



## Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 11:01 AM UTC

PDB ID : 8ZDN / pdb\_00008zdn  
EMDB ID : EMD-39995  
Title : Cryo-EM structure of Mycobacteriophage Douge genome-free tail tube (gp13)  
Authors : Maharana, J.; Wang, C.H.; Tsai, L.A.; Lowary, T.L.; Ho, M.C.  
Deposited on : 2024-05-02  
Resolution : 3.07 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

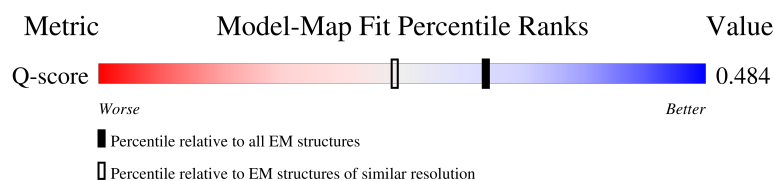
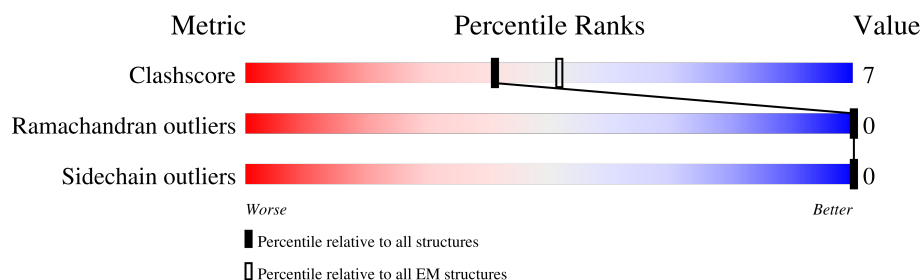
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.07 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.



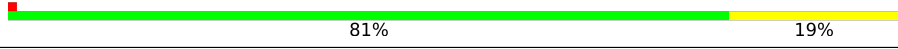
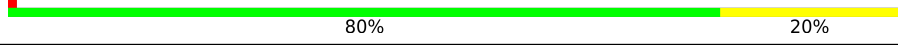
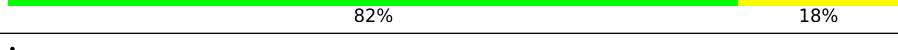
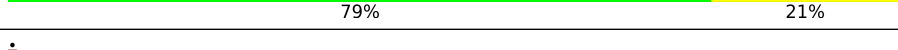
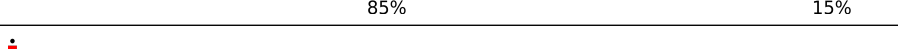
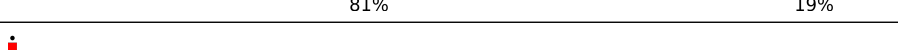
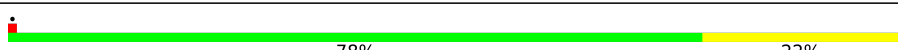
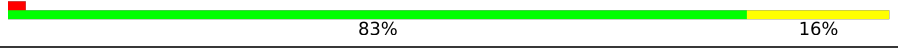
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13977 ( 2.57 - 3.57 )                                    |

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     | 300    |                  |
| 1   | B     | 300    |                  |
| 1   | C     | 300    |                  |
| 1   | D     | 300    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 300    |    |
| 1   | F     | 300    |    |
| 1   | G     | 300    |    |
| 1   | H     | 300    |    |
| 1   | I     | 300    |    |
| 1   | J     | 300    |    |
| 1   | K     | 300    |    |
| 1   | L     | 300    |    |
| 1   | M     | 300    |    |
| 1   | N     | 300    |    |
| 1   | O     | 300    |    |
| 1   | P     | 300    |  |
| 1   | Q     | 300    |  |
| 1   | R     | 300    |  |
| 1   | S     | 300    |  |
| 1   | T     | 300    |  |
| 1   | U     | 300    |  |
| 1   | V     | 300    |  |
| 1   | W     | 300    |  |
| 1   | X     | 300    |  |
| 1   | a     | 300    |  |
| 1   | b     | 300    |  |
| 1   | c     | 300    |  |
| 1   | d     | 300    |  |
| 1   | e     | 300    |  |

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| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                                                             |
|-----|-------|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | f     | 300    |  A horizontal bar chart showing the quality of the chain. The bar is divided into two segments: a green segment representing 83% and a yellow segment representing 16%. A small red square is at the beginning of the bar. |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 67680 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 Tail Tube Protein (gp13).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | B     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | C     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | D     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | E     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | F     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | G     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | H     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | I     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | J     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | K     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | L     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | M     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | N     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | O     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | P     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | Q     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |

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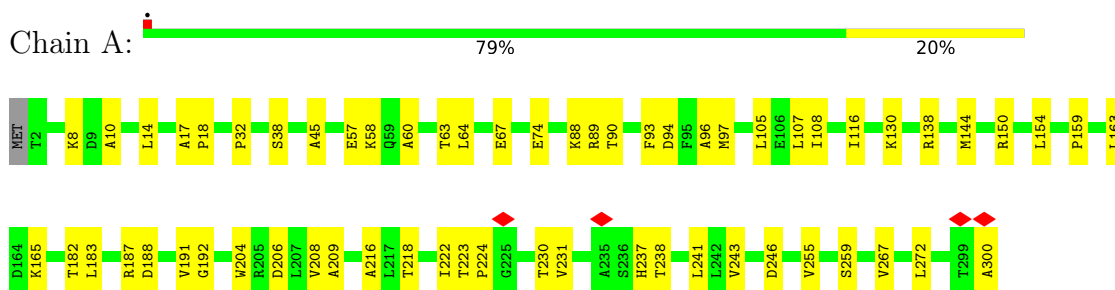
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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | R     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | S     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | T     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | U     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | V     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | W     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | X     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | a     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | b     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | c     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | d     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | e     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |
| 1   | f     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 1438 | 367 | 448 | 3 |         |       |

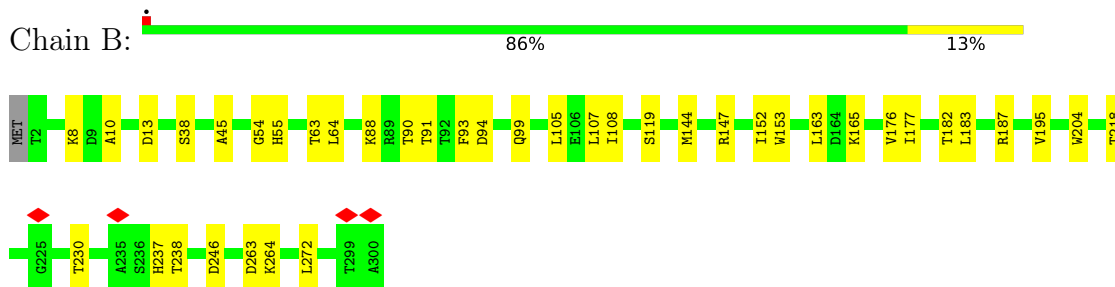
### 3 Residue-property plots

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.

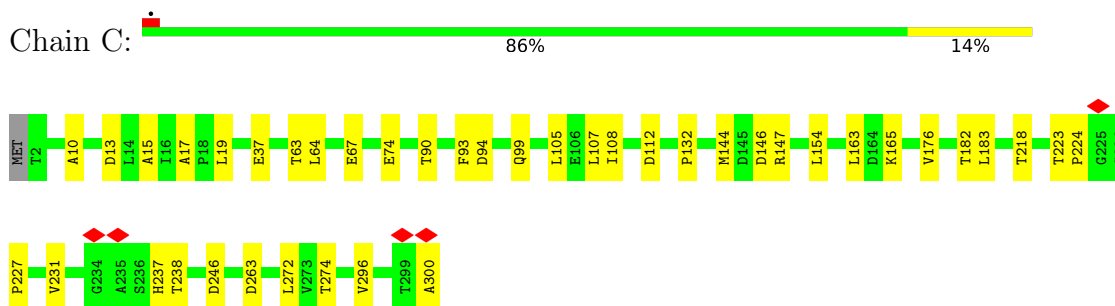
#### • Molecule 1: Tail Tube Protein (gp13)



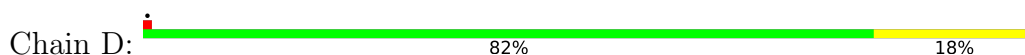
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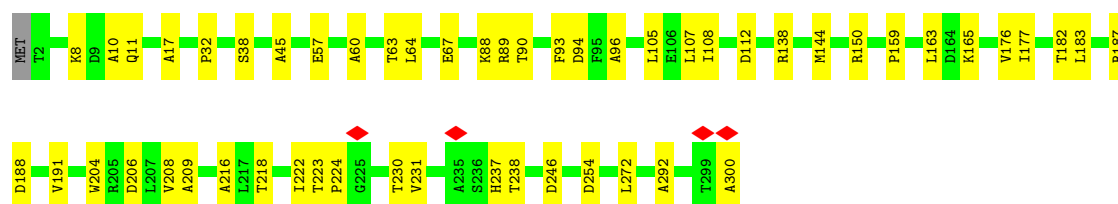


#### • Molecule 1: Tail Tube Protein (gp13)

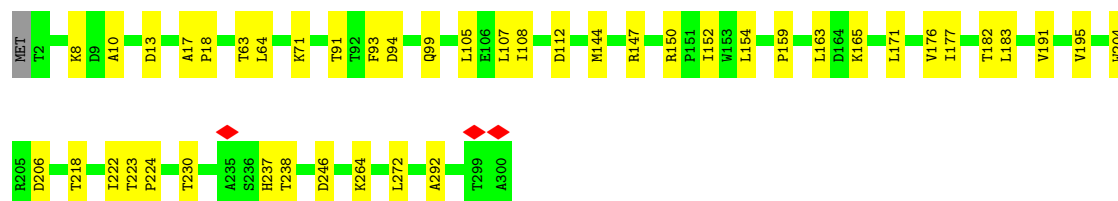
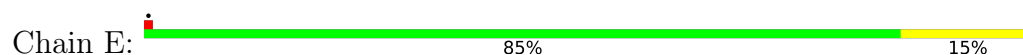


#### • Molecule 1: Tail Tube Protein (gp13)

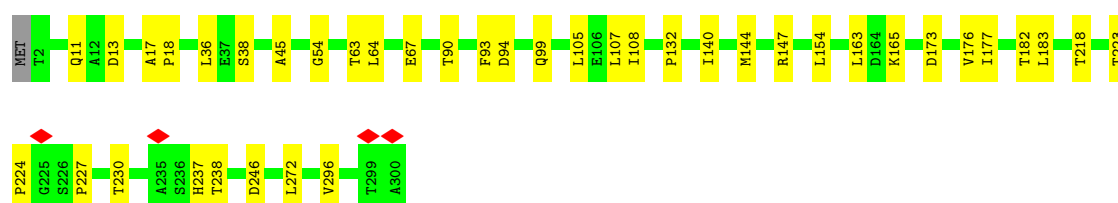
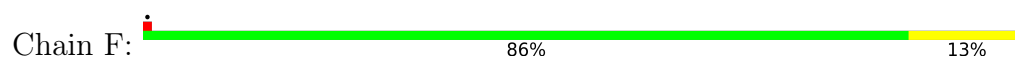




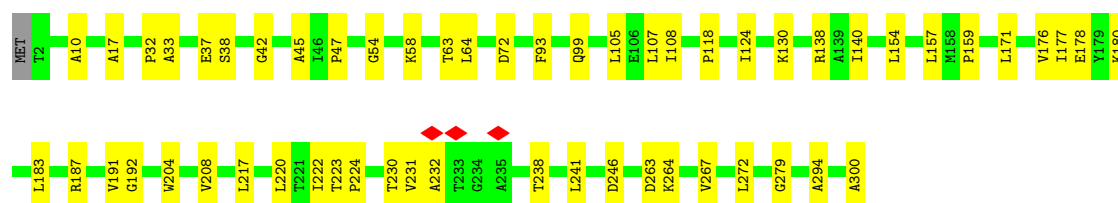
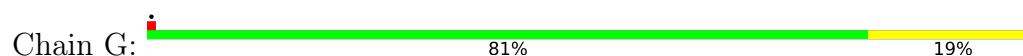
- Molecule 1: Tail Tube Protein (gp13)



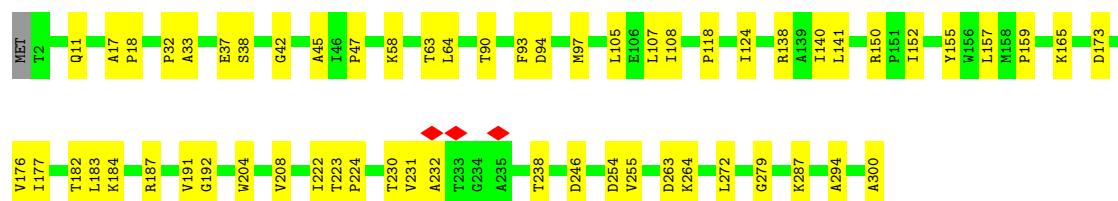
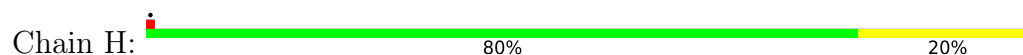
- Molecule 1: Tail Tube Protein (gp13)



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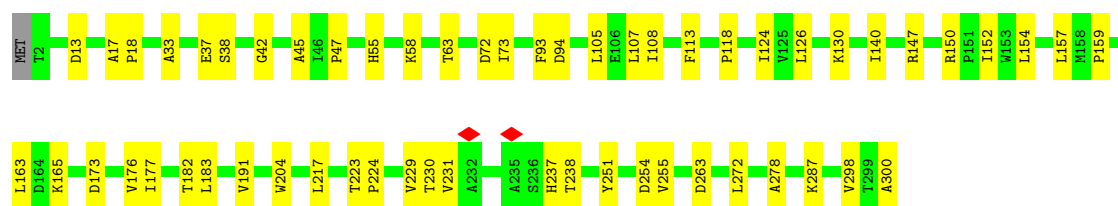
- Molecule 1: Tail Tube Protein (gp13)





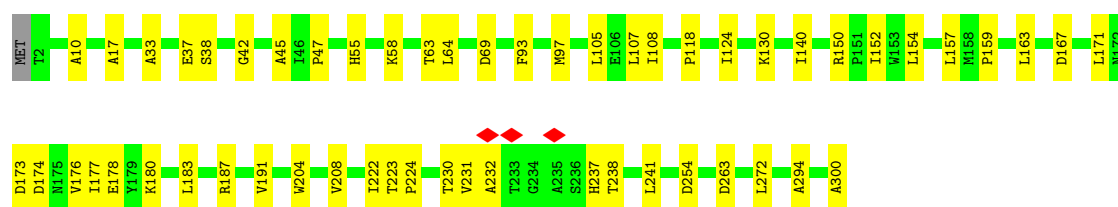
- Molecule 1: Tail Tube Protein (gp13)

Chain I:  81% 19%



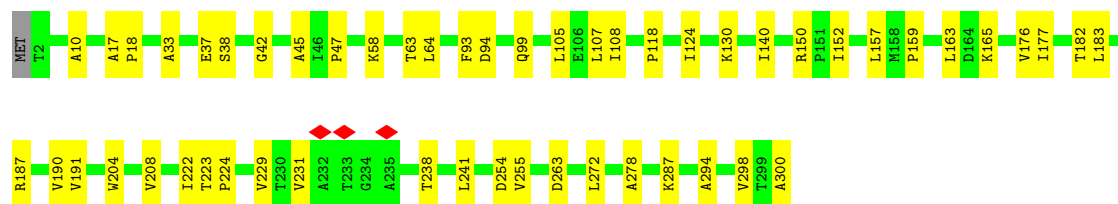
- Molecule 1: Tail Tube Protein (gp13)

Chain J:  81% 18%



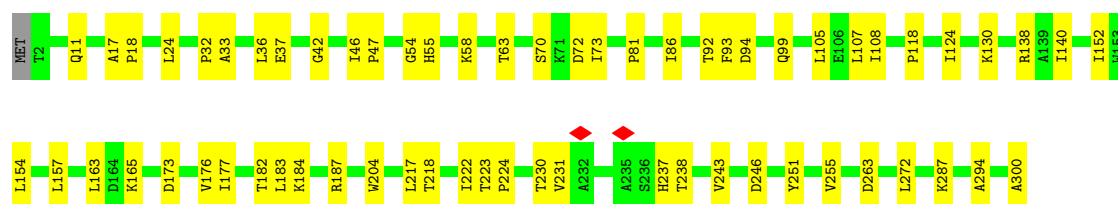
- Molecule 1: Tail Tube Protein (gp13)

Chain K:  82% 18%



- Molecule 1: Tail Tube Protein (gp13)

Chain L:  79% 21%



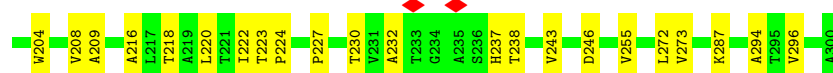
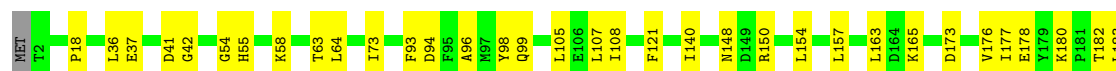
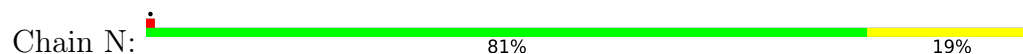
- Molecule 1: Tail Tube Protein (gp13)

Chain M:  85% 15%

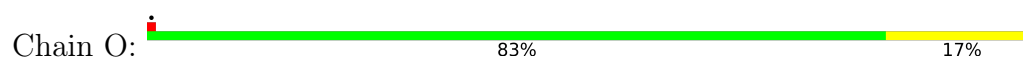




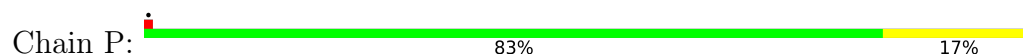
- Molecule 1: Tail Tube Protein (gp13)



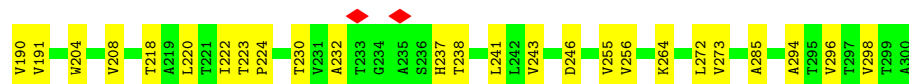
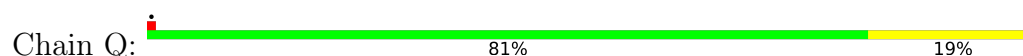
- Molecule 1: Tail Tube Protein (gp13)



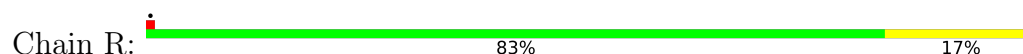
- Molecule 1: Tail Tube Protein (gp13)

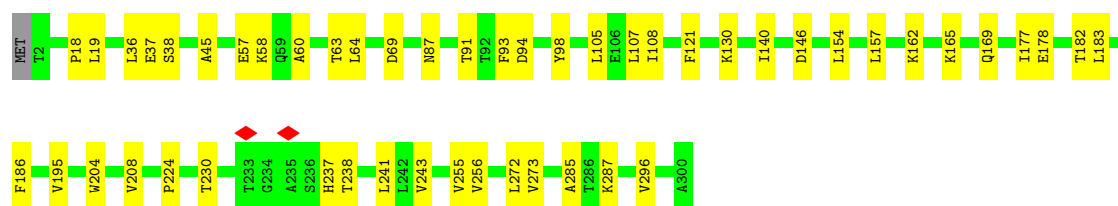


- Molecule 1: Tail Tube Protein (gp13)

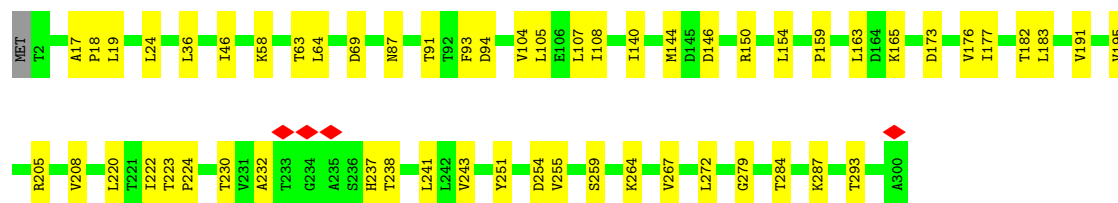
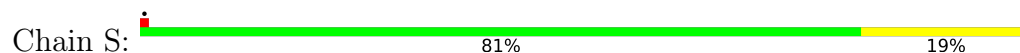


- Molecule 1: Tail Tube Protein (gp13)

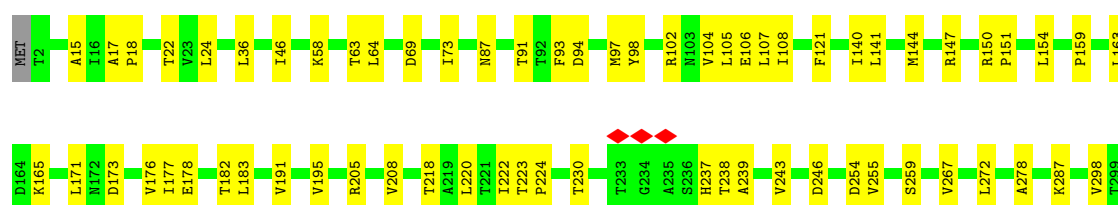
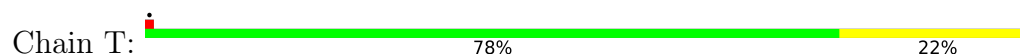




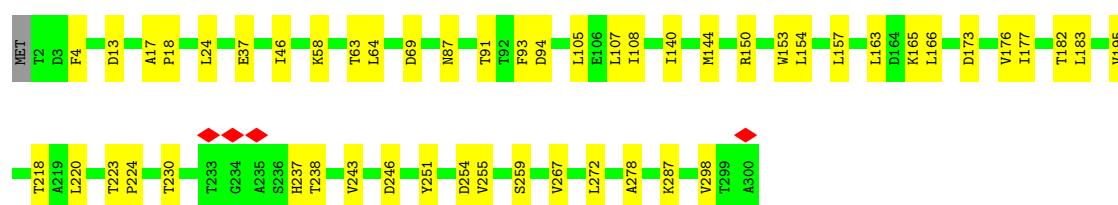
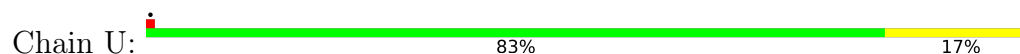
• Molecule 1: Tail Tube Protein (gp13)



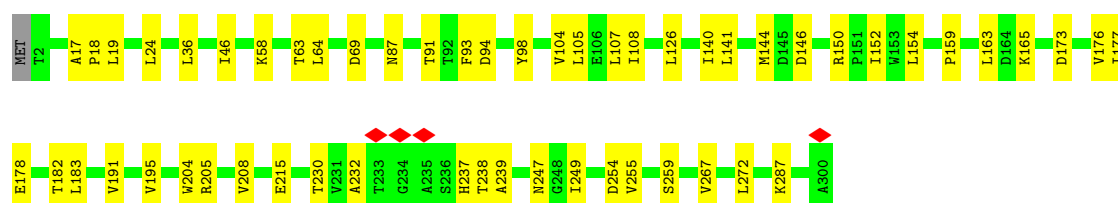
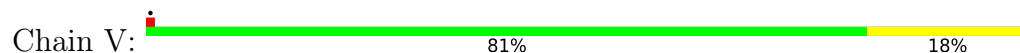
• Molecule 1: Tail Tube Protein (gp13)



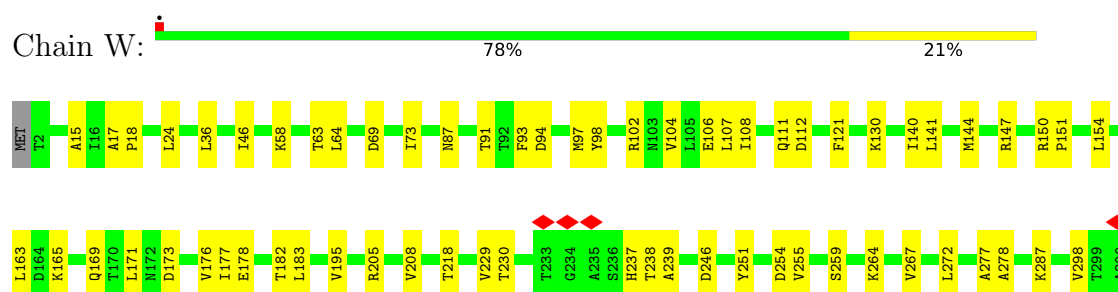
• Molecule 1: Tail Tube Protein (gp13)



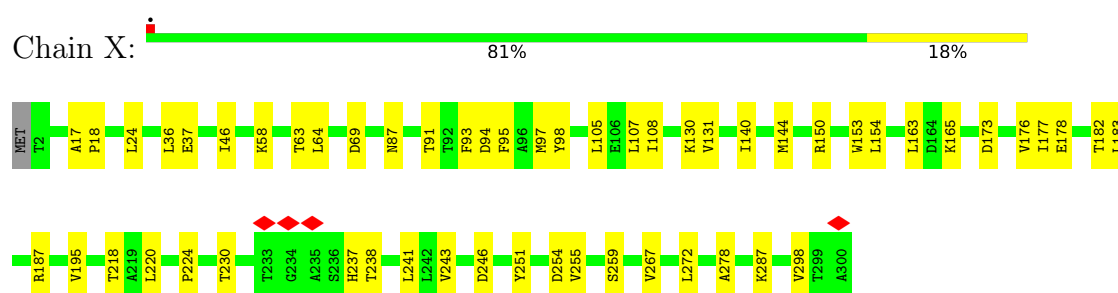
• Molecule 1: Tail Tube Protein (gp13)



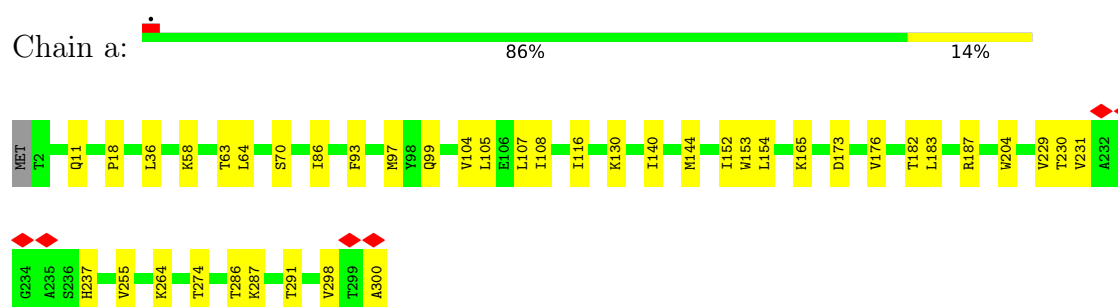
- Molecule 1: Tail Tube Protein (gp13)



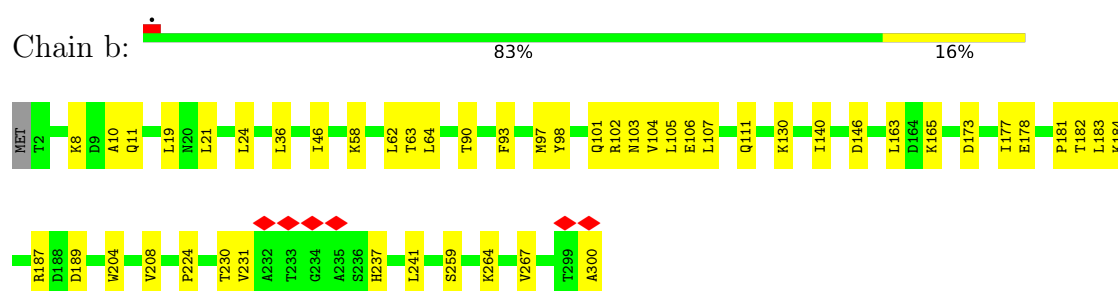
- Molecule 1: Tail Tube Protein (gp13)



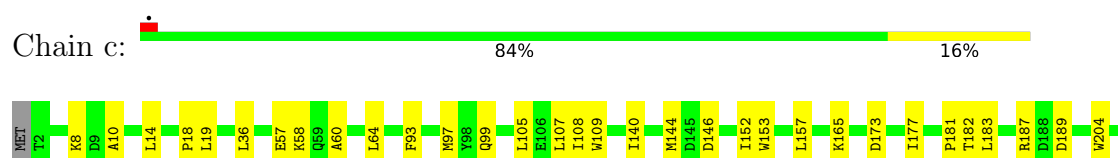
- Molecule 1: Tail Tube Protein (gp13)



- Molecule 1: Tail Tube Protein (gp13)

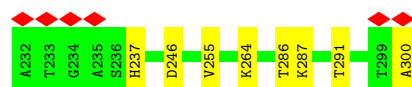
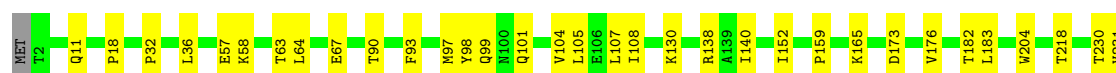
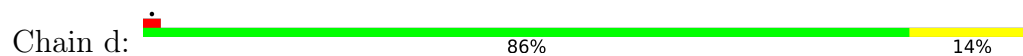


- Molecule 1: Tail Tube Protein (gp13)

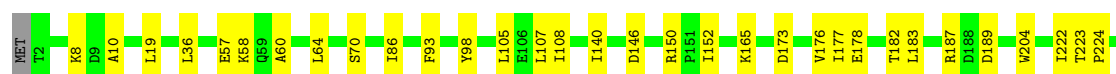
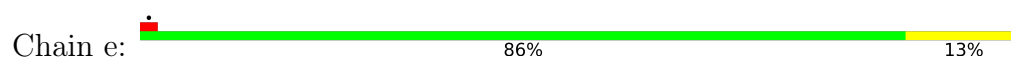




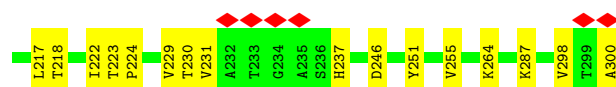
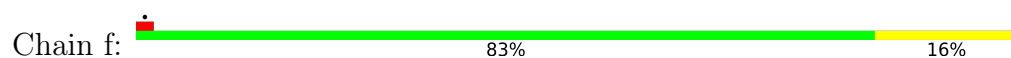
- Molecule 1: Tail Tube Protein (gp13)



- Molecule 1: Tail Tube Protein (gp13)



- Molecule 1: Tail Tube Protein (gp13)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 12010                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 430                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 2.389                                   | Depositor |
| Minimum map value                    | -1.200                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.091                                   | Depositor |
| Recommended contour level            | 0.18                                    | Depositor |
| Map size (Å)                         | 407.424, 407.424, 407.424               | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.061, 1.061, 1.061                     | 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         | 0/2306  | 0.27        | 0/3159  |
| 1   | B     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | C     | 0.11         | 0/2306  | 0.26        | 0/3159  |
| 1   | D     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | E     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| 1   | F     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| 1   | G     | 0.12         | 0/2306  | 0.29        | 0/3159  |
| 1   | H     | 0.12         | 0/2306  | 0.29        | 0/3159  |
| 1   | I     | 0.12         | 0/2306  | 0.29        | 0/3159  |
| 1   | J     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | K     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | L     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | M     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | N     | 0.12         | 0/2306  | 0.29        | 0/3159  |
| 1   | O     | 0.12         | 0/2306  | 0.29        | 0/3159  |
| 1   | P     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | Q     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | R     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | S     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | T     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| 1   | U     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | V     | 0.12         | 0/2306  | 0.28        | 0/3159  |
| 1   | W     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| 1   | X     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| 1   | a     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | b     | 0.11         | 0/2306  | 0.30        | 0/3159  |
| 1   | c     | 0.10         | 0/2306  | 0.27        | 0/3159  |
| 1   | d     | 0.11         | 0/2306  | 0.28        | 0/3159  |
| 1   | e     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| 1   | f     | 0.11         | 0/2306  | 0.27        | 0/3159  |
| All | All   | 0.11         | 0/69180 | 0.28        | 0/94770 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2256  | 0        | 2233     | 42      | 0            |
| 1   | B     | 2256  | 0        | 2233     | 28      | 0            |
| 1   | C     | 2256  | 0        | 2233     | 30      | 0            |
| 1   | D     | 2256  | 0        | 2233     | 36      | 0            |
| 1   | E     | 2256  | 0        | 2233     | 33      | 0            |
| 1   | F     | 2256  | 0        | 2233     | 32      | 0            |
| 1   | G     | 2256  | 0        | 2233     | 42      | 0            |
| 1   | H     | 2256  | 0        | 2233     | 39      | 0            |
| 1   | I     | 2256  | 0        | 2233     | 36      | 0            |
| 1   | J     | 2256  | 0        | 2233     | 39      | 0            |
| 1   | K     | 2256  | 0        | 2233     | 39      | 0            |
| 1   | L     | 2256  | 0        | 2233     | 45      | 0            |
| 1   | M     | 2256  | 0        | 2233     | 34      | 0            |
| 1   | N     | 2256  | 0        | 2233     | 40      | 0            |
| 1   | O     | 2256  | 0        | 2233     | 36      | 0            |
| 1   | P     | 2256  | 0        | 2233     | 37      | 0            |
| 1   | Q     | 2256  | 0        | 2233     | 39      | 0            |
| 1   | R     | 2256  | 0        | 2233     | 35      | 0            |
| 1   | S     | 2256  | 0        | 2233     | 37      | 0            |
| 1   | T     | 2256  | 0        | 2233     | 43      | 0            |
| 1   | U     | 2256  | 0        | 2233     | 34      | 0            |
| 1   | V     | 2256  | 0        | 2233     | 36      | 0            |
| 1   | W     | 2256  | 0        | 2233     | 44      | 0            |
| 1   | X     | 2256  | 0        | 2233     | 35      | 0            |
| 1   | a     | 2256  | 0        | 2233     | 31      | 0            |
| 1   | b     | 2256  | 0        | 2233     | 36      | 0            |
| 1   | c     | 2256  | 0        | 2233     | 34      | 0            |
| 1   | d     | 2256  | 0        | 2233     | 27      | 0            |
| 1   | e     | 2256  | 0        | 2233     | 26      | 0            |
| 1   | f     | 2256  | 0        | 2233     | 33      | 0            |
| All | All   | 67680 | 0        | 66990    | 931     | 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 7.

All (931) 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:N:107:LEU:HD11 | 1:N:183:LEU:HD21 | 1.68                     | 0.76              |
| 1:N:238:THR:HB   | 1:N:272:LEU:HD11 | 1.69                     | 0.74              |
| 1:Q:107:LEU:HD11 | 1:Q:183:LEU:HD21 | 1.70                     | 0.74              |
| 1:U:107:LEU:HD11 | 1:U:183:LEU:HD21 | 1.70                     | 0.74              |
| 1:P:255:VAL:HG12 | 1:P:287:LYS:HB2  | 1.70                     | 0.73              |
| 1:K:99:GLN:HE22  | 1:L:11:GLN:H     | 1.35                     | 0.73              |
| 1:X:107:LEU:HD11 | 1:X:183:LEU:HD21 | 1.70                     | 0.72              |
| 1:Q:238:THR:HB   | 1:Q:272:LEU:HD11 | 1.72                     | 0.72              |
| 1:A:107:LEU:HD11 | 1:A:183:LEU:HD21 | 1.72                     | 0.72              |
| 1:D:107:LEU:HD11 | 1:D:183:LEU:HD21 | 1.71                     | 0.72              |
| 1:f:107:LEU:HD11 | 1:f:183:LEU:HD21 | 1.72                     | 0.71              |
| 1:B:107:LEU:HD11 | 1:B:183:LEU:HD21 | 1.73                     | 0.71              |
| 1:M:255:VAL:HG12 | 1:M:287:LYS:HB2  | 1.71                     | 0.71              |
| 1:c:107:LEU:HD11 | 1:c:183:LEU:HD21 | 1.72                     | 0.71              |
| 1:I:173:ASP:OD2  | 1:J:58:LYS:NZ    | 2.23                     | 0.71              |
| 1:K:107:LEU:HD11 | 1:K:183:LEU:HD21 | 1.73                     | 0.71              |
| 1:M:107:LEU:HD11 | 1:M:183:LEU:HD21 | 1.72                     | 0.70              |
| 1:E:107:LEU:HD11 | 1:E:183:LEU:HD21 | 1.72                     | 0.70              |
| 1:H:107:LEU:HD11 | 1:H:183:LEU:HD21 | 1.73                     | 0.70              |
| 1:V:107:LEU:HD11 | 1:V:183:LEU:HD21 | 1.73                     | 0.69              |
| 1:S:107:LEU:HD11 | 1:S:183:LEU:HD21 | 1.73                     | 0.69              |
| 1:O:255:VAL:HG12 | 1:O:287:LYS:HB2  | 1.75                     | 0.69              |
| 1:a:58:LYS:NZ    | 1:f:173:ASP:OD2  | 2.25                     | 0.68              |
| 1:G:107:LEU:HD11 | 1:G:183:LEU:HD21 | 1.74                     | 0.68              |
| 1:O:99:GLN:HE22  | 1:P:11:GLN:H     | 1.42                     | 0.68              |
| 1:T:150:ARG:NH2  | 1:T:254:ASP:OD1  | 2.27                     | 0.68              |
| 1:P:107:LEU:HD11 | 1:P:183:LEU:HD21 | 1.76                     | 0.67              |
| 1:R:255:VAL:HG12 | 1:R:287:LYS:HB2  | 1.76                     | 0.67              |
| 1:a:107:LEU:HD11 | 1:a:183:LEU:HD21 | 1.77                     | 0.67              |
| 1:R:238:THR:HB   | 1:R:272:LEU:HD11 | 1.77                     | 0.67              |
| 1:I:130:LYS:HZ2  | 1:J:187:ARG:HD2  | 1.60                     | 0.67              |
| 1:O:107:LEU:HD11 | 1:O:183:LEU:HD21 | 1.77                     | 0.66              |
| 1:L:238:THR:HB   | 1:L:272:LEU:HD11 | 1.78                     | 0.66              |
| 1:e:177:ILE:HG13 | 1:f:18:PRO:HD3   | 1.78                     | 0.66              |
| 1:G:58:LYS:NZ    | 1:L:173:ASP:OD2  | 2.29                     | 0.66              |
| 1:O:238:THR:HB   | 1:O:272:LEU:HD11 | 1.78                     | 0.66              |
| 1:C:107:LEU:HD11 | 1:C:183:LEU:HD21 | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:107:LEU:HD11 | 1:T:183:LEU:HD21 | 1.77                     | 0.66              |
| 1:I:107:LEU:HD11 | 1:I:183:LEU:HD21 | 1.78                     | 0.66              |
| 1:T:144:MET:HE3  | 1:T:151:PRO:HB3  | 1.76                     | 0.66              |
| 1:F:107:LEU:HD11 | 1:F:183:LEU:HD21 | 1.77                     | 0.65              |
| 1:R:107:LEU:HD11 | 1:R:183:LEU:HD21 | 1.77                     | 0.65              |
| 1:V:150:ARG:NH2  | 1:V:254:ASP:OD1  | 2.29                     | 0.65              |
| 1:R:230:THR:O    | 1:R:237:HIS:ND1  | 2.28                     | 0.65              |
| 1:U:150:ARG:NH2  | 1:U:254:ASP:OD1  | 2.29                     | 0.65              |
| 1:O:230:THR:O    | 1:O:237:HIS:ND1  | 2.29                     | 0.65              |
| 1:I:238:THR:HB   | 1:I:272:LEU:HD11 | 1.78                     | 0.65              |
| 1:d:230:THR:O    | 1:d:237:HIS:ND1  | 2.30                     | 0.65              |
| 1:M:165:LYS:NZ   | 1:M:167:ASP:OD1  | 2.29                     | 0.65              |
| 1:W:107:LEU:HD11 | 1:W:183:LEU:HD21 | 1.78                     | 0.65              |
| 1:S:150:ARG:NH2  | 1:S:254:ASP:OD1  | 2.29                     | 0.65              |
| 1:E:230:THR:O    | 1:E:237:HIS:ND1  | 2.25                     | 0.65              |
| 1:W:144:MET:HE3  | 1:W:151:PRO:HB3  | 1.79                     | 0.65              |
| 1:X:150:ARG:NH2  | 1:X:254:ASP:OD1  | 2.30                     | 0.65              |
| 1:d:107:LEU:HD11 | 1:d:183:LEU:HD21 | 1.78                     | 0.64              |
| 1:D:88:LYS:NZ    | 1:D:90:THR:OG1   | 2.30                     | 0.64              |
| 1:F:238:THR:HB   | 1:F:272:LEU:HD11 | 1.80                     | 0.64              |
| 1:T:173:ASP:OD2  | 1:U:58:LYS:NZ    | 2.30                     | 0.64              |
| 1:H:37:GLU:HG3   | 1:H:42:GLY:HA2   | 1.79                     | 0.64              |
| 1:K:37:GLU:HG3   | 1:K:42:GLY:HA2   | 1.79                     | 0.64              |
| 1:c:187:ARG:NH1  | 1:c:189:ASP:OD1  | 2.31                     | 0.64              |
| 1:D:230:THR:O    | 1:D:237:HIS:ND1  | 2.27                     | 0.63              |
| 1:P:165:LYS:NZ   | 1:P:167:ASP:OD1  | 2.31                     | 0.63              |
| 1:A:230:THR:O    | 1:A:237:HIS:ND1  | 2.30                     | 0.63              |
| 1:a:230:THR:O    | 1:a:237:HIS:ND1  | 2.31                     | 0.63              |
| 1:a:255:VAL:HG12 | 1:a:287:LYS:HB2  | 1.80                     | 0.63              |
| 1:d:255:VAL:HG12 | 1:d:287:LYS:HB2  | 1.80                     | 0.63              |
| 1:D:238:THR:HB   | 1:D:272:LEU:HD11 | 1.78                     | 0.63              |
| 1:H:173:ASP:OD2  | 1:I:58:LYS:NZ    | 2.31                     | 0.63              |
| 1:J:238:THR:HB   | 1:J:272:LEU:HD11 | 1.81                     | 0.63              |
| 1:d:97:MET:HE2   | 1:d:104:VAL:HG13 | 1.80                     | 0.63              |
| 1:B:13:ASP:O     | 1:B:147:ARG:NH1  | 2.30                     | 0.63              |
| 1:G:99:GLN:HE22  | 1:H:11:GLN:H     | 1.47                     | 0.63              |
| 1:J:173:ASP:OD2  | 1:K:58:LYS:NZ    | 2.31                     | 0.62              |
| 1:A:88:LYS:NZ    | 1:A:90:THR:OG1   | 2.32                     | 0.62              |
| 1:U:173:ASP:OD2  | 1:V:58:LYS:NZ    | 2.31                     | 0.62              |
| 1:d:173:ASP:OD2  | 1:e:58:LYS:NZ    | 2.33                     | 0.62              |
| 1:G:238:THR:HB   | 1:G:272:LEU:HD11 | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:177:ILE:HD12 | 1:Q:154:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:238:THR:HB   | 1:A:272:LEU:HD11 | 1.81                     | 0.62              |
| 1:B:238:THR:HB   | 1:B:272:LEU:HD11 | 1.81                     | 0.62              |
| 1:b:177:ILE:HG13 | 1:c:18:PRO:HD3   | 1.80                     | 0.62              |
| 1:E:238:THR:HB   | 1:E:272:LEU:HD11 | 1.81                     | 0.62              |
| 1:c:255:VAL:HG12 | 1:c:287:LYS:HB2  | 1.81                     | 0.62              |
| 1:D:165:LYS:HB3  | 1:D:182:THR:HB   | 1.82                     | 0.61              |
| 1:c:231:VAL:HB   | 1:c:300:ALA:HA   | 1.82                     | 0.61              |
| 1:H:238:THR:HB   | 1:H:272:LEU:HD11 | 1.81                     | 0.61              |
| 1:e:107:LEU:HD11 | 1:e:183:LEU:HD21 | 1.83                     | 0.61              |
| 1:P:230:THR:O    | 1:P:237:HIS:ND1  | 2.33                     | 0.61              |
| 1:b:107:LEU:HD11 | 1:b:183:LEU:HD21 | 1.82                     | 0.61              |
| 1:K:238:THR:HB   | 1:K:272:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:150:ARG:NE   | 1:A:206:ASP:OD2  | 2.33                     | 0.61              |
| 1:X:36:LEU:HD11  | 1:X:140:ILE:HD13 | 1.83                     | 0.61              |
| 1:c:177:ILE:HG13 | 1:d:18:PRO:HD3   | 1.82                     | 0.61              |
| 1:U:177:ILE:HG13 | 1:V:18:PRO:HD3   | 1.83                     | 0.61              |
| 1:X:24:LEU:HD22  | 1:X:46:ILE:HG21  | 1.81                     | 0.60              |
| 1:a:173:ASP:OD2  | 1:b:58:LYS:NZ    | 2.32                     | 0.60              |
| 1:f:222:ILE:HG13 | 1:f:224:PRO:HD2  | 1.83                     | 0.60              |
| 1:E:150:ARG:NE   | 1:E:206:ASP:OD2  | 2.33                     | 0.60              |
| 1:M:238:THR:HB   | 1:M:272:LEU:HD11 | 1.82                     | 0.60              |
| 1:E:13:ASP:O     | 1:E:147:ARG:NH1  | 2.31                     | 0.60              |
| 1:L:105:LEU:HA   | 1:L:108:ILE:HG12 | 1.84                     | 0.60              |
| 1:b:173:ASP:OD2  | 1:c:58:LYS:NZ    | 2.34                     | 0.60              |
| 1:D:57:GLU:HG2   | 1:D:60:ALA:H     | 1.67                     | 0.60              |
| 1:P:173:ASP:OD2  | 1:Q:58:LYS:NZ    | 2.31                     | 0.60              |
| 1:a:99:GLN:HE22  | 1:b:11:GLN:H     | 1.48                     | 0.60              |
| 1:a:97:MET:HE2   | 1:a:104:VAL:HG13 | 1.84                     | 0.60              |
| 1:f:255:VAL:HG12 | 1:f:287:LYS:HB2  | 1.83                     | 0.60              |
| 1:B:165:LYS:HB3  | 1:B:182:THR:HB   | 1.84                     | 0.59              |
| 1:J:107:LEU:HD11 | 1:J:183:LEU:HD21 | 1.84                     | 0.59              |
| 1:U:24:LEU:HD22  | 1:U:46:ILE:HG21  | 1.82                     | 0.59              |
| 1:I:37:GLU:HG3   | 1:I:42:GLY:HA2   | 1.83                     | 0.59              |
| 1:W:150:ARG:NH2  | 1:W:254:ASP:OD1  | 2.35                     | 0.59              |
| 1:G:204:TRP:O    | 1:G:208:VAL:HG23 | 2.02                     | 0.59              |
| 1:L:70:SER:HB3   | 1:L:86:ILE:HA    | 1.83                     | 0.59              |
| 1:M:177:ILE:HD12 | 1:N:154:LEU:HD11 | 1.83                     | 0.59              |
| 1:E:177:ILE:HG13 | 1:F:18:PRO:HD3   | 1.84                     | 0.59              |
| 1:P:238:THR:HB   | 1:P:272:LEU:HD11 | 1.84                     | 0.59              |
| 1:C:238:THR:HB   | 1:C:272:LEU:HD11 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:173:ASP:OD2  | 1:f:58:LYS:NZ    | 2.35                     | 0.59              |
| 1:C:165:LYS:HB2  | 1:C:182:THR:HB   | 1.84                     | 0.59              |
| 1:H:140:ILE:HG12 | 1:H:157:LEU:HD23 | 1.85                     | 0.59              |
| 1:N:255:VAL:HG12 | 1:N:287:LYS:HB2  | 1.84                     | 0.59              |
| 1:V:259:SER:HB3  | 1:V:267:VAL:HG12 | 1.84                     | 0.59              |
| 1:H:90:THR:HG23  | 1:H:184:LYS:HE3  | 1.84                     | 0.59              |
| 1:W:176:VAL:HG12 | 1:X:17:ALA:HB2   | 1.85                     | 0.58              |
| 1:d:67:GLU:HG2   | 1:d:90:THR:HB    | 1.85                     | 0.58              |
| 1:D:150:ARG:NE   | 1:D:206:ASP:OD2  | 2.33                     | 0.58              |
| 1:F:13:ASP:HA    | 1:F:147:ARG:HH22 | 1.68                     | 0.58              |
| 1:T:163:LEU:HA   | 1:T:183:LEU:HD23 | 1.85                     | 0.58              |
| 1:e:222:ILE:HG13 | 1:e:224:PRO:HD2  | 1.84                     | 0.58              |
| 1:L:107:LEU:HD11 | 1:L:183:LEU:HD21 | 1.84                     | 0.58              |
| 1:C:67:GLU:HG3   | 1:C:90:THR:HB    | 1.85                     | 0.58              |
| 1:d:99:GLN:NE2   | 1:d:101:GLN:OE1  | 2.36                     | 0.58              |
| 1:I:140:ILE:HG12 | 1:I:157:LEU:HD23 | 1.86                     | 0.58              |
| 1:T:177:ILE:HG13 | 1:U:18:PRO:HD3   | 1.86                     | 0.58              |
| 1:K:140:ILE:HG12 | 1:K:157:LEU:HD23 | 1.84                     | 0.58              |
| 1:U:165:LYS:HB2  | 1:U:182:THR:HB   | 1.85                     | 0.58              |
| 1:e:222:ILE:HG21 | 1:e:294:ALA:HB2  | 1.84                     | 0.58              |
| 1:K:222:ILE:HG21 | 1:K:294:ALA:HB2  | 1.84                     | 0.58              |
| 1:O:99:GLN:NE2   | 1:P:11:GLN:O     | 2.37                     | 0.58              |
| 1:B:230:THR:O    | 1:B:237:HIS:ND1  | 2.25                     | 0.58              |
| 1:J:140:ILE:HG12 | 1:J:157:LEU:HD23 | 1.86                     | 0.58              |
| 1:J:177:ILE:HG13 | 1:K:18:PRO:HD3   | 1.86                     | 0.58              |
| 1:f:67:GLU:HG2   | 1:f:90:THR:HB    | 1.85                     | 0.58              |
| 1:G:140:ILE:HG12 | 1:G:157:LEU:HD23 | 1.86                     | 0.57              |
| 1:S:18:PRO:HD3   | 1:X:177:ILE:HG13 | 1.84                     | 0.57              |
| 1:T:259:SER:HB3  | 1:T:267:VAL:HG12 | 1.86                     | 0.57              |
| 1:E:165:LYS:HB3  | 1:E:182:THR:HB   | 1.85                     | 0.57              |
| 1:L:24:LEU:HD22  | 1:L:46:ILE:HG21  | 1.86                     | 0.57              |
| 1:P:165:LYS:HB3  | 1:P:182:THR:HB   | 1.86                     | 0.57              |
| 1:T:176:VAL:HG12 | 1:U:17:ALA:HB2   | 1.85                     | 0.57              |
| 1:c:173:ASP:OD2  | 1:d:58:LYS:NZ    | 2.36                     | 0.57              |
| 1:M:36:LEU:HD21  | 1:M:140:ILE:HD13 | 1.86                     | 0.57              |
| 1:W:163:LEU:HA   | 1:W:183:LEU:HD23 | 1.86                     | 0.57              |
| 1:G:177:ILE:HG13 | 1:H:18:PRO:HD3   | 1.86                     | 0.57              |
| 1:G:224:PRO:HG2  | 1:G:241:LEU:HD22 | 1.87                     | 0.57              |
| 1:D:187:ARG:NH1  | 1:D:188:ASP:O    | 2.37                     | 0.57              |
| 1:E:218:THR:OG1  | 1:E:246:ASP:OD2  | 2.23                     | 0.57              |
| 1:J:176:VAL:HG12 | 1:K:17:ALA:HB2   | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:130:LYS:HZ1  | 1:L:187:ARG:HD2  | 1.68                     | 0.57              |
| 1:L:37:GLU:HG3   | 1:L:42:GLY:HA2   | 1.86                     | 0.57              |
| 1:M:224:PRO:HG2  | 1:M:241:LEU:HA   | 1.87                     | 0.57              |
| 1:F:67:GLU:HG3   | 1:F:90:THR:HB    | 1.86                     | 0.57              |
| 1:R:57:GLU:HG2   | 1:R:60:ALA:H     | 1.70                     | 0.57              |
| 1:a:18:PRO:HD3   | 1:f:177:ILE:HG13 | 1.86                     | 0.57              |
| 1:V:177:ILE:HG13 | 1:W:18:PRO:HD3   | 1.87                     | 0.57              |
| 1:c:99:GLN:NE2   | 1:d:11:GLN:O     | 2.38                     | 0.57              |
| 1:F:230:THR:O    | 1:F:237:HIS:ND1  | 2.25                     | 0.56              |
| 1:J:105:LEU:HA   | 1:J:108:ILE:HG12 | 1.87                     | 0.56              |
| 1:K:176:VAL:HG12 | 1:L:17:ALA:HB2   | 1.87                     | 0.56              |
| 1:S:259:SER:HB3  | 1:S:267:VAL:HG12 | 1.85                     | 0.56              |
| 1:X:259:SER:HB3  | 1:X:267:VAL:HG12 | 1.87                     | 0.56              |
| 1:A:57:GLU:HG2   | 1:A:60:ALA:H     | 1.69                     | 0.56              |
| 1:M:230:THR:O    | 1:M:237:HIS:ND1  | 2.37                     | 0.56              |
| 1:P:105:LEU:HA   | 1:P:108:ILE:HG12 | 1.87                     | 0.56              |
| 1:Q:163:LEU:HA   | 1:Q:183:LEU:HD23 | 1.86                     | 0.56              |
| 1:Q:177:ILE:HD12 | 1:R:154:LEU:HD11 | 1.87                     | 0.56              |
| 1:f:231:VAL:HB   | 1:f:300:ALA:HA   | 1.87                     | 0.56              |
| 1:a:237:HIS:NE2  | 1:a:274:THR:OG1  | 2.38                     | 0.56              |
| 1:b:106:GLU:HB2  | 1:b:111:GLN:O    | 2.06                     | 0.56              |
| 1:F:165:LYS:HB2  | 1:F:182:THR:HB   | 1.87                     | 0.56              |
| 1:L:92:THR:HG22  | 1:L:184:LYS:HG2  | 1.88                     | 0.56              |
| 1:T:222:ILE:HG22 | 1:T:224:PRO:HD2  | 1.88                     | 0.56              |
| 1:S:177:ILE:HG13 | 1:T:18:PRO:HD3   | 1.88                     | 0.56              |
| 1:B:218:THR:OG1  | 1:B:246:ASP:OD2  | 2.23                     | 0.56              |
| 1:M:18:PRO:HD3   | 1:R:177:ILE:HG13 | 1.88                     | 0.56              |
| 1:O:222:ILE:HG12 | 1:O:243:VAL:HG22 | 1.88                     | 0.56              |
| 1:N:177:ILE:HD12 | 1:O:154:LEU:HD11 | 1.86                     | 0.56              |
| 1:I:105:LEU:HA   | 1:I:108:ILE:HG12 | 1.86                     | 0.55              |
| 1:J:224:PRO:HG2  | 1:J:241:LEU:HD22 | 1.86                     | 0.55              |
| 1:L:243:VAL:HG21 | 1:L:255:VAL:HG21 | 1.88                     | 0.55              |
| 1:R:273:VAL:HG11 | 1:R:296:VAL:HG11 | 1.88                     | 0.55              |
| 1:U:176:VAL:HG12 | 1:V:17:ALA:HB2   | 1.86                     | 0.55              |
| 1:W:177:ILE:HG13 | 1:X:18:PRO:HD3   | 1.87                     | 0.55              |
| 1:W:259:SER:HB3  | 1:W:267:VAL:HG12 | 1.88                     | 0.55              |
| 1:W:177:ILE:HD12 | 1:X:154:LEU:HD11 | 1.89                     | 0.55              |
| 1:F:218:THR:OG1  | 1:F:246:ASP:OD2  | 2.23                     | 0.55              |
| 1:H:152:ILE:HG23 | 1:H:204:TRP:HB2  | 1.89                     | 0.55              |
| 1:J:222:ILE:HD11 | 1:J:241:LEU:HB3  | 1.88                     | 0.55              |
| 1:O:57:GLU:HG2   | 1:O:60:ALA:H     | 1.71                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:243:VAL:HG11 | 1:O:255:VAL:HG11 | 1.87                     | 0.55              |
| 1:T:165:LYS:HB2  | 1:T:182:THR:HB   | 1.88                     | 0.55              |
| 1:N:218:THR:OG1  | 1:N:246:ASP:OD2  | 2.23                     | 0.55              |
| 1:G:187:ARG:HH11 | 1:L:130:LYS:HZ2  | 1.54                     | 0.55              |
| 1:T:73:ILE:HG13  | 1:a:176:VAL:HG13 | 1.89                     | 0.55              |
| 1:K:152:ILE:HG23 | 1:K:204:TRP:HB2  | 1.88                     | 0.55              |
| 1:S:154:LEU:HD11 | 1:X:177:ILE:HD12 | 1.89                     | 0.55              |
| 1:c:222:ILE:HG21 | 1:c:294:ALA:HB2  | 1.88                     | 0.55              |
| 1:d:152:ILE:HG23 | 1:d:204:TRP:HB2  | 1.89                     | 0.55              |
| 1:e:231:VAL:HB   | 1:e:300:ALA:HA   | 1.89                     | 0.55              |
| 1:R:243:VAL:HG11 | 1:R:255:VAL:HG11 | 1.89                     | 0.55              |
| 1:U:259:SER:HB3  | 1:U:267:VAL:HG12 | 1.88                     | 0.55              |
| 1:f:57:GLU:HG2   | 1:f:60:ALA:H     | 1.71                     | 0.55              |
| 1:A:17:ALA:HB2   | 1:F:176:VAL:HG12 | 1.89                     | 0.55              |
| 1:H:177:ILE:HG13 | 1:I:18:PRO:HD3   | 1.89                     | 0.55              |
| 1:J:204:TRP:O    | 1:J:208:VAL:HG23 | 2.07                     | 0.55              |
| 1:M:173:ASP:OD2  | 1:N:58:LYS:NZ    | 2.31                     | 0.55              |
| 1:X:105:LEU:HA   | 1:X:108:ILE:HG12 | 1.89                     | 0.54              |
| 1:b:204:TRP:O    | 1:b:208:VAL:HG23 | 2.07                     | 0.54              |
| 1:D:218:THR:OG1  | 1:D:246:ASP:OD2  | 2.23                     | 0.54              |
| 1:H:204:TRP:O    | 1:H:208:VAL:HG23 | 2.08                     | 0.54              |
| 1:D:8:LYS:HG2    | 1:D:10:ALA:HB2   | 1.88                     | 0.54              |
| 1:N:163:LEU:HA   | 1:N:183:LEU:HD23 | 1.89                     | 0.54              |
| 1:Q:224:PRO:HG2  | 1:Q:241:LEU:HA   | 1.89                     | 0.54              |
| 1:W:173:ASP:OD2  | 1:X:58:LYS:NZ    | 2.39                     | 0.54              |
| 1:c:224:PRO:HG2  | 1:c:241:LEU:HD22 | 1.89                     | 0.54              |
| 1:G:178:GLU:OE1  | 1:G:180:LYS:NZ   | 2.41                     | 0.54              |
| 1:N:222:ILE:HG13 | 1:N:224:PRO:HD2  | 1.90                     | 0.54              |
| 1:Q:63:THR:HB    | 1:Q:94:ASP:OD1   | 2.08                     | 0.54              |
| 1:b:187:ARG:NH1  | 1:b:189:ASP:OD1  | 2.39                     | 0.54              |
| 1:N:54:GLY:HA3   | 1:N:99:GLN:HG3   | 1.90                     | 0.54              |
| 1:N:63:THR:HB    | 1:N:94:ASP:OD1   | 2.08                     | 0.54              |
| 1:N:177:ILE:HG13 | 1:O:18:PRO:HD3   | 1.90                     | 0.54              |
| 1:W:218:THR:OG1  | 1:W:246:ASP:OD2  | 2.22                     | 0.54              |
| 1:b:231:VAL:HB   | 1:b:300:ALA:HA   | 1.89                     | 0.54              |
| 1:M:37:GLU:OE2   | 1:R:121:PHE:HB2  | 2.08                     | 0.54              |
| 1:M:165:LYS:HB3  | 1:M:182:THR:HB   | 1.88                     | 0.54              |
| 1:T:238:THR:HB   | 1:T:272:LEU:HD11 | 1.90                     | 0.54              |
| 1:V:177:ILE:HD12 | 1:W:154:LEU:HD11 | 1.88                     | 0.54              |
| 1:E:177:ILE:HD12 | 1:F:154:LEU:HD11 | 1.88                     | 0.54              |
| 1:G:222:ILE:HG21 | 1:G:294:ALA:HB2  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:17:ALA:HB2   | 1:X:176:VAL:HG12 | 1.89                     | 0.54              |
| 1:A:187:ARG:NH1  | 1:A:188:ASP:O    | 2.40                     | 0.54              |
| 1:K:204:TRP:O    | 1:K:208:VAL:HG23 | 2.08                     | 0.54              |
| 1:T:24:LEU:HD22  | 1:T:46:ILE:HG21  | 1.88                     | 0.54              |
| 1:C:218:THR:OG1  | 1:C:246:ASP:OD2  | 2.24                     | 0.53              |
| 1:K:222:ILE:HG13 | 1:K:224:PRO:HD2  | 1.89                     | 0.53              |
| 1:H:176:VAL:HG12 | 1:I:17:ALA:HB2   | 1.89                     | 0.53              |
| 1:S:177:ILE:HD12 | 1:T:154:LEU:HD11 | 1.90                     | 0.53              |
| 1:D:176:VAL:HG12 | 1:E:17:ALA:HB2   | 1.91                     | 0.53              |
| 1:S:224:PRO:HG2  | 1:S:241:LEU:HA   | 1.90                     | 0.53              |
| 1:H:223:THR:OG1  | 1:H:224:PRO:HD3  | 2.08                     | 0.53              |
| 1:d:57:GLU:OE1   | 1:d:98:TYR:OH    | 2.20                     | 0.53              |
| 1:d:138:ARG:NH1  | 1:d:159:PRO:O    | 2.40                     | 0.53              |
| 1:f:105:LEU:HA   | 1:f:108:ILE:HG12 | 1.90                     | 0.53              |
| 1:U:105:LEU:HA   | 1:U:108:ILE:HG12 | 1.89                     | 0.53              |
| 1:a:152:ILE:HG23 | 1:a:204:TRP:HB2  | 1.91                     | 0.53              |
| 1:a:154:LEU:HD11 | 1:f:177:ILE:HD12 | 1.89                     | 0.53              |
| 1:c:97:MET:HE1   | 1:c:181:PRO:HG3  | 1.90                     | 0.53              |
| 1:O:273:VAL:HG11 | 1:O:296:VAL:HG11 | 1.89                     | 0.53              |
| 1:W:238:THR:HB   | 1:W:272:LEU:HD11 | 1.91                     | 0.53              |
| 1:T:218:THR:OG1  | 1:T:246:ASP:OD2  | 2.23                     | 0.53              |
| 1:A:165:LYS:HB3  | 1:A:182:THR:HB   | 1.89                     | 0.53              |
| 1:A:218:THR:OG1  | 1:A:246:ASP:OD2  | 2.26                     | 0.53              |
| 1:A:57:GLU:HB3   | 1:A:96:ALA:HB3   | 1.91                     | 0.53              |
| 1:V:165:LYS:HB2  | 1:V:182:THR:HB   | 1.91                     | 0.53              |
| 1:b:130:LYS:HZ2  | 1:c:187:ARG:HE   | 1.56                     | 0.53              |
| 1:O:105:LEU:HA   | 1:O:108:ILE:HG12 | 1.91                     | 0.52              |
| 1:P:177:ILE:HG13 | 1:Q:18:PRO:HD3   | 1.91                     | 0.52              |
| 1:Q:177:ILE:HG13 | 1:R:18:PRO:HD3   | 1.91                     | 0.52              |
| 1:A:8:LYS:HG2    | 1:A:10:ALA:HB2   | 1.90                     | 0.52              |
| 1:G:176:VAL:HG12 | 1:H:17:ALA:HB2   | 1.90                     | 0.52              |
| 1:K:105:LEU:HA   | 1:K:108:ILE:HG12 | 1.91                     | 0.52              |
| 1:O:36:LEU:HD21  | 1:O:140:ILE:HD13 | 1.91                     | 0.52              |
| 1:D:57:GLU:HB3   | 1:D:96:ALA:HB3   | 1.91                     | 0.52              |
| 1:H:105:LEU:HA   | 1:H:108:ILE:HG12 | 1.91                     | 0.52              |
| 1:F:13:ASP:OD1   | 1:F:147:ARG:NH2  | 2.42                     | 0.52              |
| 1:Q:218:THR:OG1  | 1:Q:246:ASP:OD2  | 2.24                     | 0.52              |
| 1:C:237:HIS:HE1  | 1:C:274:THR:HG23 | 1.75                     | 0.52              |
| 1:O:165:LYS:HB3  | 1:O:182:THR:HB   | 1.92                     | 0.52              |
| 1:e:187:ARG:NH1  | 1:e:189:ASP:OD1  | 2.42                     | 0.52              |
| 1:J:222:ILE:HG21 | 1:J:294:ALA:HB2  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:177:ILE:HG13 | 1:L:18:PRO:HD3   | 1.92                     | 0.52              |
| 1:P:222:ILE:HG21 | 1:P:294:ALA:HB2  | 1.91                     | 0.52              |
| 1:X:64:LEU:HD23  | 1:X:93:PHE:HB3   | 1.92                     | 0.52              |
| 1:a:11:GLN:O     | 1:f:99:GLN:NE2   | 2.42                     | 0.52              |
| 1:D:67:GLU:HG3   | 1:D:90:THR:HB    | 1.92                     | 0.52              |
| 1:Q:105:LEU:HA   | 1:Q:108:ILE:HG12 | 1.90                     | 0.52              |
| 1:Q:222:ILE:HG21 | 1:Q:294:ALA:HB2  | 1.91                     | 0.52              |
| 1:U:144:MET:HG3  | 1:U:153:TRP:CD1  | 2.45                     | 0.52              |
| 1:M:105:LEU:HA   | 1:M:108:ILE:HG12 | 1.91                     | 0.52              |
| 1:N:222:ILE:HG21 | 1:N:294:ALA:HB2  | 1.91                     | 0.52              |
| 1:R:36:LEU:HD21  | 1:R:140:ILE:HD13 | 1.91                     | 0.52              |
| 1:R:165:LYS:HB3  | 1:R:182:THR:HB   | 1.93                     | 0.51              |
| 1:R:105:LEU:HA   | 1:R:108:ILE:HG12 | 1.92                     | 0.51              |
| 1:d:231:VAL:HB   | 1:d:300:ALA:HA   | 1.91                     | 0.51              |
| 1:e:57:GLU:HG2   | 1:e:60:ALA:H     | 1.75                     | 0.51              |
| 1:S:163:LEU:HA   | 1:S:183:LEU:HD23 | 1.92                     | 0.51              |
| 1:S:165:LYS:HB2  | 1:S:182:THR:HB   | 1.92                     | 0.51              |
| 1:D:223:THR:HB   | 1:D:224:PRO:HD3  | 1.92                     | 0.51              |
| 1:T:230:THR:O    | 1:T:237:HIS:ND1  | 2.44                     | 0.51              |
| 1:X:255:VAL:HA   | 1:X:287:LYS:HB2  | 1.92                     | 0.51              |
| 1:a:231:VAL:HB   | 1:a:300:ALA:HA   | 1.92                     | 0.51              |
| 1:G:105:LEU:HA   | 1:G:108:ILE:HG12 | 1.93                     | 0.51              |
| 1:W:230:THR:O    | 1:W:237:HIS:ND1  | 2.42                     | 0.51              |
| 1:B:177:ILE:HD12 | 1:C:154:LEU:HD11 | 1.92                     | 0.51              |
| 1:N:105:LEU:HA   | 1:N:108:ILE:HG12 | 1.91                     | 0.51              |
| 1:O:91:THR:HG21  | 1:O:195:VAL:HG21 | 1.92                     | 0.51              |
| 1:T:255:VAL:HA   | 1:T:287:LYS:HB2  | 1.93                     | 0.51              |
| 1:D:209:ALA:HB1  | 1:D:216:ALA:HA   | 1.92                     | 0.51              |
| 1:Q:36:LEU:HD21  | 1:Q:140:ILE:HD13 | 1.92                     | 0.51              |
| 1:e:152:ILE:HG23 | 1:e:204:TRP:HB2  | 1.93                     | 0.51              |
| 1:A:243:VAL:HG21 | 1:A:255:VAL:HG21 | 1.93                     | 0.51              |
| 1:N:173:ASP:OD2  | 1:O:58:LYS:NZ    | 2.36                     | 0.51              |
| 1:X:230:THR:O    | 1:X:237:HIS:ND1  | 2.28                     | 0.51              |
| 1:f:165:LYS:HB3  | 1:f:182:THR:HB   | 1.93                     | 0.51              |
| 1:G:37:GLU:HG3   | 1:G:42:GLY:HA2   | 1.93                     | 0.51              |
| 1:O:140:ILE:HG12 | 1:O:157:LEU:HD23 | 1.93                     | 0.51              |
| 1:c:152:ILE:HG23 | 1:c:204:TRP:HB2  | 1.92                     | 0.51              |
| 1:A:67:GLU:HG3   | 1:A:90:THR:HB    | 1.93                     | 0.51              |
| 1:F:105:LEU:HA   | 1:F:108:ILE:HG12 | 1.93                     | 0.51              |
| 1:K:165:LYS:HB3  | 1:K:182:THR:HB   | 1.93                     | 0.51              |
| 1:J:178:GLU:OE1  | 1:J:180:LYS:NZ   | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:91:THR:HG21  | 1:R:195:VAL:HG21 | 1.92                     | 0.50              |
| 1:T:177:ILE:HD12 | 1:U:154:LEU:HD11 | 1.92                     | 0.50              |
| 1:X:144:MET:HG3  | 1:X:153:TRP:CD1  | 2.46                     | 0.50              |
| 1:I:263:ASP:OD1  | 1:I:263:ASP:N    | 2.44                     | 0.50              |
| 1:P:98:TYR:HE1   | 1:P:178:GLU:HG2  | 1.76                     | 0.50              |
| 1:U:230:THR:O    | 1:U:237:HIS:ND1  | 2.27                     | 0.50              |
| 1:K:263:ASP:N    | 1:K:263:ASP:OD1  | 2.45                     | 0.50              |
| 1:U:64:LEU:HD23  | 1:U:93:PHE:HB3   | 1.92                     | 0.50              |
| 1:U:255:VAL:HA   | 1:U:287:LYS:HB2  | 1.92                     | 0.50              |
| 1:a:130:LYS:HZ2  | 1:b:187:ARG:HE   | 1.60                     | 0.50              |
| 1:A:163:LEU:HA   | 1:A:183:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:209:ALA:HB1  | 1:A:216:ALA:HA   | 1.93                     | 0.50              |
| 1:N:98:TYR:HE1   | 1:N:178:GLU:HG2  | 1.76                     | 0.50              |
| 1:Q:273:VAL:HG11 | 1:Q:296:VAL:HG11 | 1.94                     | 0.50              |
| 1:V:163:LEU:HA   | 1:V:183:LEU:HD23 | 1.92                     | 0.50              |
| 1:b:97:MET:HE1   | 1:b:181:PRO:HG3  | 1.93                     | 0.50              |
| 1:c:57:GLU:HG2   | 1:c:60:ALA:H     | 1.74                     | 0.50              |
| 1:I:165:LYS:HB3  | 1:I:182:THR:HB   | 1.94                     | 0.50              |
| 1:N:98:TYR:CE1   | 1:N:178:GLU:HG2  | 2.46                     | 0.50              |
| 1:c:99:GLN:HE22  | 1:d:11:GLN:H     | 1.58                     | 0.50              |
| 1:N:36:LEU:HD21  | 1:N:140:ILE:HD13 | 1.93                     | 0.50              |
| 1:f:152:ILE:HG23 | 1:f:204:TRP:HB2  | 1.92                     | 0.50              |
| 1:D:163:LEU:HA   | 1:D:183:LEU:HD23 | 1.92                     | 0.50              |
| 1:e:105:LEU:HA   | 1:e:108:ILE:HG12 | 1.93                     | 0.50              |
| 1:P:36:LEU:HD21  | 1:P:140:ILE:HD13 | 1.92                     | 0.50              |
| 1:X:218:THR:OG1  | 1:X:246:ASP:OD2  | 2.24                     | 0.50              |
| 1:B:176:VAL:HG12 | 1:C:17:ALA:HB2   | 1.92                     | 0.50              |
| 1:Q:165:LYS:HB3  | 1:Q:182:THR:HB   | 1.94                     | 0.50              |
| 1:R:140:ILE:HG12 | 1:R:157:LEU:HD23 | 1.93                     | 0.50              |
| 1:c:144:MET:HG3  | 1:c:153:TRP:CD1  | 2.47                     | 0.50              |
| 1:G:17:ALA:HB2   | 1:L:176:VAL:HG12 | 1.94                     | 0.49              |
| 1:H:33:ALA:HB2   | 1:H:47:PRO:HG2   | 1.94                     | 0.49              |
| 1:J:37:GLU:HG3   | 1:J:42:GLY:HA2   | 1.93                     | 0.49              |
| 1:M:64:LEU:HD23  | 1:M:93:PHE:HB3   | 1.94                     | 0.49              |
| 1:M:154:LEU:HD11 | 1:R:177:ILE:HD12 | 1.92                     | 0.49              |
| 1:M:223:THR:OG1  | 1:M:224:PRO:HD3  | 2.11                     | 0.49              |
| 1:I:33:ALA:HB2   | 1:I:47:PRO:HG2   | 1.93                     | 0.49              |
| 1:T:36:LEU:HD11  | 1:T:140:ILE:HD13 | 1.94                     | 0.49              |
| 1:K:33:ALA:HB2   | 1:K:47:PRO:HG2   | 1.94                     | 0.49              |
| 1:M:273:VAL:HG11 | 1:M:296:VAL:HG11 | 1.93                     | 0.49              |
| 1:C:105:LEU:HA   | 1:C:108:ILE:HG12 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:163:LEU:HA   | 1:C:183:LEU:HD23 | 1.94                     | 0.49              |
| 1:E:222:ILE:HD11 | 1:E:292:ALA:HB1  | 1.94                     | 0.49              |
| 1:J:167:ASP:HB3  | 1:J:180:LYS:HB2  | 1.95                     | 0.49              |
| 1:K:223:THR:OG1  | 1:K:224:PRO:HD3  | 2.12                     | 0.49              |
| 1:V:105:LEU:HD13 | 1:V:126:LEU:HD11 | 1.94                     | 0.49              |
| 1:W:165:LYS:HB2  | 1:W:182:THR:HB   | 1.94                     | 0.49              |
| 1:C:74:GLU:HG2   | 1:H:58:LYS:HB3   | 1.94                     | 0.49              |
| 1:E:176:VAL:HG12 | 1:F:17:ALA:HB2   | 1.95                     | 0.49              |
| 1:G:263:ASP:OD1  | 1:G:263:ASP:N    | 2.44                     | 0.49              |
| 1:P:169:GLN:HB3  | 1:Q:64:LEU:HB2   | 1.93                     | 0.49              |
| 1:E:99:GLN:NE2   | 1:F:11:GLN:H     | 2.10                     | 0.49              |
| 1:I:176:VAL:HG12 | 1:J:17:ALA:HB2   | 1.94                     | 0.49              |
| 1:M:98:TYR:CE1   | 1:M:178:GLU:HG2  | 2.48                     | 0.49              |
| 1:N:165:LYS:HB3  | 1:N:182:THR:HB   | 1.94                     | 0.49              |
| 1:R:224:PRO:HG2  | 1:R:241:LEU:HA   | 1.94                     | 0.49              |
| 1:H:231:VAL:HB   | 1:H:300:ALA:HA   | 1.95                     | 0.49              |
| 1:S:238:THR:HB   | 1:S:272:LEU:HD11 | 1.94                     | 0.49              |
| 1:M:177:ILE:HG13 | 1:N:18:PRO:HD3   | 1.95                     | 0.49              |
| 1:O:177:ILE:HG13 | 1:P:18:PRO:HD3   | 1.94                     | 0.49              |
| 1:P:64:LEU:HD23  | 1:P:93:PHE:HB3   | 1.94                     | 0.49              |
| 1:W:255:VAL:HA   | 1:W:287:LYS:HB2  | 1.95                     | 0.49              |
| 1:a:99:GLN:NE2   | 1:b:11:GLN:O     | 2.46                     | 0.49              |
| 1:C:246:ASP:OD1  | 1:C:246:ASP:N    | 2.46                     | 0.49              |
| 1:H:263:ASP:OD1  | 1:H:263:ASP:N    | 2.45                     | 0.49              |
| 1:J:69:ASP:OD1   | 1:J:69:ASP:N     | 2.45                     | 0.49              |
| 1:P:273:VAL:HG11 | 1:P:296:VAL:HG11 | 1.94                     | 0.49              |
| 1:R:98:TYR:HE1   | 1:R:178:GLU:HG2  | 1.78                     | 0.49              |
| 1:a:99:GLN:HE22  | 1:b:11:GLN:N     | 2.10                     | 0.49              |
| 1:d:105:LEU:HA   | 1:d:108:ILE:HG12 | 1.94                     | 0.49              |
| 1:F:163:LEU:HA   | 1:F:183:LEU:HD23 | 1.95                     | 0.48              |
| 1:Q:220:LEU:HD12 | 1:Q:243:VAL:HG12 | 1.95                     | 0.48              |
| 1:W:98:TYR:HE1   | 1:W:178:GLU:HG2  | 1.78                     | 0.48              |
| 1:e:36:LEU:HD21  | 1:e:140:ILE:HD13 | 1.95                     | 0.48              |
| 1:G:33:ALA:HB2   | 1:G:47:PRO:HG2   | 1.95                     | 0.48              |
| 1:I:72:ASP:OD1   | 1:I:72:ASP:N     | 2.45                     | 0.48              |
| 1:H:64:LEU:HD23  | 1:H:93:PHE:HB3   | 1.95                     | 0.48              |
| 1:X:163:LEU:HA   | 1:X:183:LEU:HD23 | 1.94                     | 0.48              |
| 1:f:8:LYS:HG2    | 1:f:10:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:74:GLU:HG2   | 1:L:58:LYS:HB3   | 1.95                     | 0.48              |
| 1:U:163:LEU:HA   | 1:U:183:LEU:HD23 | 1.95                     | 0.48              |
| 1:W:121:PHE:HB2  | 1:X:37:GLU:OE2   | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:54:GLY:HA3   | 1:B:99:GLN:NE2   | 2.28                     | 0.48              |
| 1:N:220:LEU:HD12 | 1:N:243:VAL:HG12 | 1.95                     | 0.48              |
| 1:X:69:ASP:O     | 1:X:87:ASN:N     | 2.46                     | 0.48              |
| 1:c:99:GLN:HE22  | 1:d:11:GLN:N     | 2.12                     | 0.48              |
| 1:e:230:THR:O    | 1:e:237:HIS:ND1  | 2.46                     | 0.48              |
| 1:f:144:MET:HG3  | 1:f:153:TRP:CD1  | 2.48                     | 0.48              |
| 1:D:177:ILE:HG13 | 1:E:18:PRO:HD3   | 1.96                     | 0.48              |
| 1:S:230:THR:O    | 1:S:237:HIS:ND1  | 2.47                     | 0.48              |
| 1:W:98:TYR:CE1   | 1:W:178:GLU:HG2  | 2.48                     | 0.48              |
| 1:b:36:LEU:HD21  | 1:b:140:ILE:HD13 | 1.95                     | 0.48              |
| 1:O:64:LEU:HD23  | 1:O:93:PHE:HB3   | 1.95                     | 0.48              |
| 1:W:36:LEU:HD11  | 1:W:140:ILE:HD13 | 1.96                     | 0.48              |
| 1:E:105:LEU:HA   | 1:E:108:ILE:HG12 | 1.96                     | 0.48              |
| 1:G:222:ILE:HD11 | 1:G:241:LEU:HB3  | 1.96                     | 0.48              |
| 1:K:63:THR:HB    | 1:K:94:ASP:OD1   | 2.14                     | 0.48              |
| 1:B:119:SER:OG   | 1:C:37:GLU:OE1   | 2.29                     | 0.47              |
| 1:J:33:ALA:HB2   | 1:J:47:PRO:HG2   | 1.95                     | 0.47              |
| 1:P:98:TYR:CE1   | 1:P:178:GLU:HG2  | 2.48                     | 0.47              |
| 1:X:278:ALA:HA   | 1:X:298:VAL:HB   | 1.96                     | 0.47              |
| 1:f:218:THR:OG1  | 1:f:246:ASP:OD2  | 2.27                     | 0.47              |
| 1:B:63:THR:HB    | 1:B:94:ASP:OD1   | 2.14                     | 0.47              |
| 1:S:255:VAL:HA   | 1:S:287:LYS:HB2  | 1.95                     | 0.47              |
| 1:T:63:THR:HB    | 1:T:94:ASP:OD1   | 2.14                     | 0.47              |
| 1:U:91:THR:HG21  | 1:U:195:VAL:HG21 | 1.96                     | 0.47              |
| 1:V:105:LEU:HA   | 1:V:108:ILE:HG12 | 1.96                     | 0.47              |
| 1:f:70:SER:HB3   | 1:f:86:ILE:HA    | 1.96                     | 0.47              |
| 1:A:224:PRO:HG2  | 1:A:241:LEU:HD22 | 1.97                     | 0.47              |
| 1:C:231:VAL:HB   | 1:C:300:ALA:HA   | 1.97                     | 0.47              |
| 1:R:64:LEU:HD23  | 1:R:93:PHE:HB3   | 1.95                     | 0.47              |
| 1:V:230:THR:O    | 1:V:237:HIS:ND1  | 2.47                     | 0.47              |
| 1:W:91:THR:HG21  | 1:W:195:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:246:ASP:OD1  | 1:A:246:ASP:N    | 2.47                     | 0.47              |
| 1:U:63:THR:HB    | 1:U:94:ASP:OD1   | 2.15                     | 0.47              |
| 1:V:64:LEU:HD23  | 1:V:93:PHE:HB3   | 1.97                     | 0.47              |
| 1:X:91:THR:HG21  | 1:X:195:VAL:HG21 | 1.97                     | 0.47              |
| 1:b:8:LYS:HG2    | 1:b:10:ALA:HB2   | 1.96                     | 0.47              |
| 1:e:19:LEU:HD12  | 1:e:146:ASP:H    | 1.80                     | 0.47              |
| 1:B:152:ILE:HG23 | 1:B:204:TRP:HB2  | 1.96                     | 0.47              |
| 1:D:63:THR:HB    | 1:D:94:ASP:OD1   | 2.14                     | 0.47              |
| 1:D:112:ASP:OD1  | 1:D:112:ASP:N    | 2.48                     | 0.47              |
| 1:E:144:MET:HE2  | 1:E:144:MET:HB3  | 1.81                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:63:THR:O     | 1:G:93:PHE:HA    | 2.15                     | 0.47              |
| 1:G:130:LYS:HZ3  | 1:H:192:GLY:C    | 2.23                     | 0.47              |
| 1:V:238:THR:HB   | 1:V:272:LEU:HD11 | 1.96                     | 0.47              |
| 1:H:222:ILE:HG21 | 1:H:294:ALA:HB2  | 1.97                     | 0.47              |
| 1:L:255:VAL:HA   | 1:L:287:LYS:HB2  | 1.97                     | 0.47              |
| 1:M:24:LEU:HD22  | 1:M:46:ILE:HG21  | 1.97                     | 0.47              |
| 1:A:14:LEU:HB2   | 1:F:99:GLN:HG2   | 1.95                     | 0.47              |
| 1:I:229:VAL:HG13 | 1:I:298:VAL:HG13 | 1.96                     | 0.47              |
| 1:L:230:THR:O    | 1:L:237:HIS:ND1  | 2.42                     | 0.47              |
| 1:M:57:GLU:HG2   | 1:M:60:ALA:H     | 1.80                     | 0.47              |
| 1:O:99:GLN:HE22  | 1:P:11:GLN:N     | 2.11                     | 0.47              |
| 1:P:163:LEU:HA   | 1:P:183:LEU:HD23 | 1.97                     | 0.47              |
| 1:S:173:ASP:OD2  | 1:T:58:LYS:NZ    | 2.44                     | 0.47              |
| 1:T:69:ASP:O     | 1:T:87:ASN:N     | 2.47                     | 0.47              |
| 1:c:222:ILE:HG13 | 1:c:224:PRO:HD2  | 1.96                     | 0.47              |
| 1:e:224:PRO:HG2  | 1:e:241:LEU:HD22 | 1.96                     | 0.47              |
| 1:Q:204:TRP:O    | 1:Q:208:VAL:N    | 2.48                     | 0.47              |
| 1:W:169:GLN:HE21 | 1:W:177:ILE:HG23 | 1.80                     | 0.47              |
| 1:X:63:THR:HB    | 1:X:94:ASP:OD1   | 2.15                     | 0.47              |
| 1:c:165:LYS:HB3  | 1:c:182:THR:HB   | 1.97                     | 0.47              |
| 1:f:64:LEU:HD23  | 1:f:93:PHE:HB3   | 1.97                     | 0.47              |
| 1:Q:230:THR:O    | 1:Q:237:HIS:ND1  | 2.47                     | 0.47              |
| 1:c:105:LEU:HA   | 1:c:108:ILE:HG12 | 1.95                     | 0.47              |
| 1:A:63:THR:HB    | 1:A:94:ASP:OD1   | 2.14                     | 0.47              |
| 1:E:63:THR:HB    | 1:E:94:ASP:OD1   | 2.14                     | 0.47              |
| 1:H:63:THR:HB    | 1:H:94:ASP:OD1   | 2.14                     | 0.47              |
| 1:J:152:ILE:HG23 | 1:J:204:TRP:HB2  | 1.96                     | 0.47              |
| 1:L:163:LEU:HA   | 1:L:183:LEU:HD23 | 1.96                     | 0.47              |
| 1:L:222:ILE:HG21 | 1:L:294:ALA:HB2  | 1.97                     | 0.47              |
| 1:S:223:THR:OG1  | 1:S:224:PRO:HD3  | 2.14                     | 0.47              |
| 1:M:144:MET:HE2  | 1:M:144:MET:HB3  | 1.86                     | 0.46              |
| 1:R:19:LEU:HD12  | 1:R:146:ASP:H    | 1.81                     | 0.46              |
| 1:R:98:TYR:CE1   | 1:R:178:GLU:HG2  | 2.50                     | 0.46              |
| 1:a:105:LEU:HA   | 1:a:108:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:64:LEU:HD23  | 1:B:93:PHE:HB3   | 1.97                     | 0.46              |
| 1:D:246:ASP:N    | 1:D:246:ASP:OD1  | 2.47                     | 0.46              |
| 1:G:99:GLN:NE2   | 1:H:11:GLN:H     | 2.11                     | 0.46              |
| 1:L:263:ASP:OD1  | 1:L:263:ASP:N    | 2.44                     | 0.46              |
| 1:S:64:LEU:HD23  | 1:S:93:PHE:HB3   | 1.98                     | 0.46              |
| 1:O:162:LYS:HB3  | 1:O:186:PHE:HE1  | 1.80                     | 0.46              |
| 1:W:63:THR:HB    | 1:W:94:ASP:OD1   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:105:LEU:HA   | 1:S:108:ILE:HG12 | 1.97                     | 0.46              |
| 1:a:64:LEU:HD23  | 1:a:93:PHE:HB3   | 1.97                     | 0.46              |
| 1:B:105:LEU:HA   | 1:B:108:ILE:HG12 | 1.96                     | 0.46              |
| 1:E:91:THR:HG21  | 1:E:195:VAL:HG21 | 1.98                     | 0.46              |
| 1:F:64:LEU:HD23  | 1:F:93:PHE:HB3   | 1.97                     | 0.46              |
| 1:N:140:ILE:HG12 | 1:N:157:LEU:HD23 | 1.98                     | 0.46              |
| 1:P:94:ASP:HB3   | 1:P:182:THR:HA   | 1.98                     | 0.46              |
| 1:V:176:VAL:HG12 | 1:W:17:ALA:HB2   | 1.97                     | 0.46              |
| 1:C:63:THR:HB    | 1:C:94:ASP:OD1   | 2.16                     | 0.46              |
| 1:E:64:LEU:HD23  | 1:E:93:PHE:HB3   | 1.97                     | 0.46              |
| 1:F:94:ASP:HB3   | 1:F:182:THR:HA   | 1.97                     | 0.46              |
| 1:K:177:ILE:HD12 | 1:L:154:LEU:HD11 | 1.97                     | 0.46              |
| 1:L:165:LYS:HB3  | 1:L:182:THR:HB   | 1.98                     | 0.46              |
| 1:M:63:THR:HB    | 1:M:94:ASP:OD1   | 2.16                     | 0.46              |
| 1:T:91:THR:HG21  | 1:T:195:VAL:HG21 | 1.97                     | 0.46              |
| 1:d:64:LEU:HD23  | 1:d:93:PHE:HB3   | 1.97                     | 0.46              |
| 1:L:218:THR:OG1  | 1:L:246:ASP:OD2  | 2.32                     | 0.46              |
| 1:R:243:VAL:HG21 | 1:R:255:VAL:HG21 | 1.98                     | 0.46              |
| 1:U:220:LEU:HD22 | 1:U:243:VAL:HG12 | 1.98                     | 0.46              |
| 1:V:19:LEU:HD12  | 1:V:146:ASP:H    | 1.81                     | 0.46              |
| 1:b:90:THR:HG23  | 1:b:184:LYS:HE2  | 1.97                     | 0.46              |
| 1:I:63:THR:O     | 1:I:93:PHE:HA    | 2.16                     | 0.46              |
| 1:R:162:LYS:HB3  | 1:R:186:PHE:HE1  | 1.80                     | 0.46              |
| 1:F:13:ASP:O     | 1:F:147:ARG:NH1  | 2.41                     | 0.46              |
| 1:M:98:TYR:HE1   | 1:M:178:GLU:HG2  | 1.81                     | 0.46              |
| 1:S:24:LEU:HD22  | 1:S:46:ILE:HG21  | 1.98                     | 0.46              |
| 1:T:121:PHE:HB2  | 1:U:37:GLU:OE2   | 2.16                     | 0.46              |
| 1:A:105:LEU:HA   | 1:A:108:ILE:HG12 | 1.98                     | 0.45              |
| 1:C:99:GLN:NE2   | 1:D:11:GLN:O     | 2.46                     | 0.45              |
| 1:K:64:LEU:HD23  | 1:K:93:PHE:HB3   | 1.98                     | 0.45              |
| 1:L:72:ASP:HB2   | 1:L:81:PRO:HB3   | 1.98                     | 0.45              |
| 1:N:37:GLU:HG2   | 1:N:42:GLY:HA2   | 1.97                     | 0.45              |
| 1:O:204:TRP:O    | 1:O:208:VAL:N    | 2.49                     | 0.45              |
| 1:V:255:VAL:HA   | 1:V:287:LYS:HB2  | 1.98                     | 0.45              |
| 1:d:130:LYS:NZ   | 1:e:187:ARG:HE   | 2.15                     | 0.45              |
| 1:f:223:THR:OG1  | 1:f:224:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:130:LYS:HG3  | 1:B:187:ARG:NE   | 2.31                     | 0.45              |
| 1:C:237:HIS:CE1  | 1:C:274:THR:HG23 | 2.51                     | 0.45              |
| 1:L:118:PRO:HA   | 1:L:124:ILE:HG22 | 1.97                     | 0.45              |
| 1:N:121:PHE:HB2  | 1:O:37:GLU:OE2   | 2.17                     | 0.45              |
| 1:N:204:TRP:O    | 1:N:208:VAL:N    | 2.48                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:24:LEU:HD22  | 1:P:46:ILE:HG21  | 1.97                     | 0.45              |
| 1:R:204:TRP:O    | 1:R:208:VAL:N    | 2.49                     | 0.45              |
| 1:T:159:PRO:HG3  | 1:T:191:VAL:HG21 | 1.99                     | 0.45              |
| 1:U:140:ILE:HG12 | 1:U:157:LEU:HD23 | 1.98                     | 0.45              |
| 1:X:130:LYS:HG3  | 1:X:131:VAL:HG23 | 1.96                     | 0.45              |
| 1:X:224:PRO:HG2  | 1:X:241:LEU:HD23 | 1.98                     | 0.45              |
| 1:b:165:LYS:HB3  | 1:b:182:THR:HB   | 1.98                     | 0.45              |
| 1:A:222:ILE:HG22 | 1:A:224:PRO:HD2  | 1.97                     | 0.45              |
| 1:I:38:SER:HB2   | 1:I:45:ALA:HB2   | 1.98                     | 0.45              |
| 1:J:63:THR:O     | 1:J:93:PHE:HA    | 2.15                     | 0.45              |
| 1:P:144:MET:HE2  | 1:P:144:MET:HB3  | 1.85                     | 0.45              |
| 1:Q:37:GLU:HG2   | 1:Q:42:GLY:HA2   | 1.98                     | 0.45              |
| 1:R:94:ASP:N     | 1:R:94:ASP:OD1   | 2.49                     | 0.45              |
| 1:S:58:LYS:NZ    | 1:X:173:ASP:OD2  | 2.49                     | 0.45              |
| 1:S:222:ILE:HG22 | 1:S:224:PRO:HD2  | 1.97                     | 0.45              |
| 1:D:94:ASP:HB3   | 1:D:182:THR:HA   | 1.98                     | 0.45              |
| 1:H:159:PRO:HG3  | 1:H:191:VAL:HG21 | 1.99                     | 0.45              |
| 1:I:255:VAL:HA   | 1:I:287:LYS:HB2  | 1.97                     | 0.45              |
| 1:L:231:VAL:HB   | 1:L:300:ALA:HA   | 1.99                     | 0.45              |
| 1:N:148:ASN:ND2  | 1:N:150:ARG:HG3  | 2.32                     | 0.45              |
| 1:V:36:LEU:HD21  | 1:V:140:ILE:HD13 | 1.98                     | 0.45              |
| 1:W:278:ALA:HA   | 1:W:298:VAL:HB   | 1.99                     | 0.45              |
| 1:b:64:LEU:HD23  | 1:b:93:PHE:HB3   | 1.98                     | 0.45              |
| 1:e:176:VAL:HG12 | 1:f:17:ALA:HB2   | 1.98                     | 0.45              |
| 1:A:187:ARG:HH12 | 1:A:192:GLY:HA2  | 1.81                     | 0.45              |
| 1:C:13:ASP:O     | 1:C:147:ARG:NH1  | 2.27                     | 0.45              |
| 1:F:63:THR:HB    | 1:F:94:ASP:OD1   | 2.16                     | 0.45              |
| 1:G:231:VAL:HB   | 1:G:300:ALA:HA   | 1.98                     | 0.45              |
| 1:L:63:THR:O     | 1:L:93:PHE:HA    | 2.17                     | 0.45              |
| 1:O:94:ASP:OD1   | 1:O:94:ASP:N     | 2.49                     | 0.45              |
| 1:S:69:ASP:O     | 1:S:87:ASN:N     | 2.48                     | 0.45              |
| 1:T:64:LEU:HD23  | 1:T:93:PHE:HB3   | 1.99                     | 0.45              |
| 1:W:64:LEU:HD23  | 1:W:93:PHE:HB3   | 1.99                     | 0.45              |
| 1:E:163:LEU:HA   | 1:E:183:LEU:HD23 | 1.98                     | 0.45              |
| 1:E:246:ASP:OD1  | 1:E:246:ASP:N    | 2.47                     | 0.45              |
| 1:I:231:VAL:HB   | 1:I:300:ALA:HA   | 1.99                     | 0.45              |
| 1:I:278:ALA:HA   | 1:I:298:VAL:HB   | 1.98                     | 0.45              |
| 1:L:223:THR:OG1  | 1:L:224:PRO:HD3  | 2.17                     | 0.45              |
| 1:D:177:ILE:HD13 | 1:E:154:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:152:ILE:HG23 | 1:E:204:TRP:HB2  | 1.99                     | 0.45              |
| 1:K:159:PRO:HG3  | 1:K:191:VAL:HG21 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:73:ILE:HG13  | 1:Q:176:VAL:HG13 | 1.98                     | 0.45              |
| 1:N:73:ILE:HG13  | 1:S:176:VAL:HG13 | 1.99                     | 0.45              |
| 1:P:140:ILE:HG12 | 1:P:157:LEU:HD23 | 1.99                     | 0.45              |
| 1:P:224:PRO:HG2  | 1:P:241:LEU:HD22 | 1.98                     | 0.45              |
| 1:V:230:THR:HG22 | 1:V:232:ALA:H    | 1.81                     | 0.45              |
| 1:P:148:ASN:ND2  | 1:P:150:ARG:HG3  | 2.31                     | 0.45              |
| 1:T:98:TYR:CE1   | 1:T:178:GLU:HG2  | 2.51                     | 0.45              |
| 1:A:144:MET:HE2  | 1:A:144:MET:HB3  | 1.83                     | 0.45              |
| 1:C:19:LEU:HD12  | 1:C:146:ASP:H    | 1.82                     | 0.45              |
| 1:C:64:LEU:HD23  | 1:C:93:PHE:HB3   | 1.98                     | 0.45              |
| 1:Q:140:ILE:HG12 | 1:Q:157:LEU:HD23 | 1.99                     | 0.45              |
| 1:a:144:MET:HG3  | 1:a:153:TRP:CD1  | 2.52                     | 0.45              |
| 1:B:91:THR:HG21  | 1:B:195:VAL:HG21 | 1.99                     | 0.45              |
| 1:K:278:ALA:HA   | 1:K:298:VAL:HB   | 1.99                     | 0.45              |
| 1:O:224:PRO:HG2  | 1:O:241:LEU:HD22 | 1.99                     | 0.45              |
| 1:Q:223:THR:OG1  | 1:Q:224:PRO:HD3  | 2.18                     | 0.45              |
| 1:J:263:ASP:OD1  | 1:J:263:ASP:N    | 2.43                     | 0.44              |
| 1:Q:121:PHE:HB2  | 1:R:37:GLU:OE2   | 2.17                     | 0.44              |
| 1:U:69:ASP:O     | 1:U:87:ASN:N     | 2.48                     | 0.44              |
| 1:e:165:LYS:HB3  | 1:e:182:THR:HB   | 1.98                     | 0.44              |
| 1:J:231:VAL:HB   | 1:J:300:ALA:HA   | 1.99                     | 0.44              |
| 1:K:229:VAL:HG13 | 1:K:298:VAL:HG13 | 1.98                     | 0.44              |
| 1:M:163:LEU:HA   | 1:M:183:LEU:HD23 | 1.99                     | 0.44              |
| 1:P:57:GLU:HG2   | 1:P:60:ALA:H     | 1.82                     | 0.44              |
| 1:T:15:ALA:O     | 1:T:147:ARG:NH2  | 2.50                     | 0.44              |
| 1:V:24:LEU:HD22  | 1:V:46:ILE:HG21  | 1.98                     | 0.44              |
| 1:V:63:THR:HB    | 1:V:94:ASP:OD1   | 2.17                     | 0.44              |
| 1:M:94:ASP:HB3   | 1:M:182:THR:HA   | 1.99                     | 0.44              |
| 1:V:69:ASP:O     | 1:V:87:ASN:N     | 2.47                     | 0.44              |
| 1:c:64:LEU:HD23  | 1:c:93:PHE:HB3   | 1.98                     | 0.44              |
| 1:c:217:LEU:HD22 | 1:c:251:TYR:CZ   | 2.52                     | 0.44              |
| 1:e:64:LEU:HD23  | 1:e:93:PHE:HB3   | 1.98                     | 0.44              |
| 1:A:58:LYS:NZ    | 1:F:173:ASP:OD2  | 2.41                     | 0.44              |
| 1:A:94:ASP:HB3   | 1:A:182:THR:HA   | 1.99                     | 0.44              |
| 1:C:176:VAL:HG12 | 1:D:17:ALA:HB2   | 1.98                     | 0.44              |
| 1:H:246:ASP:OD1  | 1:H:246:ASP:N    | 2.50                     | 0.44              |
| 1:H:255:VAL:HA   | 1:H:287:LYS:HB2  | 1.98                     | 0.44              |
| 1:L:54:GLY:HA3   | 1:L:99:GLN:NE2   | 2.33                     | 0.44              |
| 1:Q:144:MET:HE2  | 1:Q:144:MET:HB3  | 1.86                     | 0.44              |
| 1:f:140:ILE:HG12 | 1:f:157:LEU:HD23 | 1.99                     | 0.44              |
| 1:A:154:LEU:HD11 | 1:F:177:ILE:HD12 | 1.97                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:94:ASP:HB3   | 1:B:182:THR:HA   | 2.00                     | 0.44              |
| 1:H:177:ILE:HD12 | 1:I:154:LEU:HD11 | 2.00                     | 0.44              |
| 1:Q:148:ASN:ND2  | 1:Q:150:ARG:HG3  | 2.32                     | 0.44              |
| 1:T:22:THR:HG22  | 1:U:4:PHE:CZ     | 2.53                     | 0.44              |
| 1:X:165:LYS:HB2  | 1:X:182:THR:HB   | 1.99                     | 0.44              |
| 1:b:101:GLN:HG2  | 1:c:14:LEU:HD13  | 1.99                     | 0.44              |
| 1:M:140:ILE:HG12 | 1:M:157:LEU:HD23 | 2.00                     | 0.44              |
| 1:S:63:THR:HB    | 1:S:94:ASP:OD1   | 2.18                     | 0.44              |
| 1:e:223:THR:OG1  | 1:e:224:PRO:HD3  | 2.18                     | 0.44              |
| 1:H:165:LYS:HB3  | 1:H:182:THR:HB   | 1.99                     | 0.44              |
| 1:I:73:ILE:HG13  | 1:N:176:VAL:HG13 | 2.00                     | 0.44              |
| 1:J:223:THR:OG1  | 1:J:224:PRO:HD3  | 2.17                     | 0.44              |
| 1:K:231:VAL:HB   | 1:K:300:ALA:HA   | 2.00                     | 0.44              |
| 1:L:243:VAL:HG11 | 1:L:255:VAL:HG11 | 2.00                     | 0.44              |
| 1:M:222:ILE:HG21 | 1:M:294:ALA:HB2  | 1.99                     | 0.44              |
| 1:f:19:LEU:HD12  | 1:f:146:ASP:H    | 1.82                     | 0.44              |
| 1:D:105:LEU:HA   | 1:D:108:ILE:HG12 | 2.00                     | 0.44              |
| 1:E:223:THR:HB   | 1:E:224:PRO:HD3  | 1.99                     | 0.44              |
| 1:I:118:PRO:HA   | 1:I:124:ILE:HG22 | 2.00                     | 0.44              |
| 1:K:222:ILE:HD11 | 1:K:241:LEU:HB3  | 1.99                     | 0.44              |
| 1:N:230:THR:O    | 1:N:237:HIS:ND1  | 2.50                     | 0.44              |
| 1:O:98:TYR:HE1   | 1:O:178:GLU:HG2  | 1.83                     | 0.44              |
| 1:X:220:LEU:HD22 | 1:X:243:VAL:HG12 | 2.00                     | 0.44              |
| 1:e:98:TYR:CE1   | 1:e:178:GLU:HG2  | 2.53                     | 0.44              |
| 1:C:94:ASP:HB3   | 1:C:182:THR:HA   | 1.99                     | 0.44              |
| 1:E:94:ASP:HB3   | 1:E:182:THR:HA   | 2.00                     | 0.44              |
| 1:M:222:ILE:HD11 | 1:M:241:LEU:HB3  | 1.99                     | 0.44              |
| 1:P:37:GLU:HG2   | 1:P:42:GLY:HA2   | 2.00                     | 0.44              |
| 1:P:63:THR:HB    | 1:P:94:ASP:OD1   | 2.18                     | 0.44              |
| 1:T:98:TYR:HE1   | 1:T:178:GLU:HG2  | 1.83                     | 0.44              |
| 1:a:63:THR:O     | 1:a:93:PHE:HA    | 2.17                     | 0.44              |
| 1:D:64:LEU:HD23  | 1:D:93:PHE:HB3   | 1.99                     | 0.43              |
| 1:J:118:PRO:HA   | 1:J:124:ILE:HG22 | 2.00                     | 0.43              |
| 1:N:273:VAL:HG11 | 1:N:296:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:112:ASP:OD1  | 1:C:112:ASP:N    | 2.52                     | 0.43              |
| 1:H:230:THR:HG22 | 1:H:232:ALA:H    | 1.84                     | 0.43              |
| 1:I:163:LEU:HA   | 1:I:183:LEU:HD23 | 1.99                     | 0.43              |
| 1:J:38:SER:HB2   | 1:J:45:ALA:HB2   | 2.00                     | 0.43              |
| 1:J:55:HIS:CD2   | 1:K:10:ALA:HB1   | 2.53                     | 0.43              |
| 1:R:169:GLN:NE2  | 1:R:178:GLU:O    | 2.50                     | 0.43              |
| 1:S:19:LEU:HD12  | 1:S:146:ASP:H    | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:246:ASP:N    | 1:B:246:ASP:OD1  | 2.50                     | 0.43              |
| 1:D:159:PRO:HG3  | 1:D:191:VAL:HG21 | 2.00                     | 0.43              |
| 1:F:227:PRO:HD2  | 1:F:296:VAL:HG22 | 2.00                     | 0.43              |
| 1:G:154:LEU:HD11 | 1:L:177:ILE:HD13 | 2.01                     | 0.43              |
| 1:L:36:LEU:HD21  | 1:L:140:ILE:HD13 | 2.00                     | 0.43              |
| 1:N:96:ALA:HB2   | 1:N:180:LYS:HE2  | 1.99                     | 0.43              |
| 1:S:91:THR:HG21  | 1:S:195:VAL:HG21 | 2.00                     | 0.43              |
| 1:S:144:MET:HE2  | 1:S:144:MET:HB3  | 1.90                     | 0.43              |
| 1:W:229:VAL:HG23 | 1:W:298:VAL:HG13 | 1.99                     | 0.43              |
| 1:G:54:GLY:HA3   | 1:G:99:GLN:OE1   | 2.18                     | 0.43              |
| 1:G:130:LYS:HA   | 1:G:130:LYS:HD2  | 1.77                     | 0.43              |
| 1:G:223:THR:HB   | 1:G:224:PRO:HD3  | 2.01                     | 0.43              |
| 1:H:118:PRO:HA   | 1:H:124:ILE:HG22 | 2.00                     | 0.43              |
| 1:d:218:THR:OG1  | 1:d:246:ASP:OD2  | 2.31                     | 0.43              |
| 1:B:163:LEU:HA   | 1:B:183:LEU:HD23 | 1.99                     | 0.43              |
| 1:C:144:MET:HE2  | 1:C:144:MET:HB3  | 1.92                     | 0.43              |
| 1:D:38:SER:HB2   | 1:D:45:ALA:HB2   | 2.01                     | 0.43              |
| 1:H:264:LYS:NZ   | 1:H:279:GLY:HA3  | 2.34                     | 0.43              |
| 1:K:190:VAL:HG13 | 1:K:191:VAL:HG13 | 2.01                     | 0.43              |
| 1:P:247:ASN:ND2  | 1:P:249:ILE:HD12 | 2.32                     | 0.43              |
| 1:c:218:THR:OG1  | 1:c:246:ASP:OD2  | 2.28                     | 0.43              |
| 1:F:246:ASP:OD1  | 1:F:246:ASP:N    | 2.51                     | 0.43              |
| 1:I:217:LEU:HD22 | 1:I:251:TYR:CZ   | 2.53                     | 0.43              |
| 1:L:217:LEU:HD22 | 1:L:251:TYR:CZ   | 2.54                     | 0.43              |
| 1:V:205:ARG:HA   | 1:V:208:VAL:HG23 | 2.01                     | 0.43              |
| 1:b:19:LEU:HD12  | 1:b:146:ASP:H    | 1.83                     | 0.43              |
| 1:c:230:THR:O    | 1:c:237:HIS:ND1  | 2.52                     | 0.43              |
| 1:d:286:THR:HG22 | 1:d:291:THR:HG22 | 2.01                     | 0.43              |
| 1:e:264:LYS:HA   | 1:e:264:LYS:HD3  | 1.80                     | 0.43              |
| 1:f:230:THR:O    | 1:f:237:HIS:ND1  | 2.51                     | 0.43              |
| 1:I:177:ILE:HD13 | 1:J:154:LEU:HD11 | 2.00                     | 0.43              |
| 1:T:223:THR:OG1  | 1:T:224:PRO:HD3  | 2.19                     | 0.43              |
| 1:G:187:ARG:NH1  | 1:L:130:LYS:HZ2  | 2.16                     | 0.43              |
| 1:K:99:GLN:NE2   | 1:L:11:GLN:O     | 2.52                     | 0.43              |
| 1:W:69:ASP:O     | 1:W:87:ASN:N     | 2.46                     | 0.43              |
| 1:B:144:MET:HE2  | 1:B:144:MET:HB3  | 1.85                     | 0.43              |
| 1:D:144:MET:HE2  | 1:D:144:MET:HB3  | 1.83                     | 0.43              |
| 1:G:38:SER:HB2   | 1:G:45:ALA:HB2   | 2.00                     | 0.43              |
| 1:G:64:LEU:HD23  | 1:G:93:PHE:HB3   | 2.01                     | 0.43              |
| 1:I:150:ARG:NH2  | 1:I:254:ASP:OD1  | 2.52                     | 0.43              |
| 1:N:63:THR:O     | 1:N:93:PHE:HA    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:159:PRO:HG3  | 1:S:191:VAL:HG21 | 2.01                     | 0.43              |
| 1:V:93:PHE:CD2   | 1:V:141:LEU:HD21 | 2.54                     | 0.43              |
| 1:b:130:LYS:HZ2  | 1:c:187:ARG:NE   | 2.16                     | 0.43              |
| 1:A:159:PRO:HG3  | 1:A:191:VAL:HG21 | 2.00                     | 0.43              |
| 1:B:264:LYS:HA   | 1:B:264:LYS:HD3  | 1.85                     | 0.43              |
| 1:I:159:PRO:HG3  | 1:I:191:VAL:HG21 | 1.99                     | 0.43              |
| 1:K:38:SER:HB2   | 1:K:45:ALA:HB2   | 2.01                     | 0.43              |
| 1:K:118:PRO:HA   | 1:K:124:ILE:HG22 | 2.00                     | 0.43              |
| 1:L:152:ILE:HG23 | 1:L:204:TRP:HB2  | 2.01                     | 0.43              |
| 1:S:36:LEU:HD21  | 1:S:140:ILE:HD13 | 2.01                     | 0.43              |
| 1:S:264:LYS:HD2  | 1:S:279:GLY:HA3  | 2.00                     | 0.43              |
| 1:b:98:TYR:CE1   | 1:b:178:GLU:HG2  | 2.54                     | 0.43              |
| 1:F:223:THR:OG1  | 1:F:224:PRO:HD3  | 2.18                     | 0.42              |
| 1:J:159:PRO:HG3  | 1:J:191:VAL:HG21 | 2.00                     | 0.42              |
| 1:N:41:ASP:N     | 1:N:41:ASP:OD1   | 2.51                     | 0.42              |
| 1:N:230:THR:HG22 | 1:N:232:ALA:H    | 1.83                     | 0.42              |
| 1:Q:32:PRO:HG3   | 1:Q:138:ARG:CZ   | 2.49                     | 0.42              |
| 1:Q:63:THR:O     | 1:Q:93:PHE:HA    | 2.19                     | 0.42              |
| 1:W:15:ALA:O     | 1:W:147:ARG:NH2  | 2.51                     | 0.42              |
| 1:a:11:GLN:N     | 1:f:99:GLN:HE22  | 2.16                     | 0.42              |
| 1:K:224:PRO:HG2  | 1:K:241:LEU:HA   | 2.01                     | 0.42              |
| 1:N:223:THR:OG1  | 1:N:224:PRO:HD3  | 2.19                     | 0.42              |
| 1:R:63:THR:HB    | 1:R:94:ASP:OD1   | 2.19                     | 0.42              |
| 1:T:171:LEU:HD22 | 1:T:177:ILE:HG12 | 2.01                     | 0.42              |
| 1:c:8:LYS:HG2    | 1:c:10:ALA:HB2   | 2.02                     | 0.42              |
| 1:d:32:PRO:HG3   | 1:d:138:ARG:CZ   | 2.48                     | 0.42              |
| 1:A:64:LEU:HD23  | 1:A:93:PHE:HB3   | 1.99                     | 0.42              |
| 1:G:159:PRO:HG3  | 1:G:191:VAL:HG21 | 2.02                     | 0.42              |
| 1:S:205:ARG:HA   | 1:S:208:VAL:HG23 | 2.01                     | 0.42              |
| 1:c:36:LEU:HD11  | 1:c:140:ILE:HD13 | 2.01                     | 0.42              |
| 1:f:217:LEU:HD22 | 1:f:251:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:231:VAL:HB   | 1:A:300:ALA:HA   | 2.01                     | 0.42              |
| 1:C:227:PRO:HG2  | 1:C:296:VAL:HG22 | 2.01                     | 0.42              |
| 1:D:222:ILE:HD11 | 1:D:292:ALA:HB1  | 2.01                     | 0.42              |
| 1:G:192:GLY:HA2  | 1:L:130:LYS:HZ1  | 1.85                     | 0.42              |
| 1:H:38:SER:HB2   | 1:H:45:ALA:HB2   | 2.01                     | 0.42              |
| 1:R:69:ASP:O     | 1:R:87:ASN:N     | 2.51                     | 0.42              |
| 1:U:223:THR:OG1  | 1:U:224:PRO:HD3  | 2.18                     | 0.42              |
| 1:V:98:TYR:CE1   | 1:V:178:GLU:HG2  | 2.54                     | 0.42              |
| 1:V:144:MET:HE2  | 1:V:144:MET:HB3  | 1.90                     | 0.42              |
| 1:W:251:TYR:O    | 1:W:255:VAL:HG13 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:102:ARG:O    | 1:b:105:LEU:N    | 2.52                     | 0.42              |
| 1:e:177:ILE:CD1  | 1:f:154:LEU:HD11 | 2.50                     | 0.42              |
| 1:A:18:PRO:HD3   | 1:F:177:ILE:HG13 | 2.01                     | 0.42              |
| 1:I:223:THR:HB   | 1:I:224:PRO:HD3  | 2.01                     | 0.42              |
| 1:J:64:LEU:HD23  | 1:J:93:PHE:HB3   | 2.01                     | 0.42              |
| 1:N:227:PRO:HD2  | 1:N:296:VAL:HG22 | 2.01                     | 0.42              |
| 1:O:177:ILE:HD12 | 1:P:154:LEU:HD11 | 2.01                     | 0.42              |
| 1:T:220:LEU:HD22 | 1:T:243:VAL:HG12 | 2.02                     | 0.42              |
| 1:U:177:ILE:CD1  | 1:V:154:LEU:HD11 | 2.50                     | 0.42              |
| 1:V:159:PRO:HG3  | 1:V:191:VAL:HG21 | 2.01                     | 0.42              |
| 1:A:223:THR:OG1  | 1:A:224:PRO:HD3  | 2.20                     | 0.42              |
| 1:G:118:PRO:HA   | 1:G:124:ILE:HG22 | 2.02                     | 0.42              |
| 1:V:104:VAL:O    | 1:V:108:ILE:HG23 | 2.20                     | 0.42              |
| 1:a:70:SER:HB3   | 1:a:86:ILE:HA    | 2.02                     | 0.42              |
| 1:d:165:LYS:HB3  | 1:d:182:THR:HB   | 2.01                     | 0.42              |
| 1:Q:41:ASP:OD1   | 1:Q:41:ASP:N     | 2.51                     | 0.42              |
| 1:Q:173:ASP:OD2  | 1:R:58:LYS:NZ    | 2.36                     | 0.42              |
| 1:d:63:THR:O     | 1:d:93:PHE:HA    | 2.19                     | 0.42              |
| 1:C:223:THR:HB   | 1:C:224:PRO:HD3  | 2.02                     | 0.42              |
| 1:E:99:GLN:HE22  | 1:F:11:GLN:H     | 1.65                     | 0.42              |
| 1:E:264:LYS:HA   | 1:E:264:LYS:HD3  | 1.86                     | 0.42              |
| 1:I:230:THR:O    | 1:I:237:HIS:ND1  | 2.46                     | 0.42              |
| 1:K:130:LYS:HA   | 1:K:130:LYS:HD2  | 1.81                     | 0.42              |
| 1:O:132:PRO:HG3  | 1:P:89:ARG:HB2   | 2.01                     | 0.42              |
| 1:T:104:VAL:O    | 1:T:108:ILE:HG23 | 2.20                     | 0.42              |
| 1:W:102:ARG:O    | 1:W:106:GLU:HG3  | 2.20                     | 0.42              |
| 1:a:165:LYS:HB3  | 1:a:182:THR:HB   | 2.02                     | 0.42              |
| 1:f:108:ILE:HG13 | 1:f:109:TRP:N    | 2.35                     | 0.42              |
| 1:B:38:SER:HB2   | 1:B:45:ALA:HB2   | 2.01                     | 0.42              |
| 1:L:33:ALA:HB2   | 1:L:47:PRO:HG2   | 2.00                     | 0.42              |
| 1:M:169:GLN:HB3  | 1:N:64:LEU:HB2   | 2.01                     | 0.42              |
| 1:O:63:THR:HB    | 1:O:94:ASP:OD1   | 2.20                     | 0.42              |
| 1:W:93:PHE:CD2   | 1:W:141:LEU:HD21 | 2.55                     | 0.42              |
| 1:W:97:MET:HE3   | 1:W:97:MET:HB2   | 1.81                     | 0.42              |
| 1:W:104:VAL:O    | 1:W:108:ILE:HG23 | 2.20                     | 0.42              |
| 1:a:11:GLN:H     | 1:f:99:GLN:HE22  | 1.68                     | 0.42              |
| 1:c:19:LEU:HD12  | 1:c:146:ASP:H    | 1.84                     | 0.42              |
| 1:A:97:MET:HE3   | 1:A:97:MET:HB2   | 1.95                     | 0.42              |
| 1:B:55:HIS:CD2   | 1:C:10:ALA:HB1   | 2.55                     | 0.42              |
| 1:D:150:ARG:NH2  | 1:D:254:ASP:OD1  | 2.53                     | 0.42              |
| 1:E:94:ASP:OD1   | 1:E:94:ASP:N     | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:144:MET:HE2  | 1:F:144:MET:HB3  | 1.92                     | 0.42              |
| 1:I:55:HIS:CD2   | 1:J:10:ALA:HB1   | 2.55                     | 0.42              |
| 1:W:264:LYS:HA   | 1:W:277:ALA:HB3  | 2.02                     | 0.42              |
| 1:X:238:THR:HB   | 1:X:272:LEU:HD11 | 2.01                     | 0.42              |
| 1:b:259:SER:HB3  | 1:b:267:VAL:HG12 | 2.02                     | 0.42              |
| 1:I:63:THR:HB    | 1:I:94:ASP:OD1   | 2.20                     | 0.41              |
| 1:Q:222:ILE:HG13 | 1:Q:224:PRO:HD2  | 2.01                     | 0.41              |
| 1:S:176:VAL:HG12 | 1:T:17:ALA:HB2   | 2.01                     | 0.41              |
| 1:W:205:ARG:HA   | 1:W:208:VAL:HG23 | 2.01                     | 0.41              |
| 1:D:231:VAL:HB   | 1:D:300:ALA:HA   | 2.02                     | 0.41              |
| 1:E:159:PRO:HG3  | 1:E:191:VAL:HG21 | 2.01                     | 0.41              |
| 1:F:38:SER:HB2   | 1:F:45:ALA:HB2   | 2.01                     | 0.41              |
| 1:N:243:VAL:HG21 | 1:N:255:VAL:HG21 | 2.02                     | 0.41              |
| 1:P:41:ASP:N     | 1:P:41:ASP:OD1   | 2.52                     | 0.41              |
| 1:Q:230:THR:HG22 | 1:Q:232:ALA:H    | 1.85                     | 0.41              |
| 1:T:205:ARG:HA   | 1:T:208:VAL:HG23 | 2.00                     | 0.41              |
| 1:A:259:SER:HB3  | 1:A:267:VAL:HG12 | 2.02                     | 0.41              |
| 1:E:112:ASP:OD1  | 1:E:112:ASP:N    | 2.47                     | 0.41              |
| 1:J:230:THR:O    | 1:J:237:HIS:ND1  | 2.47                     | 0.41              |
| 1:O:108:ILE:HD13 | 1:O:179:TYR:CD1  | 2.56                     | 0.41              |
| 1:Q:83:ARG:NH1   | 1:W:147:ARG:HH21 | 2.19                     | 0.41              |
| 1:U:278:ALA:HA   | 1:U:298:VAL:HB   | 2.02                     | 0.41              |
| 1:W:130:LYS:HE2  | 1:X:187:ARG:NH2  | 2.34                     | 0.41              |
| 1:W:171:LEU:HD22 | 1:W:177:ILE:HG12 | 2.02                     | 0.41              |
| 1:b:103:ASN:HA   | 1:b:106:GLU:OE2  | 2.20                     | 0.41              |
| 1:E:71:LYS:HD2   | 1:J:174:ASP:O    | 2.19                     | 0.41              |
| 1:H:97:MET:HE1   | 1:H:107:LEU:HD23 | 2.02                     | 0.41              |
| 1:M:263:ASP:OD1  | 1:M:263:ASP:N    | 2.52                     | 0.41              |
| 1:O:69:ASP:O     | 1:O:87:ASN:N     | 2.51                     | 0.41              |
| 1:P:263:ASP:N    | 1:P:263:ASP:OD1  | 2.53                     | 0.41              |
| 1:T:239:ALA:O    | 1:T:272:LEU:HD12 | 2.21                     | 0.41              |
| 1:V:91:THR:HG21  | 1:V:195:VAL:HG21 | 2.02                     | 0.41              |
| 1:V:173:ASP:OD2  | 1:W:58:LYS:NZ    | 2.44                     | 0.41              |
| 1:W:73:ILE:HG13  | 1:d:176:VAL:HG13 | 2.02                     | 0.41              |
| 1:a:36:LEU:HD21  | 1:a:140:ILE:HD13 | 2.01                     | 0.41              |
| 1:c:264:LYS:HA   | 1:c:264:LYS:HD3  | 1.79                     | 0.41              |
| 1:G:217:LEU:HD21 | 1:G:220:LEU:HD11 | 2.01                     | 0.41              |
| 1:R:63:THR:O     | 1:R:93:PHE:HA    | 2.21                     | 0.41              |
| 1:B:144:MET:HG3  | 1:B:153:TRP:CD1  | 2.56                     | 0.41              |
| 1:C:263:ASP:N    | 1:C:263:ASP:OD1  | 2.53                     | 0.41              |
| 1:G:230:THR:HG22 | 1:G:232:ALA:H    | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:150:ARG:NH2  | 1:H:254:ASP:OD1  | 2.53                     | 0.41              |
| 1:K:255:VAL:HA   | 1:K:287:LYS:HB2  | 2.02                     | 0.41              |
| 1:M:19:LEU:HD12  | 1:M:146:ASP:H    | 1.85                     | 0.41              |
| 1:T:93:PHE:CD2   | 1:T:141:LEU:HD21 | 2.55                     | 0.41              |
| 1:b:21:LEU:HD21  | 1:b:62:LEU:HD13  | 2.03                     | 0.41              |
| 1:b:97:MET:O     | 1:b:178:GLU:HA   | 2.21                     | 0.41              |
| 1:c:108:ILE:HG13 | 1:c:109:TRP:N    | 2.34                     | 0.41              |
| 1:f:264:LYS:HD3  | 1:f:264:LYS:HA   | 1.79                     | 0.41              |
| 1:A:38:SER:HB2   | 1:A:45:ALA:HB2   | 2.01                     | 0.41              |
| 1:D:204:TRP:O    | 1:D:208:VAL:N    | 2.54                     | 0.41              |
| 1:G:246:ASP:N    | 1:G:246:ASP:OD1  | 2.53                     | 0.41              |
| 1:I:152:ILE:HG23 | 1:I:204:TRP:HB2  | 2.03                     | 0.41              |
| 1:L:63:THR:HB    | 1:L:94:ASP:OD1   | 2.19                     | 0.41              |
| 1:T:102:ARG:O    | 1:T:106:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:204:TRP:O    | 1:A:208:VAL:N    | 2.53                     | 0.41              |
| 1:D:94:ASP:OD1   | 1:D:94:ASP:N     | 2.54                     | 0.41              |
| 1:G:171:LEU:HD22 | 1:G:177:ILE:HG12 | 2.03                     | 0.41              |
| 1:J:130:LYS:HZ2  | 1:K:187:ARG:HD2  | 1.85                     | 0.41              |
| 1:P:223:THR:HB   | 1:P:224:PRO:HD3  | 2.03                     | 0.41              |
| 1:Q:243:VAL:HG21 | 1:Q:255:VAL:HG21 | 2.01                     | 0.41              |
| 1:R:256:VAL:O    | 1:R:285:ALA:HA   | 2.21                     | 0.41              |
| 1:X:98:TYR:CE1   | 1:X:178:GLU:HG2  | 2.56                     | 0.41              |
| 1:B:8:LYS:HG2    | 1:B:10:ALA:HB2   | 2.03                     | 0.41              |
| 1:E:171:LEU:HD22 | 1:E:177:ILE:HG12 | 2.03                     | 0.41              |
| 1:G:264:LYS:NZ   | 1:G:279:GLY:HA3  | 2.36                     | 0.41              |
| 1:H:32:PRO:HG3   | 1:H:138:ARG:CZ   | 2.51                     | 0.41              |
| 1:J:150:ARG:NH2  | 1:J:254:ASP:OD1  | 2.52                     | 0.41              |
| 1:J:171:LEU:HD22 | 1:J:177:ILE:HG12 | 2.03                     | 0.41              |
| 1:K:150:ARG:NH2  | 1:K:254:ASP:OD1  | 2.53                     | 0.41              |
| 1:L:140:ILE:HG12 | 1:L:157:LEU:HD23 | 2.03                     | 0.41              |
| 1:M:73:ILE:HG13  | 1:X:176:VAL:HG13 | 2.03                     | 0.41              |
| 1:N:209:ALA:HB1  | 1:N:216:ALA:HA   | 2.03                     | 0.41              |
| 1:O:256:VAL:O    | 1:O:285:ALA:HA   | 2.21                     | 0.41              |
| 1:S:104:VAL:O    | 1:S:108:ILE:HG23 | 2.20                     | 0.41              |
| 1:S:251:TYR:O    | 1:S:255:VAL:HG13 | 2.21                     | 0.41              |
| 1:T:105:LEU:HA   | 1:T:108:ILE:HG12 | 2.02                     | 0.41              |
| 1:U:218:THR:OG1  | 1:U:246:ASP:OD2  | 2.25                     | 0.41              |
| 1:W:239:ALA:O    | 1:W:272:LEU:HD12 | 2.21                     | 0.41              |
| 1:c:140:ILE:HG12 | 1:c:157:LEU:HD23 | 2.02                     | 0.41              |
| 1:c:223:THR:HB   | 1:c:224:PRO:HD3  | 2.03                     | 0.41              |
| 1:d:264:LYS:HA   | 1:d:264:LYS:HD3  | 1.78                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:150:ARG:NH2  | 1:e:254:ASP:OD1  | 2.54                     | 0.41              |
| 1:f:229:VAL:HG23 | 1:f:298:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:94:ASP:OD1   | 1:B:94:ASP:N     | 2.54                     | 0.41              |
| 1:C:15:ALA:O     | 1:C:147:ARG:NH2  | 2.52                     | 0.41              |
| 1:G:72:ASP:OD1   | 1:G:72:ASP:N     | 2.47                     | 0.41              |
| 1:O:63:THR:O     | 1:O:93:PHE:HA    | 2.21                     | 0.41              |
| 1:Q:256:VAL:O    | 1:Q:285:ALA:HA   | 2.21                     | 0.41              |
| 1:a:116:ILE:HD13 | 1:a:116:ILE:HA   | 1.93                     | 0.41              |
| 1:d:36:LEU:HD21  | 1:d:140:ILE:HD13 | 2.01                     | 0.41              |
| 1:A:89:ARG:HB2   | 1:F:132:PRO:HG3  | 2.03                     | 0.40              |
| 1:A:94:ASP:OD1   | 1:A:94:ASP:N     | 2.54                     | 0.40              |
| 1:C:132:PRO:HG3  | 1:D:89:ARG:HB2   | 2.02                     | 0.40              |
| 1:J:97:MET:HE1   | 1:J:107:LEU:HD23 | 2.03                     | 0.40              |
| 1:K:163:LEU:HA   | 1:K:183:LEU:HD23 | 2.03                     | 0.40              |
| 1:O:218:THR:OG1  | 1:O:246:ASP:OD2  | 2.27                     | 0.40              |
| 1:Q:264:LYS:O    | 1:Q:298:VAL:HG21 | 2.21                     | 0.40              |
| 1:U:238:THR:HB   | 1:U:272:LEU:HD11 | 2.02                     | 0.40              |
| 1:V:215:GLU:N    | 1:V:215:GLU:OE1  | 2.54                     | 0.40              |
| 1:a:264:LYS:HD3  | 1:a:264:LYS:HA   | 1.78                     | 0.40              |
| 1:b:63:THR:O     | 1:b:93:PHE:HA    | 2.21                     | 0.40              |
| 1:b:264:LYS:HA   | 1:b:264:LYS:HD3  | 1.79                     | 0.40              |
| 1:e:8:LYS:HG2    | 1:e:10:ALA:HB2   | 2.03                     | 0.40              |
| 1:e:70:SER:HB3   | 1:e:86:ILE:HA    | 2.02                     | 0.40              |
| 1:A:116:ILE:HD13 | 1:A:116:ILE:HA   | 1.94                     | 0.40              |
| 1:B:263:ASP:N    | 1:B:263:ASP:OD1  | 2.54                     | 0.40              |
| 1:D:32:PRO:HG3   | 1:D:138:ARG:CZ   | 2.52                     | 0.40              |
| 1:E:8:LYS:HG2    | 1:E:10:ALA:HB2   | 2.02                     | 0.40              |
| 1:G:32:PRO:HG3   | 1:G:138:ARG:CZ   | 2.51                     | 0.40              |
| 1:I:113:PHE:CD1  | 1:I:126:LEU:HD22 | 2.55                     | 0.40              |
| 1:T:97:MET:HE3   | 1:T:97:MET:HB2   | 1.81                     | 0.40              |
| 1:V:152:ILE:HG23 | 1:V:204:TRP:HB2  | 2.03                     | 0.40              |
| 1:W:111:GLN:HG3  | 1:W:112:ASP:N    | 2.36                     | 0.40              |
| 1:X:251:TYR:O    | 1:X:255:VAL:HG13 | 2.22                     | 0.40              |
| 1:b:224:PRO:HG2  | 1:b:241:LEU:HD22 | 2.02                     | 0.40              |
| 1:F:36:LEU:HD21  | 1:F:140:ILE:HD13 | 2.02                     | 0.40              |
| 1:G:130:LYS:HE3  | 1:H:187:ARG:NH2  | 2.37                     | 0.40              |
| 1:G:267:VAL:HA   | 1:G:272:LEU:O    | 2.21                     | 0.40              |
| 1:H:141:LEU:O    | 1:H:155:TYR:HA   | 2.21                     | 0.40              |
| 1:M:94:ASP:OD1   | 1:M:94:ASP:N     | 2.54                     | 0.40              |
| 1:N:55:HIS:CD2   | 1:O:10:ALA:HB1   | 2.57                     | 0.40              |
| 1:Q:69:ASP:O     | 1:Q:87:ASN:N     | 2.52                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:130:LYS:HB2  | 1:R:130:LYS:HE2  | 1.79                     | 0.40              |
| 1:V:247:ASN:ND2  | 1:V:249:ILE:HD12 | 2.36                     | 0.40              |
| 1:F:54:GLY:HA3   | 1:F:99:GLN:OE1   | 2.21                     | 0.40              |
| 1:H:63:THR:O     | 1:H:93:PHE:HA    | 2.22                     | 0.40              |
| 1:J:163:LEU:HA   | 1:J:183:LEU:HD23 | 2.04                     | 0.40              |
| 1:J:230:THR:HG22 | 1:J:232:ALA:H    | 1.85                     | 0.40              |
| 1:L:173:ASP:N    | 1:L:173:ASP:OD1  | 2.54                     | 0.40              |
| 1:S:220:LEU:HD22 | 1:S:243:VAL:HG12 | 2.03                     | 0.40              |
| 1:U:105:LEU:HD23 | 1:U:108:ILE:HD11 | 2.03                     | 0.40              |
| 1:U:251:TYR:O    | 1:U:255:VAL:HG13 | 2.22                     | 0.40              |
| 1:W:24:LEU:HD22  | 1:W:46:ILE:HG21  | 2.03                     | 0.40              |
| 1:a:286:THR:HG22 | 1:a:291:THR:HG22 | 2.04                     | 0.40              |
| 1:b:97:MET:HE2   | 1:b:104:VAL:HG13 | 2.04                     | 0.40              |
| 1:b:230:THR:O    | 1:b:237:HIS:ND1  | 2.54                     | 0.40              |
| 1:A:32:PRO:HG3   | 1:A:138:ARG:CZ   | 2.52                     | 0.40              |
| 1:B:88:LYS:HE3   | 1:B:90:THR:OG1   | 2.22                     | 0.40              |
| 1:G:10:ALA:HB1   | 1:L:55:HIS:CD2   | 2.57                     | 0.40              |
| 1:I:13:ASP:O     | 1:I:147:ARG:NH1  | 2.37                     | 0.40              |
| 1:L:32:PRO:HG3   | 1:L:138:ARG:CZ   | 2.52                     | 0.40              |
| 1:Q:190:VAL:HG13 | 1:Q:191:VAL:HG23 | 2.04                     | 0.40              |
| 1:R:38:SER:HB2   | 1:R:45:ALA:HB2   | 2.04                     | 0.40              |
| 1:S:230:THR:HG22 | 1:S:232:ALA:H    | 1.85                     | 0.40              |
| 1:S:284:THR:HG23 | 1:S:293:THR:HG22 | 2.03                     | 0.40              |
| 1:T:278:ALA:HA   | 1:T:298:VAL:HB   | 2.03                     | 0.40              |
| 1:U:13:ASP:OD1   | 1:U:13:ASP:N     | 2.53                     | 0.40              |
| 1:U:166:LEU:HD12 | 1:U:166:LEU:HA   | 1.97                     | 0.40              |
| 1:V:239:ALA:O    | 1:V:272:LEU:HD12 | 2.22                     | 0.40              |
| 1:X:95:PHE:CE2   | 1:X:97:MET:HE2   | 2.57                     | 0.40              |
| 1:a:187:ARG:NH2  | 1:f:130:LYS:HD2  | 2.37                     | 0.40              |
| 1:a:229:VAL:HG23 | 1:a:298:VAL:HG22 | 2.04                     | 0.40              |
| 1:b:24:LEU:HD22  | 1:b:46:ILE:HG21  | 2.04                     | 0.40              |
| 1:b:103:ASN:HA   | 1:b:106:GLU:CD   | 2.47                     | 0.40              |
| 1:b:163:LEU:HA   | 1:b:183:LEU:HD23 | 2.03                     | 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     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | B     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | C     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | D     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | E     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | F     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | G     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | H     | 297/300 (99%) | 292 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | I     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | J     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | K     | 297/300 (99%) | 291 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | L     | 297/300 (99%) | 292 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | M     | 297/300 (99%) | 292 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | N     | 297/300 (99%) | 292 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | O     | 297/300 (99%) | 291 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | P     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | Q     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | R     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | S     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | T     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | U     | 297/300 (99%) | 292 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | V     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | W     | 297/300 (99%) | 294 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | X     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 1   | a     | 297/300 (99%) | 293 (99%) | 4 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | b     | 297/300 (99%)   | 293 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | c     | 297/300 (99%)   | 293 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | d     | 297/300 (99%)   | 293 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | e     | 297/300 (99%)   | 293 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | f     | 297/300 (99%)   | 293 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| All | All   | 8910/9000 (99%) | 8789 (99%) | 121 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | B     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | C     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | D     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | E     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | F     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | G     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | H     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | I     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | J     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | K     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | L     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | M     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | N     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | O     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |
| 1   | P     | 242/243 (100%) | 242 (100%) | 0        | 100         | 100 |

*Continued on next page...*

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | Q     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | R     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | S     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | T     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | U     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | V     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | W     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | X     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | a     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | b     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | c     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | d     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | e     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| 1   | f     | 242/243 (100%)   | 242 (100%)  | 0        | 100         | 100 |
| All | All   | 7260/7290 (100%) | 7260 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 101 | GLN  |
| 1   | C     | 99  | GLN  |
| 1   | C     | 237 | HIS  |
| 1   | G     | 172 | ASN  |
| 1   | G     | 240 | GLN  |
| 1   | H     | 172 | ASN  |
| 1   | H     | 240 | GLN  |
| 1   | I     | 172 | ASN  |
| 1   | I     | 240 | GLN  |
| 1   | J     | 66  | ASN  |
| 1   | J     | 240 | GLN  |
| 1   | K     | 99  | GLN  |
| 1   | K     | 134 | ASN  |
| 1   | K     | 172 | ASN  |
| 1   | K     | 240 | GLN  |
| 1   | L     | 101 | GLN  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 134 | ASN  |
| 1   | L     | 172 | ASN  |
| 1   | L     | 240 | GLN  |
| 1   | M     | 87  | ASN  |
| 1   | M     | 148 | ASN  |
| 1   | M     | 172 | ASN  |
| 1   | N     | 148 | ASN  |
| 1   | N     | 168 | ASN  |
| 1   | N     | 172 | ASN  |
| 1   | O     | 87  | ASN  |
| 1   | O     | 99  | GLN  |
| 1   | O     | 101 | GLN  |
| 1   | P     | 87  | ASN  |
| 1   | P     | 148 | ASN  |
| 1   | P     | 172 | ASN  |
| 1   | Q     | 148 | ASN  |
| 1   | Q     | 168 | ASN  |
| 1   | Q     | 172 | ASN  |
| 1   | R     | 101 | GLN  |
| 1   | R     | 172 | ASN  |
| 1   | S     | 111 | GLN  |
| 1   | U     | 172 | ASN  |
| 1   | V     | 111 | GLN  |
| 1   | V     | 117 | GLN  |
| 1   | a     | 99  | GLN  |
| 1   | a     | 172 | ASN  |
| 1   | b     | 169 | GLN  |
| 1   | b     | 172 | ASN  |
| 1   | c     | 99  | GLN  |
| 1   | c     | 169 | GLN  |
| 1   | c     | 172 | ASN  |
| 1   | d     | 172 | ASN  |
| 1   | e     | 101 | GLN  |
| 1   | e     | 172 | ASN  |
| 1   | f     | 99  | GLN  |
| 1   | f     | 172 | ASN  |

### 5.3.3 RNA ⓘ

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.

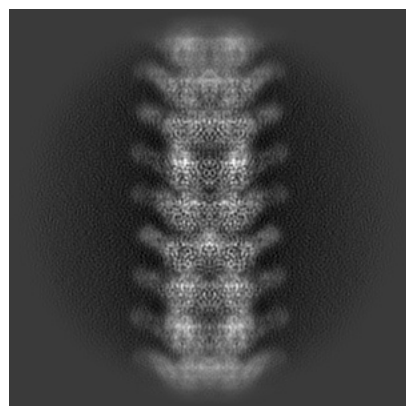
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39995. These allow visual inspection of the internal detail of the map and identification of artifacts.

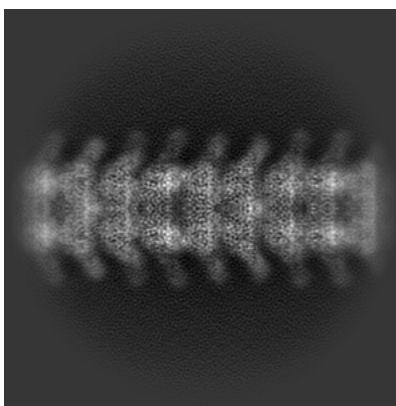
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

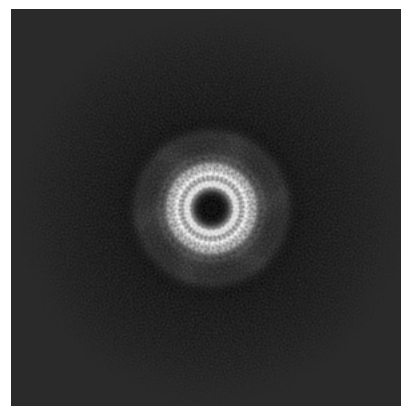
#### 6.1.1 Primary map



X

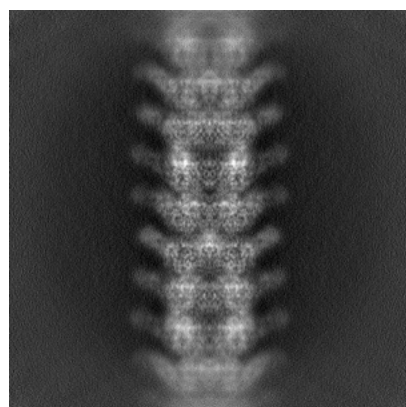


Y

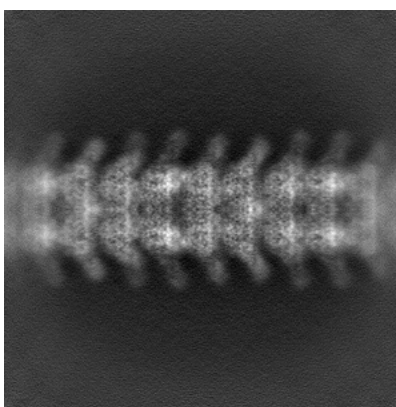


Z

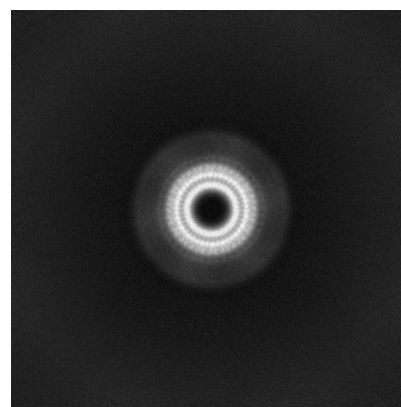
#### 6.1.2 Raw map



X



Y

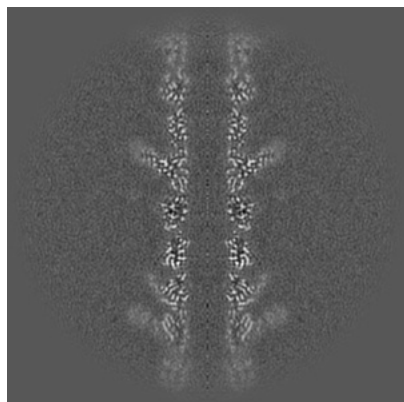


Z

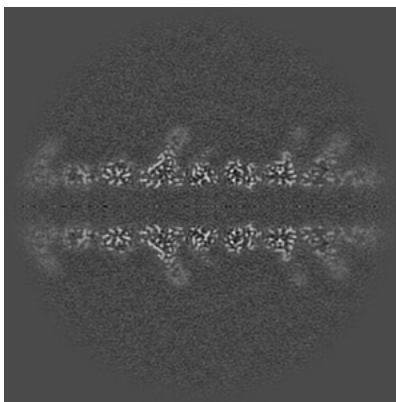
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

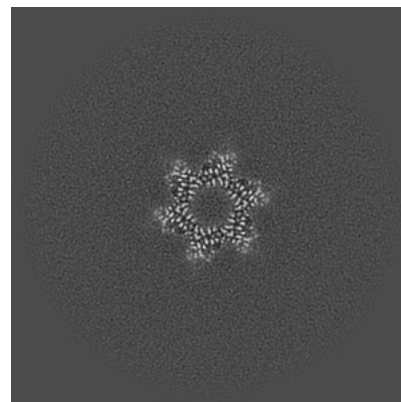
### 6.2.1 Primary map



X Index: 192

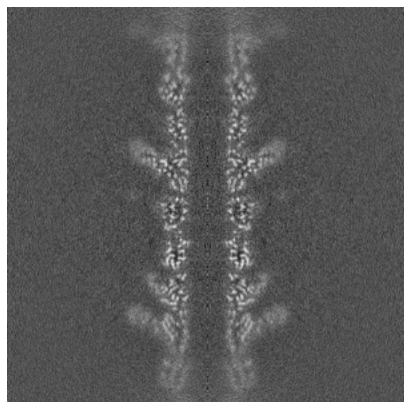


Y Index: 192

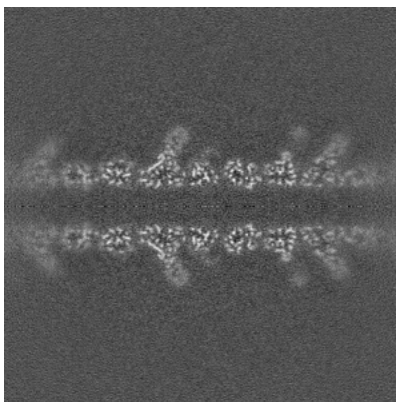


Z Index: 192

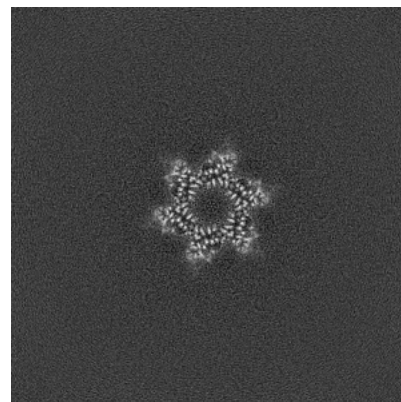
### 6.2.2 Raw map



X Index: 192



Y Index: 192



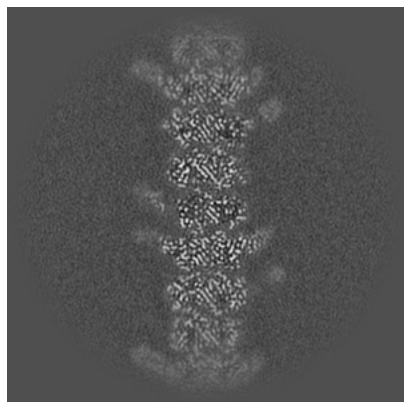
Z Index: 192

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

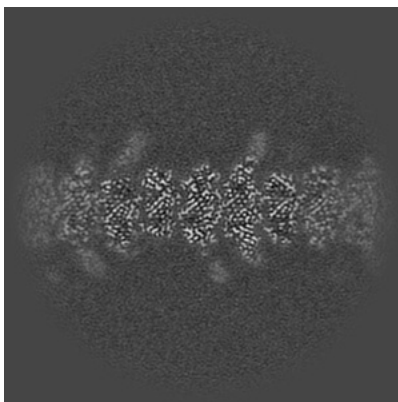


## 6.3 Largest variance slices [i](#)

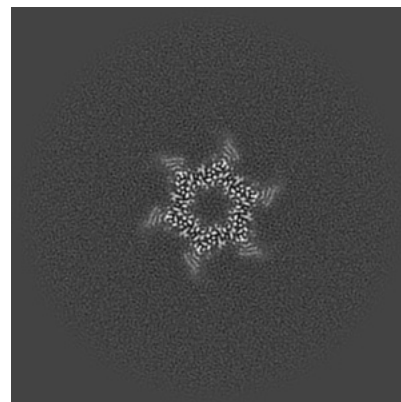
### 6.3.1 Primary map



X Index: 169

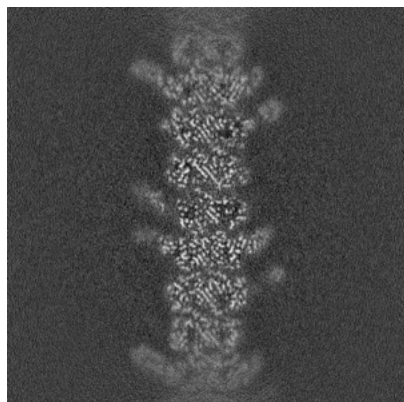


Y Index: 168

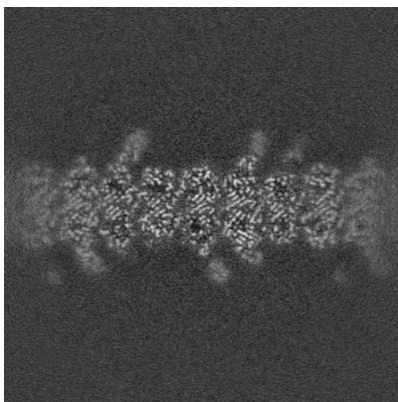


Z Index: 196

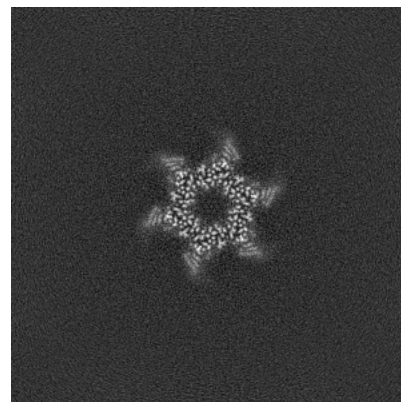
### 6.3.2 Raw map



X Index: 169



Y Index: 170

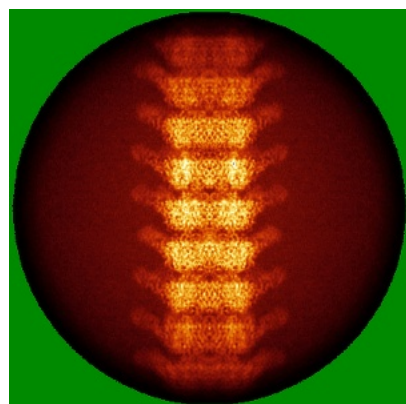


Z Index: 196

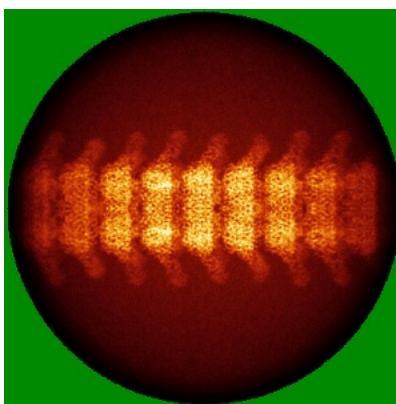
The images above show the largest variance slices of the map in three orthogonal directions.

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

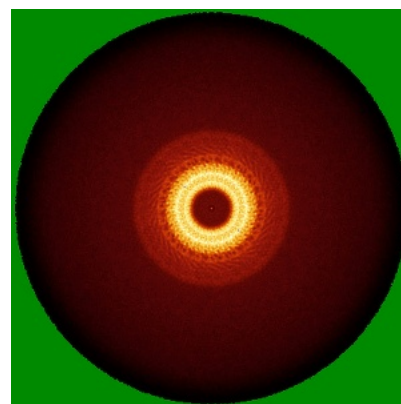
### 6.4.1 Primary map



X

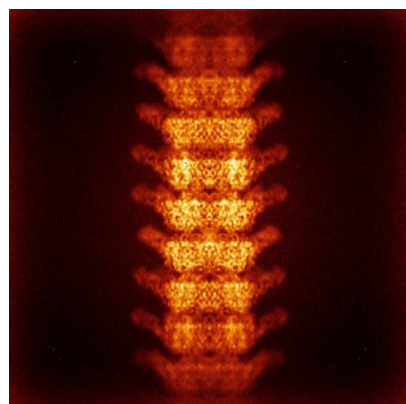


Y

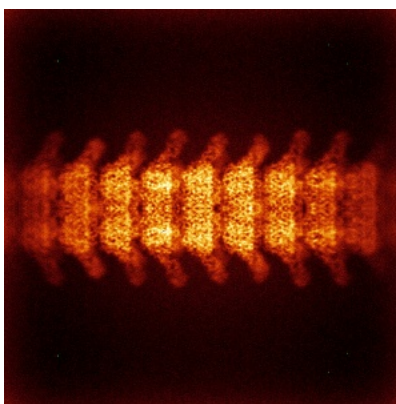


Z

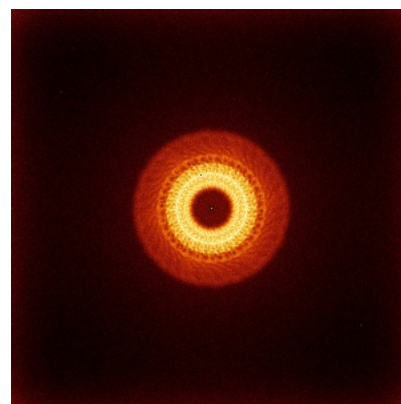
### 6.4.2 Raw map



X



Y



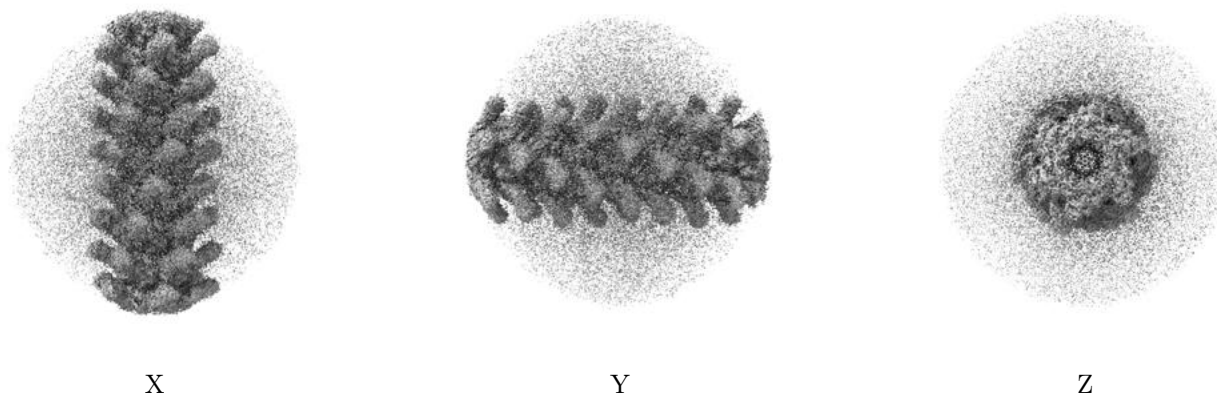
Z

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.



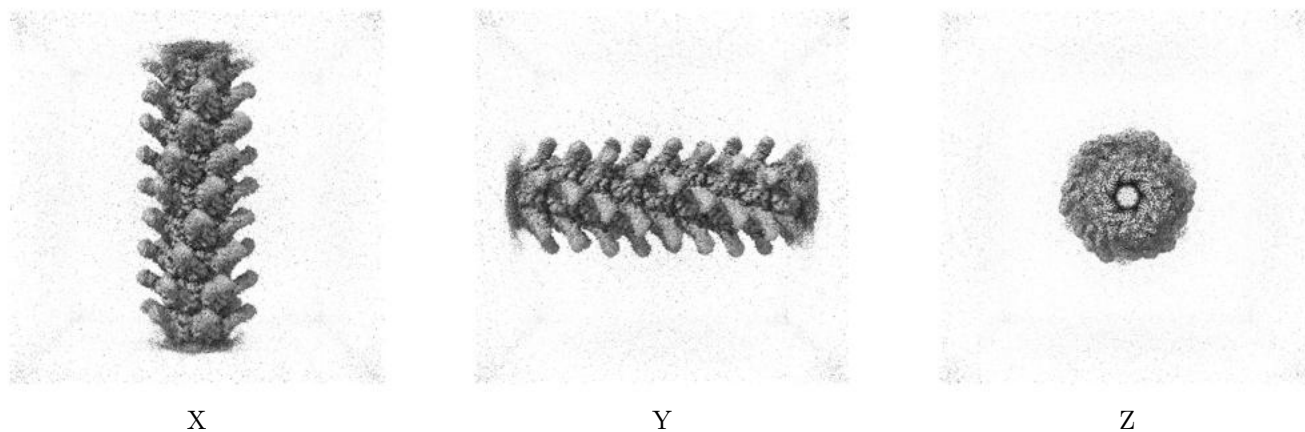
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

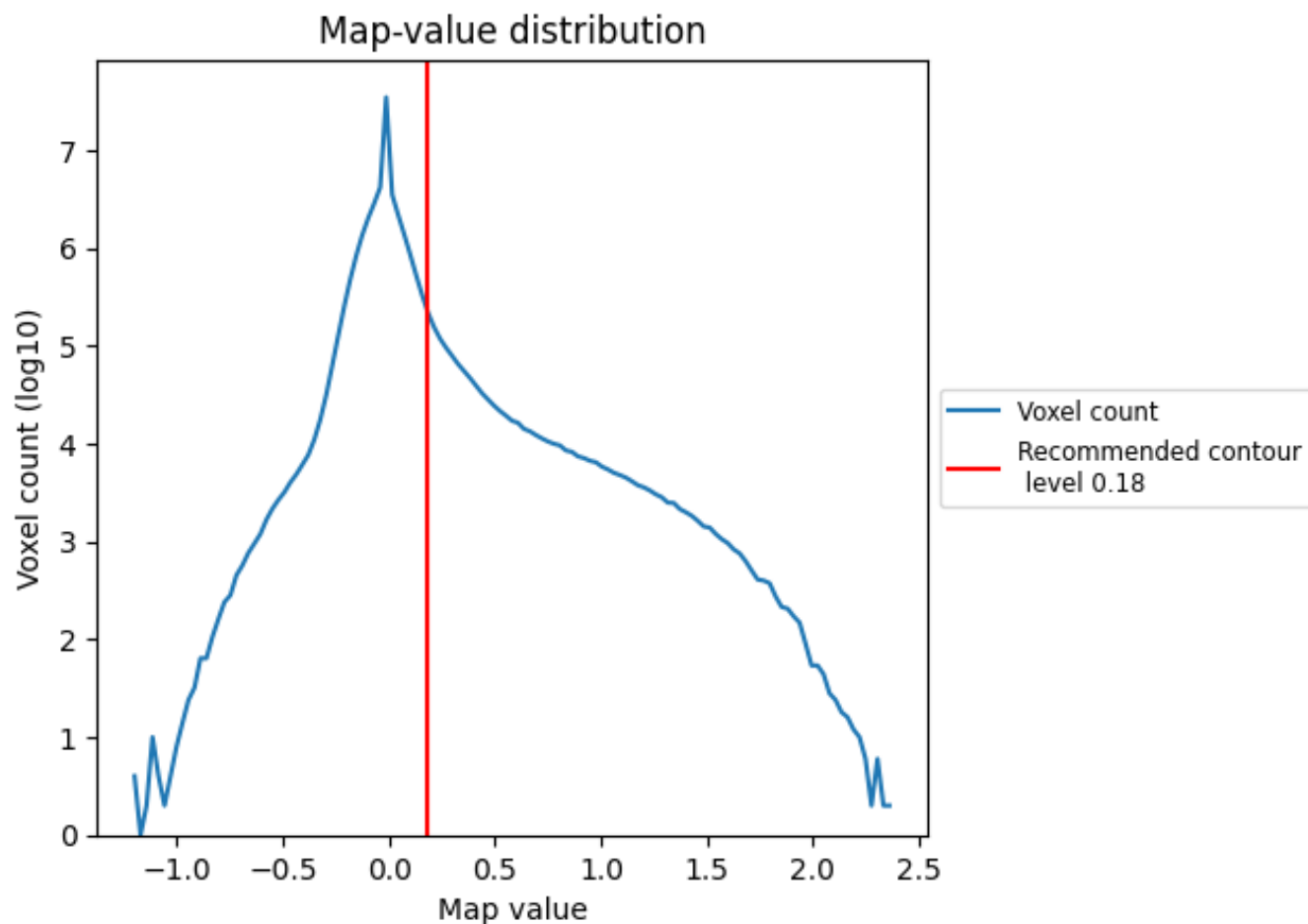
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

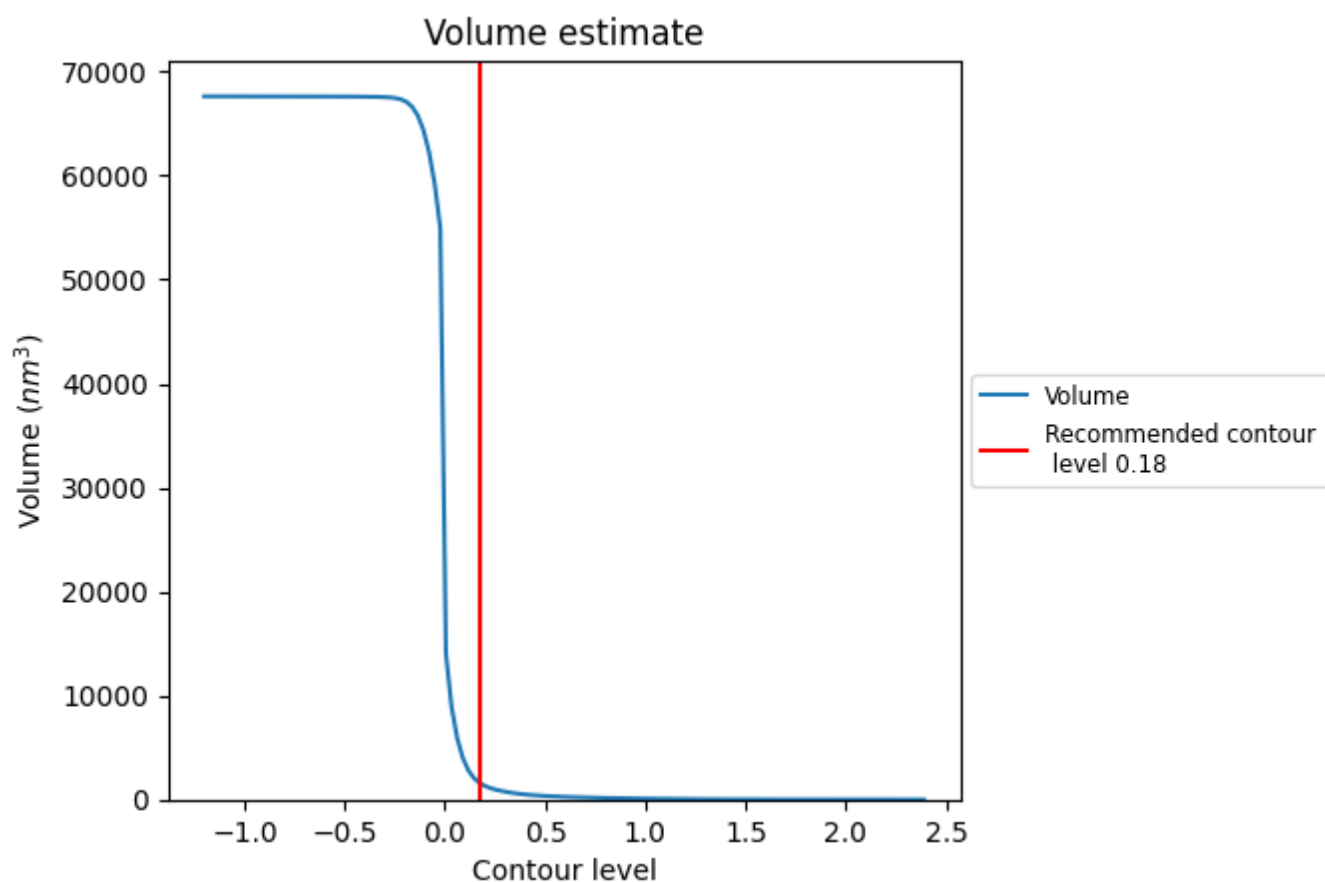
This section contains the results of statistical analysis of the map.

### 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.

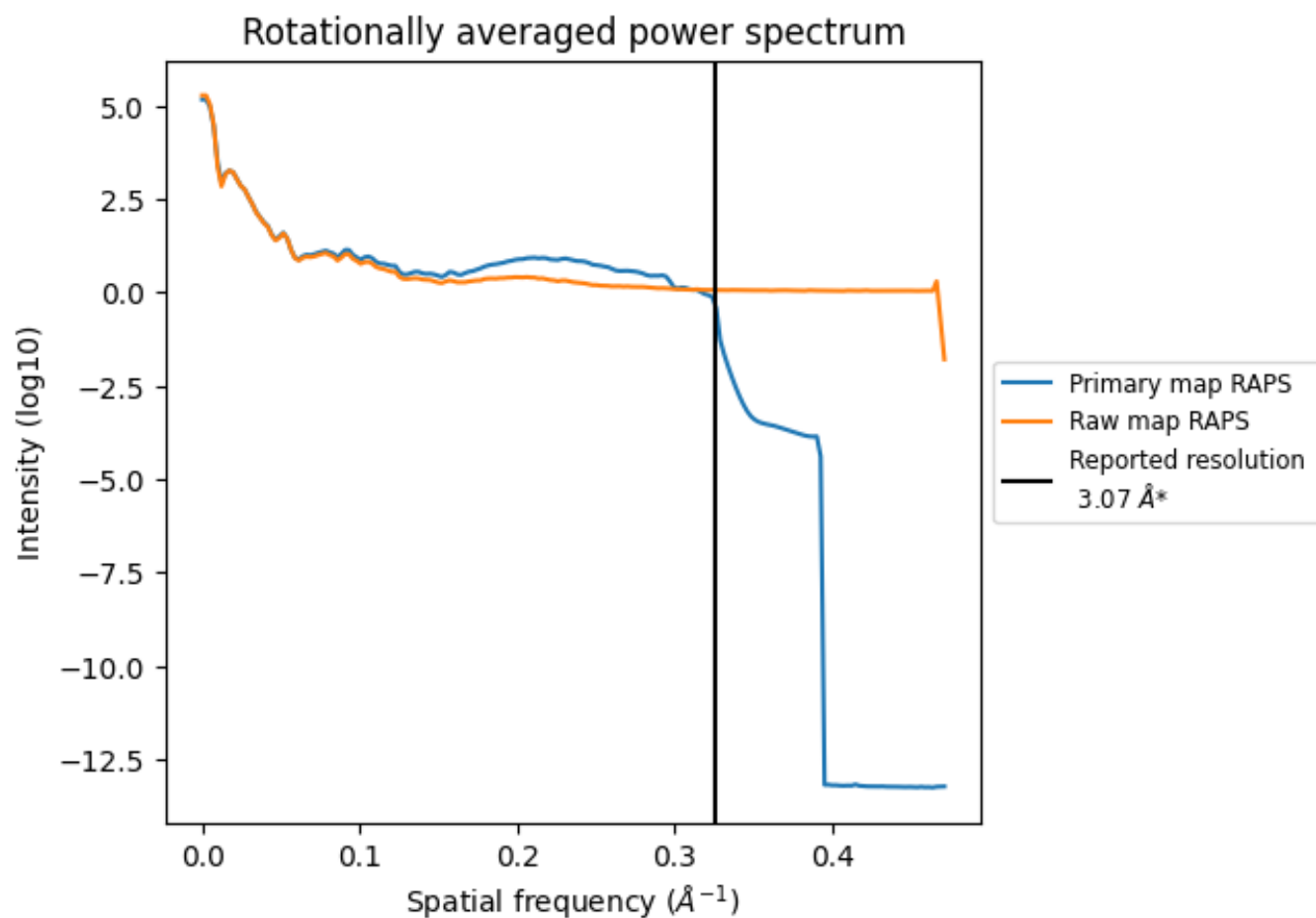
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1527 nm<sup>3</sup>; this corresponds to an approximate mass of 1380 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 ⓘ

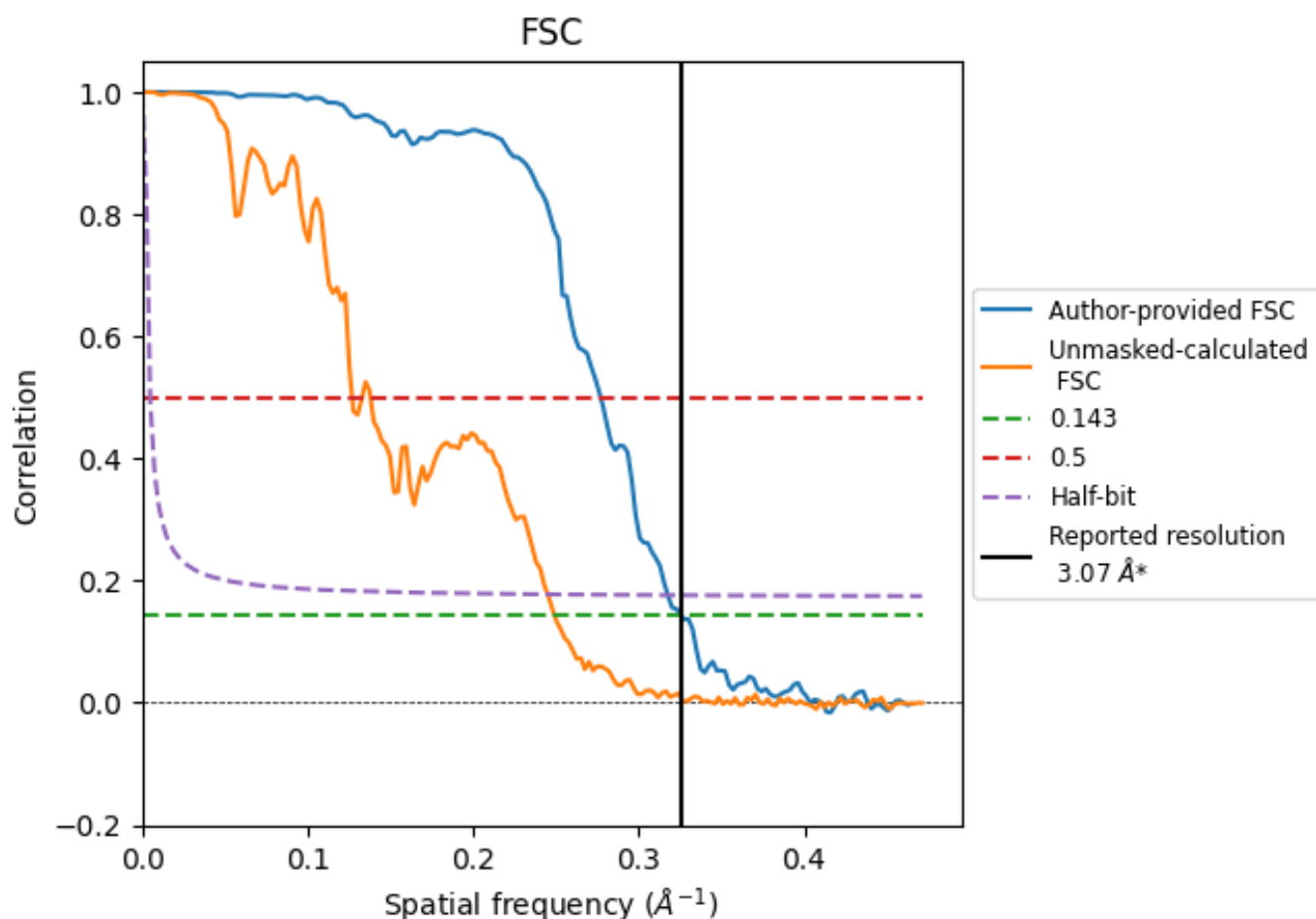


\*Reported resolution corresponds to spatial frequency of 0.326 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

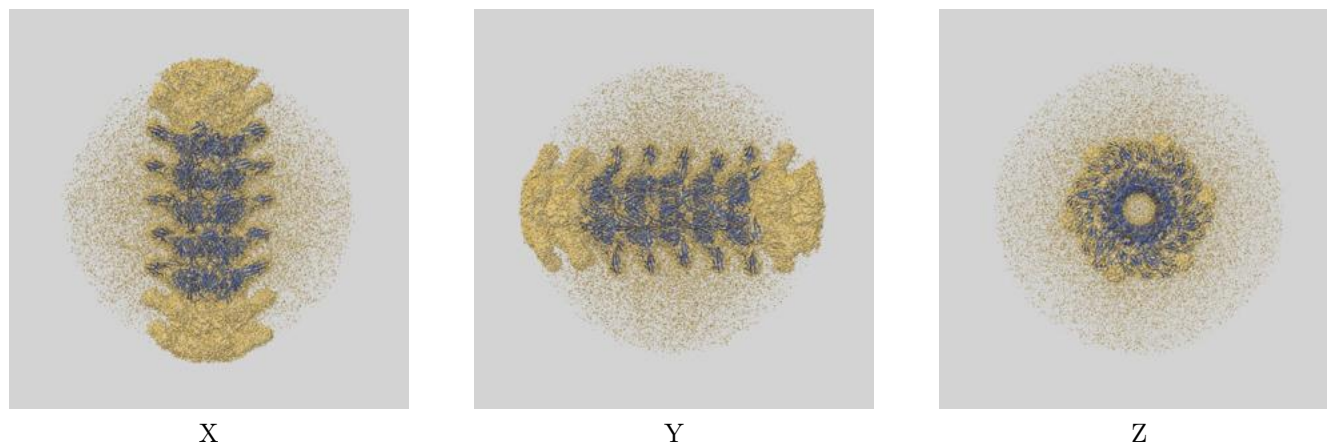
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.07                               | -    | -        |
| Author-provided FSC curve | 3.07                               | 3.61 | 3.15     |
| Unmasked-calculated*      | 4.01                               | 7.88 | 4.08     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.07 by more than 10 %

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

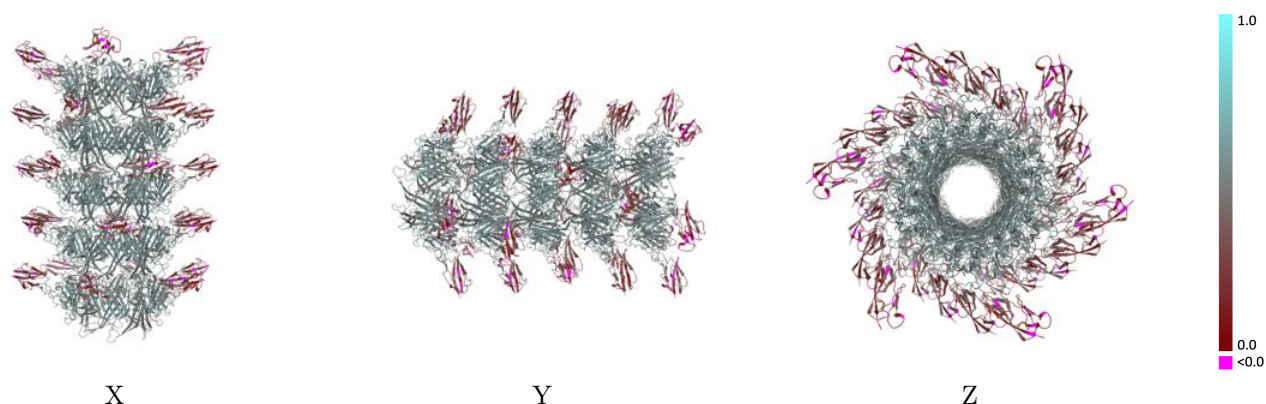
This section contains information regarding the fit between EMDB map EMD-39995 and PDB model 8ZDN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



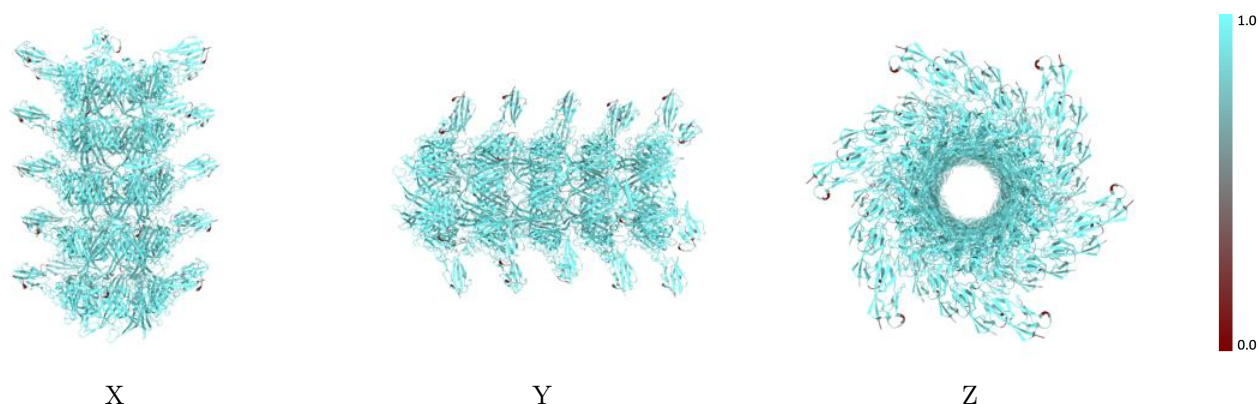
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

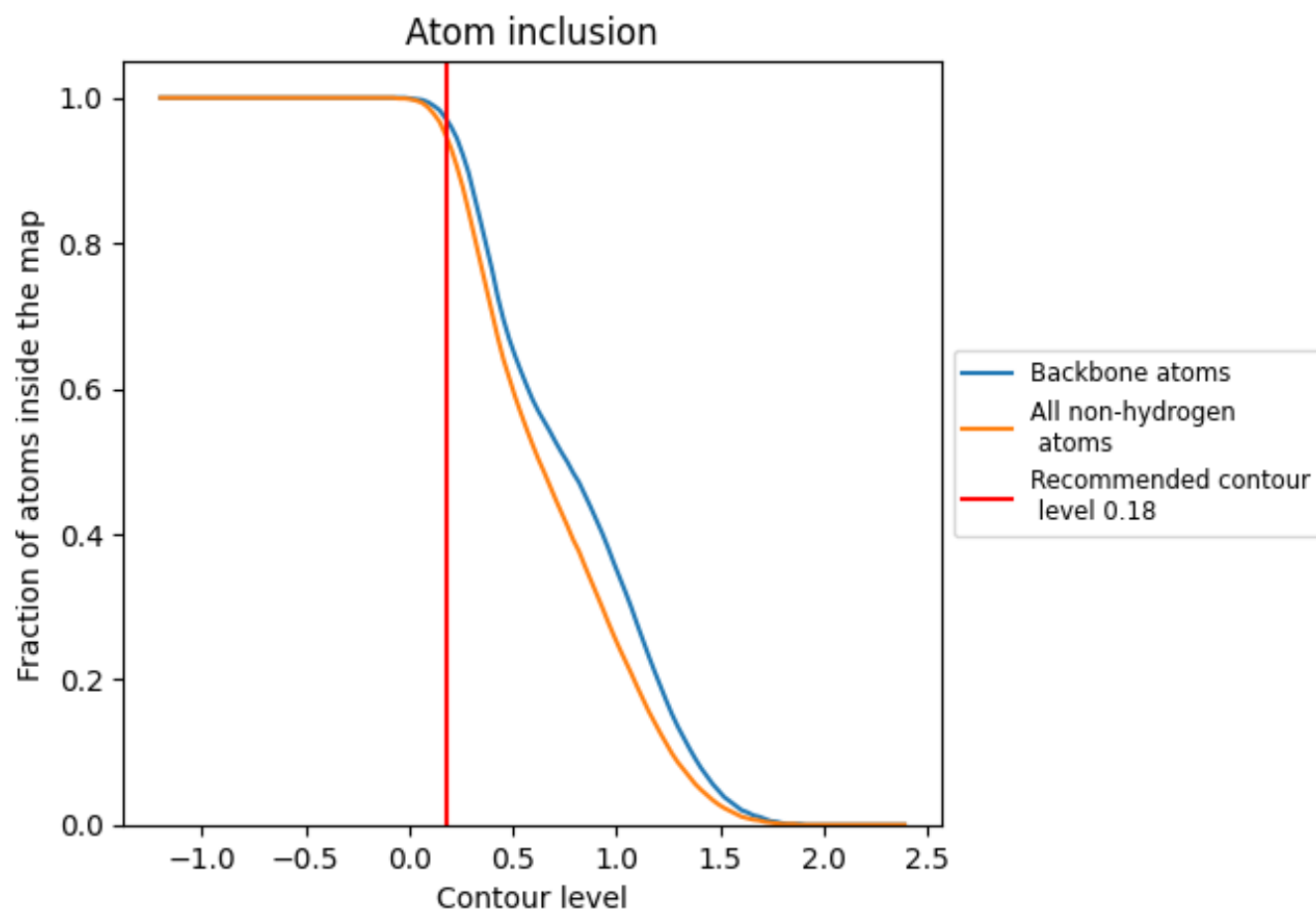
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.18) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9460   |  0.4840   |
| A     |  0.9400   |  0.4700   |
| B     |  0.9430   |  0.4710   |
| C     |  0.9410   |  0.4720   |
| D     |  0.9410   |  0.4720   |
| E     |  0.9390   |  0.4710   |
| F     |  0.9430   |  0.4710   |
| G     |  0.9480   |  0.4930   |
| H     |  0.9480   |  0.4900   |
| I     |  0.9470   |  0.4920   |
| J     |  0.9480   |  0.4920   |
| K     |  0.9490   |  0.4930   |
| L     |  0.9500   |  0.4900   |
| M     |  0.9560   |  0.4930   |
| N     |  0.9540  |  0.4910  |
| O     |  0.9560 |  0.4920 |
| P     |  0.9540 |  0.4940 |
| Q     |  0.9530 |  0.4940 |
| R     |  0.9560 |  0.4920 |
| S     |  0.9460 |  0.4890 |
| T     |  0.9460 |  0.4900 |
| U     |  0.9460 |  0.4910 |
| V     |  0.9430 |  0.4870 |
| W     |  0.9420 |  0.4900 |
| X     |  0.9440 |  0.4910 |
| a     |  0.9360 |  0.4730 |
| b     |  0.9410 |  0.4740 |
| c     |  0.9420 |  0.4750 |
| d     |  0.9370 |  0.4730 |
| e     |  0.9430 |  0.4730 |
| f     |  0.9390 |  0.4740 |

