L:295:HIS:CD2  | 4:L:297:PRO:HG2  | 2.46                     | 0.51              |
| 1:d:95:LYS:O     | 1:d:99:SER:OG    | 2.23                     | 0.51              |
| 1:A:28:VAL:HG12  | 1:A:105:VAL:HG12 | 1.93                     | 0.51              |
| 1:T:77:ILE:HD13  | 1:T:107:ILE:HD11 | 1.93                     | 0.51              |
| 1:Z:72:MET:HB3   | 1:o:66:LYS:HE2   | 1.93                     | 0.51              |
| 1:e:30:ASN:OD1   | 1:e:33:GLY:N     | 2.39                     | 0.51              |
| 1:B:125:ASP:HB3  | 1:B:141:LYS:HB3  | 1.93                     | 0.51              |
| 3:X:113:ARG:NH1  | 1:f:60:ASP:OD1   | 2.39                     | 0.51              |
| 1:B:113:LYS:HB3  | 1:B:160:MET:HE3  | 1.91                     | 0.51              |
| 1:T:2:ALA:HB3    | 1:U:33:GLY:HA3   | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:125:ASP:HB3  | 1:Z:141:LYS:HB3  | 1.92                     | 0.51              |
| 1:p:4:GLU:OE1    | 1:p:8:TYR:OH     | 2.24                     | 0.51              |
| 1:D:72:MET:HA    | 1:D:72:MET:HE3   | 1.93                     | 0.51              |
| 1:H:51:LYS:HZ1   | 1:q:123:VAL:HG13 | 1.76                     | 0.51              |
| 3:K:99:GLY:HA3   | 3:K:150:GLN:HG2  | 1.92                     | 0.51              |
| 1:B:108:ILE:HG22 | 1:B:115:GLY:HA2  | 1.93                     | 0.51              |
| 1:S:10:ASP:OD1   | 1:S:10:ASP:N     | 2.43                     | 0.51              |
| 1:Y:133:ASP:OD1  | 1:Y:133:ASP:N    | 2.44                     | 0.51              |
| 1:b:75:TRP:CE2   | 1:b:144:GLY:HA3  | 2.46                     | 0.51              |
| 1:V:122:ILE:HG12 | 1:V:145:MET:HE1  | 1.93                     | 0.51              |
| 1:h:107:ILE:HG22 | 1:h:116:LEU:HB2  | 1.92                     | 0.51              |
| 1:D:95:LYS:O     | 1:D:99:SER:OG    | 2.24                     | 0.51              |
| 1:d:79:ASN:ND2   | 1:d:140:VAL:HB   | 2.25                     | 0.51              |
| 4:Q:201:ASP:OD2  | 4:Q:329:ARG:NH2  | 2.43                     | 0.51              |
| 4:l:211:GLY:N    | 4:l:228:ALA:O    | 2.38                     | 0.51              |
| 1:S:125:ASP:HB3  | 1:S:141:LYS:HB3  | 1.93                     | 0.50              |
| 3:X:87:ARG:NH1   | 3:j:52:THR:O     | 2.45                     | 0.50              |
| 3:s:116:ASP:N    | 3:s:116:ASP:OD1  | 2.44                     | 0.50              |
| 1:h:58:SER:OG    | 1:h:60:ASP:OD1   | 2.28                     | 0.50              |
| 1:A:83:TYR:HB2   | 1:A:138:TYR:HB3  | 1.93                     | 0.50              |
| 1:D:47:VAL:HG22  | 1:D:77:ILE:HG12  | 1.94                     | 0.50              |
| 4:L:146:ASN:ND2  | 4:L:149:GLU:OE1  | 2.44                     | 0.50              |
| 3:k:35:SER:HB3   | 3:k:53:GLN:HG3   | 1.93                     | 0.50              |
| 1:N:86:ASP:OD2   | 1:N:86:ASP:N     | 2.33                     | 0.50              |
| 1:Z:84:VAL:HG23  | 1:Z:87:ALA:HB2   | 1.93                     | 0.50              |
| 1:a:10:ASP:OD1   | 1:a:10:ASP:N     | 2.44                     | 0.50              |
| 4:Q:214:LYS:HG3  | 4:Q:227:MET:HE3  | 1.94                     | 0.50              |
| 4:Q:295:HIS:CD2  | 4:Q:297:PRO:HG2  | 2.47                     | 0.50              |
| 3:X:254:GLU:OE2  | 3:X:256:LYS:NZ   | 2.40                     | 0.50              |
| 4:l:19:ASP:OD2   | 4:l:44:THR:OG1   | 2.23                     | 0.50              |
| 5:m:83:PHE:CZ    | 5:m:87:VAL:HG11  | 2.47                     | 0.50              |
| 3:s:103:GLU:OE1  | 3:s:129:LYS:NZ   | 2.34                     | 0.50              |
| 1:N:143:ASP:N    | 1:N:143:ASP:OD1  | 2.43                     | 0.50              |
| 3:P:195:ASN:OD1  | 3:P:217:LYS:N    | 2.44                     | 0.50              |
| 4:Q:19:ASP:OD2   | 4:Q:44:THR:OG1   | 2.22                     | 0.50              |
| 1:V:56:ILE:HD13  | 1:V:69:ILE:HG13  | 1.92                     | 0.50              |
| 1:V:85:ALA:O     | 1:V:91:LYS:NZ    | 2.44                     | 0.50              |
| 1:Z:80:ASP:OD1   | 1:Z:81:GLY:N     | 2.45                     | 0.50              |
| 3:j:226:ILE:HG22 | 3:j:243:ILE:HG21 | 1.94                     | 0.50              |
| 4:l:295:HIS:CD2  | 4:l:297:PRO:HG2  | 2.47                     | 0.50              |
| 1:F:72:MET:HG3   | 1:c:66:LYS:HB3   | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:87:ALA:O     | 1:h:91:LYS:HG3   | 2.12                     | 0.50              |
| 3:s:11:LYS:HE3   | 3:s:13:HIS:HE2   | 1.76                     | 0.50              |
| 1:F:68:LYS:NZ    | 1:p:74:GLU:OE1   | 2.31                     | 0.50              |
| 1:N:23:ASP:HA    | 1:N:110:GLN:NE2  | 2.25                     | 0.50              |
| 1:N:79:ASN:HB3   | 1:N:140:VAL:HG23 | 1.94                     | 0.50              |
| 1:Z:108:ILE:HG22 | 1:Z:115:GLY:HA2  | 1.93                     | 0.50              |
| 4:L:214:LYS:HG3  | 4:L:227:MET:HE3  | 1.92                     | 0.49              |
| 1:b:30:ASN:ND2   | 1:b:35:LYS:H     | 2.10                     | 0.49              |
| 1:H:75:TRP:CZ2   | 1:H:144:GLY:HA3  | 2.47                     | 0.49              |
| 4:L:20:ILE:HG12  | 4:L:41:VAL:HG13  | 1.94                     | 0.49              |
| 4:l:52:ASP:OD1   | 4:l:52:ASP:N     | 2.46                     | 0.49              |
| 1:A:86:ASP:N     | 1:A:86:ASP:OD1   | 2.43                     | 0.49              |
| 3:s:104:VAL:HG12 | 3:s:127:VAL:HG22 | 1.95                     | 0.49              |
| 2:J:593:ASP:OD2  | 2:J:594:ASP:N    | 2.45                     | 0.49              |
| 1:V:143:ASP:OD1  | 1:V:143:ASP:N    | 2.44                     | 0.49              |
| 1:W:34:ASP:OD1   | 1:W:34:ASP:N     | 2.45                     | 0.49              |
| 3:X:116:ASP:N    | 3:X:116:ASP:OD1  | 2.44                     | 0.49              |
| 1:E:125:ASP:HB3  | 1:E:141:LYS:HB3  | 1.95                     | 0.49              |
| 1:H:64:GLY:O     | 1:q:73:LYS:NZ    | 2.38                     | 0.49              |
| 3:k:75:LEU:HD21  | 3:P:152:GLY:HA3  | 1.93                     | 0.49              |
| 2:O:575:ARG:HH22 | 2:O:576:VAL:HG22 | 1.78                     | 0.49              |
| 5:R:94:LYS:HZ2   | 5:R:94:LYS:HB2   | 1.78                     | 0.49              |
| 1:h:23:ASP:HA    | 1:h:110:GLN:NE2  | 2.26                     | 0.49              |
| 4:l:214:LYS:HG3  | 4:l:227:MET:HE3  | 1.94                     | 0.49              |
| 3:K:14:SER:HB3   | 3:K:17:GLU:HB2   | 1.95                     | 0.49              |
| 1:Y:58:SER:OG    | 1:Y:60:ASP:OD1   | 2.21                     | 0.49              |
| 1:q:115:GLY:N    | 1:q:158:ASP:OD1  | 2.45                     | 0.49              |
| 3:s:202:ASN:O    | 3:s:206:GLY:N    | 2.46                     | 0.49              |
| 1:F:83:TYR:HB2   | 1:F:138:TYR:HB3  | 1.94                     | 0.49              |
| 4:Q:112:GLN:HG3  | 4:Q:130:ILE:HD12 | 1.93                     | 0.49              |
| 1:n:33:GLY:HA3   | 1:r:2:ALA:HB3    | 1.94                     | 0.49              |
| 1:c:135:ALA:HA   | 1:C:20:ALA:HA    | 1.95                     | 0.49              |
| 1:A:75:TRP:CE2   | 1:A:148:LEU:HB2  | 2.48                     | 0.49              |
| 3:X:146:VAL:HG23 | 3:X:147:ASP:N    | 2.28                     | 0.49              |
| 1:e:43:GLN:HB2   | 1:e:81:GLY:HA2   | 1.95                     | 0.49              |
| 1:n:4:GLU:OE1    | 1:n:8:TYR:OH     | 2.25                     | 0.49              |
| 3:K:45:ASP:CG    | 3:j:87:ARG:HH22  | 2.21                     | 0.49              |
| 1:b:28:VAL:HG12  | 1:b:105:VAL:HG12 | 1.95                     | 0.49              |
| 1:d:113:LYS:HA   | 1:d:160:MET:HE1  | 1.95                     | 0.49              |
| 1:N:30:ASN:CG    | 1:N:33:GLY:H     | 2.20                     | 0.49              |
| 4:Q:211:GLY:HA3  | 4:Q:228:ALA:HB3  | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:s:146:VAL:HG23 | 3:s:147:ASP:N    | 2.27                     | 0.49              |
| 3:k:104:VAL:HG12 | 3:k:127:VAL:HG22 | 1.93                     | 0.49              |
| 1:T:102:PRO:HB3  | 1:T:145:MET:SD   | 2.53                     | 0.49              |
| 1:f:99:SER:O     | 1:f:101:SER:OG   | 2.24                     | 0.49              |
| 3:j:202:ASN:ND2  | 3:j:245:THR:O    | 2.46                     | 0.49              |
| 4:l:218:ASP:OD1  | 4:l:219:LYS:NZ   | 2.31                     | 0.49              |
| 1:r:113:LYS:C    | 1:r:160:MET:HE1  | 2.37                     | 0.49              |
| 2:J:575:ARG:HH22 | 2:J:576:VAL:HG23 | 1.78                     | 0.48              |
| 1:N:75:TRP:CE2   | 1:N:144:GLY:HA3  | 2.47                     | 0.48              |
| 1:U:4:GLU:OE1    | 1:U:8:TYR:OH     | 2.28                     | 0.48              |
| 1:U:30:ASN:HD22  | 1:U:35:LYS:HB2   | 1.78                     | 0.48              |
| 1:V:151:LEU:HA   | 1:V:154:THR:HG22 | 1.93                     | 0.48              |
| 4:l:330:ASP:OD1  | 4:l:331:MET:N    | 2.46                     | 0.48              |
| 3:k:150:GLN:NE2  | 3:k:175:ALA:O    | 2.46                     | 0.48              |
| 3:k:183:LEU:HD21 | 4:Q:186:ARG:HD2  | 1.95                     | 0.48              |
| 3:k:254:GLU:OE2  | 3:k:256:LYS:NZ   | 2.40                     | 0.48              |
| 1:I:113:LYS:HA   | 1:I:160:MET:HE1  | 1.93                     | 0.48              |
| 1:T:113:LYS:HA   | 1:T:160:MET:HE2  | 1.94                     | 0.48              |
| 1:H:87:ALA:O     | 1:H:91:LYS:HG3   | 2.14                     | 0.48              |
| 1:d:43:GLN:HB2   | 1:d:81:GLY:HA2   | 1.94                     | 0.48              |
| 5:m:84:LYS:HG3   | 5:m:85:ILE:HD12  | 1.95                     | 0.48              |
| 1:r:25:ILE:HG13  | 1:r:108:ILE:HG23 | 1.96                     | 0.48              |
| 1:W:154:THR:OG1  | 1:W:155:GLU:N    | 2.46                     | 0.48              |
| 1:Z:45:LEU:HD21  | 1:Z:107:ILE:HD13 | 1.95                     | 0.48              |
| 4:l:211:GLY:HA3  | 4:l:228:ALA:HB3  | 1.95                     | 0.48              |
| 4:L:211:GLY:HA3  | 4:L:228:ALA:HB3  | 1.95                     | 0.48              |
| 2:i:575:ARG:HA   | 2:i:578:ASN:HB3  | 1.95                     | 0.48              |
| 3:j:14:SER:HB3   | 3:j:17:GLU:HB2   | 1.95                     | 0.48              |
| 4:L:75:LYS:HD3   | 4:L:77:ILE:HD11  | 1.96                     | 0.48              |
| 5:M:84:LYS:O     | 5:M:88:THR:HG23  | 2.14                     | 0.48              |
| 1:c:26:LEU:HD23  | 1:c:79:ASN:HD22  | 1.79                     | 0.48              |
| 1:d:143:ASP:OD1  | 1:d:143:ASP:N    | 2.45                     | 0.48              |
| 4:Q:95:GLN:HB3   | 4:Q:148:LEU:HB2  | 1.95                     | 0.48              |
| 1:h:75:TRP:CZ2   | 1:h:144:GLY:HA3  | 2.48                     | 0.48              |
| 3:k:159:ASP:OD1  | 3:k:159:ASP:N    | 2.37                     | 0.48              |
| 1:N:30:ASN:ND2   | 1:N:35:LYS:H     | 2.10                     | 0.48              |
| 1:W:29:PHE:HB2   | 1:W:104:CYS:HB3  | 1.95                     | 0.48              |
| 1:n:107:ILE:HG22 | 1:n:116:LEU:HB2  | 1.96                     | 0.48              |
| 1:H:143:ASP:OD1  | 1:H:143:ASP:N    | 2.45                     | 0.48              |
| 3:K:113:ARG:NH1  | 1:g:60:ASP:OD1   | 2.45                     | 0.48              |
| 4:L:283:GLU:OE2  | 3:s:227:TYR:OH   | 2.27                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:44:GLY:O     | 1:a:79:ASN:ND2   | 2.46                     | 0.48              |
| 1:a:147:ALA:HA   | 1:A:65:TRP:CG    | 2.49                     | 0.48              |
| 1:d:59:LYS:HG2   | 1:p:22:LYS:HA    | 1.96                     | 0.48              |
| 1:T:125:ASP:OD1  | 1:T:127:SER:OG   | 2.27                     | 0.48              |
| 1:Y:3:PHE:O      | 1:Y:4:GLU:HB2    | 2.13                     | 0.48              |
| 1:h:159:GLN:HB3  | 1:h:161:PRO:HD2  | 1.96                     | 0.48              |
| 3:j:202:ASN:O    | 3:j:206:GLY:N    | 2.43                     | 0.48              |
| 4:l:363:TYR:O    | 4:l:367:ILE:HG12 | 2.14                     | 0.48              |
| 1:p:75:TRP:CE2   | 1:p:148:LEU:HB2  | 2.49                     | 0.48              |
| 1:r:34:ASP:OD1   | 1:r:34:ASP:N     | 2.46                     | 0.48              |
| 1:g:102:PRO:HB3  | 1:g:145:MET:HE1  | 1.95                     | 0.48              |
| 3:P:14:SER:HB3   | 3:P:17:GLU:HB2   | 1.96                     | 0.48              |
| 1:S:33:GLY:HA3   | 1:W:2:ALA:HB3    | 1.96                     | 0.48              |
| 1:T:75:TRP:CE2   | 1:T:148:LEU:HB2  | 2.49                     | 0.48              |
| 1:V:132:PHE:HB2  | 1:h:43:GLN:OE1   | 2.14                     | 0.48              |
| 1:H:103:VAL:HG13 | 1:H:105:VAL:HG23 | 1.96                     | 0.47              |
| 4:L:57:GLU:OE1   | 4:Q:243:ARG:NH2  | 2.42                     | 0.47              |
| 1:A:3:PHE:O      | 1:A:4:GLU:HB2    | 2.14                     | 0.47              |
| 1:q:143:ASP:OD1  | 1:q:143:ASP:N    | 2.47                     | 0.47              |
| 1:D:3:PHE:O      | 1:D:4:GLU:HB2    | 2.13                     | 0.47              |
| 1:H:4:GLU:O      | 1:H:5:GLU:HG3    | 2.14                     | 0.47              |
| 1:A:149:VAL:HB   | 1:I:8:TYR:HB3    | 1.96                     | 0.47              |
| 1:N:26:LEU:HD21  | 1:N:105:VAL:HG12 | 1.96                     | 0.47              |
| 1:e:114:LYS:HD2  | 1:e:114:LYS:HA   | 1.74                     | 0.47              |
| 1:H:106:LYS:HZ3  | 1:H:159:GLN:H    | 1.62                     | 0.47              |
| 3:K:211:TYR:CZ   | 3:K:213:LYS:HB2  | 2.49                     | 0.47              |
| 1:b:102:PRO:HB3  | 1:b:145:MET:SD   | 2.55                     | 0.47              |
| 1:g:34:ASP:OD1   | 1:g:34:ASP:N     | 2.45                     | 0.47              |
| 1:C:43:GLN:HB2   | 1:C:81:GLY:HA2   | 1.95                     | 0.47              |
| 4:Q:358:ILE:HA   | 4:Q:361:ASN:HB2  | 1.95                     | 0.47              |
| 1:S:74:GLU:HB3   | 1:Y:66:LYS:HD2   | 1.96                     | 0.47              |
| 1:W:30:ASN:OD1   | 1:W:31:ALA:N     | 2.47                     | 0.47              |
| 1:Y:75:TRP:CE2   | 1:Y:148:LEU:HB2  | 2.49                     | 0.47              |
| 1:o:30:ASN:ND2   | 1:o:35:LYS:H     | 2.12                     | 0.47              |
| 1:r:29:PHE:HB2   | 1:r:104:CYS:HB3  | 1.96                     | 0.47              |
| 1:G:75:TRP:CE2   | 1:G:148:LEU:HB2  | 2.49                     | 0.47              |
| 3:K:105:HIS:ND1  | 3:k:36:MET:SD    | 2.88                     | 0.47              |
| 3:K:204:THR:HG23 | 3:K:252:ASP:H    | 1.78                     | 0.47              |
| 4:Q:57:GLU:OE1   | 4:l:243:ARG:NH2  | 2.36                     | 0.47              |
| 1:U:27:ALA:HB1   | 1:U:36:LEU:HG    | 1.96                     | 0.47              |
| 1:e:109:ASN:HB2  | 1:e:116:LEU:HD11 | 1.95                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:10:ASP:OD1   | 1:n:10:ASP:N     | 2.43                     | 0.47              |
| 1:n:109:ASN:ND2  | 1:n:109:ASN:C    | 2.71                     | 0.47              |
| 1:H:9:CYS:SG     | 1:H:10:ASP:N     | 2.87                     | 0.47              |
| 1:H:79:ASN:HB3   | 1:H:140:VAL:HG23 | 1.96                     | 0.47              |
| 3:X:227:TYR:OH   | 4:l:283:GLU:OE2  | 2.25                     | 0.47              |
| 1:e:125:ASP:HB3  | 1:e:141:LYS:HB3  | 1.96                     | 0.47              |
| 1:r:30:ASN:OD1   | 1:r:31:ALA:N     | 2.48                     | 0.47              |
| 1:a:113:LYS:HD2  | 1:a:113:LYS:HA   | 1.71                     | 0.47              |
| 1:d:30:ASN:ND2   | 1:d:35:LYS:H     | 2.11                     | 0.47              |
| 1:A:4:GLU:OE2    | 1:B:106:LYS:NZ   | 2.46                     | 0.47              |
| 1:A:72:MET:HB3   | 1:S:66:LYS:HE2   | 1.97                     | 0.47              |
| 1:C:3:PHE:HE2    | 1:N:33:GLY:HA3   | 1.80                     | 0.47              |
| 3:P:202:ASN:ND2  | 3:P:245:THR:O    | 2.47                     | 0.47              |
| 4:Q:70:LYS:HA    | 4:Q:70:LYS:HD3   | 1.71                     | 0.47              |
| 3:X:241:HIS:O    | 4:l:186:ARG:NH2  | 2.35                     | 0.47              |
| 1:h:75:TRP:CE2   | 1:h:144:GLY:HA3  | 2.49                     | 0.47              |
| 1:E:72:MET:HB3   | 1:b:66:LYS:HE2   | 1.95                     | 0.47              |
| 1:E:75:TRP:CD2   | 1:E:148:LEU:HD12 | 2.50                     | 0.47              |
| 1:F:108:ILE:HG22 | 1:F:115:GLY:HA2  | 1.96                     | 0.47              |
| 1:G:113:LYS:HA   | 1:G:160:MET:HE1  | 1.95                     | 0.47              |
| 4:L:335:GLN:HE22 | 4:l:335:GLN:NE2  | 2.12                     | 0.47              |
| 1:C:77:ILE:HD13  | 1:C:107:ILE:HD11 | 1.97                     | 0.47              |
| 1:N:75:TRP:CZ2   | 1:N:144:GLY:HA3  | 2.50                     | 0.47              |
| 1:Y:55:GLU:HG2   | 1:Y:57:THR:HG22  | 1.96                     | 0.47              |
| 1:e:30:ASN:ND2   | 1:e:35:LYS:O     | 2.48                     | 0.47              |
| 2:i:575:ARG:O    | 2:i:575:ARG:NH1  | 2.48                     | 0.47              |
| 1:o:121:ALA:HA   | 1:o:144:GLY:HA2  | 1.96                     | 0.47              |
| 1:H:145:MET:SD   | 1:H:145:MET:N    | 2.83                     | 0.47              |
| 2:J:605:GLN:HB3  | 4:L:331:MET:HE3  | 1.96                     | 0.47              |
| 4:L:182:GLU:HG3  | 3:s:234:ARG:HB3  | 1.97                     | 0.47              |
| 1:g:74:GLU:HB3   | 1:I:66:LYS:HD3   | 1.97                     | 0.47              |
| 1:Z:91:LYS:O     | 1:Z:95:LYS:NZ    | 2.46                     | 0.47              |
| 2:i:577:GLU:CD   | 5:m:75:LEU:HB3   | 2.40                     | 0.47              |
| 4:L:180:ARG:HH11 | 4:L:180:ARG:HB2  | 1.80                     | 0.47              |
| 1:c:30:ASN:HD22  | 1:c:35:LYS:HB2   | 1.80                     | 0.47              |
| 1:C:9:CYS:HB3    | 1:C:11:TYR:CE2   | 2.49                     | 0.47              |
| 4:Q:206:GLU:OE1  | 4:Q:233:THR:OG1  | 2.33                     | 0.47              |
| 1:T:30:ASN:ND2   | 1:T:35:LYS:H     | 2.13                     | 0.47              |
| 2:i:605:GLN:HB3  | 4:l:331:MET:HE3  | 1.97                     | 0.47              |
| 5:m:82:ASN:OD1   | 5:m:83:PHE:N     | 2.47                     | 0.47              |
| 1:c:27:ALA:HB1   | 1:c:36:LEU:HG    | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Q:204:LYS:HG3  | 4:Q:245:ALA:HB2  | 1.95                     | 0.47              |
| 1:h:74:GLU:HB3   | 1:q:66:LYS:HD2   | 1.97                     | 0.47              |
| 1:o:30:ASN:ND2   | 1:o:34:ASP:OD1   | 2.40                     | 0.47              |
| 1:q:30:ASN:ND2   | 1:q:35:LYS:H     | 2.11                     | 0.47              |
| 1:E:2:ALA:HB3    | 1:F:33:GLY:HA3   | 1.96                     | 0.46              |
| 3:k:146:VAL:HG23 | 3:k:147:ASP:N    | 2.28                     | 0.46              |
| 3:P:113:ARG:NH1  | 1:W:60:ASP:OD1   | 2.48                     | 0.46              |
| 1:V:30:ASN:ND2   | 1:V:35:LYS:H     | 2.12                     | 0.46              |
| 3:j:41:ILE:O     | 3:j:44:THR:OG1   | 2.33                     | 0.46              |
| 1:H:37:LEU:HG    | 1:H:89:SER:HB3   | 1.96                     | 0.46              |
| 1:d:132:PHE:HB2  | 1:N:43:GLN:O     | 2.15                     | 0.46              |
| 3:P:211:TYR:CZ   | 3:P:213:LYS:HB2  | 2.50                     | 0.46              |
| 1:h:45:LEU:HD11  | 1:h:107:ILE:HD11 | 1.98                     | 0.46              |
| 1:h:83:TYR:HB3   | 1:h:136:MET:SD   | 2.55                     | 0.46              |
| 5:m:79:ASN:HA    | 5:m:82:ASN:ND2   | 2.29                     | 0.46              |
| 3:K:148:LEU:HD23 | 3:K:148:LEU:HA   | 1.82                     | 0.46              |
| 1:N:113:LYS:HD2  | 1:N:113:LYS:HA   | 1.69                     | 0.46              |
| 1:Z:147:ALA:HA   | 1:o:65:TRP:CG    | 2.50                     | 0.46              |
| 1:D:65:TRP:CG    | 1:n:147:ALA:HA   | 2.51                     | 0.46              |
| 1:H:44:GLY:O     | 1:H:79:ASN:ND2   | 2.48                     | 0.46              |
| 1:N:123:VAL:HA   | 1:N:142:LEU:HG   | 1.97                     | 0.46              |
| 1:N:159:GLN:HB3  | 1:N:161:PRO:HD2  | 1.97                     | 0.46              |
| 1:h:129:GLU:HA   | 1:q:46:THR:HA    | 1.98                     | 0.46              |
| 4:l:207:ILE:HD13 | 4:l:245:ALA:HB3  | 1.96                     | 0.46              |
| 4:l:340:ASN:OD1  | 4:l:341:GLN:N    | 2.49                     | 0.46              |
| 1:N:58:SER:OG    | 1:N:60:ASP:OD1   | 2.31                     | 0.46              |
| 2:O:594:ASP:OD1  | 2:O:595:LYS:N    | 2.48                     | 0.46              |
| 1:W:113:LYS:C    | 1:W:160:MET:HE1  | 2.41                     | 0.46              |
| 2:i:575:ARG:NH1  | 2:i:579:LEU:HD23 | 2.31                     | 0.46              |
| 1:H:65:TRP:HZ3   | 1:q:75:TRP:HB3   | 1.80                     | 0.46              |
| 1:d:75:TRP:HB3   | 1:N:65:TRP:HZ3   | 1.80                     | 0.46              |
| 3:k:116:ASP:OD1  | 3:k:116:ASP:N    | 2.45                     | 0.46              |
| 1:C:147:ALA:HA   | 1:U:65:TRP:CG    | 2.50                     | 0.46              |
| 4:Q:75:LYS:HD3   | 4:Q:77:ILE:HD11  | 1.96                     | 0.46              |
| 1:U:125:ASP:HB3  | 1:U:141:LYS:HB3  | 1.98                     | 0.46              |
| 1:A:55:GLU:HG2   | 1:A:57:THR:HG22  | 1.96                     | 0.46              |
| 1:N:52:ASP:OD1   | 1:N:52:ASP:N     | 2.47                     | 0.46              |
| 3:P:217:LYS:NZ   | 3:P:260:ASP:O    | 2.45                     | 0.46              |
| 1:V:30:ASN:HD22  | 1:V:35:LYS:H     | 1.63                     | 0.46              |
| 1:V:43:GLN:HB2   | 1:V:81:GLY:HA2   | 1.97                     | 0.46              |
| 1:f:4:GLU:OE1    | 1:f:8:TYR:OH     | 2.27                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:28:VAL:HG12  | 1:f:105:VAL:HG12 | 1.96                     | 0.46              |
| 1:h:29:PHE:CD1   | 1:h:36:LEU:HD13  | 2.51                     | 0.46              |
| 4:l:95:GLN:HB3   | 4:l:148:LEU:HB2  | 1.97                     | 0.46              |
| 1:q:85:ALA:O     | 1:q:91:LYS:NZ    | 2.48                     | 0.46              |
| 1:r:105:VAL:HG21 | 1:r:142:LEU:HD13 | 1.98                     | 0.46              |
| 1:c:22:LYS:HA    | 1:V:59:LYS:HG2   | 1.97                     | 0.46              |
| 2:O:589:VAL:HA   | 5:R:91:GLY:HA3   | 1.98                     | 0.46              |
| 4:Q:331:MET:O    | 4:Q:335:GLN:HG2  | 2.15                     | 0.46              |
| 1:V:75:TRP:HB3   | 1:h:65:TRP:HZ3   | 1.81                     | 0.46              |
| 1:V:77:ILE:HD11  | 1:V:142:LEU:HB2  | 1.97                     | 0.46              |
| 1:h:30:ASN:ND2   | 1:h:35:LYS:H     | 2.12                     | 0.46              |
| 1:h:45:LEU:HB2   | 1:h:79:ASN:HD22  | 1.80                     | 0.46              |
| 1:h:47:VAL:HG12  | 1:h:77:ILE:HG22  | 1.98                     | 0.46              |
| 3:j:113:ARG:HG2  | 1:r:59:LYS:HD3   | 1.98                     | 0.46              |
| 1:H:107:ILE:HG22 | 1:H:116:LEU:HB2  | 1.98                     | 0.46              |
| 3:K:115:SER:OG   | 3:K:116:ASP:N    | 2.48                     | 0.46              |
| 5:M:95:ALA:HB3   | 5:M:97:LYS:HZ1   | 1.81                     | 0.46              |
| 1:N:30:ASN:ND2   | 1:N:35:LYS:O     | 2.37                     | 0.46              |
| 1:N:147:ALA:HA   | 1:V:65:TRP:CG    | 2.51                     | 0.46              |
| 1:e:147:ALA:HA   | 1:p:65:TRP:CG    | 2.50                     | 0.46              |
| 1:h:147:ALA:HA   | 1:q:65:TRP:CG    | 2.51                     | 0.46              |
| 1:D:75:TRP:CE2   | 1:D:148:LEU:HB2  | 2.50                     | 0.46              |
| 1:F:66:LYS:HD2   | 1:p:74:GLU:HB3   | 1.98                     | 0.46              |
| 3:K:25:GLN:OE1   | 3:K:64:ASN:ND2   | 2.43                     | 0.46              |
| 4:L:115:LEU:HD12 | 4:L:130:ILE:HD11 | 1.98                     | 0.46              |
| 1:g:30:ASN:OD1   | 1:g:31:ALA:N     | 2.49                     | 0.46              |
| 1:N:130:ALA:N    | 1:V:45:LEU:O     | 2.43                     | 0.46              |
| 1:S:113:LYS:HD2  | 1:S:113:LYS:HA   | 1.72                     | 0.46              |
| 1:Y:4:GLU:OE2    | 1:Z:106:LYS:NZ   | 2.43                     | 0.46              |
| 4:l:70:LYS:HD3   | 4:l:70:LYS:HA    | 1.71                     | 0.46              |
| 4:L:116:GLU:OE1  | 4:L:128:TYR:OH   | 2.29                     | 0.45              |
| 1:d:30:ASN:HD22  | 1:d:35:LYS:H     | 1.62                     | 0.45              |
| 1:A:47:VAL:HG22  | 1:A:77:ILE:HG12  | 1.98                     | 0.45              |
| 1:A:133:ASP:OD1  | 1:A:133:ASP:N    | 2.49                     | 0.45              |
| 1:D:147:ALA:HA   | 1:a:65:TRP:CG    | 2.52                     | 0.45              |
| 1:H:36:LEU:HD23  | 1:H:161:PRO:HG2  | 1.97                     | 0.45              |
| 1:V:73:LYS:NZ    | 1:h:64:GLY:O     | 2.39                     | 0.45              |
| 1:W:3:PHE:O      | 1:W:4:GLU:HB2    | 2.16                     | 0.45              |
| 1:e:129:GLU:OE2  | 1:p:46:THR:OG1   | 2.33                     | 0.45              |
| 1:f:159:GLN:OE1  | 1:f:160:MET:N    | 2.49                     | 0.45              |
| 4:L:330:ASP:OD1  | 4:L:331:MET:N    | 2.49                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:q:43:GLN:HB2   | 1:q:81:GLY:HA2   | 1.97                     | 0.45              |
| 1:F:72:MET:HE2   | 1:F:72:MET:HA    | 1.98                     | 0.45              |
| 1:H:30:ASN:ND2   | 1:H:35:LYS:H     | 2.13                     | 0.45              |
| 3:k:215:LEU:HD23 | 3:k:215:LEU:HA   | 1.82                     | 0.45              |
| 1:S:113:LYS:HZ3  | 1:S:161:PRO:HD3  | 1.81                     | 0.45              |
| 1:T:28:VAL:HG12  | 1:T:105:VAL:HG12 | 1.99                     | 0.45              |
| 1:U:74:GLU:HB3   | 1:e:66:LYS:HD2   | 1.98                     | 0.45              |
| 4:L:19:ASP:OD2   | 4:L:44:THR:OG1   | 2.24                     | 0.45              |
| 1:N:36:LEU:HD23  | 1:N:161:PRO:HG2  | 1.98                     | 0.45              |
| 1:W:113:LYS:HA   | 1:W:113:LYS:HD3  | 1.67                     | 0.45              |
| 1:f:72:MET:HE2   | 1:r:59:LYS:HG3   | 1.98                     | 0.45              |
| 1:H:121:ALA:HA   | 1:H:144:GLY:HA2  | 1.98                     | 0.45              |
| 4:L:108:LYS:HG2  | 4:L:138:GLU:HB3  | 1.99                     | 0.45              |
| 1:f:113:LYS:HA   | 1:f:113:LYS:HD2  | 1.79                     | 0.45              |
| 2:i:595:LYS:NZ   | 2:i:595:LYS:HB3  | 2.31                     | 0.45              |
| 1:G:75:TRP:CE2   | 1:G:144:GLY:HA3  | 2.52                     | 0.45              |
| 1:G:99:SER:O     | 1:G:101:SER:OG   | 2.27                     | 0.45              |
| 1:a:149:VAL:HB   | 1:g:8:TYR:HB3    | 1.99                     | 0.45              |
| 1:c:43:GLN:HG3   | 1:c:81:GLY:HA2   | 1.98                     | 0.45              |
| 1:d:73:LYS:NZ    | 1:N:64:GLY:O     | 2.43                     | 0.45              |
| 1:S:17:LYS:HB2   | 1:S:17:LYS:HE3   | 1.76                     | 0.45              |
| 3:s:215:LEU:HD23 | 3:s:215:LEU:HA   | 1.82                     | 0.45              |
| 4:L:90:ILE:O     | 4:L:93:THR:OG1   | 2.15                     | 0.45              |
| 1:b:30:ASN:ND2   | 1:b:34:ASP:OD1   | 2.39                     | 0.45              |
| 1:h:77:ILE:HD11  | 1:h:142:LEU:HB2  | 1.99                     | 0.45              |
| 2:i:584:LEU:HG   | 5:m:82:ASN:HB2   | 1.99                     | 0.45              |
| 3:j:211:TYR:CZ   | 3:j:213:LYS:HB2  | 2.52                     | 0.45              |
| 4:l:355:PHE:O    | 4:l:358:ILE:HG13 | 2.17                     | 0.45              |
| 1:D:78:GLU:HB3   | 1:D:141:LYS:HB2  | 1.98                     | 0.45              |
| 4:L:340:ASN:OD1  | 4:L:341:GLN:N    | 2.49                     | 0.45              |
| 1:c:30:ASN:ND2   | 1:c:35:LYS:H     | 2.15                     | 0.45              |
| 1:I:75:TRP:CE2   | 1:I:148:LEU:HB2  | 2.52                     | 0.45              |
| 1:N:4:GLU:O      | 1:N:5:GLU:HG3    | 2.17                     | 0.45              |
| 1:T:77:ILE:HB    | 1:T:142:LEU:HD12 | 1.98                     | 0.45              |
| 1:U:25:ILE:HD11  | 1:U:108:ILE:HD11 | 1.99                     | 0.45              |
| 3:X:33:GLN:HB2   | 3:X:55:LYS:HB2   | 1.99                     | 0.45              |
| 1:D:16:ALA:C     | 1:D:18:ALA:H     | 2.25                     | 0.45              |
| 3:K:217:LYS:NZ   | 3:K:260:ASP:OD2  | 2.46                     | 0.45              |
| 4:L:244:MET:HE3  | 4:l:98:VAL:H     | 1.81                     | 0.45              |
| 1:g:122:ILE:CG2  | 1:g:145:MET:HE2  | 2.47                     | 0.45              |
| 1:C:75:TRP:CE2   | 1:C:148:LEU:HB2  | 2.52                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:99:SER:O     | 1:I:101:SER:OG   | 2.24                     | 0.45              |
| 4:l:116:GLU:OE1  | 4:l:128:TYR:OH   | 2.30                     | 0.45              |
| 1:n:149:VAL:HB   | 1:r:8:TYR:HB3    | 1.99                     | 0.45              |
| 4:L:186:ARG:HD2  | 3:s:183:LEU:HD21 | 1.98                     | 0.44              |
| 4:L:335:GLN:NE2  | 4:Q:335:GLN:HE22 | 2.16                     | 0.44              |
| 3:k:88:ASP:OD1   | 3:k:88:ASP:N     | 2.48                     | 0.44              |
| 3:P:204:THR:HG23 | 3:P:252:ASP:H    | 1.82                     | 0.44              |
| 1:U:96:TYR:CE1   | 1:U:103:VAL:HG13 | 2.52                     | 0.44              |
| 1:V:47:VAL:HG22  | 1:V:77:ILE:HG22  | 1.99                     | 0.44              |
| 1:e:108:ILE:HG22 | 1:e:115:GLY:HA2  | 1.97                     | 0.44              |
| 4:L:211:GLY:N    | 4:L:228:ALA:O    | 2.37                     | 0.44              |
| 1:C:114:LYS:HA   | 1:C:114:LYS:HD2  | 1.79                     | 0.44              |
| 2:O:582:ARG:O    | 2:O:585:GLN:HB3  | 2.17                     | 0.44              |
| 1:V:95:LYS:O     | 1:V:99:SER:OG    | 2.28                     | 0.44              |
| 2:i:593:ASP:OD2  | 2:i:595:LYS:N    | 2.46                     | 0.44              |
| 4:l:201:ASP:OD1  | 4:l:201:ASP:N    | 2.47                     | 0.44              |
| 1:D:133:ASP:OD1  | 1:D:133:ASP:N    | 2.49                     | 0.44              |
| 1:F:9:CYS:HB3    | 1:F:11:TYR:CE2   | 2.50                     | 0.44              |
| 1:F:147:ALA:HA   | 1:c:65:TRP:CG    | 2.52                     | 0.44              |
| 1:G:25:ILE:HG22  | 1:A:59:LYS:HD3   | 1.99                     | 0.44              |
| 3:K:29:ARG:HE    | 3:s:78:ARG:NH2   | 2.16                     | 0.44              |
| 1:n:102:PRO:HB3  | 1:n:145:MET:SD   | 2.58                     | 0.44              |
| 1:r:113:LYS:HA   | 1:r:113:LYS:HD3  | 1.72                     | 0.44              |
| 4:L:373:GLY:HA3  | 4:l:374:VAL:HG22 | 1.99                     | 0.44              |
| 5:M:84:LYS:HZ2   | 5:R:83:PHE:HD2   | 1.65                     | 0.44              |
| 1:I:4:GLU:OE1    | 1:I:8:TYR:OH     | 2.25                     | 0.44              |
| 1:e:73:LYS:HB2   | 1:p:64:GLY:O     | 2.17                     | 0.44              |
| 1:r:36:LEU:HD21  | 1:r:160:MET:C    | 2.43                     | 0.44              |
| 1:d:123:VAL:HG13 | 1:N:51:LYS:HZ1   | 1.81                     | 0.44              |
| 4:Q:223:ASP:HB2  | 4:Q:229:VAL:HG21 | 2.00                     | 0.44              |
| 1:h:84:VAL:HG23  | 1:h:87:ALA:HB2   | 1.98                     | 0.44              |
| 1:p:30:ASN:HD22  | 1:p:35:LYS:HB2   | 1.82                     | 0.44              |
| 1:H:59:LYS:NZ    | 1:e:21:GLY:O     | 2.36                     | 0.44              |
| 1:b:34:ASP:OD1   | 1:b:34:ASP:N     | 2.50                     | 0.44              |
| 1:C:108:ILE:HD13 | 1:C:108:ILE:HA   | 1.87                     | 0.44              |
| 3:P:115:SER:OG   | 3:P:116:ASP:N    | 2.49                     | 0.44              |
| 4:Q:340:ASN:OD1  | 4:Q:341:GLN:N    | 2.50                     | 0.44              |
| 1:U:113:LYS:HA   | 1:U:160:MET:HE2  | 2.00                     | 0.44              |
| 1:V:25:ILE:HD11  | 1:V:42:GLN:NE2   | 2.32                     | 0.44              |
| 3:j:52:THR:O     | 3:j:53:GLN:NE2   | 2.36                     | 0.44              |
| 3:j:204:THR:HG23 | 3:j:252:ASP:H    | 1.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:l:333:ARG:H    | 4:l:333:ARG:HG2  | 1.58                     | 0.44              |
| 4:L:343:LYS:O    | 4:L:347:VAL:HG13 | 2.17                     | 0.44              |
| 1:c:75:TRP:CE2   | 1:c:148:LEU:HB2  | 2.53                     | 0.44              |
| 3:k:247:GLU:OE1  | 3:k:248:LYS:N    | 2.43                     | 0.44              |
| 1:N:84:VAL:HG23  | 1:N:87:ALA:HB2   | 2.00                     | 0.44              |
| 4:Q:353:ASN:HA   | 4:l:352:ILE:HD11 | 2.00                     | 0.44              |
| 5:m:95:ALA:HB3   | 5:m:97:LYS:NZ    | 2.33                     | 0.44              |
| 1:q:95:LYS:O     | 1:q:99:SER:OG    | 2.25                     | 0.44              |
| 3:s:177:SER:HB3  | 3:s:271:TYR:HA   | 2.00                     | 0.44              |
| 4:L:1:MET:HB3    | 4:L:1:MET:HE2    | 1.74                     | 0.44              |
| 4:L:95:GLN:HB3   | 4:L:148:LEU:HB2  | 2.00                     | 0.44              |
| 1:A:147:ALA:HA   | 1:S:65:TRP:CG    | 2.53                     | 0.44              |
| 1:N:37:LEU:HG    | 1:N:89:SER:HB3   | 1.99                     | 0.44              |
| 4:Q:227:MET:SD   | 4:Q:227:MET:N    | 2.80                     | 0.44              |
| 4:Q:269:ASP:OD1  | 4:Q:269:ASP:N    | 2.50                     | 0.44              |
| 1:V:58:SER:OG    | 1:V:59:LYS:N     | 2.50                     | 0.44              |
| 3:j:193:THR:HB   | 3:j:217:LYS:HD2  | 2.00                     | 0.44              |
| 1:n:113:LYS:HD2  | 1:n:113:LYS:HA   | 1.71                     | 0.44              |
| 1:a:34:ASP:OD1   | 1:a:34:ASP:N     | 2.50                     | 0.44              |
| 1:b:129:GLU:HG3  | 1:B:46:THR:HG22  | 2.00                     | 0.44              |
| 1:I:130:ALA:HB2  | 1:I:136:MET:HG3  | 2.00                     | 0.44              |
| 1:U:22:LYS:HA    | 1:q:59:LYS:HG2   | 2.00                     | 0.44              |
| 3:X:215:LEU:HD23 | 3:X:215:LEU:HA   | 1.82                     | 0.44              |
| 1:Y:95:LYS:O     | 1:Y:99:SER:OG    | 2.24                     | 0.44              |
| 4:l:187:TYR:CZ   | 4:l:188:LEU:HG   | 2.53                     | 0.44              |
| 1:o:102:PRO:HB3  | 1:o:145:MET:SD   | 2.57                     | 0.44              |
| 1:p:133:ASP:OD1  | 1:p:133:ASP:N    | 2.50                     | 0.44              |
| 1:D:75:TRP:CE2   | 1:D:144:GLY:HA3  | 2.53                     | 0.43              |
| 1:E:84:VAL:HG13  | 1:E:87:ALA:HB2   | 1.99                     | 0.43              |
| 2:J:594:ASP:OD1  | 2:J:595:LYS:N    | 2.51                     | 0.43              |
| 4:L:210:TYR:HD1  | 4:L:229:VAL:HG22 | 1.83                     | 0.43              |
| 1:d:75:TRP:CE2   | 1:d:148:LEU:HB2  | 2.53                     | 0.43              |
| 4:Q:363:TYR:CE2  | 4:l:366:ARG:HD2  | 2.53                     | 0.43              |
| 1:S:72:MET:HE3   | 1:Y:64:GLY:C     | 2.43                     | 0.43              |
| 1:T:75:TRP:CZ2   | 1:T:144:GLY:HA3  | 2.53                     | 0.43              |
| 1:V:115:GLY:N    | 1:V:158:ASP:OD1  | 2.51                     | 0.43              |
| 1:D:102:PRO:HB3  | 1:D:145:MET:SD   | 2.58                     | 0.43              |
| 1:D:102:PRO:O    | 1:G:11:TYR:OH    | 2.36                     | 0.43              |
| 2:J:589:VAL:HA   | 5:M:91:GLY:HA3   | 2.00                     | 0.43              |
| 4:L:206:GLU:OE1  | 4:L:233:THR:OG1  | 2.36                     | 0.43              |
| 1:d:102:PRO:HB2  | 1:d:120:LEU:HD11 | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:84:VAL:HG13  | 1:n:87:ALA:HB2   | 2.00                     | 0.43              |
| 1:c:74:GLU:HB3   | 1:C:66:LYS:HD2   | 2.00                     | 0.43              |
| 1:C:73:LYS:HB2   | 1:U:64:GLY:O     | 2.18                     | 0.43              |
| 2:O:595:LYS:NZ   | 2:O:595:LYS:HB3  | 2.33                     | 0.43              |
| 1:T:87:ALA:O     | 1:T:91:LYS:HG3   | 2.19                     | 0.43              |
| 3:X:202:ASN:O    | 3:X:206:GLY:N    | 2.50                     | 0.43              |
| 1:h:30:ASN:CG    | 1:h:33:GLY:H     | 2.25                     | 0.43              |
| 1:h:123:VAL:HA   | 1:h:142:LEU:HG   | 1.99                     | 0.43              |
| 5:m:75:LEU:HD12  | 5:m:75:LEU:H     | 1.83                     | 0.43              |
| 3:s:248:LYS:HE2  | 3:s:248:LYS:HB3  | 1.74                     | 0.43              |
| 4:Q:242:LYS:HE3  | 4:Q:242:LYS:HB3  | 1.86                     | 0.43              |
| 1:T:34:ASP:OD1   | 1:T:34:ASP:N     | 2.50                     | 0.43              |
| 1:T:72:MET:HE3   | 1:T:72:MET:HA    | 2.00                     | 0.43              |
| 1:U:110:GLN:OE1  | 1:U:110:GLN:HA   | 2.17                     | 0.43              |
| 1:f:52:ASP:O     | 1:f:71:GLY:N     | 2.51                     | 0.43              |
| 1:h:93:LEU:HD12  | 1:h:93:LEU:HA    | 1.82                     | 0.43              |
| 1:q:23:ASP:HB3   | 1:q:111:ALA:HB3  | 2.01                     | 0.43              |
| 1:q:58:SER:OG    | 1:q:59:LYS:N     | 2.52                     | 0.43              |
| 3:s:11:LYS:HE3   | 3:s:13:HIS:NE2   | 2.33                     | 0.43              |
| 1:F:37:LEU:HD13  | 1:F:88:GLU:HG2   | 2.01                     | 0.43              |
| 1:d:151:LEU:HA   | 1:d:154:THR:HG22 | 2.00                     | 0.43              |
| 4:l:227:MET:SD   | 4:l:227:MET:N    | 2.81                     | 0.43              |
| 1:E:65:TRP:CG    | 1:o:147:ALA:HA   | 2.53                     | 0.43              |
| 4:L:362:ALA:O    | 4:l:363:TYR:OH   | 2.34                     | 0.43              |
| 5:R:75:LEU:HD12  | 5:R:75:LEU:HA    | 1.83                     | 0.43              |
| 1:h:25:ILE:HG23  | 1:h:42:GLN:HE22  | 1.83                     | 0.43              |
| 3:j:33:GLN:HB2   | 3:j:55:LYS:HB2   | 2.00                     | 0.43              |
| 4:l:115:LEU:HD12 | 4:l:130:ILE:HD11 | 2.00                     | 0.43              |
| 4:L:333:ARG:O    | 4:L:337:GLN:HG2  | 2.18                     | 0.43              |
| 4:L:365:SER:O    | 4:L:369:THR:HG23 | 2.19                     | 0.43              |
| 1:c:147:ALA:HA   | 1:C:65:TRP:CG    | 2.54                     | 0.43              |
| 1:N:23:ASP:O     | 1:N:109:ASN:HA   | 2.18                     | 0.43              |
| 1:S:147:ALA:HA   | 1:Y:65:TRP:CG    | 2.53                     | 0.43              |
| 2:i:612:TYR:O    | 2:i:616:MET:HG3  | 2.19                     | 0.43              |
| 1:n:75:TRP:CE2   | 1:n:148:LEU:HB2  | 2.54                     | 0.43              |
| 1:p:5:GLU:N      | 1:p:5:GLU:OE2    | 2.52                     | 0.43              |
| 1:F:136:MET:HE3  | 1:F:136:MET:HB2  | 1.71                     | 0.43              |
| 4:L:202:ASN:OD1  | 4:L:202:ASN:N    | 2.52                     | 0.43              |
| 4:L:237:GLU:O    | 4:L:241:GLY:N    | 2.42                     | 0.43              |
| 1:a:75:TRP:CE2   | 1:a:148:LEU:HB2  | 2.54                     | 0.43              |
| 1:S:133:ASP:OD1  | 1:S:133:ASP:N    | 2.51                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:i:579:LEU:HD12 | 2:i:580:LEU:N    | 2.34                     | 0.43              |
| 4:l:333:ARG:O    | 4:l:337:GLN:HG2  | 2.19                     | 0.43              |
| 5:m:97:LYS:HE2   | 5:m:97:LYS:H     | 1.83                     | 0.43              |
| 1:q:30:ASN:HD22  | 1:q:35:LYS:H     | 1.66                     | 0.43              |
| 5:M:97:LYS:HE2   | 5:M:97:LYS:H     | 1.84                     | 0.43              |
| 1:b:26:LEU:HD23  | 1:b:107:ILE:HD12 | 2.01                     | 0.43              |
| 1:b:147:ALA:HA   | 1:B:65:TRP:CG    | 2.54                     | 0.43              |
| 3:P:139:LEU:HD23 | 3:P:139:LEU:HA   | 1.85                     | 0.43              |
| 5:R:84:LYS:HB2   | 2:i:583:LEU:HD21 | 2.00                     | 0.43              |
| 3:X:83:PHE:O     | 3:X:86:GLN:NE2   | 2.35                     | 0.43              |
| 1:Y:47:VAL:HG22  | 1:Y:77:ILE:HG12  | 2.00                     | 0.43              |
| 1:p:102:PRO:HB2  | 1:p:120:LEU:HD22 | 2.00                     | 0.43              |
| 1:F:130:ALA:HB2  | 1:F:136:MET:HE2  | 2.01                     | 0.43              |
| 4:L:363:TYR:HA   | 4:l:363:TYR:OH   | 2.18                     | 0.43              |
| 1:g:108:ILE:HG23 | 1:g:160:MET:HE2  | 2.00                     | 0.43              |
| 3:k:202:ASN:O    | 3:k:206:GLY:N    | 2.52                     | 0.43              |
| 2:O:592:MET:SD   | 5:R:94:LYS:HE3   | 2.59                     | 0.43              |
| 3:P:41:ILE:O     | 3:P:44:THR:OG1   | 2.37                     | 0.43              |
| 1:Y:44:GLY:O     | 1:Y:79:ASN:HB2   | 2.19                     | 0.43              |
| 5:m:84:LYS:HD2   | 5:m:84:LYS:O     | 2.18                     | 0.43              |
| 1:F:20:ALA:HA    | 1:p:135:ALA:HA   | 2.00                     | 0.42              |
| 1:H:30:ASN:CG    | 1:H:33:GLY:H     | 2.27                     | 0.42              |
| 2:O:593:ASP:OD1  | 2:O:594:ASP:N    | 2.52                     | 0.42              |
| 1:Y:83:TYR:HB2   | 1:Y:138:TYR:HB3  | 2.00                     | 0.42              |
| 1:o:125:ASP:OD1  | 1:o:127:SER:OG   | 2.28                     | 0.42              |
| 1:p:27:ALA:HB1   | 1:p:36:LEU:HG    | 2.01                     | 0.42              |
| 1:E:3:PHE:HB3    | 1:E:4:GLU:H      | 1.75                     | 0.42              |
| 1:G:4:GLU:OE1    | 1:G:8:TYR:OH     | 2.27                     | 0.42              |
| 1:H:113:LYS:HD2  | 1:H:113:LYS:HA   | 1.71                     | 0.42              |
| 1:C:29:PHE:CE1   | 1:C:36:LEU:HB2   | 2.54                     | 0.42              |
| 1:N:25:ILE:HD11  | 1:N:110:GLN:NE2  | 2.34                     | 0.42              |
| 2:O:584:LEU:HD23 | 5:R:83:PHE:HA    | 2.00                     | 0.42              |
| 3:P:202:ASN:O    | 3:P:206:GLY:N    | 2.49                     | 0.42              |
| 3:j:3:ASP:OD2    | 3:j:14:SER:OG    | 2.35                     | 0.42              |
| 1:r:75:TRP:CE2   | 1:r:144:GLY:HA3  | 2.54                     | 0.42              |
| 1:D:59:LYS:HG2   | 1:f:22:LYS:HA    | 2.01                     | 0.42              |
| 1:H:75:TRP:CE2   | 1:H:144:GLY:HA3  | 2.54                     | 0.42              |
| 1:H:103:VAL:O    | 1:H:120:LEU:HD12 | 2.19                     | 0.42              |
| 4:L:70:LYS:HA    | 4:L:70:LYS:HD3   | 1.72                     | 0.42              |
| 1:U:75:TRP:CE2   | 1:U:148:LEU:HB2  | 2.55                     | 0.42              |
| 1:Y:147:ALA:HA   | 1:n:65:TRP:CG    | 2.53                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:23:ASP:O     | 1:h:109:ASN:HA   | 2.19                     | 0.42              |
| 2:i:610:ASP:OD2  | 4:l:329:ARG:NE   | 2.32                     | 0.42              |
| 3:j:243:ILE:HD12 | 3:j:243:ILE:O    | 2.19                     | 0.42              |
| 4:l:230:VAL:HG21 | 4:l:260:LEU:HD13 | 2.01                     | 0.42              |
| 1:q:75:TRP:CZ2   | 1:q:144:GLY:HA3  | 2.54                     | 0.42              |
| 1:q:102:PRO:HB2  | 1:q:120:LEU:HD11 | 2.00                     | 0.42              |
| 1:F:3:PHE:HE1    | 1:H:33:GLY:HA3   | 1.84                     | 0.42              |
| 5:M:92:GLU:O     | 5:M:92:GLU:HG2   | 2.19                     | 0.42              |
| 1:b:75:TRP:CZ2   | 1:b:144:GLY:HA3  | 2.55                     | 0.42              |
| 1:c:5:GLU:N      | 1:c:5:GLU:OE2    | 2.52                     | 0.42              |
| 1:d:109:ASN:HB2  | 1:d:116:LEU:HD11 | 2.00                     | 0.42              |
| 3:k:11:LYS:HE3   | 3:k:13:HIS:NE2   | 2.34                     | 0.42              |
| 3:P:123:ILE:H    | 3:P:123:ILE:HG13 | 1.69                     | 0.42              |
| 4:Q:304:VAL:HB   | 4:Q:324:PHE:CD2  | 2.54                     | 0.42              |
| 5:R:83:PHE:CE1   | 5:R:84:LYS:HG2   | 2.54                     | 0.42              |
| 1:T:3:PHE:O      | 1:T:4:GLU:HB2    | 2.19                     | 0.42              |
| 1:V:77:ILE:CD1   | 1:V:142:LEU:HB2  | 2.50                     | 0.42              |
| 1:h:37:LEU:HG    | 1:h:89:SER:HB3   | 2.01                     | 0.42              |
| 4:l:223:ASP:HB2  | 4:l:229:VAL:HG21 | 2.02                     | 0.42              |
| 2:J:595:LYS:NZ   | 2:J:595:LYS:HB3  | 2.34                     | 0.42              |
| 1:A:44:GLY:O     | 1:A:79:ASN:HB2   | 2.19                     | 0.42              |
| 1:V:147:ALA:HA   | 1:h:65:TRP:CG    | 2.55                     | 0.42              |
| 1:W:29:PHE:HE2   | 1:W:106:LYS:HE3  | 1.85                     | 0.42              |
| 1:W:129:GLU:HG2  | 1:f:46:THR:HG23  | 2.01                     | 0.42              |
| 1:h:25:ILE:HD11  | 1:h:110:GLN:NE2  | 2.34                     | 0.42              |
| 3:j:139:LEU:HD23 | 3:j:139:LEU:HA   | 1.87                     | 0.42              |
| 3:j:217:LYS:NZ   | 3:j:260:ASP:O    | 2.46                     | 0.42              |
| 1:n:125:ASP:HB3  | 1:n:141:LYS:HB3  | 2.00                     | 0.42              |
| 3:k:227:TYR:OH   | 4:Q:283:GLU:OE2  | 2.26                     | 0.42              |
| 1:N:124:ALA:HB3  | 1:N:141:LYS:HG2  | 2.00                     | 0.42              |
| 4:Q:115:LEU:HD12 | 4:Q:130:ILE:HD11 | 2.02                     | 0.42              |
| 4:Q:116:GLU:OE1  | 4:Q:128:TYR:OH   | 2.34                     | 0.42              |
| 1:U:30:ASN:ND2   | 1:U:35:LYS:H     | 2.18                     | 0.42              |
| 1:Y:149:VAL:HB   | 1:f:8:TYR:HB3    | 2.02                     | 0.42              |
| 1:n:35:LYS:HD2   | 1:n:37:LEU:HD21  | 2.01                     | 0.42              |
| 1:H:129:GLU:HA   | 1:d:46:THR:HA    | 2.00                     | 0.42              |
| 3:K:3:ASP:OD2    | 3:K:14:SER:OG    | 2.37                     | 0.42              |
| 3:K:241:HIS:NE2  | 4:L:14:GLU:HG2   | 2.35                     | 0.42              |
| 1:d:45:LEU:HD23  | 1:d:79:ASN:HB3   | 2.02                     | 0.42              |
| 1:A:16:ALA:C     | 1:A:18:ALA:H     | 2.26                     | 0.42              |
| 5:R:84:LYS:HE3   | 2:i:586:LYS:HE3  | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:75:TRP:CE2   | 1:V:148:LEU:HB2  | 2.54                     | 0.42              |
| 1:W:150:ASP:O    | 1:W:154:THR:HG22 | 2.20                     | 0.42              |
| 3:X:195:ASN:OD1  | 3:X:217:LYS:N    | 2.53                     | 0.42              |
| 1:e:75:TRP:CE2   | 1:e:148:LEU:HB2  | 2.55                     | 0.42              |
| 1:h:26:LEU:H     | 1:h:42:GLN:CD    | 2.28                     | 0.42              |
| 1:h:106:LYS:HZ3  | 1:h:159:GLN:H    | 1.67                     | 0.42              |
| 3:j:53:GLN:NE2   | 3:j:53:GLN:HA    | 2.35                     | 0.42              |
| 3:j:258:VAL:HG23 | 3:j:261:VAL:HG22 | 2.01                     | 0.42              |
| 1:o:3:PHE:O      | 1:o:4:GLU:HB2    | 2.19                     | 0.42              |
| 1:p:47:VAL:HG22  | 1:p:77:ILE:HG12  | 2.02                     | 0.42              |
| 1:p:83:TYR:HD2   | 1:p:136:MET:HE3  | 1.84                     | 0.42              |
| 1:D:149:VAL:HB   | 1:G:8:TYR:HB3    | 2.02                     | 0.42              |
| 1:F:29:PHE:CE1   | 1:F:36:LEU:HB2   | 2.54                     | 0.42              |
| 3:K:97:MET:HE3   | 3:s:78:ARG:HD2   | 2.01                     | 0.42              |
| 1:b:3:PHE:O      | 1:b:4:GLU:HB2    | 2.20                     | 0.42              |
| 1:C:75:TRP:HZ3   | 1:C:77:ILE:HG13  | 1.85                     | 0.42              |
| 2:O:580:LEU:HD23 | 2:O:580:LEU:HA   | 1.85                     | 0.42              |
| 5:R:99:GLU:HG2   | 2:i:592:MET:HB3  | 2.02                     | 0.42              |
| 1:S:43:GLN:NE2   | 1:o:57:THR:O     | 2.43                     | 0.42              |
| 1:V:23:ASP:HB3   | 1:V:111:ALA:HB3  | 2.02                     | 0.42              |
| 3:X:88:ASP:OD1   | 3:X:88:ASP:N     | 2.49                     | 0.42              |
| 1:Y:78:GLU:HB3   | 1:Y:141:LYS:HB2  | 2.02                     | 0.42              |
| 1:f:75:TRP:CE2   | 1:f:148:LEU:HB2  | 2.55                     | 0.42              |
| 1:h:26:LEU:HB2   | 1:h:45:LEU:CD1   | 2.49                     | 0.42              |
| 1:H:43:GLN:O     | 1:q:132:PHE:HB3  | 2.19                     | 0.42              |
| 1:H:96:TYR:CE2   | 1:H:103:VAL:HG23 | 2.55                     | 0.42              |
| 4:L:363:TYR:O    | 4:L:367:ILE:HG13 | 2.20                     | 0.42              |
| 5:M:85:ILE:O     | 5:M:88:THR:OG1   | 2.21                     | 0.42              |
| 1:B:76:SER:OG    | 1:B:141:LYS:NZ   | 2.51                     | 0.42              |
| 4:Q:280:LYS:HD3  | 4:Q:280:LYS:HA   | 1.80                     | 0.42              |
| 1:W:26:LEU:HD11  | 1:W:105:VAL:HG22 | 2.02                     | 0.42              |
| 1:Y:102:PRO:HB3  | 1:Y:145:MET:SD   | 2.60                     | 0.42              |
| 1:f:107:ILE:HG22 | 1:f:116:LEU:HB2  | 2.00                     | 0.42              |
| 1:h:160:MET:SD   | 1:h:161:PRO:HD3  | 2.59                     | 0.42              |
| 3:s:177:SER:N    | 3:s:270:ILE:O    | 2.42                     | 0.42              |
| 1:G:28:VAL:HG12  | 1:G:105:VAL:HG12 | 2.01                     | 0.42              |
| 1:b:87:ALA:O     | 1:b:91:LYS:HG3   | 2.20                     | 0.42              |
| 1:c:73:LYS:HG2   | 1:C:64:GLY:O     | 2.20                     | 0.42              |
| 1:c:153:ILE:H    | 1:c:153:ILE:HG13 | 1.75                     | 0.42              |
| 1:I:28:VAL:HG12  | 1:I:105:VAL:HG12 | 2.00                     | 0.42              |
| 4:Q:1:MET:HE2    | 4:Q:1:MET:HB3    | 1.73                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:Q:210:TYR:HD1 | 4:Q:229:VAL:HG22 | 1.85                     | 0.42              |
| 3:X:211:TYR:CZ  | 3:X:213:LYS:HB2  | 2.55                     | 0.42              |
| 1:Z:16:ALA:O    | 1:Z:17:LYS:HG2   | 2.19                     | 0.42              |
| 4:l:365:SER:O   | 4:l:369:THR:HG23 | 2.19                     | 0.42              |
| 1:o:87:ALA:O    | 1:o:91:LYS:HG3   | 2.20                     | 0.42              |
| 1:c:23:ASP:O    | 1:c:110:GLN:N    | 2.49                     | 0.41              |
| 3:k:3:ASP:OD2   | 3:k:14:SER:OG    | 2.38                     | 0.41              |
| 2:O:591:LYS:HD2 | 2:O:591:LYS:C    | 2.44                     | 0.41              |
| 1:f:36:LEU:HB3  | 1:f:161:PRO:HA   | 2.01                     | 0.41              |
| 1:E:45:LEU:HB2  | 1:E:79:ASN:HD22  | 1.84                     | 0.41              |
| 1:H:123:VAL:HA  | 1:H:142:LEU:HG   | 2.00                     | 0.41              |
| 4:L:349:THR:HA  | 4:L:352:ILE:HG22 | 2.02                     | 0.41              |
| 3:k:23:SER:OG   | 3:k:64:ASN:OD1   | 2.37                     | 0.41              |
| 1:N:43:GLN:HB2  | 1:N:81:GLY:CA    | 2.50                     | 0.41              |
| 1:N:47:VAL:HG12 | 1:N:77:ILE:HG22  | 2.01                     | 0.41              |
| 2:O:593:ASP:OD1 | 2:O:593:ASP:C    | 2.63                     | 0.41              |
| 1:V:25:ILE:HD11 | 1:V:42:GLN:CD    | 2.45                     | 0.41              |
| 1:o:34:ASP:OD1  | 1:o:34:ASP:N     | 2.50                     | 0.41              |
| 1:H:30:ASN:ND2  | 1:H:35:LYS:O     | 2.35                     | 0.41              |
| 4:L:31:LYS:HB2  | 4:L:31:LYS:HE3   | 1.75                     | 0.41              |
| 4:L:51:PHE:O    | 4:L:83:LYS:NZ    | 2.53                     | 0.41              |
| 1:a:133:ASP:OD1 | 1:a:133:ASP:N    | 2.48                     | 0.41              |
| 1:g:106:LYS:HG2 | 1:g:108:ILE:HD11 | 2.02                     | 0.41              |
| 1:U:97:PHE:CZ   | 1:e:73:LYS:HE2   | 2.56                     | 0.41              |
| 3:X:248:LYS:HB3 | 3:X:248:LYS:HE2  | 1.77                     | 0.41              |
| 3:s:153:MET:SD  | 3:s:158:ARG:HD2  | 2.60                     | 0.41              |
| 1:F:143:ASP:OD1 | 1:F:143:ASP:N    | 2.54                     | 0.41              |
| 5:M:95:ALA:HB3  | 5:M:97:LYS:NZ    | 2.35                     | 0.41              |
| 1:d:58:SER:OG   | 1:d:60:ASP:OD1   | 2.29                     | 0.41              |
| 1:I:113:LYS:C   | 1:I:160:MET:HE1  | 2.45                     | 0.41              |
| 4:Q:216:ASN:OD1 | 4:Q:216:ASN:N    | 2.52                     | 0.41              |
| 1:S:3:PHE:HD1   | 1:S:3:PHE:HA     | 1.75                     | 0.41              |
| 1:Y:75:TRP:CE2  | 1:Y:144:GLY:HA3  | 2.55                     | 0.41              |
| 4:l:210:TYR:HD1 | 4:l:229:VAL:HG22 | 1.84                     | 0.41              |
| 5:m:83:PHE:O    | 5:m:87:VAL:HG12  | 2.20                     | 0.41              |
| 1:p:113:LYS:HD2 | 1:p:113:LYS:HA   | 1.83                     | 0.41              |
| 1:q:29:PHE:CD1  | 1:q:36:LEU:HD13  | 2.56                     | 0.41              |
| 1:r:113:LYS:HA  | 1:r:160:MET:HE1  | 2.01                     | 0.41              |
| 1:F:83:TYR:HB3  | 1:F:136:MET:HG2  | 2.02                     | 0.41              |
| 1:H:31:ALA:N    | 1:H:92:GLU:OE2   | 2.45                     | 0.41              |
| 2:J:592:MET:HA  | 5:m:99:GLU:HG2   | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:180:ARG:HB2  | 4:L:180:ARG:NH1  | 2.35                     | 0.41              |
| 1:a:107:ILE:HG22 | 1:a:116:LEU:HB2  | 2.02                     | 0.41              |
| 3:k:236:GLY:N    | 4:Q:182:GLU:OE2  | 2.53                     | 0.41              |
| 1:N:24:VAL:C     | 1:N:25:ILE:HD12  | 2.46                     | 0.41              |
| 4:Q:219:LYS:HE3  | 4:Q:219:LYS:HB3  | 1.83                     | 0.41              |
| 1:S:34:ASP:OD1   | 1:S:34:ASP:N     | 2.50                     | 0.41              |
| 1:e:29:PHE:CE1   | 1:e:36:LEU:HB2   | 2.55                     | 0.41              |
| 5:m:84:LYS:NZ    | 5:m:85:ILE:HD12  | 2.34                     | 0.41              |
| 1:p:30:ASN:ND2   | 1:p:35:LYS:H     | 2.18                     | 0.41              |
| 4:L:204:LYS:HG3  | 4:L:245:ALA:HB2  | 2.01                     | 0.41              |
| 5:M:94:LYS:HG2   | 5:M:99:GLU:O     | 2.21                     | 0.41              |
| 1:N:51:LYS:HB3   | 1:N:73:LYS:HG2   | 2.02                     | 0.41              |
| 5:R:84:LYS:O     | 5:R:88:THR:HG23  | 2.21                     | 0.41              |
| 4:l:325:SER:O    | 4:l:326:ASN:ND2  | 2.54                     | 0.41              |
| 5:m:84:LYS:HZ2   | 5:m:85:ILE:HA    | 1.86                     | 0.41              |
| 1:E:75:TRP:CE3   | 1:E:148:LEU:HD12 | 2.56                     | 0.41              |
| 1:F:21:GLY:HA3   | 1:p:131:PRO:O    | 2.20                     | 0.41              |
| 1:G:96:TYR:HD1   | 1:G:101:SER:HB2  | 1.84                     | 0.41              |
| 3:K:41:ILE:O     | 3:K:44:THR:OG1   | 2.38                     | 0.41              |
| 4:L:57:GLU:OE2   | 4:L:70:LYS:NZ    | 2.42                     | 0.41              |
| 4:L:216:ASN:OD1  | 4:L:216:ASN:N    | 2.52                     | 0.41              |
| 1:b:143:ASP:OD1  | 1:b:143:ASP:N    | 2.51                     | 0.41              |
| 1:A:75:TRP:CE2   | 1:A:144:GLY:HA3  | 2.55                     | 0.41              |
| 1:C:131:PRO:O    | 1:U:21:GLY:HA3   | 2.20                     | 0.41              |
| 1:I:122:ILE:O    | 1:I:142:LEU:HA   | 2.21                     | 0.41              |
| 4:Q:335:GLN:NE2  | 4:l:335:GLN:HE22 | 2.18                     | 0.41              |
| 1:U:130:ALA:HB2  | 1:U:136:MET:HG3  | 2.02                     | 0.41              |
| 1:U:133:ASP:OD1  | 1:U:133:ASP:N    | 2.49                     | 0.41              |
| 3:X:153:MET:HE3  | 3:X:153:MET:HB2  | 1.79                     | 0.41              |
| 3:K:192:MET:HE2  | 3:K:221:LEU:HD23 | 2.03                     | 0.41              |
| 3:K:215:LEU:HD23 | 3:K:215:LEU:HA   | 1.91                     | 0.41              |
| 5:M:84:LYS:HE3   | 2:O:586:LYS:HZ2  | 1.85                     | 0.41              |
| 1:a:160:MET:HE2  | 1:a:160:MET:C    | 2.46                     | 0.41              |
| 1:b:133:ASP:OD1  | 1:b:133:ASP:N    | 2.54                     | 0.41              |
| 1:N:77:ILE:HD11  | 1:N:142:LEU:HB2  | 2.03                     | 0.41              |
| 5:R:89:ASN:OD1   | 5:R:89:ASN:N     | 2.54                     | 0.41              |
| 3:X:78:ARG:NH2   | 3:j:272:ARG:O    | 2.54                     | 0.41              |
| 1:Y:16:ALA:C     | 1:Y:18:ALA:H     | 2.27                     | 0.41              |
| 1:e:75:TRP:HZ3   | 1:e:77:ILE:HG13  | 1.86                     | 0.41              |
| 1:f:75:TRP:CE2   | 1:f:144:GLY:HA3  | 2.56                     | 0.41              |
| 1:h:26:LEU:HD21  | 1:h:105:VAL:CG1  | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:117:PHE:HB3  | 1:E:148:LEU:HD21 | 2.03                     | 0.41              |
| 1:G:26:LEU:HD12  | 1:G:107:ILE:HD11 | 2.02                     | 0.41              |
| 1:a:75:TRP:CE2   | 1:a:144:GLY:HA3  | 2.56                     | 0.41              |
| 1:d:23:ASP:HB3   | 1:d:111:ALA:HB3  | 2.02                     | 0.41              |
| 3:k:194:ALA:HB2  | 3:k:261:VAL:HA   | 2.01                     | 0.41              |
| 1:C:83:TYR:HD2   | 1:C:136:MET:HE1  | 1.85                     | 0.41              |
| 1:I:75:TRP:CE2   | 1:I:144:GLY:HA3  | 2.55                     | 0.41              |
| 1:N:26:LEU:HD21  | 1:N:105:VAL:CG1  | 2.51                     | 0.41              |
| 3:P:237:LYS:H    | 3:P:237:LYS:HG2  | 1.67                     | 0.41              |
| 1:U:131:PRO:O    | 1:e:21:GLY:HA3   | 2.20                     | 0.41              |
| 1:W:75:TRP:CE2   | 1:W:144:GLY:HA3  | 2.56                     | 0.41              |
| 3:X:230:VAL:HG23 | 3:X:235:VAL:HG21 | 2.03                     | 0.41              |
| 1:h:24:VAL:C     | 1:h:25:ILE:HD12  | 2.46                     | 0.41              |
| 2:i:584:LEU:HD13 | 2:i:584:LEU:O    | 2.21                     | 0.41              |
| 1:o:26:LEU:HD21  | 1:o:105:VAL:HB   | 2.02                     | 0.41              |
| 1:p:103:VAL:O    | 1:p:120:LEU:HD23 | 2.20                     | 0.41              |
| 1:q:47:VAL:HA    | 1:q:77:ILE:HG22  | 2.02                     | 0.41              |
| 1:r:16:ALA:C     | 1:r:18:ALA:H     | 2.28                     | 0.41              |
| 1:E:3:PHE:HD1    | 1:E:3:PHE:HA     | 1.80                     | 0.41              |
| 3:K:46:GLY:HA2   | 3:s:56:PRO:HD3   | 2.03                     | 0.41              |
| 5:M:84:LYS:HD2   | 5:R:83:PHE:CD2   | 2.56                     | 0.41              |
| 1:c:113:LYS:HA   | 1:c:113:LYS:HD2  | 1.88                     | 0.41              |
| 1:T:4:GLU:OE2    | 1:T:8:TYR:OH     | 2.36                     | 0.41              |
| 1:W:69:ILE:HD11  | 3:X:118:VAL:HG11 | 2.03                     | 0.41              |
| 1:o:4:GLU:OE2    | 1:o:8:TYR:OH     | 2.30                     | 0.41              |
| 1:q:93:LEU:HD23  | 1:q:93:LEU:HA    | 1.95                     | 0.41              |
| 3:s:83:PHE:O     | 3:s:86:GLN:NE2   | 2.36                     | 0.41              |
| 1:G:159:GLN:OE1  | 1:G:160:MET:N    | 2.54                     | 0.40              |
| 4:L:227:MET:H    | 4:L:227:MET:CE   | 2.33                     | 0.40              |
| 4:Q:333:ARG:O    | 4:Q:337:GLN:HG2  | 2.21                     | 0.40              |
| 1:Z:76:SER:OG    | 1:Z:141:LYS:NZ   | 2.55                     | 0.40              |
| 3:j:241:HIS:NE2  | 4:l:14:GLU:HG2   | 2.36                     | 0.40              |
| 4:l:187:TYR:HB2  | 4:l:295:HIS:ND1  | 2.36                     | 0.40              |
| 1:q:151:LEU:HA   | 1:q:154:THR:HG22 | 2.02                     | 0.40              |
| 3:K:226:ILE:HG22 | 3:K:243:ILE:HG21 | 2.03                     | 0.40              |
| 4:Q:115:LEU:HD23 | 4:Q:115:LEU:HA   | 1.86                     | 0.40              |
| 4:Q:187:TYR:CZ   | 4:Q:188:LEU:HG   | 2.56                     | 0.40              |
| 1:U:153:ILE:H    | 1:U:153:ILE:HG13 | 1.75                     | 0.40              |
| 3:X:192:MET:HE3  | 3:X:263:ILE:HD12 | 2.03                     | 0.40              |
| 1:Z:16:ALA:C     | 1:Z:18:ALA:H     | 2.29                     | 0.40              |
| 1:p:155:GLU:OE2  | 1:p:156:GLY:N    | 2.54                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:d:47:VAL:HG22 | 1:d:77:ILE:HG22  | 2.04                     | 0.40              |
| 1:d:77:ILE:HD12 | 1:d:77:ILE:C     | 2.47                     | 0.40              |
| 1:g:72:MET:HE2  | 3:k:115:SER:HB2  | 2.03                     | 0.40              |
| 1:B:133:ASP:OD1 | 1:B:133:ASP:N    | 2.54                     | 0.40              |
| 1:N:73:LYS:O    | 1:V:66:LYS:HG2   | 2.20                     | 0.40              |
| 4:l:175:LYS:HA  | 4:l:175:LYS:HD2  | 1.91                     | 0.40              |
| 1:p:131:PRO:HG2 | 1:p:134:GLU:HG3  | 2.03                     | 0.40              |
| 1:q:39:VAL:HG13 | 1:q:42:GLN:HE21  | 1.86                     | 0.40              |
| 4:L:223:ASP:HB2 | 4:L:229:VAL:HG21 | 2.03                     | 0.40              |
| 1:g:75:TRP:CE2  | 1:g:144:GLY:HA3  | 2.56                     | 0.40              |
| 1:N:35:LYS:HZ1  | 1:N:161:PRO:HB3  | 1.87                     | 0.40              |
| 1:V:73:LYS:HD2  | 1:h:65:TRP:CZ2   | 2.57                     | 0.40              |
| 1:Y:131:PRO:O   | 1:n:21:GLY:HA3   | 2.22                     | 0.40              |
| 1:e:9:CYS:HB3   | 1:e:11:TYR:CE2   | 2.47                     | 0.40              |
| 1:p:75:TRP:CE2  | 1:p:144:GLY:HA3  | 2.57                     | 0.40              |
| 1:F:12:THR:HA   | 1:F:13:PRO:HD3   | 1.96                     | 0.40              |
| 1:F:65:TRP:CG   | 1:p:147:ALA:HA   | 2.57                     | 0.40              |
| 3:K:29:ARG:HE   | 3:s:78:ARG:HH21  | 1.69                     | 0.40              |
| 4:L:325:SER:O   | 4:L:326:ASN:ND2  | 2.54                     | 0.40              |
| 5:M:77:SER:HB2  | 2:O:576:VAL:HG22 | 2.04                     | 0.40              |
| 1:a:125:ASP:HB3 | 1:a:141:LYS:HB3  | 2.03                     | 0.40              |
| 1:d:30:ASN:O    | 1:d:96:TYR:OH    | 2.40                     | 0.40              |
| 1:d:51:LYS:HG3  | 1:d:73:LYS:HB3   | 2.03                     | 0.40              |
| 1:d:121:ALA:HA  | 1:d:145:MET:HE3  | 2.04                     | 0.40              |
| 3:k:158:ARG:NH2 | 3:k:160:ASP:OD2  | 2.42                     | 0.40              |
| 1:A:102:PRO:HB3 | 1:A:145:MET:SD   | 2.61                     | 0.40              |
| 1:I:147:ALA:HA  | 1:W:65:TRP:CD2   | 2.57                     | 0.40              |
| 3:P:180:VAL:HB  | 3:P:246:LEU:HB2  | 2.03                     | 0.40              |
| 3:j:115:SER:OG  | 3:j:116:ASP:N    | 2.54                     | 0.40              |
| 4:l:31:LYS:HB2  | 4:l:31:LYS:HE3   | 1.75                     | 0.40              |
| 1:r:3:PHE:HB3   | 1:r:4:GLU:H      | 1.78                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 159/170 (94%) | 151 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | B     | 159/170 (94%) | 153 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | C     | 159/170 (94%) | 152 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | D     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | E     | 159/170 (94%) | 152 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | F     | 159/170 (94%) | 152 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | G     | 159/170 (94%) | 146 (92%) | 13 (8%) | 0        | 100         | 100 |
| 1   | H     | 158/170 (93%) | 151 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | I     | 159/170 (94%) | 148 (93%) | 11 (7%) | 0        | 100         | 100 |
| 1   | N     | 158/170 (93%) | 151 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | S     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | T     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | U     | 159/170 (94%) | 149 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | V     | 158/170 (93%) | 153 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | W     | 158/170 (93%) | 152 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | Y     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | Z     | 159/170 (94%) | 151 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | a     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | b     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | c     | 159/170 (94%) | 149 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | d     | 158/170 (93%) | 153 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | e     | 159/170 (94%) | 153 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | f     | 159/170 (94%) | 148 (93%) | 11 (7%) | 0        | 100         | 100 |
| 1   | g     | 158/170 (93%) | 152 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | h     | 158/170 (93%) | 149 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | n     | 159/170 (94%) | 149 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | o     | 159/170 (94%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | p     | 159/170 (94%) | 149 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | q     | 158/170 (93%) | 153 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | r     | 158/170 (93%) | 152 (96%) | 6 (4%)  | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 2   | J     | 48/622 (8%)      | 46 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 2   | O     | 48/622 (8%)      | 46 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 2   | i     | 48/622 (8%)      | 46 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 3   | K     | 270/272 (99%)    | 265 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 3   | P     | 270/272 (99%)    | 265 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 3   | X     | 270/272 (99%)    | 263 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 3   | j     | 270/272 (99%)    | 264 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 3   | k     | 270/272 (99%)    | 261 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 3   | s     | 270/272 (99%)    | 261 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 4   | L     | 376/378 (100%)   | 363 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 4   | Q     | 376/378 (100%)   | 363 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 4   | l     | 376/378 (100%)   | 364 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 5   | M     | 25/99 (25%)      | 20 (80%)   | 5 (20%)  | 0        | 100         | 100 |
| 5   | R     | 25/99 (25%)      | 20 (80%)   | 5 (20%)  | 0        | 100         | 100 |
| 5   | m     | 25/99 (25%)      | 21 (84%)   | 4 (16%)  | 0        | 100         | 100 |
| All | All   | 7728/10029 (77%) | 7386 (96%) | 342 (4%) | 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     | 124/131 (95%) | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | B     | 124/131 (95%) | 116 (94%) | 8 (6%)   | 15          | 41 |
| 1   | C     | 124/131 (95%) | 116 (94%) | 8 (6%)   | 15          | 41 |
| 1   | D     | 124/131 (95%) | 118 (95%) | 6 (5%)   | 23          | 53 |
| 1   | E     | 124/131 (95%) | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | F     | 124/131 (95%) | 115 (93%) | 9 (7%)   | 13          | 35 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | G     | 124/131 (95%)  | 114 (92%) | 10 (8%)  | 11          | 30 |
| 1   | H     | 124/131 (95%)  | 116 (94%) | 8 (6%)   | 15          | 41 |
| 1   | I     | 124/131 (95%)  | 116 (94%) | 8 (6%)   | 15          | 41 |
| 1   | N     | 124/131 (95%)  | 116 (94%) | 8 (6%)   | 15          | 41 |
| 1   | S     | 124/131 (95%)  | 119 (96%) | 5 (4%)   | 28          | 60 |
| 1   | T     | 124/131 (95%)  | 119 (96%) | 5 (4%)   | 28          | 60 |
| 1   | U     | 124/131 (95%)  | 121 (98%) | 3 (2%)   | 43          | 73 |
| 1   | V     | 124/131 (95%)  | 112 (90%) | 12 (10%) | 8           | 23 |
| 1   | W     | 124/131 (95%)  | 114 (92%) | 10 (8%)  | 11          | 30 |
| 1   | Y     | 124/131 (95%)  | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | Z     | 124/131 (95%)  | 118 (95%) | 6 (5%)   | 23          | 53 |
| 1   | a     | 124/131 (95%)  | 119 (96%) | 5 (4%)   | 28          | 60 |
| 1   | b     | 124/131 (95%)  | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | c     | 124/131 (95%)  | 118 (95%) | 6 (5%)   | 23          | 53 |
| 1   | d     | 124/131 (95%)  | 115 (93%) | 9 (7%)   | 13          | 35 |
| 1   | e     | 124/131 (95%)  | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | f     | 124/131 (95%)  | 116 (94%) | 8 (6%)   | 15          | 41 |
| 1   | g     | 124/131 (95%)  | 115 (93%) | 9 (7%)   | 13          | 35 |
| 1   | h     | 124/131 (95%)  | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | n     | 124/131 (95%)  | 117 (94%) | 7 (6%)   | 19          | 47 |
| 1   | o     | 124/131 (95%)  | 115 (93%) | 9 (7%)   | 13          | 35 |
| 1   | p     | 124/131 (95%)  | 118 (95%) | 6 (5%)   | 23          | 53 |
| 1   | q     | 124/131 (95%)  | 114 (92%) | 10 (8%)  | 11          | 30 |
| 1   | r     | 124/131 (95%)  | 118 (95%) | 6 (5%)   | 23          | 53 |
| 2   | J     | 43/510 (8%)    | 41 (95%)  | 2 (5%)   | 23          | 54 |
| 2   | O     | 43/510 (8%)    | 42 (98%)  | 1 (2%)   | 44          | 74 |
| 2   | i     | 43/510 (8%)    | 42 (98%)  | 1 (2%)   | 44          | 74 |
| 3   | K     | 245/245 (100%) | 229 (94%) | 16 (6%)  | 15          | 41 |
| 3   | P     | 245/245 (100%) | 233 (95%) | 12 (5%)  | 22          | 51 |
| 3   | X     | 245/245 (100%) | 235 (96%) | 10 (4%)  | 27          | 59 |
| 3   | j     | 245/245 (100%) | 231 (94%) | 14 (6%)  | 18          | 47 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 3   | k     | 245/245 (100%)  | 239 (98%)  | 6 (2%)   | 43          | 73  |
| 3   | s     | 245/245 (100%)  | 233 (95%)  | 12 (5%)  | 22          | 51  |
| 4   | L     | 339/339 (100%)  | 329 (97%)  | 10 (3%)  | 37          | 68  |
| 4   | Q     | 339/339 (100%)  | 327 (96%)  | 12 (4%)  | 32          | 63  |
| 4   | l     | 339/339 (100%)  | 329 (97%)  | 10 (3%)  | 37          | 68  |
| 5   | M     | 22/83 (26%)     | 21 (96%)   | 1 (4%)   | 24          | 55  |
| 5   | R     | 22/83 (26%)     | 21 (96%)   | 1 (4%)   | 24          | 55  |
| 5   | m     | 22/83 (26%)     | 22 (100%)  | 0        | 100         | 100 |
| All | All   | 6402/8196 (78%) | 6071 (95%) | 331 (5%) | 22          | 50  |

All (331) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 42  | GLN  |
| 1   | D     | 57  | THR  |
| 1   | D     | 89  | SER  |
| 1   | D     | 103 | VAL  |
| 1   | D     | 137 | THR  |
| 1   | D     | 142 | LEU  |
| 1   | E     | 3   | PHE  |
| 1   | E     | 42  | GLN  |
| 1   | E     | 58  | SER  |
| 1   | E     | 84  | VAL  |
| 1   | E     | 101 | SER  |
| 1   | E     | 133 | ASP  |
| 1   | E     | 142 | LEU  |
| 1   | F     | 45  | LEU  |
| 1   | F     | 46  | THR  |
| 1   | F     | 66  | LYS  |
| 1   | F     | 89  | SER  |
| 1   | F     | 101 | SER  |
| 1   | F     | 103 | VAL  |
| 1   | F     | 112 | SER  |
| 1   | F     | 127 | SER  |
| 1   | F     | 149 | VAL  |
| 1   | G     | 11  | TYR  |
| 1   | G     | 50  | SER  |
| 1   | G     | 58  | SER  |
| 1   | G     | 62  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 84  | VAL  |
| 1   | G     | 89  | SER  |
| 1   | G     | 101 | SER  |
| 1   | G     | 103 | VAL  |
| 1   | G     | 108 | ILE  |
| 1   | G     | 114 | LYS  |
| 1   | H     | 24  | VAL  |
| 1   | H     | 39  | VAL  |
| 1   | H     | 52  | ASP  |
| 1   | H     | 58  | SER  |
| 1   | H     | 86  | ASP  |
| 1   | H     | 93  | LEU  |
| 1   | H     | 140 | VAL  |
| 1   | H     | 152 | THR  |
| 2   | J     | 578 | ASN  |
| 2   | J     | 621 | TYR  |
| 3   | K     | 9   | ASN  |
| 3   | K     | 28  | SER  |
| 3   | K     | 35  | SER  |
| 3   | K     | 40  | GLU  |
| 3   | K     | 48  | ILE  |
| 3   | K     | 60  | SER  |
| 3   | K     | 63  | CYS  |
| 3   | K     | 105 | HIS  |
| 3   | K     | 115 | SER  |
| 3   | K     | 118 | VAL  |
| 3   | K     | 127 | VAL  |
| 3   | K     | 146 | VAL  |
| 3   | K     | 159 | ASP  |
| 3   | K     | 162 | PHE  |
| 3   | K     | 218 | THR  |
| 3   | K     | 229 | LEU  |
| 4   | L     | 13  | VAL  |
| 4   | L     | 41  | VAL  |
| 4   | L     | 54  | VAL  |
| 4   | L     | 80  | THR  |
| 4   | L     | 169 | LEU  |
| 4   | L     | 201 | ASP  |
| 4   | L     | 226 | TYR  |
| 4   | L     | 239 | ILE  |
| 4   | L     | 270 | VAL  |
| 4   | L     | 285 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 76  | VAL  |
| 1   | a     | 7   | LEU  |
| 1   | a     | 57  | THR  |
| 1   | a     | 89  | SER  |
| 1   | a     | 108 | ILE  |
| 1   | a     | 142 | LEU  |
| 1   | b     | 8   | TYR  |
| 1   | b     | 9   | CYS  |
| 1   | b     | 26  | LEU  |
| 1   | b     | 36  | LEU  |
| 1   | b     | 86  | ASP  |
| 1   | b     | 103 | VAL  |
| 1   | b     | 142 | LEU  |
| 1   | c     | 12  | THR  |
| 1   | c     | 28  | VAL  |
| 1   | c     | 42  | GLN  |
| 1   | c     | 84  | VAL  |
| 1   | c     | 137 | THR  |
| 1   | c     | 142 | LEU  |
| 1   | d     | 28  | VAL  |
| 1   | d     | 46  | THR  |
| 1   | d     | 48  | ASN  |
| 1   | d     | 50  | SER  |
| 1   | d     | 58  | SER  |
| 1   | d     | 61  | THR  |
| 1   | d     | 79  | ASN  |
| 1   | d     | 103 | VAL  |
| 1   | d     | 123 | VAL  |
| 1   | g     | 3   | PHE  |
| 1   | g     | 8   | TYR  |
| 1   | g     | 26  | LEU  |
| 1   | g     | 37  | LEU  |
| 1   | g     | 47  | VAL  |
| 1   | g     | 84  | VAL  |
| 1   | g     | 103 | VAL  |
| 1   | g     | 112 | SER  |
| 1   | g     | 137 | THR  |
| 3   | k     | 2   | SER  |
| 3   | k     | 27  | VAL  |
| 3   | k     | 63  | CYS  |
| 3   | k     | 95  | ASP  |
| 3   | k     | 239 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | k     | 261 | VAL  |
| 1   | A     | 42  | GLN  |
| 1   | A     | 46  | THR  |
| 1   | A     | 72  | MET  |
| 1   | A     | 86  | ASP  |
| 1   | A     | 137 | THR  |
| 1   | A     | 140 | VAL  |
| 1   | A     | 142 | LEU  |
| 1   | B     | 17  | LYS  |
| 1   | B     | 42  | GLN  |
| 1   | B     | 46  | THR  |
| 1   | B     | 61  | THR  |
| 1   | B     | 86  | ASP  |
| 1   | B     | 101 | SER  |
| 1   | B     | 133 | ASP  |
| 1   | B     | 142 | LEU  |
| 1   | C     | 23  | ASP  |
| 1   | C     | 36  | LEU  |
| 1   | C     | 46  | THR  |
| 1   | C     | 66  | LYS  |
| 1   | C     | 101 | SER  |
| 1   | C     | 112 | SER  |
| 1   | C     | 143 | ASP  |
| 1   | C     | 149 | VAL  |
| 1   | I     | 12  | THR  |
| 1   | I     | 26  | LEU  |
| 1   | I     | 50  | SER  |
| 1   | I     | 58  | SER  |
| 1   | I     | 84  | VAL  |
| 1   | I     | 89  | SER  |
| 1   | I     | 101 | SER  |
| 1   | I     | 103 | VAL  |
| 1   | N     | 24  | VAL  |
| 1   | N     | 39  | VAL  |
| 1   | N     | 52  | ASP  |
| 1   | N     | 58  | SER  |
| 1   | N     | 86  | ASP  |
| 1   | N     | 101 | SER  |
| 1   | N     | 140 | VAL  |
| 1   | N     | 152 | THR  |
| 2   | O     | 579 | LEU  |
| 3   | P     | 9   | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | P     | 28  | SER  |
| 3   | P     | 35  | SER  |
| 3   | P     | 63  | CYS  |
| 3   | P     | 88  | ASP  |
| 3   | P     | 115 | SER  |
| 3   | P     | 118 | VAL  |
| 3   | P     | 127 | VAL  |
| 3   | P     | 159 | ASP  |
| 3   | P     | 172 | VAL  |
| 3   | P     | 222 | LEU  |
| 3   | P     | 226 | ILE  |
| 4   | Q     | 41  | VAL  |
| 4   | Q     | 54  | VAL  |
| 4   | Q     | 113 | THR  |
| 4   | Q     | 162 | LEU  |
| 4   | Q     | 169 | LEU  |
| 4   | Q     | 201 | ASP  |
| 4   | Q     | 202 | ASN  |
| 4   | Q     | 226 | TYR  |
| 4   | Q     | 268 | LEU  |
| 4   | Q     | 285 | VAL  |
| 4   | Q     | 302 | THR  |
| 4   | Q     | 352 | ILE  |
| 5   | R     | 87  | VAL  |
| 1   | S     | 26  | LEU  |
| 1   | S     | 45  | LEU  |
| 1   | S     | 57  | THR  |
| 1   | S     | 84  | VAL  |
| 1   | S     | 89  | SER  |
| 1   | T     | 26  | LEU  |
| 1   | T     | 36  | LEU  |
| 1   | T     | 86  | ASP  |
| 1   | T     | 103 | VAL  |
| 1   | T     | 142 | LEU  |
| 1   | U     | 12  | THR  |
| 1   | U     | 42  | GLN  |
| 1   | U     | 84  | VAL  |
| 1   | V     | 28  | VAL  |
| 1   | V     | 39  | VAL  |
| 1   | V     | 46  | THR  |
| 1   | V     | 48  | ASN  |
| 1   | V     | 52  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 58  | SER  |
| 1   | V     | 103 | VAL  |
| 1   | V     | 108 | ILE  |
| 1   | V     | 123 | VAL  |
| 1   | V     | 149 | VAL  |
| 1   | V     | 153 | ILE  |
| 1   | V     | 160 | MET  |
| 1   | W     | 37  | LEU  |
| 1   | W     | 39  | VAL  |
| 1   | W     | 47  | VAL  |
| 1   | W     | 84  | VAL  |
| 1   | W     | 86  | ASP  |
| 1   | W     | 103 | VAL  |
| 1   | W     | 105 | VAL  |
| 1   | W     | 112 | SER  |
| 1   | W     | 122 | ILE  |
| 1   | W     | 137 | THR  |
| 3   | X     | 2   | SER  |
| 3   | X     | 27  | VAL  |
| 3   | X     | 63  | CYS  |
| 3   | X     | 65  | LEU  |
| 3   | X     | 95  | ASP  |
| 3   | X     | 97  | MET  |
| 3   | X     | 159 | ASP  |
| 3   | X     | 220 | VAL  |
| 3   | X     | 239 | THR  |
| 3   | X     | 261 | VAL  |
| 1   | Y     | 42  | GLN  |
| 1   | Y     | 72  | MET  |
| 1   | Y     | 86  | ASP  |
| 1   | Y     | 89  | SER  |
| 1   | Y     | 112 | SER  |
| 1   | Y     | 137 | THR  |
| 1   | Y     | 142 | LEU  |
| 1   | Z     | 26  | LEU  |
| 1   | Z     | 42  | GLN  |
| 1   | Z     | 61  | THR  |
| 1   | Z     | 86  | ASP  |
| 1   | Z     | 101 | SER  |
| 1   | Z     | 133 | ASP  |
| 1   | e     | 37  | LEU  |
| 1   | e     | 46  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 50  | SER  |
| 1   | e     | 55  | GLU  |
| 1   | e     | 112 | SER  |
| 1   | e     | 127 | SER  |
| 1   | e     | 149 | VAL  |
| 1   | f     | 3   | PHE  |
| 1   | f     | 26  | LEU  |
| 1   | f     | 50  | SER  |
| 1   | f     | 58  | SER  |
| 1   | f     | 62  | VAL  |
| 1   | f     | 84  | VAL  |
| 1   | f     | 101 | SER  |
| 1   | f     | 103 | VAL  |
| 1   | h     | 39  | VAL  |
| 1   | h     | 48  | ASN  |
| 1   | h     | 52  | ASP  |
| 1   | h     | 86  | ASP  |
| 1   | h     | 101 | SER  |
| 1   | h     | 105 | VAL  |
| 1   | h     | 152 | THR  |
| 2   | i     | 621 | TYR  |
| 3   | j     | 9   | ASN  |
| 3   | j     | 60  | SER  |
| 3   | j     | 63  | CYS  |
| 3   | j     | 97  | MET  |
| 3   | j     | 105 | HIS  |
| 3   | j     | 115 | SER  |
| 3   | j     | 118 | VAL  |
| 3   | j     | 127 | VAL  |
| 3   | j     | 159 | ASP  |
| 3   | j     | 162 | PHE  |
| 3   | j     | 172 | VAL  |
| 3   | j     | 178 | ASP  |
| 3   | j     | 193 | THR  |
| 3   | j     | 218 | THR  |
| 4   | l     | 13  | VAL  |
| 4   | l     | 52  | ASP  |
| 4   | l     | 54  | VAL  |
| 4   | l     | 80  | THR  |
| 4   | l     | 140 | GLU  |
| 4   | l     | 162 | LEU  |
| 4   | l     | 169 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | l     | 226 | TYR  |
| 4   | l     | 285 | VAL  |
| 4   | l     | 352 | ILE  |
| 1   | n     | 3   | PHE  |
| 1   | n     | 7   | LEU  |
| 1   | n     | 26  | LEU  |
| 1   | n     | 45  | LEU  |
| 1   | n     | 46  | THR  |
| 1   | n     | 109 | ASN  |
| 1   | n     | 142 | LEU  |
| 1   | o     | 8   | TYR  |
| 1   | o     | 9   | CYS  |
| 1   | o     | 26  | LEU  |
| 1   | o     | 36  | LEU  |
| 1   | o     | 86  | ASP  |
| 1   | o     | 103 | VAL  |
| 1   | o     | 141 | LYS  |
| 1   | o     | 142 | LEU  |
| 1   | o     | 160 | MET  |
| 1   | p     | 12  | THR  |
| 1   | p     | 42  | GLN  |
| 1   | p     | 61  | THR  |
| 1   | p     | 84  | VAL  |
| 1   | p     | 137 | THR  |
| 1   | p     | 142 | LEU  |
| 1   | q     | 6   | ASN  |
| 1   | q     | 28  | VAL  |
| 1   | q     | 39  | VAL  |
| 1   | q     | 46  | THR  |
| 1   | q     | 48  | ASN  |
| 1   | q     | 50  | SER  |
| 1   | q     | 58  | SER  |
| 1   | q     | 103 | VAL  |
| 1   | q     | 108 | ILE  |
| 1   | q     | 123 | VAL  |
| 1   | r     | 47  | VAL  |
| 1   | r     | 50  | SER  |
| 1   | r     | 84  | VAL  |
| 1   | r     | 103 | VAL  |
| 1   | r     | 105 | VAL  |
| 1   | r     | 137 | THR  |
| 3   | s     | 2   | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | s     | 27  | VAL  |
| 3   | s     | 62  | LYS  |
| 3   | s     | 63  | CYS  |
| 3   | s     | 65  | LEU  |
| 3   | s     | 88  | ASP  |
| 3   | s     | 95  | ASP  |
| 3   | s     | 97  | MET  |
| 3   | s     | 177 | SER  |
| 3   | s     | 220 | VAL  |
| 3   | s     | 239 | THR  |
| 3   | s     | 261 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 79  | ASN  |
| 1   | H     | 109 | ASN  |
| 3   | K     | 74  | HIS  |
| 3   | K     | 96  | GLN  |
| 4   | L     | 7   | GLN  |
| 4   | L     | 42  | ASN  |
| 4   | L     | 88  | GLN  |
| 4   | L     | 266 | GLN  |
| 4   | L     | 337 | GLN  |
| 1   | a     | 109 | ASN  |
| 1   | d     | 79  | ASN  |
| 1   | g     | 43  | GLN  |
| 1   | g     | 48  | ASN  |
| 3   | k     | 168 | ASN  |
| 1   | B     | 109 | ASN  |
| 1   | N     | 110 | GLN  |
| 3   | P     | 74  | HIS  |
| 3   | P     | 96  | GLN  |
| 3   | P     | 266 | ASN  |
| 4   | Q     | 7   | GLN  |
| 4   | Q     | 42  | ASN  |
| 4   | Q     | 88  | GLN  |
| 4   | Q     | 266 | GLN  |
| 4   | Q     | 335 | GLN  |
| 1   | S     | 109 | ASN  |
| 1   | W     | 48  | ASN  |
| 1   | W     | 109 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 79  | ASN  |
| 1   | h     | 48  | ASN  |
| 1   | h     | 110 | GLN  |
| 3   | j     | 74  | HIS  |
| 3   | j     | 96  | GLN  |
| 3   | j     | 150 | GLN  |
| 3   | j     | 266 | ASN  |
| 4   | l     | 7   | GLN  |
| 4   | l     | 42  | ASN  |
| 4   | l     | 88  | GLN  |
| 4   | l     | 335 | GLN  |
| 3   | s     | 202 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [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.

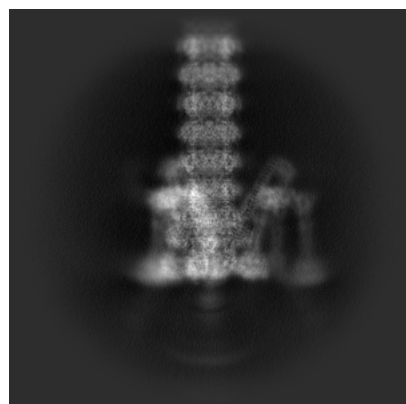
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61074. These allow visual inspection of the internal detail of the map and identification of artifacts.

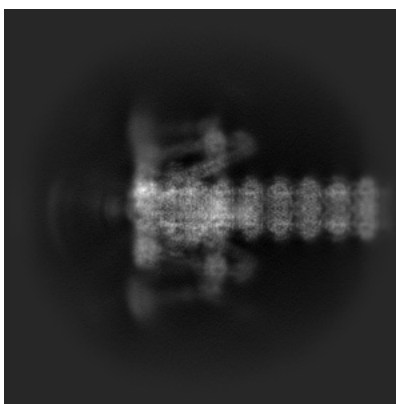
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

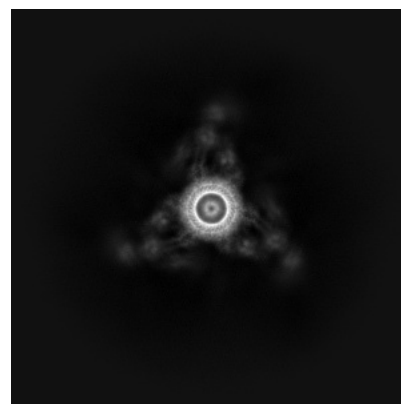
#### 6.1.1 Primary map



X

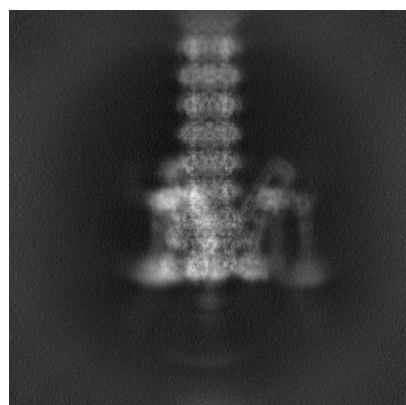


Y

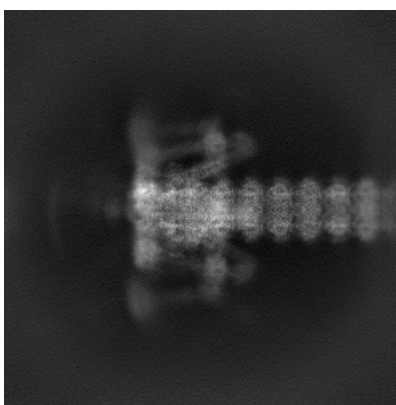


Z

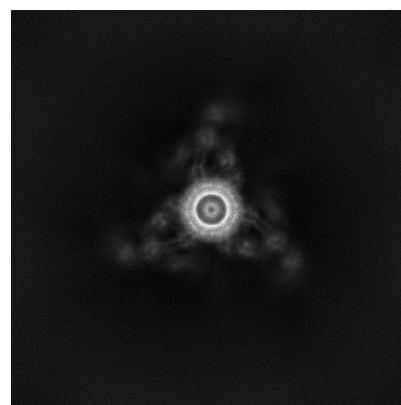
#### 6.1.2 Raw map



X



Y

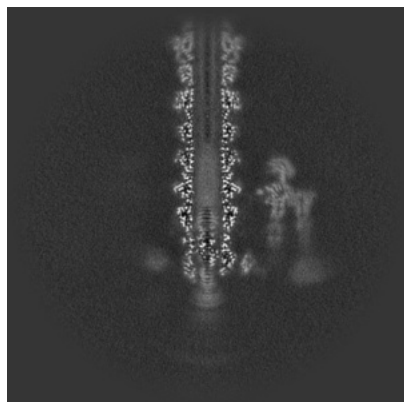


Z

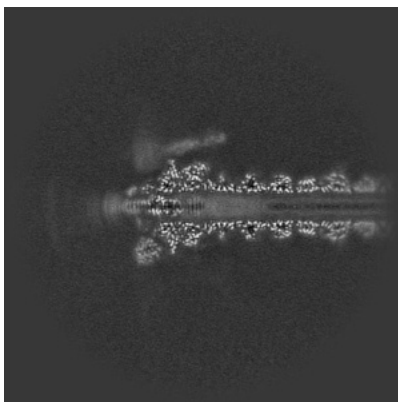
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

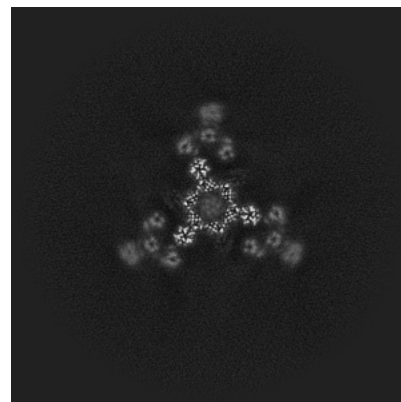
### 6.2.1 Primary map



X Index: 256

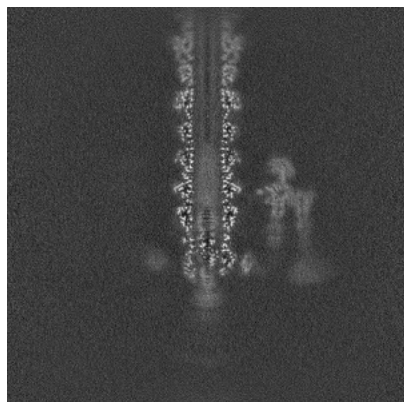


Y Index: 256

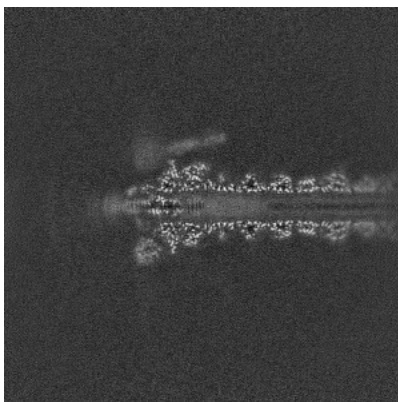


Z Index: 256

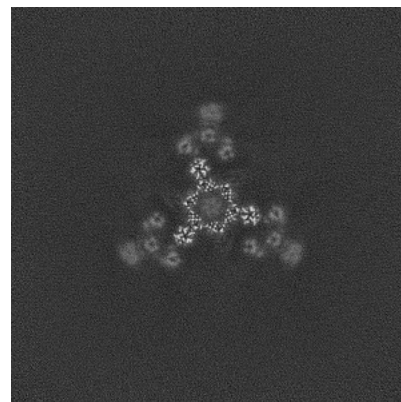
### 6.2.2 Raw map



X Index: 256



Y Index: 256

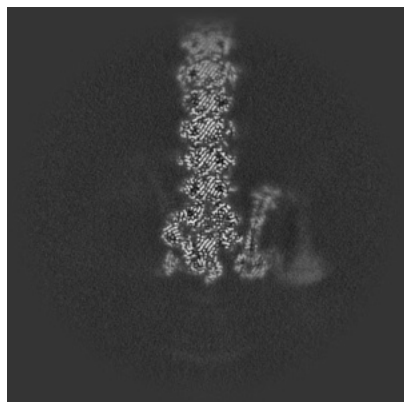


Z Index: 256

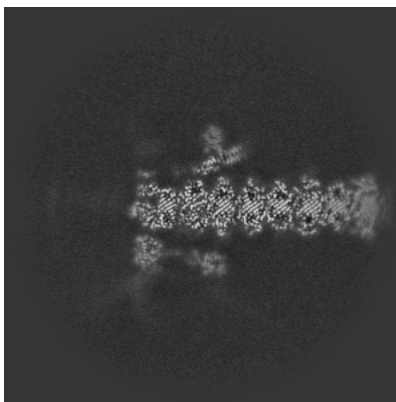
The images above show central slices of the map in three orthogonal directions.

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

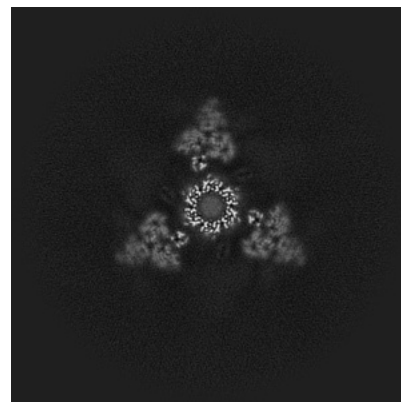
### 6.3.1 Primary map



X Index: 276

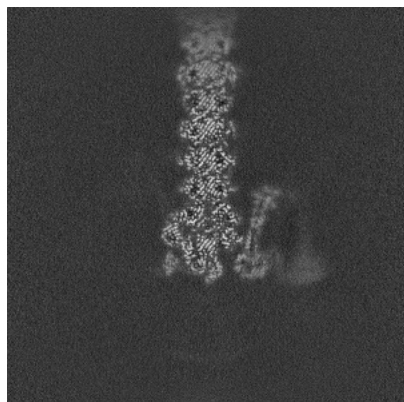


Y Index: 235

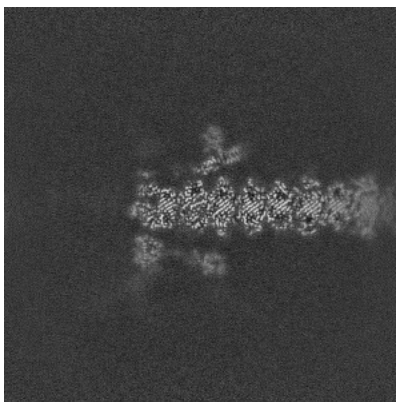


Z Index: 273

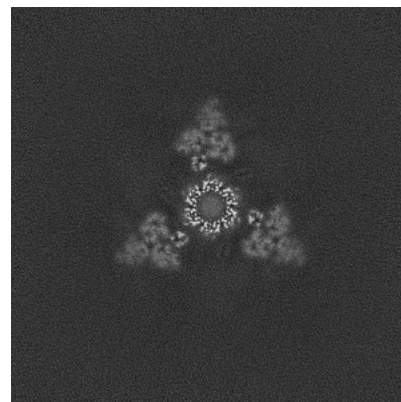
### 6.3.2 Raw map



X Index: 276



Y Index: 235

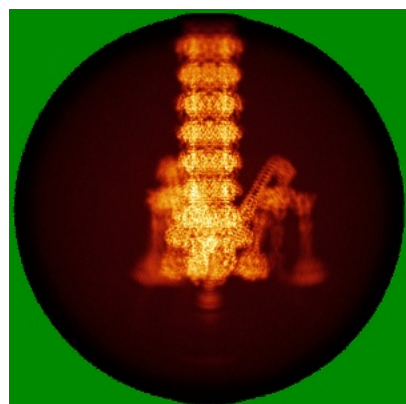


Z Index: 273

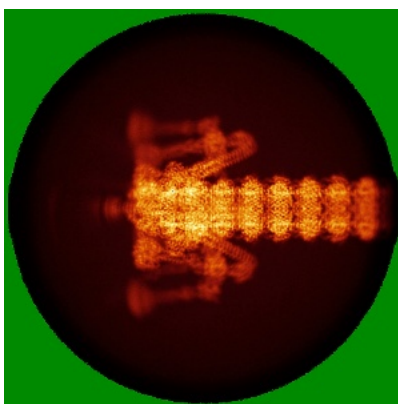
The images above show the largest variance slices of the map in three orthogonal directions.

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

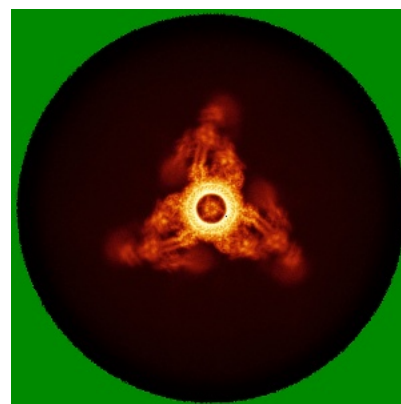
### 6.4.1 Primary map



X

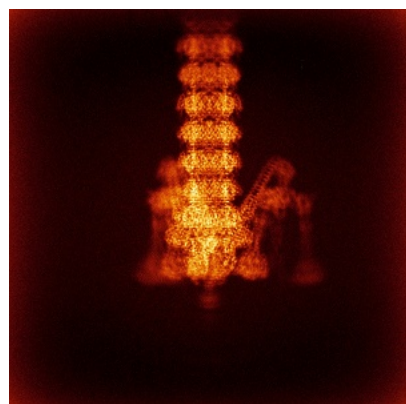


Y

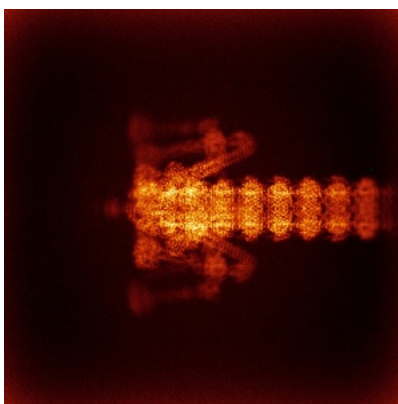


Z

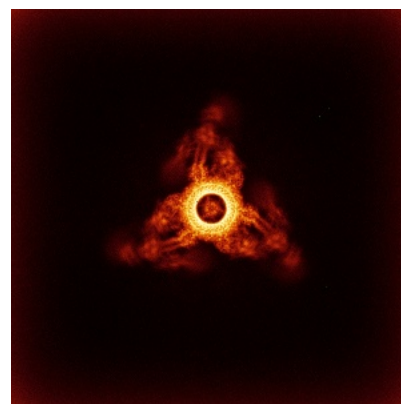
### 6.4.2 Raw map



X



Y

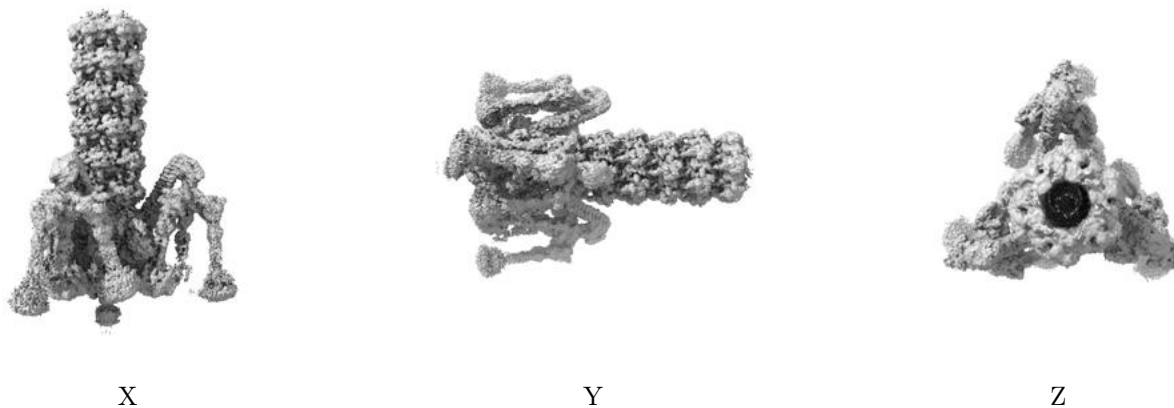


Z

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.

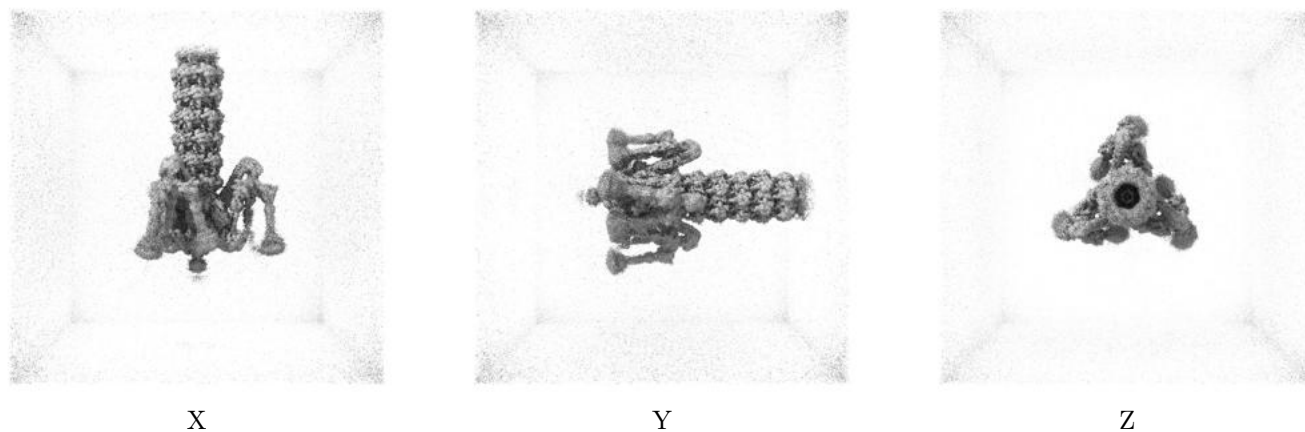
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

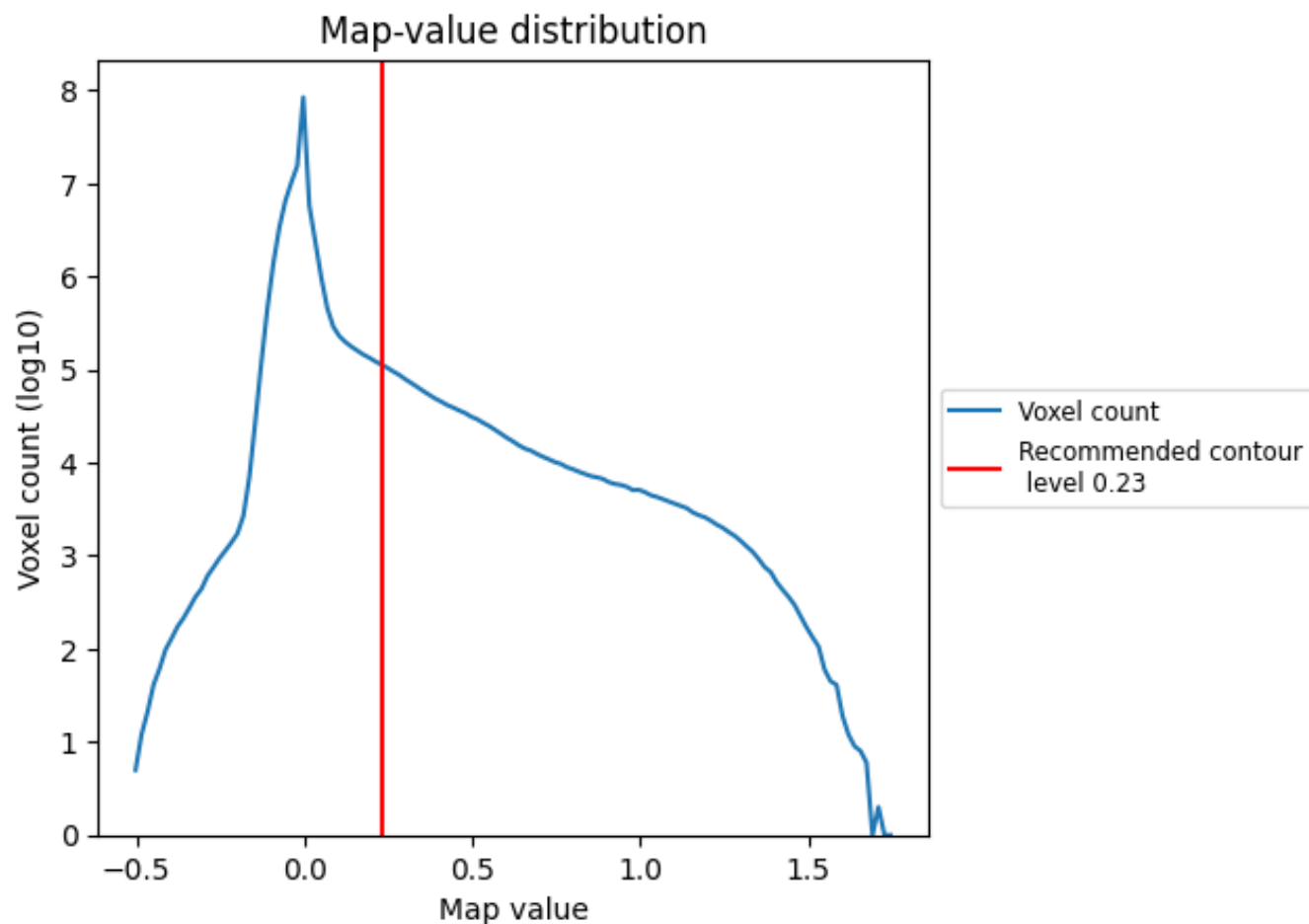
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

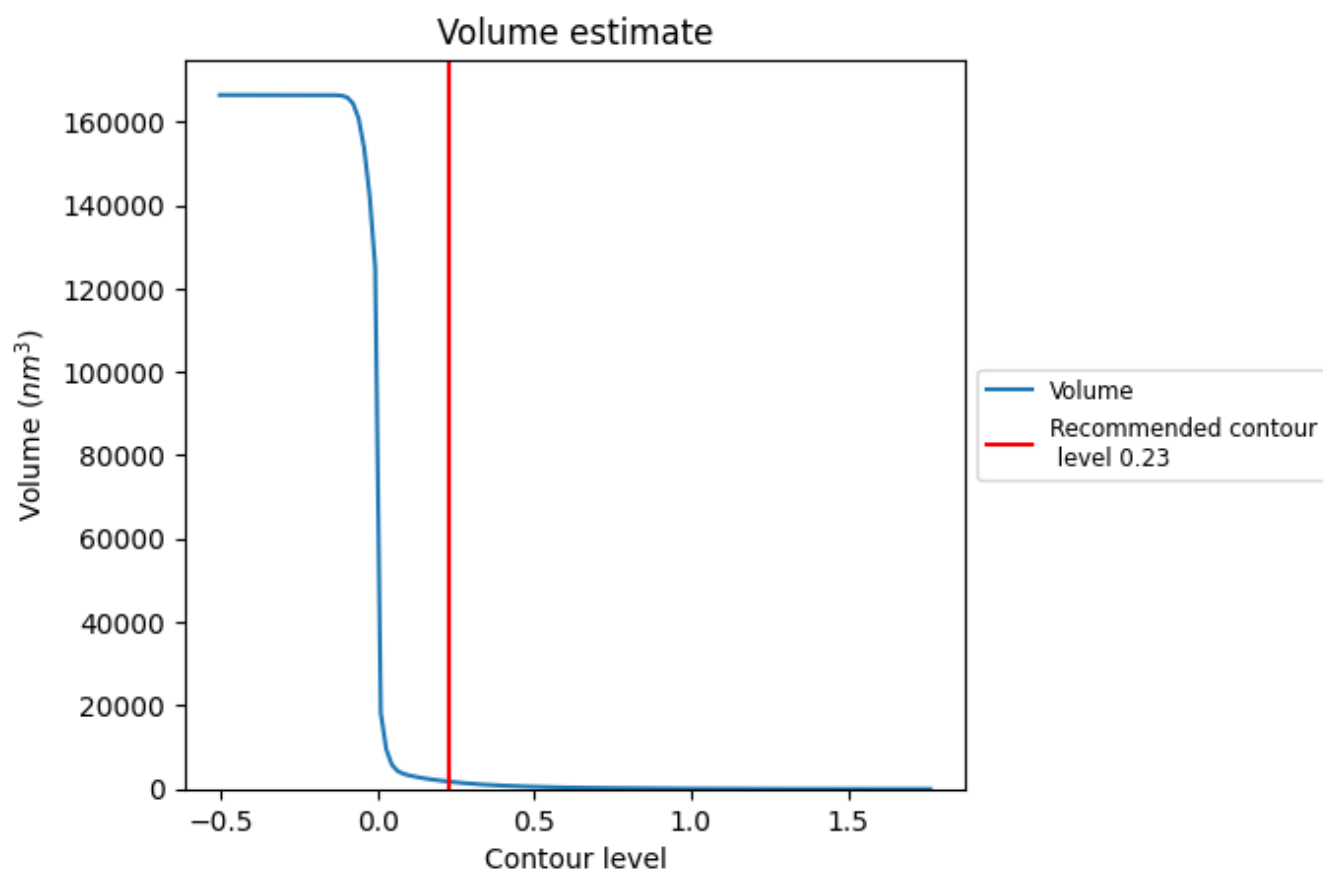
This section contains the results of statistical analysis of the map.

### 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.

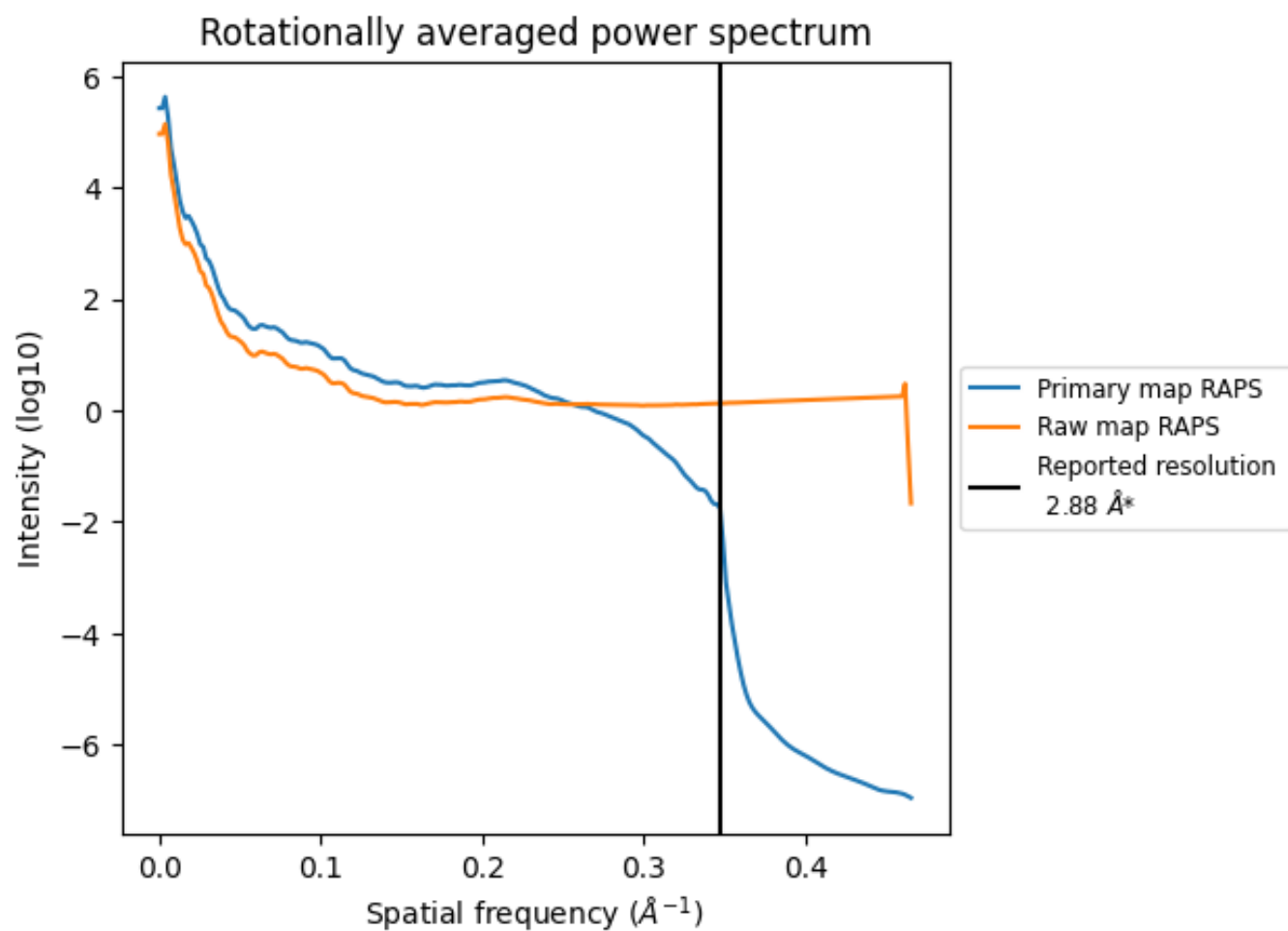
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1737  $\text{nm}^3$ ; this corresponds to an approximate mass of 1569 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 ⓘ

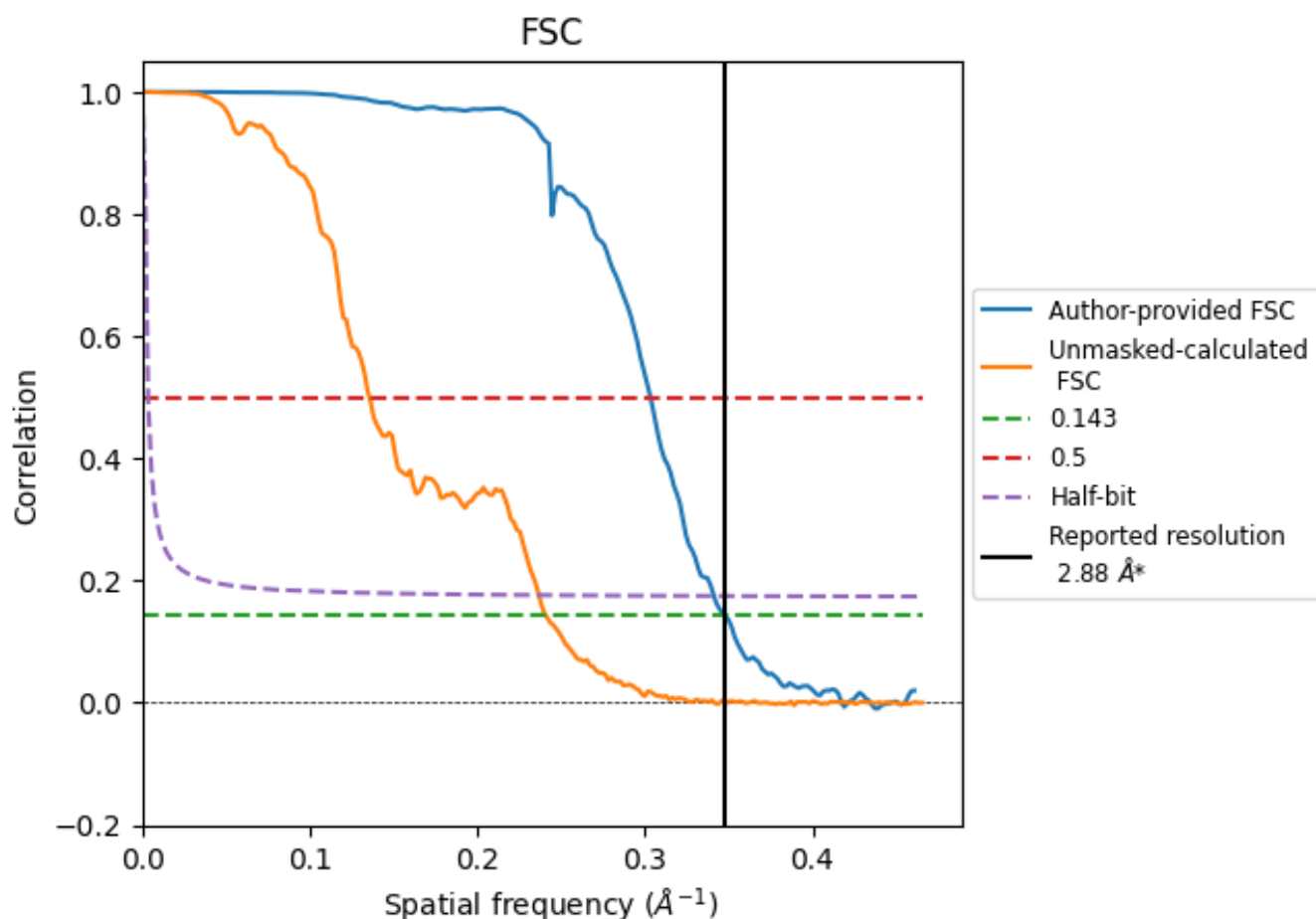


\*Reported resolution corresponds to spatial frequency of 0.347 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.347  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

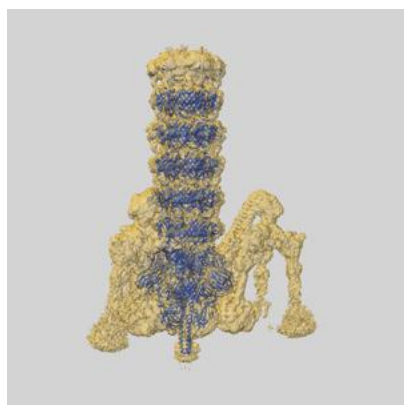
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.88                               | -    | -        |
| Author-provided FSC curve | 2.88                               | 3.30 | 2.93     |
| Unmasked-calculated*      | 4.15                               | 7.37 | 4.22     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 2.88 by more than 10 %

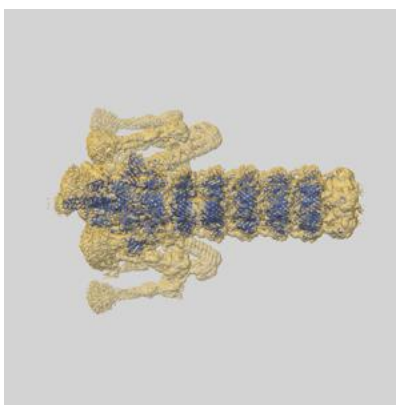
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61074 and PDB model 9J1K. Per-residue inclusion information can be found in section [3](#) on page [8](#).

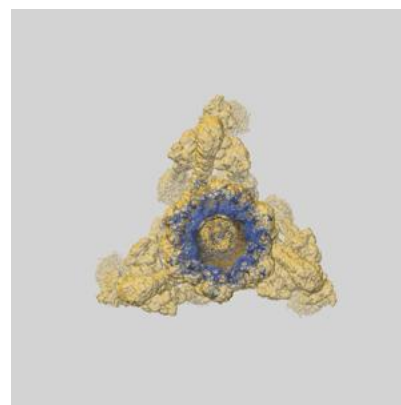
### 9.1 Map-model overlay [i](#)



X



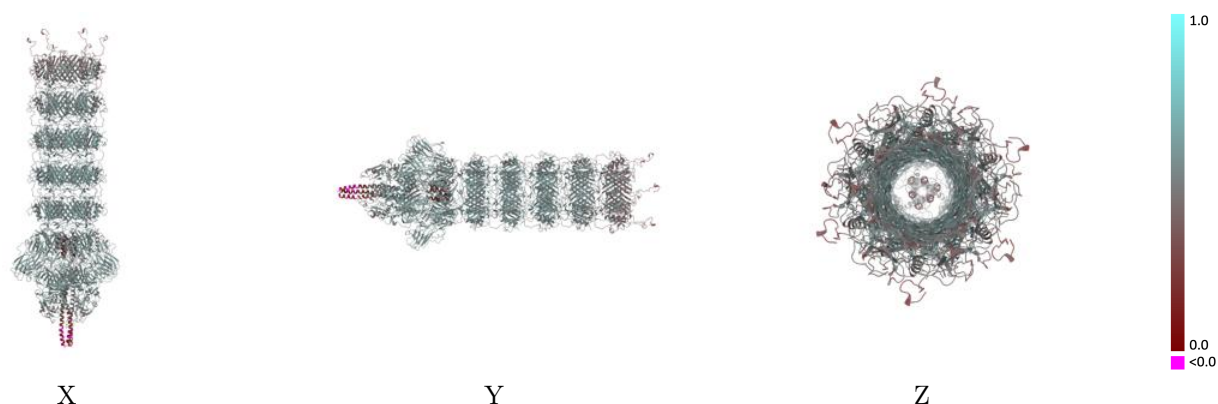
Y



Z

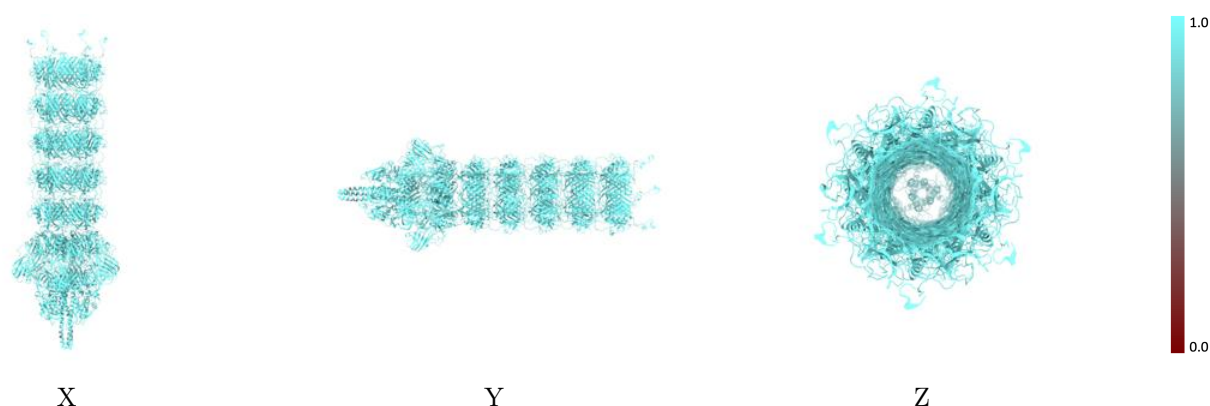
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



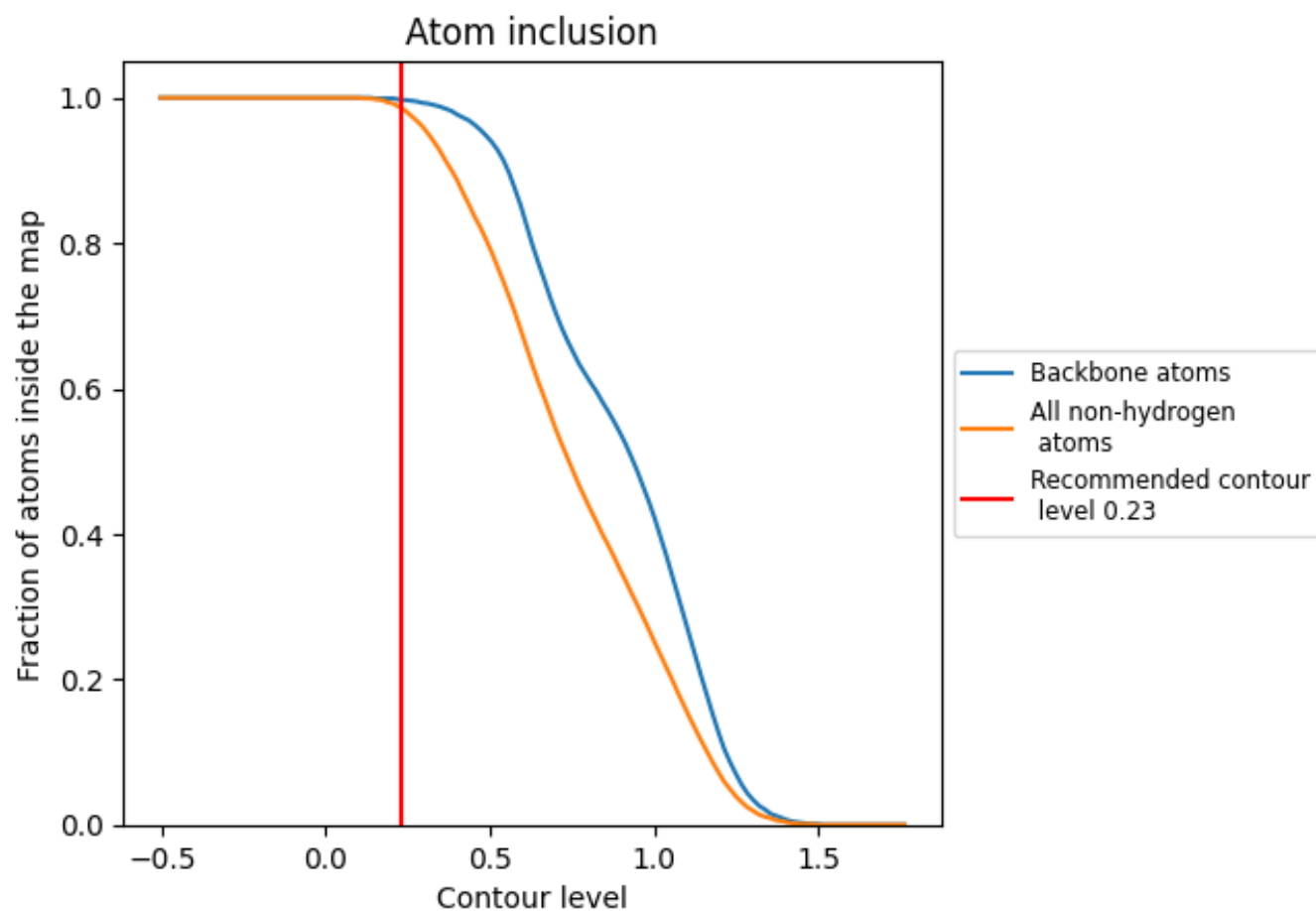
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.23) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9860   |  0.5150   |
| A     |  0.9860   |  0.5450   |
| B     |  0.9890   |  0.5370   |
| C     |  0.9870   |  0.5060   |
| D     |  0.9870   |  0.5440   |
| E     |  0.9880   |  0.5380   |
| F     |  0.9880   |  0.5060   |
| G     |  0.9870   |  0.5380   |
| H     |  0.9810   |  0.4390   |
| I     |  0.9880   |  0.5390   |
| J     |  0.9850   |  0.4420   |
| K     |  0.9880   |  0.5460   |
| L     |  0.9830   |  0.5020   |
| M     |  0.9750   |  0.3240   |
| N     |  0.9820  |  0.4370  |
| O     |  0.9820 |  0.4420 |
| P     |  0.9880 |  0.5440 |
| Q     |  0.9830 |  0.5020 |
| R     |  0.9800 |  0.3280 |
| S     |  0.9820 |  0.5420 |
| T     |  0.9860 |  0.5360 |
| U     |  0.9870 |  0.5080 |
| V     |  0.9850 |  0.4380 |
| W     |  0.9870 |  0.5340 |
| X     |  0.9910 |  0.5440 |
| Y     |  0.9870 |  0.5440 |
| Z     |  0.9890 |  0.5370 |
| a     |  0.9850 |  0.5420 |
| b     |  0.9890 |  0.5370 |
| c     |  0.9880 |  0.5120 |
| d     |  0.9850 |  0.4400 |
| e     |  0.9870 |  0.5080 |
| f     |  0.9890 |  0.5410 |
| g     |  0.9870 |  0.5350 |
| h     |  0.9820 |  0.4390 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.9850 |  0.4360 |
| j     |  0.9890 |  0.5460 |
| k     |  0.9910 |  0.5450 |
| l     |  0.9820 |  0.5010 |
| m     |  0.9850 |  0.3190 |
| n     |  0.9840 |  0.5410 |
| o     |  0.9860 |  0.5360 |
| p     |  0.9900 |  0.5070 |
| q     |  0.9820 |  0.4410 |
| r     |  0.9870 |  0.5350 |
| s     |  0.9920 |  0.5440 |