



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:50 PM UTC

PDB ID : 7Z46 / pdb\_00007z46  
EMDB ID : EMD-14485  
Title : Top part (C5) of bacteriophage SU10 capsid  
Authors : Siborova, M.; Fuzik, T.; Prochazkova, M.; Novacek, J.; Plevka, P.  
Deposited on : 2022-03-03  
Resolution : 3.40 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:

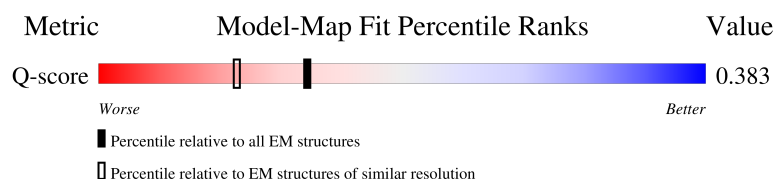
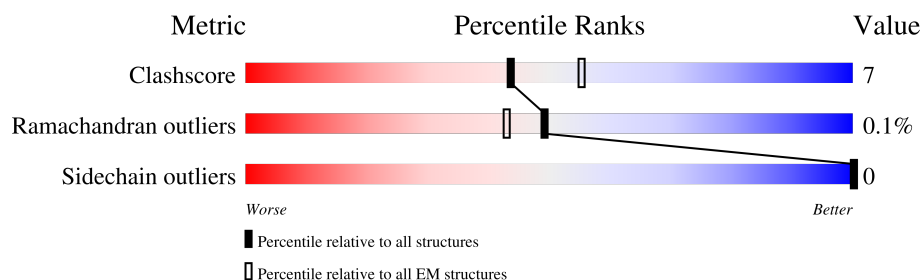
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.40 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                       | 14717 ( 2.90 - 3.90 )                                    |

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     | 352    |                  |
| 1   | B     | 352    |                  |
| 1   | C     | 352    |                  |
| 1   | D     | 352    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 352    |                  |
| 1   | F     | 352    |                  |
| 1   | G     | 352    |                  |
| 1   | H     | 352    |                  |
| 1   | I     | 352    |                  |
| 1   | J     | 352    |                  |
| 1   | K     | 352    |                  |
| 1   | L     | 352    |                  |
| 1   | M     | 352    |                  |
| 1   | N     | 352    |                  |
| 1   | O     | 352    |                  |
| 1   | P     | 352    |                  |
| 1   | Q     | 352    |                  |
| 1   | R     | 352    |                  |
| 1   | S     | 352    |                  |
| 1   | T     | 352    |                  |
| 1   | U     | 352    |                  |
| 1   | V     | 352    |                  |
| 1   | W     | 352    |                  |
| 1   | X     | 352    |                  |
| 1   | Y     | 352    |                  |
| 1   | Z     | 352    |                  |
| 1   | a     | 352    |                  |
| 1   | b     | 352    |                  |
| 1   | c     | 352    |                  |

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| Mol | Chain | Length | Quality of chain                                                            |
|-----|-------|--------|-----------------------------------------------------------------------------|
| 1   | d     | 352    | <div><div></div><div>10%</div><div>77%</div><div>22%</div><div></div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 80206 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 Major head protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 345      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2672  | 1676 | 467 | 519 | 10 |         |       |
| 1   | B     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2677  | 1680 | 468 | 519 | 10 |         |       |
| 1   | C     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | D     | 345      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2670  | 1675 | 467 | 518 | 10 |         |       |
| 1   | E     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2677  | 1680 | 468 | 519 | 10 |         |       |
| 1   | F     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |
| 1   | G     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | H     | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2657  | 1668 | 465 | 514 | 10 |         |       |
| 1   | I     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |
| 1   | J     | 342      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2644  | 1656 | 464 | 514 | 10 |         |       |
| 1   | K     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | L     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | M     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |
| 1   | N     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | O     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | P     | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2654  | 1665 | 464 | 515 | 10 |         |       |
| 1   | Q     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |

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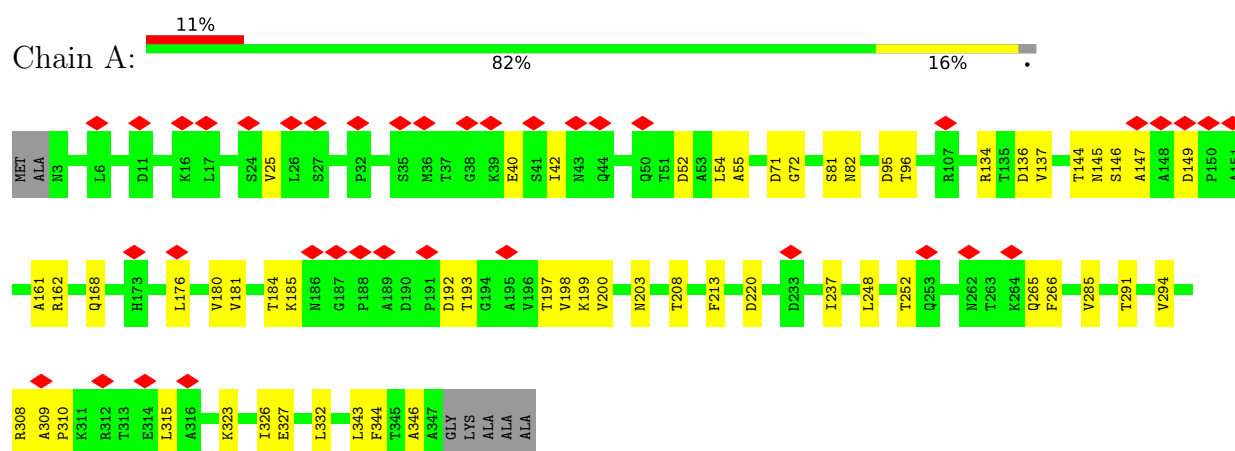
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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | R     | 342      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2644  | 1656 | 464 | 514 | 10 |         |       |
| 1   | S     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2637  | 1651 | 463 | 513 | 10 |         |       |
| 1   | T     | 345      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2668  | 1674 | 466 | 518 | 10 |         |       |
| 1   | U     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |
| 1   | V     | 345      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2670  | 1675 | 467 | 518 | 10 |         |       |
| 1   | W     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | X     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2677  | 1680 | 468 | 519 | 10 |         |       |
| 1   | Y     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |
| 1   | Z     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | a     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2677  | 1680 | 468 | 519 | 10 |         |       |
| 1   | b     | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1678 | 468 | 520 | 10 |         |       |
| 1   | c     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |
| 1   | d     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1684 | 470 | 521 | 10 |         |       |

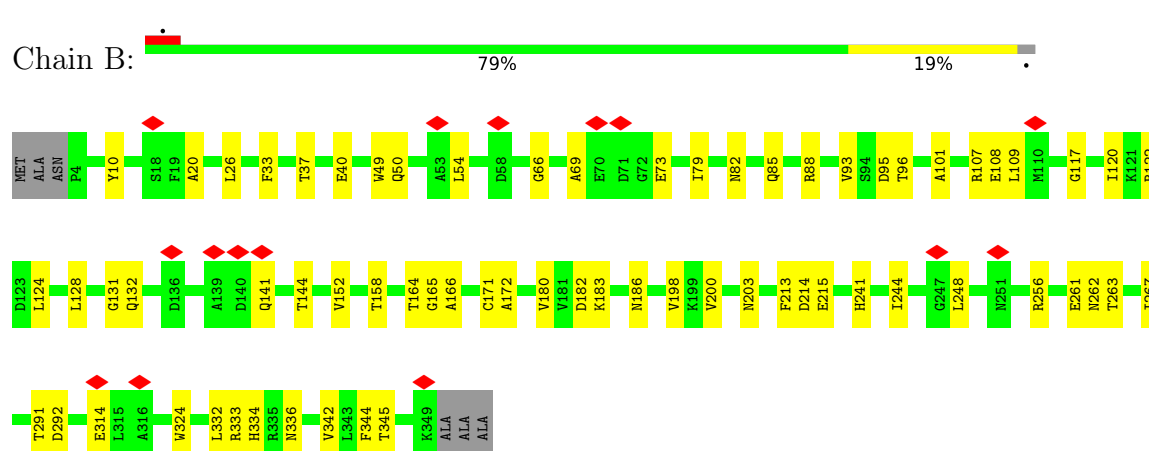
### 3 Residue-property plots [i](#)

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

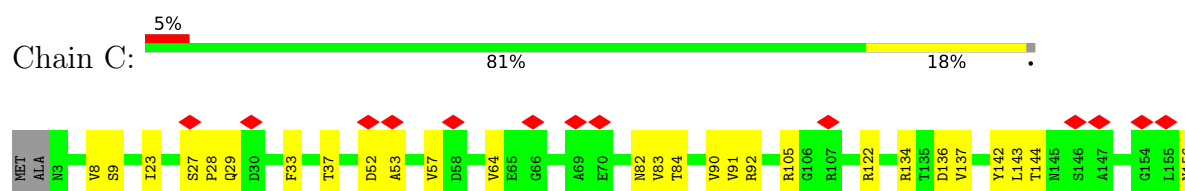
- Molecule 1: Major head protein



- Molecule 1: Major head protein

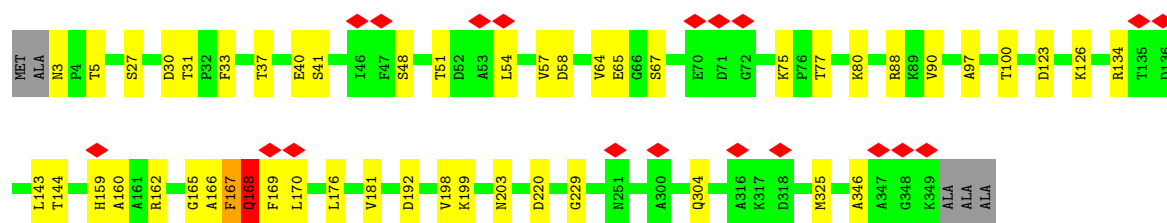


- Molecule 1: Major head protein



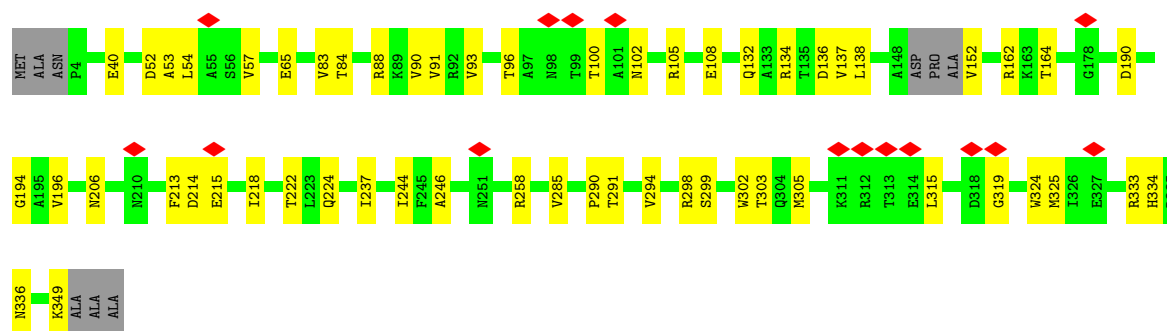


Chain G: 



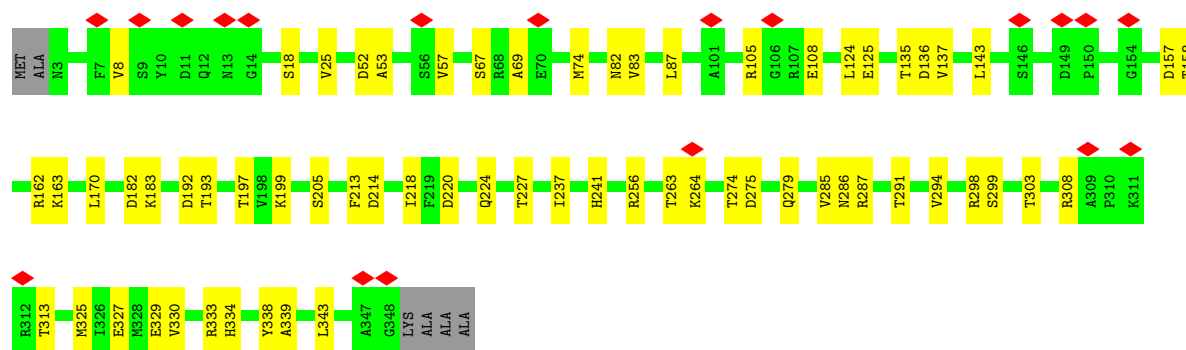
• Molecule 1: Major head protein

Chain H: 



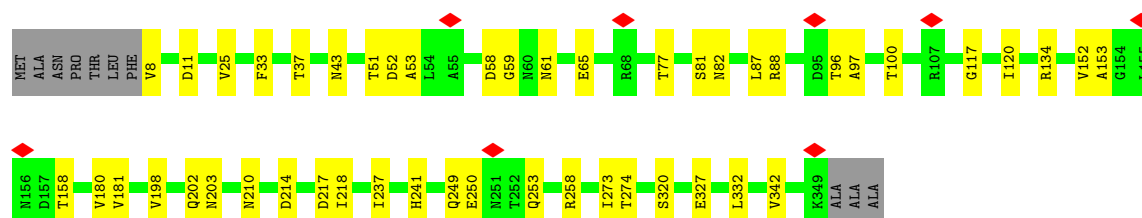
• Molecule 1: Major head protein

Chain I: 

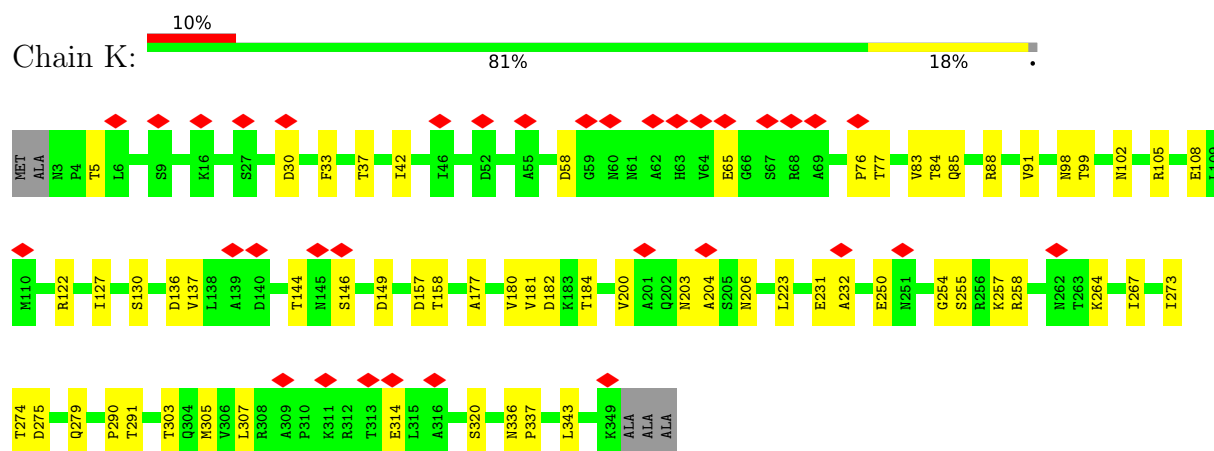


• Molecule 1: Major head protein

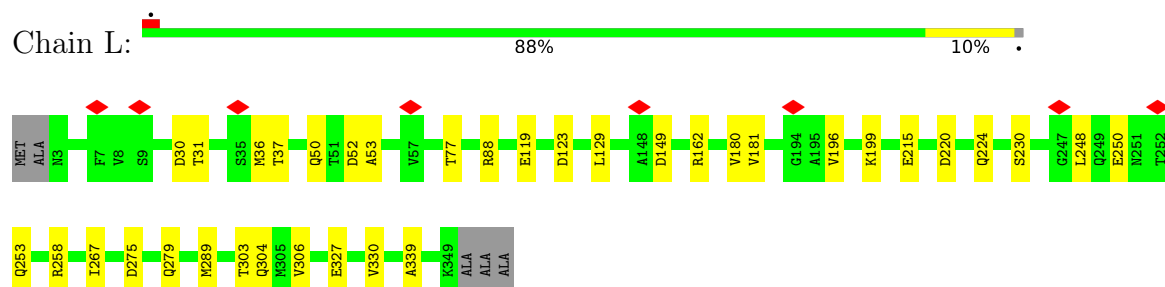
Chain J: 



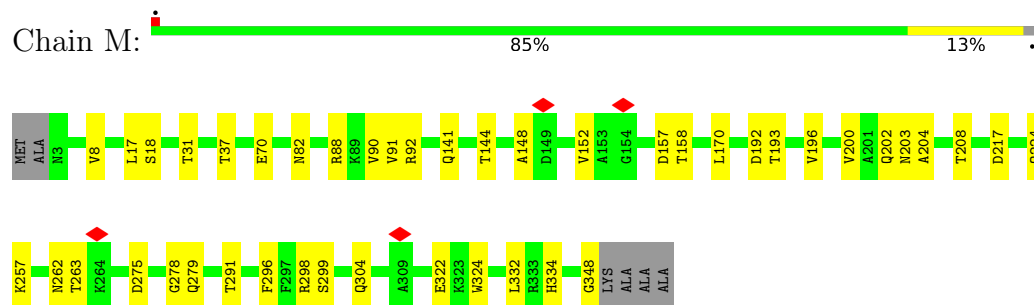
- Molecule 1: Major head protein



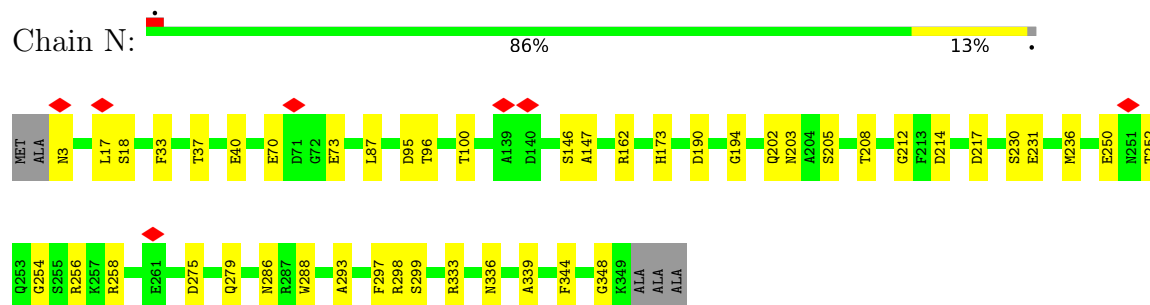
- Molecule 1: Major head protein



- Molecule 1: Major head protein

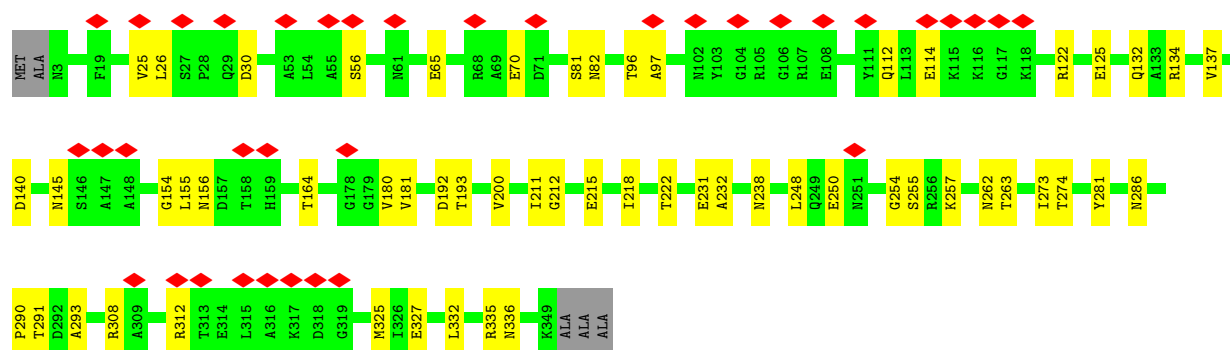


- Molecule 1: Major head protein



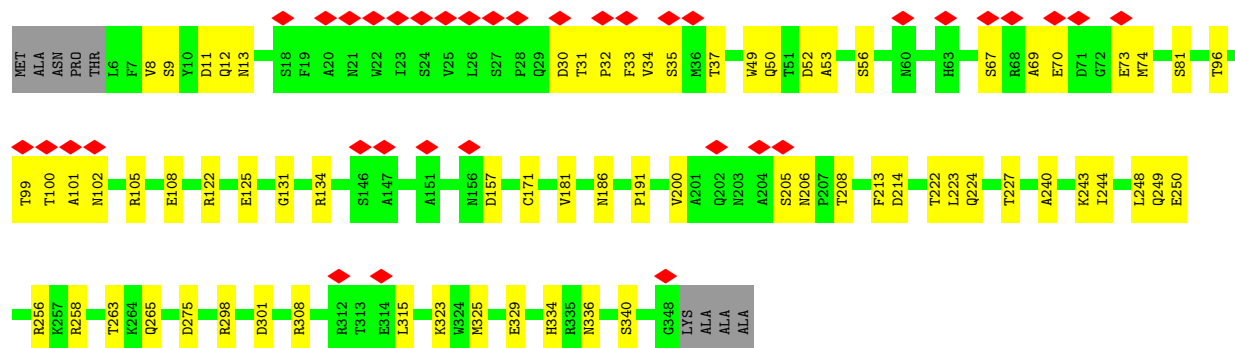
- Molecule 1: Major head protein

Chain O: 



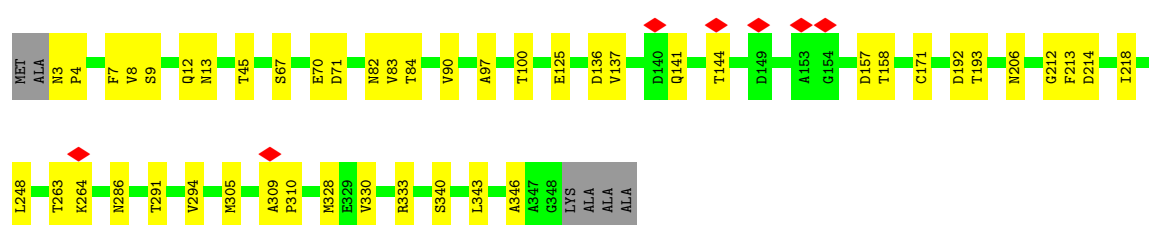
• Molecule 1: Major head protein

Chain P: 



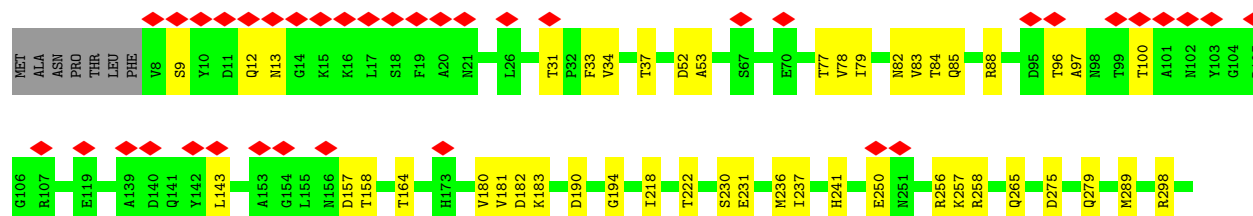
• Molecule 1: Major head protein

Chain Q: 



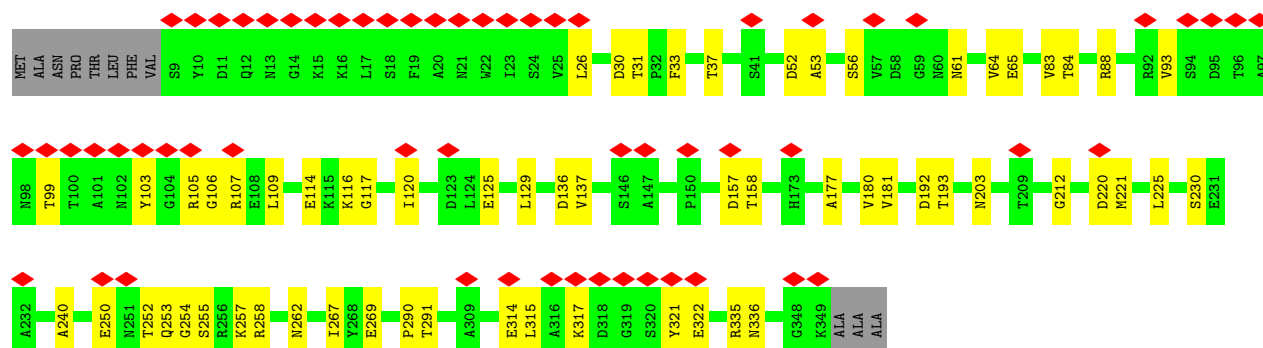
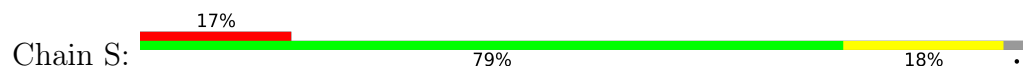
• Molecule 1: Major head protein

Chain R: 

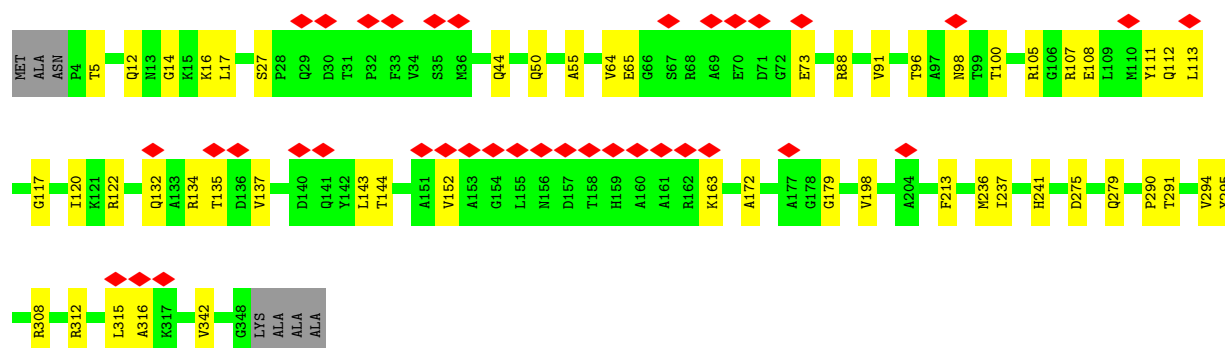
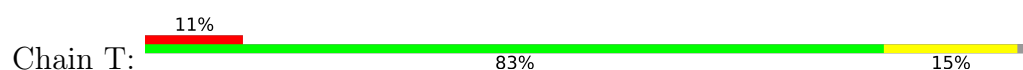




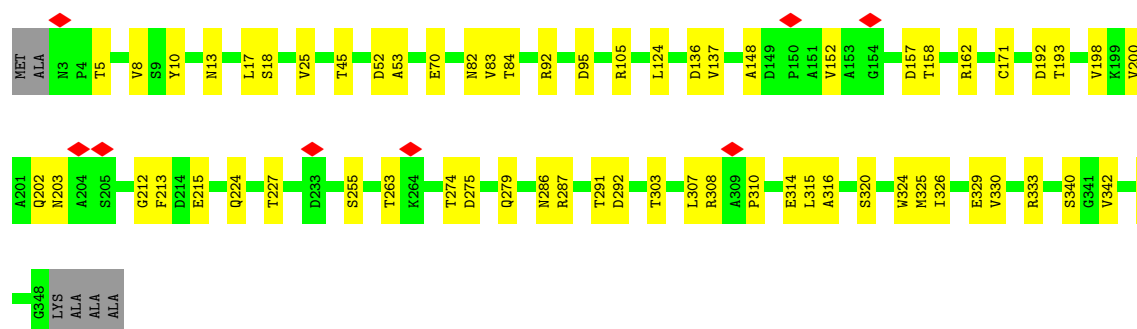
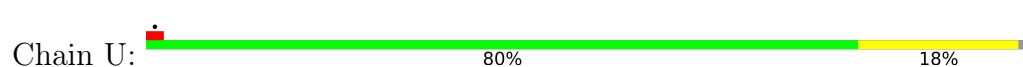
- Molecule 1: Major head protein



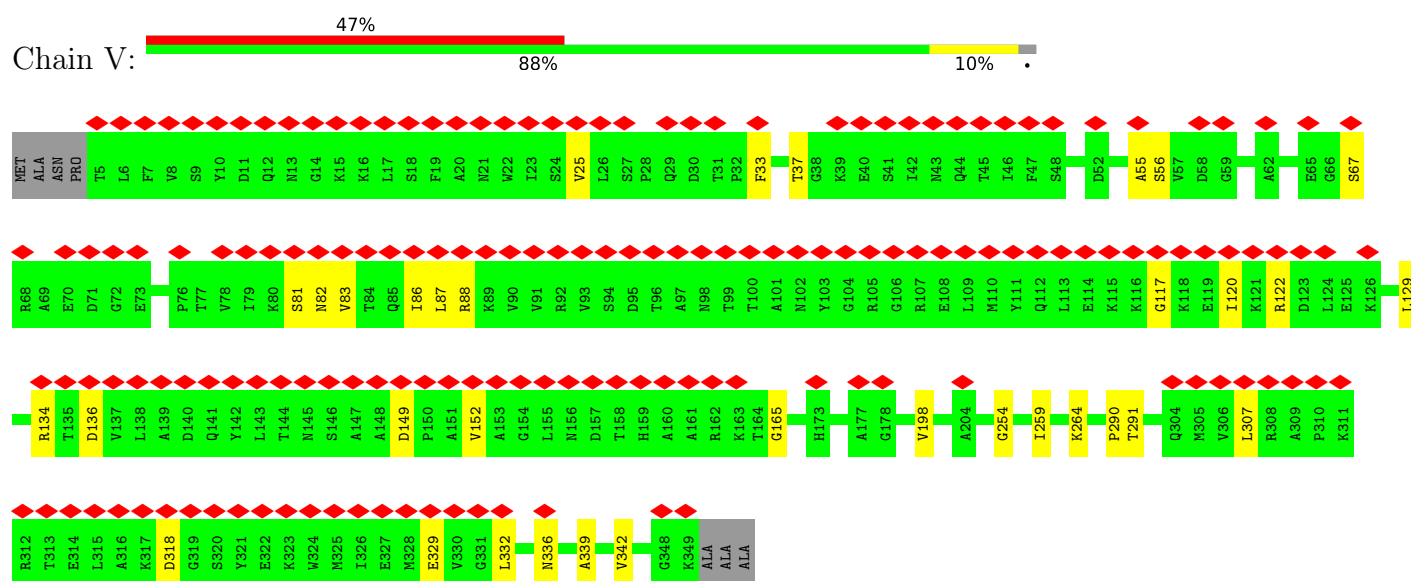
- Molecule 1: Major head protein



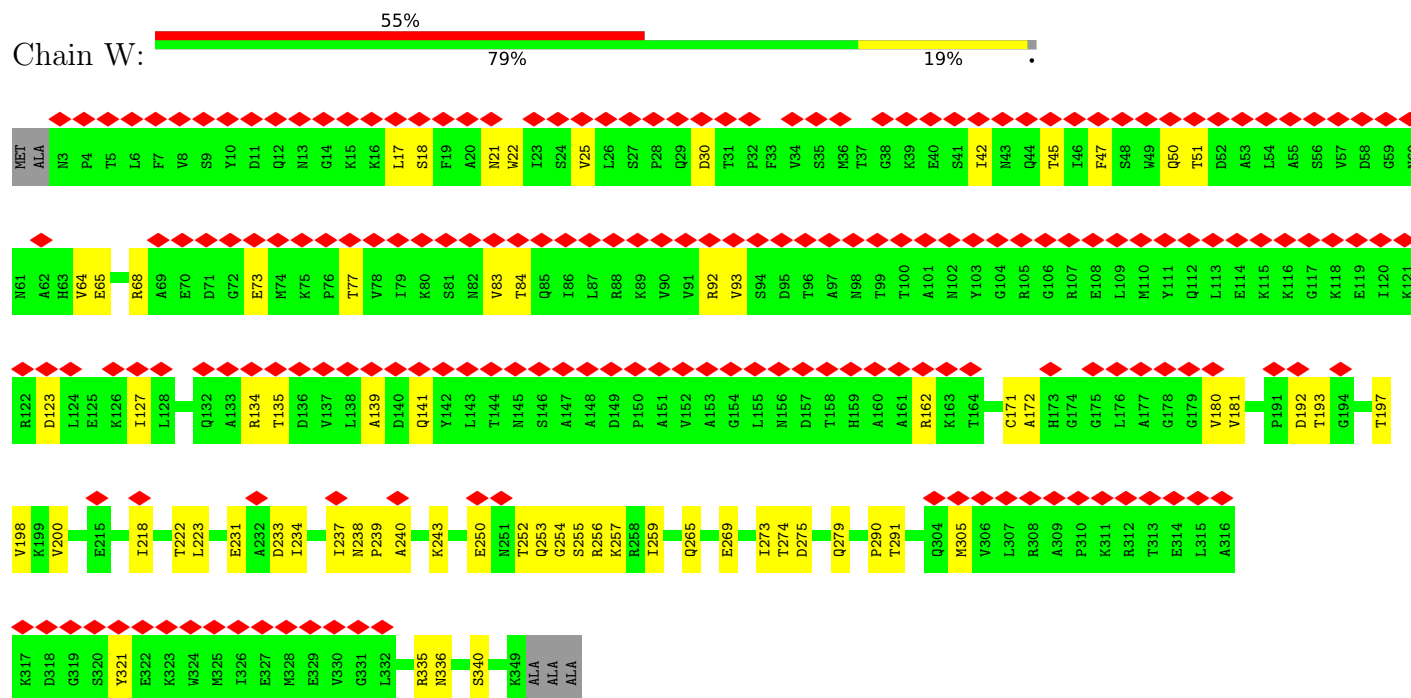
- Molecule 1: Major head protein



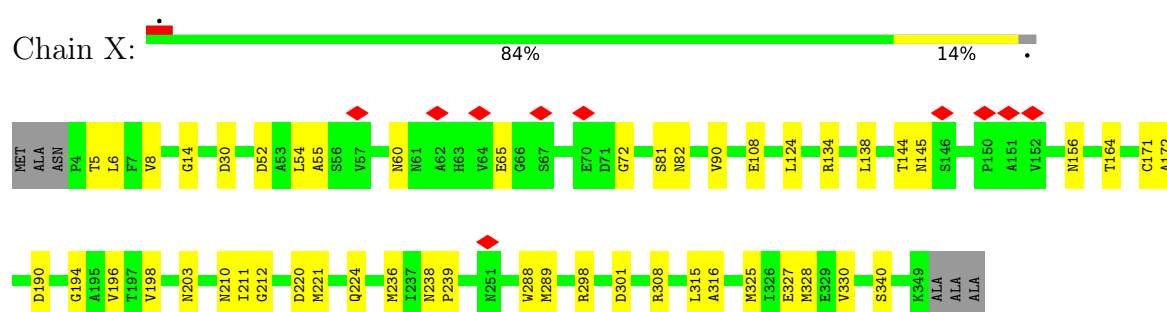
- Molecule 1: Major head protein



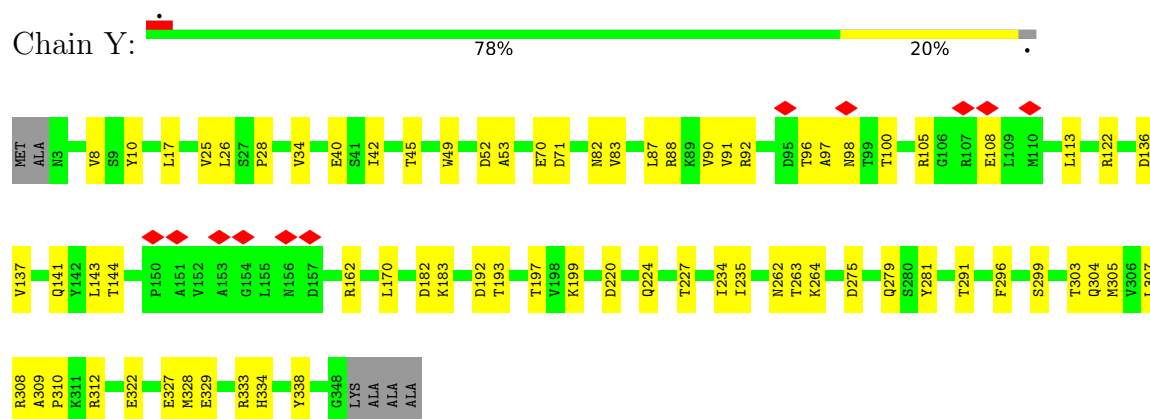
• Molecule 1: Major head protein



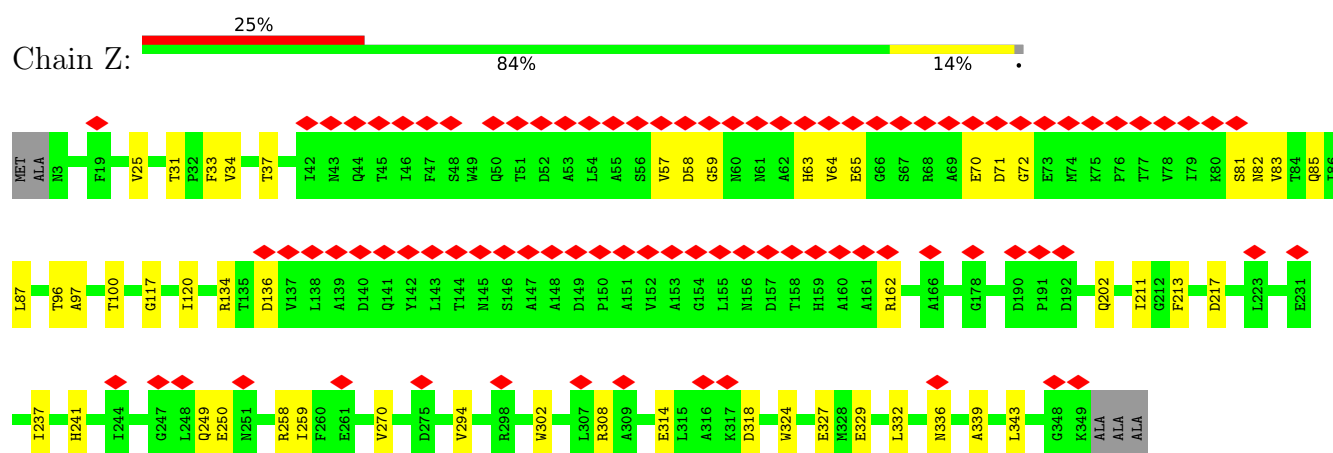
• Molecule 1: Major head protein



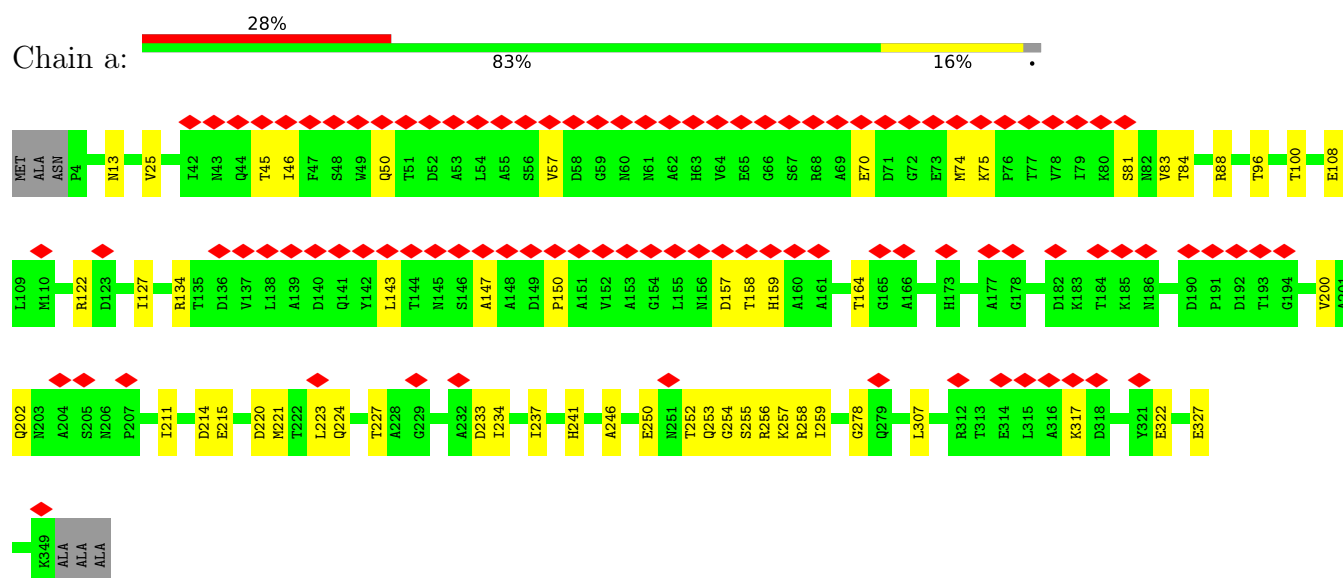
- Molecule 1: Major head protein



- Molecule 1: Major head protein

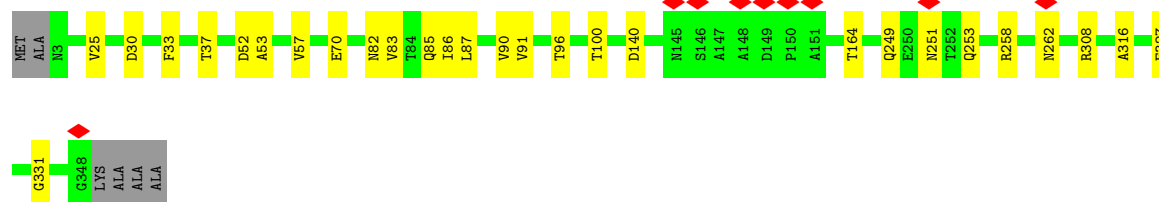


- Molecule 1: Major head protein



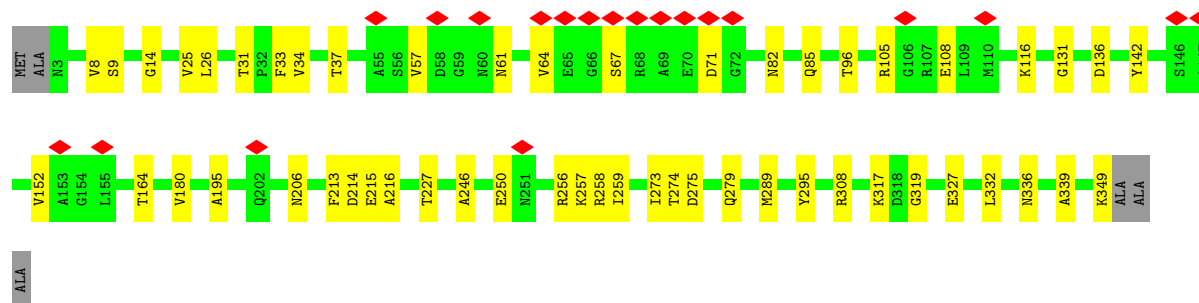
- Molecule 1: Major head protein

Chain b:  90% 8% .



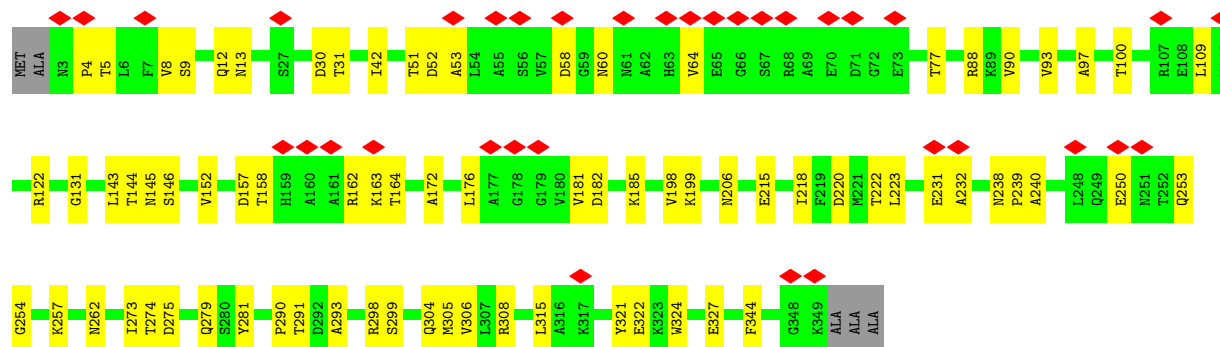
- Molecule 1: Major head protein

Chain c:  6% 84% 15% .



- Molecule 1: Major head protein

Chain d:  10% 77% 22% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C5                               | Depositor |
| Number of particles used             | 22146                                   | 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 ( $e^-/\text{\AA}^2$ ) | 49                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2700                                    | Depositor |
| Magnification                        | 59000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.239                                   | Depositor |
| Minimum map value                    | -0.136                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.011                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size (Å)                         | 552.0, 552.0, 552.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.38, 1.38, 1.38                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.13         | 0/2723      | 0.36        | 0/3690      |
| 1   | B     | 0.11         | 0/2728      | 0.33        | 0/3694      |
| 1   | C     | 0.12         | 0/2736      | 0.31        | 0/3706      |
| 1   | D     | 0.12         | 0/2720      | 0.31        | 0/3683      |
| 1   | E     | 0.12         | 0/2728      | 0.37        | 0/3694      |
| 1   | F     | 0.13         | 0/2727      | 0.33        | 0/3695      |
| 1   | G     | 0.13         | 0/2736      | 0.34        | 0/3706      |
| 1   | H     | 0.12         | 0/2706      | 0.31        | 0/3661      |
| 1   | I     | 0.12         | 0/2727      | 0.30        | 0/3695      |
| 1   | J     | 0.12         | 0/2693      | 0.30        | 0/3646      |
| 1   | K     | 0.13         | 0/2736      | 0.35        | 0/3706      |
| 1   | L     | 0.12         | 0/2736      | 0.29        | 0/3706      |
| 1   | M     | 0.11         | 0/2727      | 0.30        | 0/3695      |
| 1   | N     | 0.11         | 0/2736      | 0.28        | 0/3706      |
| 1   | O     | 0.13         | 0/2736      | 0.35        | 0/3706      |
| 1   | P     | 0.12         | 0/2704      | 0.31        | 0/3662      |
| 1   | Q     | 0.12         | 0/2727      | 0.30        | 0/3695      |
| 1   | R     | 0.12         | 0/2693      | 0.31        | 0/3646      |
| 1   | S     | 0.12         | 0/2686      | 0.34        | 0/3636      |
| 1   | T     | 0.12         | 0/2719      | 0.30        | 0/3683      |
| 1   | U     | 0.12         | 0/2727      | 0.33        | 0/3695      |
| 1   | V     | 0.12         | 0/2720      | 0.31        | 0/3683      |
| 1   | W     | 0.13         | 0/2736      | 0.33        | 0/3706      |
| 1   | X     | 0.12         | 0/2728      | 0.29        | 0/3694      |
| 1   | Y     | 0.12         | 0/2727      | 0.30        | 0/3695      |
| 1   | Z     | 0.11         | 0/2736      | 0.30        | 0/3706      |
| 1   | a     | 0.12         | 0/2728      | 0.34        | 0/3694      |
| 1   | b     | 0.13         | 0/2727      | 0.29        | 0/3695      |
| 1   | c     | 0.12         | 0/2736      | 0.29        | 0/3706      |
| 1   | d     | 0.12         | 0/2736      | 0.35        | 0/3706      |
| All | All   | 0.12         | 0/81725     | 0.32        | 0/110691    |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 0                   | 1                   |
| 1   | G     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 144 | THR  | Peptide |
| 1   | G     | 167 | PHE  | Peptide |
| 1   | G     | 168 | GLN  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2672  | 0        | 2635     | 42      | 0            |
| 1   | B     | 2677  | 0        | 2646     | 53      | 0            |
| 1   | C     | 2685  | 0        | 2651     | 43      | 0            |
| 1   | D     | 2670  | 0        | 2638     | 35      | 0            |
| 1   | E     | 2677  | 0        | 2646     | 46      | 0            |
| 1   | F     | 2676  | 0        | 2638     | 41      | 0            |
| 1   | G     | 2685  | 0        | 2651     | 37      | 0            |
| 1   | H     | 2657  | 0        | 2629     | 43      | 0            |
| 1   | I     | 2676  | 0        | 2638     | 46      | 0            |
| 1   | J     | 2644  | 0        | 2611     | 34      | 0            |
| 1   | K     | 2685  | 0        | 2651     | 42      | 0            |
| 1   | L     | 2685  | 0        | 2651     | 23      | 0            |
| 1   | M     | 2676  | 0        | 2638     | 30      | 0            |
| 1   | N     | 2685  | 0        | 2651     | 29      | 0            |
| 1   | O     | 2685  | 0        | 2651     | 45      | 0            |
| 1   | P     | 2654  | 0        | 2618     | 45      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Q     | 2676  | 0        | 2638     | 31      | 0            |
| 1   | R     | 2644  | 0        | 2611     | 33      | 0            |
| 1   | S     | 2637  | 0        | 2602     | 43      | 0            |
| 1   | T     | 2668  | 0        | 2633     | 38      | 0            |
| 1   | U     | 2676  | 0        | 2638     | 47      | 0            |
| 1   | V     | 2670  | 0        | 2638     | 26      | 0            |
| 1   | W     | 2685  | 0        | 2651     | 51      | 0            |
| 1   | X     | 2677  | 0        | 2646     | 38      | 0            |
| 1   | Y     | 2676  | 0        | 2638     | 51      | 0            |
| 1   | Z     | 2685  | 0        | 2651     | 36      | 0            |
| 1   | a     | 2677  | 0        | 2646     | 41      | 0            |
| 1   | b     | 2676  | 0        | 2638     | 21      | 0            |
| 1   | c     | 2685  | 0        | 2651     | 37      | 0            |
| 1   | d     | 2685  | 0        | 2651     | 53      | 0            |
| All | All   | 80206 | 0        | 79175    | 1043    | 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 (1043) 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:P:206:ASN:ND2 | 1:P:214:ASP:OD2 | 2.04                     | 0.91              |
| 1:H:96:THR:O    | 1:H:100:THR:OG1 | 1.91                     | 0.89              |
| 1:W:93:VAL:O    | 1:W:321:TYR:OH  | 1.90                     | 0.89              |
| 1:d:51:THR:O    | 1:d:77:THR:OG1  | 1.94                     | 0.86              |
| 1:B:88:ARG:NH1  | 1:G:64:VAL:O    | 2.09                     | 0.86              |
| 1:K:250:GLU:OE1 | 1:K:258:ARG:NH2 | 2.09                     | 0.85              |
| 1:G:51:THR:O    | 1:G:77:THR:OG1  | 1.94                     | 0.85              |
| 1:B:88:ARG:NH2  | 1:G:67:SER:O    | 2.09                     | 0.84              |
| 1:N:250:GLU:OE1 | 1:N:258:ARG:NH2 | 2.12                     | 0.83              |
| 1:d:308:ARG:NH1 | 1:d:327:GLU:OE1 | 2.12                     | 0.83              |
| 1:R:257:LYS:NZ  | 1:V:254:GLY:O   | 2.11                     | 0.82              |
| 1:S:252:THR:OG1 | 1:S:255:SER:O   | 1.97                     | 0.82              |
| 1:a:254:GLY:O   | 1:a:257:LYS:NZ  | 2.12                     | 0.82              |
| 1:W:51:THR:O    | 1:W:77:THR:OG1  | 1.97                     | 0.81              |
| 1:K:122:ARG:NH2 | 1:S:56:SER:OG   | 2.15                     | 0.80              |
| 1:S:203:ASN:ND2 | 1:S:212:GLY:O   | 2.14                     | 0.80              |
| 1:K:254:GLY:O   | 1:K:257:LYS:NZ  | 2.14                     | 0.80              |
| 1:N:203:ASN:ND2 | 1:N:212:GLY:O   | 2.15                     | 0.79              |
| 1:R:77:THR:O    | 1:a:13:ASN:ND2  | 2.15                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:199:LYS:NZ   | 1:I:220:ASP:OD2  | 2.15                     | 0.79              |
| 1:F:143:LEU:O    | 1:F:144:THR:HG22 | 1.82                     | 0.79              |
| 1:T:135:THR:OG1  | 1:T:163:LYS:O    | 2.00                     | 0.79              |
| 1:U:171:CYS:SG   | 1:U:340:SER:OG   | 2.41                     | 0.79              |
| 1:Y:308:ARG:NH1  | 1:Y:329:GLU:OE2  | 2.16                     | 0.78              |
| 1:d:254:GLY:O    | 1:d:257:LYS:NZ   | 2.16                     | 0.78              |
| 1:B:292:ASP:OD1  | 1:B:345:THR:OG1  | 2.01                     | 0.77              |
| 1:b:249:GLN:OE1  | 1:b:258:ARG:NH1  | 2.18                     | 0.77              |
| 1:B:215:GLU:HA   | 1:B:248:LEU:HD11 | 1.67                     | 0.76              |
| 1:I:308:ARG:NH2  | 1:I:327:GLU:OE1  | 2.19                     | 0.76              |
| 1:J:65:GLU:OE2   | 1:N:162:ARG:NH1  | 2.18                     | 0.76              |
| 1:S:254:GLY:O    | 1:S:257:LYS:NZ   | 2.18                     | 0.76              |
| 1:G:3:ASN:OD1    | 1:G:5:THR:OG1    | 2.02                     | 0.75              |
| 1:C:28:PRO:O     | 1:C:122:ARG:NH2  | 2.21                     | 0.74              |
| 1:T:12:GLN:O     | 1:X:145:ASN:ND2  | 2.20                     | 0.74              |
| 1:b:308:ARG:NH1  | 1:b:327:GLU:OE1  | 2.20                     | 0.74              |
| 1:D:90:VAL:HG21  | 1:E:71:ASP:HB3   | 1.67                     | 0.74              |
| 1:Z:81:SER:O     | 1:Z:134:ARG:NH2  | 2.19                     | 0.74              |
| 1:D:249:GLN:OE1  | 1:D:258:ARG:NH1  | 2.22                     | 0.73              |
| 1:T:105:ARG:NH1  | 1:U:13:ASN:O     | 2.21                     | 0.73              |
| 1:P:105:ARG:O    | 1:T:50:GLN:NE2   | 2.21                     | 0.73              |
| 1:R:218:ILE:O    | 1:R:222:THR:HG23 | 1.88                     | 0.72              |
| 1:L:306:VAL:HG22 | 1:L:330:VAL:HG12 | 1.71                     | 0.72              |
| 1:a:74:MET:SD    | 1:a:75:LYS:NZ    | 2.62                     | 0.72              |
| 1:O:134:ARG:NH1  | 1:O:140:ASP:OD2  | 2.23                     | 0.72              |
| 1:U:320:SER:OG   | 1:X:327:GLU:OE2  | 2.04                     | 0.72              |
| 1:Q:212:GLY:N    | 1:Q:346:ALA:O    | 2.23                     | 0.72              |
| 1:c:33:PHE:O     | 1:c:37:THR:HG23  | 1.90                     | 0.71              |
| 1:K:85:GLN:NE2   | 1:S:61:ASN:O     | 2.23                     | 0.71              |
| 1:T:237:ILE:HD13 | 1:T:294:VAL:HG22 | 1.72                     | 0.71              |
| 1:A:237:ILE:HG22 | 1:A:294:VAL:HG22 | 1.72                     | 0.71              |
| 1:E:154:GLY:O    | 1:E:159:HIS:NE2  | 2.24                     | 0.71              |
| 1:S:114:GLU:N    | 1:S:114:GLU:OE1  | 2.22                     | 0.71              |
| 1:O:81:SER:O     | 1:O:134:ARG:NH2  | 2.23                     | 0.71              |
| 1:U:192:ASP:OD1  | 1:U:193:THR:N    | 2.22                     | 0.71              |
| 1:D:52:ASP:OD1   | 1:D:53:ALA:N     | 2.23                     | 0.71              |
| 1:M:192:ASP:OD1  | 1:M:193:THR:N    | 2.23                     | 0.70              |
| 1:I:192:ASP:OD1  | 1:I:193:THR:N    | 2.24                     | 0.70              |
| 1:V:83:VAL:HG21  | 1:V:136:ASP:HB3  | 1.73                     | 0.70              |
| 1:A:203:ASN:ND2  | 1:A:346:ALA:O    | 2.25                     | 0.70              |
| 1:a:253:GLN:N    | 1:a:253:GLN:OE1  | 2.24                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:200:VAL:O    | 1:a:202:GLN:NE2  | 2.25                     | 0.70              |
| 1:Y:105:ARG:NH1  | 1:c:14:GLY:O     | 2.25                     | 0.69              |
| 1:S:64:VAL:HG12  | 1:S:65:GLU:H     | 1.56                     | 0.69              |
| 1:Y:192:ASP:OD1  | 1:Y:193:THR:N    | 2.26                     | 0.69              |
| 1:G:143:LEU:O    | 1:G:144:THR:OG1  | 2.05                     | 0.69              |
| 1:J:33:PHE:O     | 1:J:37:THR:HG23  | 1.91                     | 0.69              |
| 1:U:5:THR:OG1    | 1:X:72:GLY:O     | 2.03                     | 0.69              |
| 1:O:56:SER:OG    | 1:d:122:ARG:NH1  | 2.25                     | 0.69              |
| 1:E:102:ASN:OD1  | 1:E:103:TYR:N    | 2.26                     | 0.68              |
| 1:a:81:SER:O     | 1:a:134:ARG:NH2  | 2.26                     | 0.68              |
| 1:A:40:GLU:N     | 1:A:40:GLU:OE1   | 2.27                     | 0.68              |
| 1:D:88:ARG:NH2   | 1:D:327:GLU:OE1  | 2.26                     | 0.68              |
| 1:E:155:LEU:O    | 1:E:158:THR:OG1  | 2.12                     | 0.68              |
| 1:a:250:GLU:OE1  | 1:a:258:ARG:NH2  | 2.25                     | 0.68              |
| 1:O:145:ASN:ND2  | 1:d:13:ASN:OD1   | 2.27                     | 0.68              |
| 1:Q:305:MET:SD   | 1:Q:333:ARG:NH2  | 2.67                     | 0.68              |
| 1:d:253:GLN:N    | 1:d:253:GLN:OE1  | 2.27                     | 0.68              |
| 1:R:96:THR:O     | 1:R:100:THR:HG23 | 1.93                     | 0.68              |
| 1:N:202:GLN:NE2  | 1:N:217:ASP:OD1  | 2.27                     | 0.67              |
| 1:Y:28:PRO:O     | 1:Y:122:ARG:NH2  | 2.27                     | 0.67              |
| 1:B:203:ASN:N    | 1:B:214:ASP:OD2  | 2.27                     | 0.67              |
| 1:W:192:ASP:OD1  | 1:W:193:THR:N    | 2.28                     | 0.67              |
| 1:E:143:LEU:O    | 1:E:144:THR:OG1  | 2.12                     | 0.67              |
| 1:S:314:GLU:OE2  | 1:S:317:LYS:N    | 2.28                     | 0.67              |
| 1:P:81:SER:O     | 1:P:134:ARG:NH2  | 2.28                     | 0.67              |
| 1:X:144:THR:OG1  | 1:Y:143:LEU:O    | 2.09                     | 0.67              |
| 1:A:168:GLN:HB3  | 1:A:180:VAL:HG21 | 1.77                     | 0.67              |
| 1:S:33:PHE:O     | 1:S:37:THR:HG23  | 1.95                     | 0.66              |
| 1:O:82:ASN:ND2   | 1:O:332:LEU:O    | 2.27                     | 0.66              |
| 1:H:52:ASP:OD1   | 1:H:53:ALA:N     | 2.29                     | 0.66              |
| 1:E:83:VAL:HG11  | 1:E:164:THR:HA   | 1.76                     | 0.66              |
| 1:N:3:ASN:ND2    | 1:T:73:GLU:OE1   | 2.28                     | 0.66              |
| 1:N:33:PHE:O     | 1:N:37:THR:HG23  | 1.95                     | 0.66              |
| 1:a:252:THR:OG1  | 1:a:255:SER:O    | 2.04                     | 0.66              |
| 1:O:222:THR:HG22 | 1:O:281:TYR:CE2  | 2.31                     | 0.65              |
| 1:A:136:ASP:OD1  | 1:A:162:ARG:NH2  | 2.29                     | 0.65              |
| 1:H:298:ARG:O    | 1:H:299:SER:OG   | 2.15                     | 0.65              |
| 1:J:214:ASP:O    | 1:J:218:ILE:HD12 | 1.96                     | 0.65              |
| 1:W:231:GLU:OE1  | 1:W:231:GLU:N    | 2.30                     | 0.65              |
| 1:O:218:ILE:O    | 1:O:222:THR:HG23 | 1.96                     | 0.65              |
| 1:W:254:GLY:O    | 1:W:257:LYS:NZ   | 2.29                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:157:ASP:O    | 1:K:158:THR:OG1  | 2.12                     | 0.65              |
| 1:W:17:LEU:HD22  | 1:a:143:LEU:HD22 | 1.78                     | 0.65              |
| 1:T:91:VAL:HG21  | 1:T:112:GLN:HB3  | 1.79                     | 0.65              |
| 1:E:143:LEU:N    | 1:E:146:SER:OG   | 2.28                     | 0.65              |
| 1:K:98:ASN:OD1   | 1:K:99:THR:N     | 2.29                     | 0.65              |
| 1:O:254:GLY:O    | 1:O:257:LYS:NZ   | 2.28                     | 0.65              |
| 1:L:230:SER:OG   | 1:L:339:ALA:O    | 2.13                     | 0.64              |
| 1:W:252:THR:OG1  | 1:W:255:SER:O    | 2.09                     | 0.64              |
| 1:Q:213:PHE:CZ   | 1:Q:218:ILE:HD11 | 2.32                     | 0.64              |
| 1:I:182:ASP:OD1  | 1:I:183:LYS:N    | 2.29                     | 0.64              |
| 1:K:127:ILE:O    | 1:K:130:SER:OG   | 2.16                     | 0.64              |
| 1:S:99:THR:O     | 1:S:107:ARG:NH1  | 2.30                     | 0.64              |
| 1:H:88:ARG:NH2   | 1:H:325:MET:SD   | 2.69                     | 0.64              |
| 1:R:182:ASP:OD1  | 1:R:183:LYS:N    | 2.30                     | 0.64              |
| 1:D:29:GLN:OE1   | 1:D:29:GLN:N     | 2.31                     | 0.64              |
| 1:K:303:THR:OG1  | 1:K:305:MET:SD   | 2.55                     | 0.64              |
| 1:C:250:GLU:OE2  | 1:C:258:ARG:NH2  | 2.31                     | 0.64              |
| 1:V:198:VAL:HG22 | 1:V:342:VAL:HB   | 1.80                     | 0.64              |
| 1:E:102:ASN:ND2  | 1:X:14:GLY:O     | 2.30                     | 0.64              |
| 1:M:88:ARG:NH1   | 1:Q:67:SER:OG    | 2.31                     | 0.64              |
| 1:Y:52:ASP:OD1   | 1:Y:53:ALA:N     | 2.31                     | 0.64              |
| 1:a:220:ASP:OD1  | 1:a:221:MET:N    | 2.31                     | 0.64              |
| 1:d:199:LYS:NZ   | 1:d:220:ASP:OD2  | 2.31                     | 0.64              |
| 1:M:224:GLN:O    | 1:M:227:THR:OG1  | 2.15                     | 0.64              |
| 1:T:98:ASN:OD1   | 1:T:107:ARG:NH1  | 2.30                     | 0.64              |
| 1:K:255:SER:OG   | 1:O:250:GLU:O    | 2.16                     | 0.63              |
| 1:M:37:THR:OG1   | 1:M:304:GLN:NE2  | 2.32                     | 0.63              |
| 1:O:222:THR:HG22 | 1:O:281:TYR:HE2  | 1.63                     | 0.63              |
| 1:T:132:GLN:NE2  | 1:X:60:ASN:OD1   | 2.32                     | 0.63              |
| 1:T:275:ASP:OD1  | 1:T:279:GLN:N    | 2.32                     | 0.63              |
| 1:A:81:SER:O     | 1:A:134:ARG:NH2  | 2.31                     | 0.63              |
| 1:H:137:VAL:HG23 | 1:H:138:LEU:HD12 | 1.81                     | 0.63              |
| 1:J:65:GLU:OE1   | 1:J:65:GLU:N     | 2.32                     | 0.63              |
| 1:H:105:ARG:NH2  | 1:P:50:GLN:OE1   | 2.32                     | 0.63              |
| 1:H:334:HIS:NE2  | 1:H:336:ASN:O    | 2.31                     | 0.63              |
| 1:U:198:VAL:HG23 | 1:U:342:VAL:HB   | 1.81                     | 0.63              |
| 1:G:33:PHE:O     | 1:G:37:THR:HG23  | 1.98                     | 0.62              |
| 1:W:237:ILE:HG23 | 1:W:238:ASN:H    | 1.65                     | 0.62              |
| 1:I:308:ARG:NH1  | 1:I:329:GLU:OE2  | 2.32                     | 0.62              |
| 1:E:105:ARG:NE   | 1:E:108:GLU:OE1  | 2.30                     | 0.62              |
| 1:J:52:ASP:OD1   | 1:J:53:ALA:N     | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:314:GLU:OE2  | 1:Z:324:TRP:NE1  | 2.33                     | 0.62              |
| 1:c:317:LYS:NZ   | 1:c:319:GLY:O    | 2.33                     | 0.62              |
| 1:H:137:VAL:HG23 | 1:H:138:LEU:CD1  | 2.29                     | 0.61              |
| 1:N:230:SER:OG   | 1:N:339:ALA:O    | 2.10                     | 0.61              |
| 1:P:315:LEU:HD12 | 1:P:323:LYS:HG2  | 1.81                     | 0.61              |
| 1:Y:40:GLU:OE1   | 1:Y:333:ARG:NH2  | 2.33                     | 0.61              |
| 1:O:96:THR:HG22  | 1:O:97:ALA:H     | 1.65                     | 0.61              |
| 1:a:158:THR:O    | 1:a:159:HIS:ND1  | 2.33                     | 0.61              |
| 1:L:196:VAL:N    | 1:L:224:GLN:OE1  | 2.32                     | 0.61              |
| 1:T:143:LEU:O    | 1:T:144:THR:OG1  | 2.07                     | 0.61              |
| 1:X:90:VAL:HG11  | 1:b:70:GLU:O     | 2.00                     | 0.61              |
| 1:A:308:ARG:NH2  | 1:A:327:GLU:OE1  | 2.32                     | 0.61              |
| 1:C:254:GLY:O    | 1:C:257:LYS:NZ   | 2.33                     | 0.61              |
| 1:F:307:LEU:HD23 | 1:F:329:GLU:CD   | 2.26                     | 0.61              |
| 1:P:99:THR:O     | 1:P:100:THR:OG1  | 2.19                     | 0.61              |
| 1:J:320:SER:OG   | 1:O:65:GLU:O     | 2.19                     | 0.61              |
| 1:T:44:GLN:OE1   | 1:T:44:GLN:N     | 2.33                     | 0.61              |
| 1:V:83:VAL:HG21  | 1:V:136:ASP:CB   | 2.30                     | 0.61              |
| 1:d:176:LEU:CD2  | 1:d:181:VAL:HG13 | 2.30                     | 0.61              |
| 1:C:262:ASN:ND2  | 1:D:265:GLN:O    | 2.32                     | 0.61              |
| 1:M:148:ALA:O    | 1:M:152:VAL:HG22 | 2.00                     | 0.61              |
| 1:W:17:LEU:HD22  | 1:a:143:LEU:CD2  | 2.31                     | 0.61              |
| 1:c:8:VAL:HG13   | 1:c:9:SER:H      | 1.65                     | 0.61              |
| 1:P:334:HIS:NE2  | 1:P:336:ASN:O    | 2.34                     | 0.60              |
| 1:U:213:PHE:CE1  | 1:U:345:THR:HG22 | 2.36                     | 0.60              |
| 1:d:42:ILE:HD12  | 1:d:305:MET:HB3  | 1.83                     | 0.60              |
| 1:S:157:ASP:O    | 1:S:158:THR:OG1  | 2.13                     | 0.60              |
| 1:I:67:SER:OG    | 1:Y:88:ARG:NH1   | 2.33                     | 0.60              |
| 1:I:213:PHE:CD1  | 1:I:218:ILE:HD11 | 2.37                     | 0.60              |
| 1:J:82:ASN:ND2   | 1:J:332:LEU:O    | 2.34                     | 0.60              |
| 1:d:182:ASP:OD2  | 1:d:185:LYS:NZ   | 2.31                     | 0.60              |
| 1:I:82:ASN:OD1   | 1:I:83:VAL:N     | 2.34                     | 0.60              |
| 1:P:34:VAL:HG21  | 1:P:125:GLU:OE1  | 2.01                     | 0.60              |
| 1:R:250:GLU:OE1  | 1:R:258:ARG:NH2  | 2.35                     | 0.60              |
| 1:Z:71:ASP:OD1   | 1:Z:72:GLY:N     | 2.35                     | 0.60              |
| 1:S:64:VAL:HG12  | 1:S:65:GLU:N     | 2.17                     | 0.60              |
| 1:V:81:SER:O     | 1:V:134:ARG:NH2  | 2.35                     | 0.60              |
| 1:Y:170:LEU:HD23 | 1:Y:334:HIS:HB2  | 1.83                     | 0.60              |
| 1:b:33:PHE:O     | 1:b:37:THR:HG23  | 2.02                     | 0.60              |
| 1:T:213:PHE:CE1  | 1:T:294:VAL:HG21 | 2.36                     | 0.60              |
| 1:U:82:ASN:OD1   | 1:U:83:VAL:N     | 2.34                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:52:ASP:OD1   | 1:I:53:ALA:N     | 2.35                     | 0.59              |
| 1:H:54:LEU:HD12  | 1:L:119:GLU:HG3  | 1.83                     | 0.59              |
| 1:N:95:ASP:OD1   | 1:T:308:ARG:NH2  | 2.36                     | 0.59              |
| 1:P:250:GLU:OE2  | 1:P:258:ARG:NH2  | 2.35                     | 0.59              |
| 1:D:88:ARG:NH1   | 1:D:327:GLU:OE2  | 2.36                     | 0.59              |
| 1:F:146:SER:O    | 1:F:149:ASP:N    | 2.30                     | 0.59              |
| 1:U:70:GLU:OE1   | 1:U:70:GLU:N     | 2.35                     | 0.59              |
| 1:Y:322:GLU:OE1  | 1:Y:322:GLU:N    | 2.35                     | 0.59              |
| 1:c:206:ASN:O    | 1:c:349:LYS:N    | 2.35                     | 0.59              |
| 1:U:215:GLU:N    | 1:U:215:GLU:OE1  | 2.36                     | 0.59              |
| 1:T:111:TYR:OH   | 1:X:52:ASP:OD2   | 2.20                     | 0.59              |
| 1:A:82:ASN:ND2   | 1:A:332:LEU:O    | 2.36                     | 0.59              |
| 1:D:30:ASP:O     | 1:D:31:THR:OG1   | 2.19                     | 0.59              |
| 1:E:190:ASP:O    | 1:E:194:GLY:N    | 2.35                     | 0.59              |
| 1:G:48:SER:OG    | 1:G:80:LYS:O     | 2.07                     | 0.58              |
| 1:C:136:ASP:OD1  | 1:C:137:VAL:N    | 2.35                     | 0.58              |
| 1:E:78:VAL:HG12  | 1:E:78:VAL:O     | 2.03                     | 0.58              |
| 1:H:237:ILE:HD13 | 1:H:294:VAL:HG22 | 1.85                     | 0.58              |
| 1:d:304:GLN:O    | 1:d:306:VAL:HG13 | 2.03                     | 0.58              |
| 1:Q:70:GLU:N     | 1:Q:70:GLU:OE1   | 2.37                     | 0.58              |
| 1:T:5:THR:OG1    | 1:X:156:ASN:ND2  | 2.37                     | 0.58              |
| 1:Y:82:ASN:OD1   | 1:Y:83:VAL:N     | 2.37                     | 0.58              |
| 1:H:246:ALA:O    | 1:H:258:ARG:NH1  | 2.36                     | 0.58              |
| 1:I:237:ILE:HG13 | 1:I:285:VAL:HG12 | 1.86                     | 0.58              |
| 1:E:44:GLN:HG2   | 1:E:45:THR:H     | 1.68                     | 0.58              |
| 1:d:218:ILE:O    | 1:d:222:THR:HG23 | 2.04                     | 0.58              |
| 1:B:95:ASP:O     | 1:B:96:THR:OG1   | 2.16                     | 0.58              |
| 1:Q:8:VAL:O      | 1:Q:9:SER:OG     | 2.19                     | 0.58              |
| 1:R:157:ASP:O    | 1:R:158:THR:OG1  | 2.15                     | 0.58              |
| 1:B:261:GLU:OE1  | 1:B:262:ASN:N    | 2.37                     | 0.58              |
| 1:T:163:LYS:NZ   | 1:T:179:GLY:O    | 2.30                     | 0.58              |
| 1:L:250:GLU:OE2  | 1:L:258:ARG:NH2  | 2.36                     | 0.57              |
| 1:I:157:ASP:O    | 1:I:158:THR:OG1  | 2.15                     | 0.57              |
| 1:d:222:THR:HG22 | 1:d:281:TYR:HE2  | 1.69                     | 0.57              |
| 1:B:26:LEU:HD11  | 1:G:229:GLY:O    | 2.05                     | 0.57              |
| 1:G:159:HIS:ND1  | 1:G:159:HIS:O    | 2.37                     | 0.57              |
| 1:A:265:GLN:OE1  | 1:A:266:PHE:CE2  | 2.58                     | 0.57              |
| 1:I:303:THR:OG1  | 1:I:333:ARG:NH1  | 2.37                     | 0.57              |
| 1:P:249:GLN:OE1  | 1:P:258:ARG:NE   | 2.37                     | 0.57              |
| 1:Q:157:ASP:O    | 1:Q:158:THR:OG1  | 2.16                     | 0.57              |
| 1:S:52:ASP:OD1   | 1:S:53:ALA:N     | 2.37                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:25:VAL:HG12  | 1:a:25:VAL:O     | 2.02                     | 0.57              |
| 1:a:83:VAL:HG22  | 1:a:84:THR:H     | 1.70                     | 0.57              |
| 1:M:235:ILE:HG23 | 1:M:296:PHE:CE1  | 2.39                     | 0.57              |
| 1:M:275:ASP:OD1  | 1:M:279:GLN:N    | 2.37                     | 0.57              |
| 1:S:253:GLN:N    | 1:S:253:GLN:OE1  | 2.37                     | 0.57              |
| 1:P:157:ASP:OD1  | 1:d:321:TYR:OH   | 2.21                     | 0.57              |
| 1:d:222:THR:HG22 | 1:d:281:TYR:CE2  | 2.39                     | 0.57              |
| 1:E:224:GLN:O    | 1:E:227:THR:OG1  | 2.22                     | 0.57              |
| 1:I:329:GLU:OE2  | 1:c:96:THR:OG1   | 2.16                     | 0.57              |
| 1:U:314:GLU:OE1  | 1:U:324:TRP:NE1  | 2.38                     | 0.57              |
| 1:a:122:ARG:NH2  | 1:d:58:ASP:OD1   | 2.37                     | 0.57              |
| 1:c:308:ARG:NH1  | 1:c:327:GLU:OE1  | 2.37                     | 0.57              |
| 1:F:240:ALA:O    | 1:F:243:LYS:NZ   | 2.37                     | 0.56              |
| 1:O:132:GLN:NE2  | 1:O:164:THR:O    | 2.38                     | 0.56              |
| 1:P:308:ARG:NH2  | 1:P:329:GLU:OE1  | 2.38                     | 0.56              |
| 1:X:6:LEU:O      | 1:X:8:VAL:HG13   | 2.05                     | 0.56              |
| 1:c:25:VAL:HG13  | 1:c:25:VAL:O     | 2.05                     | 0.56              |
| 1:X:5:THR:C      | 1:X:6:LEU:HD23   | 2.30                     | 0.56              |
| 1:J:153:ALA:O    | 1:J:158:THR:HG21 | 2.05                     | 0.56              |
| 1:O:114:GLU:OE2  | 1:O:312:ARG:NH2  | 2.39                     | 0.56              |
| 1:a:83:VAL:O     | 1:a:164:THR:HG22 | 2.06                     | 0.56              |
| 1:B:49:TRP:NE1   | 1:B:334:HIS:O    | 2.38                     | 0.56              |
| 1:W:134:ARG:O    | 1:W:135:THR:OG1  | 2.17                     | 0.56              |
| 1:D:105:ARG:NH2  | 1:D:108:GLU:OE2  | 2.38                     | 0.56              |
| 1:H:290:PRO:O    | 1:H:291:THR:HG22 | 2.05                     | 0.56              |
| 1:Y:8:VAL:HG13   | 1:Y:8:VAL:O      | 2.06                     | 0.56              |
| 1:A:192:ASP:OD1  | 1:A:193:THR:N    | 2.37                     | 0.56              |
| 1:B:186:ASN:OD1  | 1:B:200:VAL:N    | 2.39                     | 0.56              |
| 1:W:238:ASN:ND2  | 1:W:239:PRO:O    | 2.36                     | 0.56              |
| 1:X:171:CYS:SG   | 1:X:340:SER:OG   | 2.52                     | 0.56              |
| 1:M:263:THR:O    | 1:M:263:THR:HG22 | 2.06                     | 0.56              |
| 1:V:86:ILE:HG21  | 1:V:88:ARG:NH2   | 2.20                     | 0.56              |
| 1:Z:63:HIS:NE2   | 1:Z:70:GLU:OE2   | 2.39                     | 0.56              |
| 1:Z:202:GLN:N    | 1:Z:217:ASP:OD2  | 2.39                     | 0.56              |
| 1:C:214:ASP:OD2  | 1:C:217:ASP:N    | 2.39                     | 0.55              |
| 1:D:200:VAL:HG12 | 1:D:344:PHE:HB2  | 1.88                     | 0.55              |
| 1:I:8:VAL:HG13   | 1:I:8:VAL:O      | 2.06                     | 0.55              |
| 1:Q:192:ASP:OD1  | 1:Q:193:THR:N    | 2.39                     | 0.55              |
| 1:b:83:VAL:O     | 1:b:164:THR:HG22 | 2.07                     | 0.55              |
| 1:A:147:ALA:O    | 1:A:149:ASP:N    | 2.39                     | 0.55              |
| 1:A:252:THR:O    | 1:A:252:THR:HG23 | 2.05                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:257:LYS:NZ   | 1:M:278:GLY:O    | 2.37                     | 0.55              |
| 1:O:192:ASP:OD1  | 1:O:193:THR:N    | 2.39                     | 0.55              |
| 1:K:267:ILE:HD12 | 1:O:262:ASN:HB3  | 1.88                     | 0.55              |
| 1:U:124:LEU:HD13 | 1:U:330:VAL:HG21 | 1.88                     | 0.55              |
| 1:N:254:GLY:O    | 1:c:257:LYS:NZ   | 2.38                     | 0.55              |
| 1:F:33:PHE:O     | 1:F:37:THR:HG23  | 2.06                     | 0.55              |
| 1:O:215:GLU:OE1  | 1:O:248:LEU:HD13 | 2.07                     | 0.55              |
| 1:V:264:LYS:O    | 1:Z:270:VAL:HG13 | 2.06                     | 0.55              |
| 1:I:57:VAL:HG21  | 1:Y:122:ARG:HE   | 1.72                     | 0.55              |
| 1:M:31:THR:HG23  | 1:M:31:THR:O     | 2.06                     | 0.55              |
| 1:c:195:ALA:HB2  | 1:c:227:THR:HG23 | 1.89                     | 0.55              |
| 1:c:246:ALA:O    | 1:c:258:ARG:NH1  | 2.36                     | 0.55              |
| 1:B:33:PHE:O     | 1:B:37:THR:HG23  | 2.06                     | 0.55              |
| 1:I:308:ARG:NH1  | 1:c:96:THR:OG1   | 2.39                     | 0.55              |
| 1:U:45:THR:OG1   | 1:U:162:ARG:NH2  | 2.40                     | 0.55              |
| 1:W:93:VAL:HG13  | 1:W:321:TYR:OH   | 2.06                     | 0.55              |
| 1:H:196:VAL:N    | 1:H:224:GLN:OE1  | 2.39                     | 0.55              |
| 1:a:246:ALA:O    | 1:a:258:ARG:NH1  | 2.39                     | 0.55              |
| 1:d:206:ASN:ND2  | 1:d:215:GLU:OE2  | 2.40                     | 0.55              |
| 1:M:196:VAL:HG23 | 1:M:196:VAL:O    | 2.07                     | 0.54              |
| 1:Q:97:ALA:O     | 1:Q:100:THR:OG1  | 2.24                     | 0.54              |
| 1:R:237:ILE:HD11 | 1:R:241:HIS:CB   | 2.37                     | 0.54              |
| 1:Y:303:THR:OG1  | 1:Y:333:ARG:NH1  | 2.40                     | 0.54              |
| 1:Z:31:THR:HB    | 1:Z:34:VAL:HG12  | 1.89                     | 0.54              |
| 1:a:50:GLN:N     | 1:a:50:GLN:OE1   | 2.40                     | 0.54              |
| 1:b:82:ASN:OD1   | 1:b:83:VAL:N     | 2.39                     | 0.54              |
| 1:C:64:VAL:HG13  | 1:G:160:ALA:HA   | 1.89                     | 0.54              |
| 1:G:199:LYS:NZ   | 1:G:220:ASP:OD2  | 2.37                     | 0.54              |
| 1:H:102:ASN:OD1  | 1:H:105:ARG:NH1  | 2.41                     | 0.54              |
| 1:J:202:GLN:N    | 1:J:217:ASP:OD2  | 2.40                     | 0.54              |
| 1:X:203:ASN:ND2  | 1:X:212:GLY:O    | 2.40                     | 0.54              |
| 1:d:97:ALA:O     | 1:d:100:THR:OG1  | 2.25                     | 0.54              |
| 1:B:82:ASN:OD1   | 1:B:165:GLY:N    | 2.41                     | 0.54              |
| 1:G:167:PHE:N    | 1:G:169:PHE:O    | 2.35                     | 0.54              |
| 1:P:208:THR:HG22 | 1:P:208:THR:O    | 2.06                     | 0.54              |
| 1:B:85:GLN:HB2   | 1:B:164:THR:HG23 | 1.89                     | 0.54              |
| 1:C:82:ASN:ND2   | 1:C:332:LEU:O    | 2.36                     | 0.54              |
| 1:C:334:HIS:NE2  | 1:C:336:ASN:O    | 2.41                     | 0.54              |
| 1:X:82:ASN:ND2   | 1:X:164:THR:O    | 2.41                     | 0.54              |
| 1:B:82:ASN:ND2   | 1:B:332:LEU:O    | 2.38                     | 0.54              |
| 1:Z:249:GLN:OE1  | 1:Z:258:ARG:NH1  | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:LEU:HD11 | 1:B:128:LEU:HD11 | 1.89                     | 0.54              |
| 1:D:233:ASP:C    | 1:D:234:ILE:HD12 | 2.33                     | 0.54              |
| 1:E:118:LYS:HB2  | 1:F:54:LEU:HD21  | 1.88                     | 0.54              |
| 1:F:144:THR:HG23 | 1:F:144:THR:O    | 2.08                     | 0.54              |
| 1:K:99:THR:N     | 1:K:108:GLU:OE2  | 2.41                     | 0.54              |
| 1:a:88:ARG:NE    | 1:a:327:GLU:OE2  | 2.38                     | 0.54              |
| 1:Y:70:GLU:N     | 1:Y:70:GLU:OE1   | 2.41                     | 0.54              |
| 1:c:275:ASP:OD1  | 1:c:279:GLN:N    | 2.41                     | 0.54              |
| 1:B:215:GLU:OE2  | 1:B:256:ARG:NH1  | 2.41                     | 0.53              |
| 1:O:215:GLU:HG3  | 1:O:248:LEU:HD13 | 1.90                     | 0.53              |
| 1:Q:82:ASN:OD1   | 1:Q:83:VAL:N     | 2.38                     | 0.53              |
| 1:R:97:ALA:O     | 1:R:100:THR:OG1  | 2.25                     | 0.53              |
| 1:D:171:CYS:SG   | 1:D:342:VAL:HG21 | 2.49                     | 0.53              |
| 1:D:240:ALA:O    | 1:D:243:LYS:NZ   | 2.39                     | 0.53              |
| 1:E:44:GLN:O     | 1:E:46:ILE:HG22  | 2.07                     | 0.53              |
| 1:G:54:LEU:HD22  | 1:G:75:LYS:HB3   | 1.89                     | 0.53              |
| 1:N:208:THR:HG22 | 1:N:348:GLY:O    | 2.08                     | 0.53              |
| 1:P:33:PHE:O     | 1:P:37:THR:HG23  | 2.08                     | 0.53              |
| 1:S:83:VAL:HG12  | 1:S:84:THR:N     | 2.23                     | 0.53              |
| 1:X:124:LEU:HD13 | 1:X:330:VAL:HG21 | 1.90                     | 0.53              |
| 1:I:275:ASP:OD1  | 1:I:279:GLN:N    | 2.40                     | 0.53              |
| 1:J:87:LEU:HB2   | 1:J:120:ILE:HD11 | 1.90                     | 0.53              |
| 1:S:30:ASP:OD1   | 1:S:31:THR:N     | 2.39                     | 0.53              |
| 1:Y:45:THR:OG1   | 1:Y:162:ARG:NH2  | 2.42                     | 0.53              |
| 1:C:192:ASP:OD2  | 1:G:27:SER:OG    | 2.27                     | 0.53              |
| 1:P:122:ARG:NH1  | 1:T:55:ALA:O     | 2.42                     | 0.53              |
| 1:S:258:ARG:NH2  | 1:S:267:ILE:O    | 2.42                     | 0.53              |
| 1:Y:182:ASP:OD1  | 1:Y:183:LYS:N    | 2.42                     | 0.53              |
| 1:T:64:VAL:HG12  | 1:T:64:VAL:O     | 2.07                     | 0.53              |
| 1:W:218:ILE:O    | 1:W:222:THR:HG23 | 2.09                     | 0.53              |
| 1:X:288:TRP:CZ3  | 1:b:57:VAL:HG11  | 2.44                     | 0.53              |
| 1:Y:308:ARG:NH2  | 1:Y:327:GLU:OE1  | 2.41                     | 0.53              |
| 1:A:54:LEU:HD23  | 1:A:55:ALA:O     | 2.08                     | 0.53              |
| 1:A:25:VAL:HG23  | 1:A:25:VAL:O     | 2.09                     | 0.53              |
| 1:B:69:ALA:HB1   | 1:F:90:VAL:HG21  | 1.90                     | 0.53              |
| 1:B:131:GLY:CA   | 1:B:180:VAL:HG13 | 2.39                     | 0.53              |
| 1:C:182:ASP:OD2  | 1:C:185:LYS:NZ   | 2.40                     | 0.53              |
| 1:I:125:GLU:OE2  | 1:I:286:ASN:ND2  | 2.42                     | 0.53              |
| 1:R:237:ILE:HD11 | 1:R:241:HIS:HB2  | 1.90                     | 0.53              |
| 1:A:315:LEU:HD23 | 1:C:318:ASP:OD2  | 2.08                     | 0.53              |
| 1:J:237:ILE:HD11 | 1:J:241:HIS:CB   | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:157:ASP:O    | 1:U:158:THR:OG1  | 2.19                     | 0.53              |
| 1:c:31:THR:HB    | 1:c:34:VAL:HG12  | 1.91                     | 0.53              |
| 1:K:180:VAL:HG22 | 1:K:181:VAL:H    | 1.74                     | 0.52              |
| 1:S:26:LEU:HD12  | 1:W:336:ASN:HB3  | 1.90                     | 0.52              |
| 1:S:240:ALA:H    | 1:W:223:LEU:HD11 | 1.74                     | 0.52              |
| 1:B:241:HIS:NE2  | 1:B:291:THR:O    | 2.40                     | 0.52              |
| 1:E:237:ILE:HG22 | 1:E:285:VAL:HA   | 1.90                     | 0.52              |
| 1:I:263:THR:HG22 | 1:I:263:THR:O    | 2.10                     | 0.52              |
| 1:P:298:ARG:NH1  | 1:P:301:ASP:OD1  | 2.42                     | 0.52              |
| 1:X:196:VAL:N    | 1:X:224:GLN:OE1  | 2.42                     | 0.52              |
| 1:Y:262:ASN:OD1  | 1:Y:263:THR:N    | 2.43                     | 0.52              |
| 1:G:134:ARG:NH1  | 1:G:168:GLN:OE1  | 2.43                     | 0.52              |
| 1:N:205:SER:OG   | 1:N:214:ASP:OD2  | 2.28                     | 0.52              |
| 1:Q:213:PHE:CE1  | 1:Q:218:ILE:HD11 | 2.44                     | 0.52              |
| 1:T:236:MET:O    | 1:T:294:VAL:HG13 | 2.10                     | 0.52              |
| 1:Y:96:THR:O     | 1:Y:96:THR:HG22  | 2.10                     | 0.52              |
| 1:I:124:LEU:HD13 | 1:I:330:VAL:HG21 | 1.91                     | 0.52              |
| 1:Y:263:THR:O    | 1:Y:263:THR:HG22 | 2.10                     | 0.52              |
| 1:B:132:GLN:OE1  | 1:B:164:THR:N    | 2.42                     | 0.52              |
| 1:B:267:ILE:HD12 | 1:F:262:ASN:HB3  | 1.90                     | 0.52              |
| 1:P:30:ASP:O     | 1:P:31:THR:OG1   | 2.19                     | 0.52              |
| 1:U:224:GLN:O    | 1:U:227:THR:OG1  | 2.27                     | 0.52              |
| 1:W:250:GLU:OE2  | 1:a:256:ARG:NH1  | 2.43                     | 0.52              |
| 1:I:197:THR:HG21 | 1:I:338:TYR:HA   | 1.92                     | 0.52              |
| 1:K:33:PHE:O     | 1:K:37:THR:HG23  | 2.09                     | 0.52              |
| 1:Y:224:GLN:O    | 1:Y:227:THR:OG1  | 2.28                     | 0.52              |
| 1:J:198:VAL:HG22 | 1:J:342:VAL:HB   | 1.92                     | 0.52              |
| 1:R:83:VAL:O     | 1:R:164:THR:HG22 | 2.10                     | 0.52              |
| 1:U:307:LEU:HD22 | 1:U:329:GLU:OE1  | 2.10                     | 0.52              |
| 1:H:315:LEU:HD13 | 1:H:324:TRP:HA   | 1.92                     | 0.51              |
| 1:K:290:PRO:O    | 1:K:291:THR:HG22 | 2.10                     | 0.51              |
| 1:O:231:GLU:O    | 1:O:232:ALA:HB3  | 2.10                     | 0.51              |
| 1:O:255:SER:OG   | 1:d:250:GLU:O    | 2.23                     | 0.51              |
| 1:Z:82:ASN:ND2   | 1:Z:332:LEU:O    | 2.43                     | 0.51              |
| 1:W:42:ILE:CD1   | 1:W:305:MET:HE2  | 2.40                     | 0.51              |
| 1:H:218:ILE:O    | 1:H:222:THR:HG23 | 2.10                     | 0.51              |
| 1:J:88:ARG:NH1   | 1:J:327:GLU:OE2  | 2.42                     | 0.51              |
| 1:J:249:GLN:OE1  | 1:J:258:ARG:NH1  | 2.43                     | 0.51              |
| 1:Z:82:ASN:OD1   | 1:Z:83:VAL:N     | 2.43                     | 0.51              |
| 1:A:161:ALA:O    | 1:A:162:ARG:HG2  | 2.11                     | 0.51              |
| 1:C:92:ARG:NH1   | 1:D:71:ASP:OD2   | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:83:VAL:HG12  | 1:K:84:THR:N     | 2.26                     | 0.51              |
| 1:P:49:TRP:NE1   | 1:P:334:HIS:O    | 2.43                     | 0.51              |
| 1:P:70:GLU:OE2   | 1:P:70:GLU:N     | 2.39                     | 0.51              |
| 1:U:203:ASN:ND2  | 1:U:212:GLY:O    | 2.43                     | 0.51              |
| 1:N:40:GLU:OE1   | 1:N:333:ARG:NH1  | 2.43                     | 0.51              |
| 1:D:145:ASN:O    | 1:D:146:SER:OG   | 2.22                     | 0.51              |
| 1:E:41:SER:OG    | 1:E:42:ILE:N     | 2.44                     | 0.51              |
| 1:G:203:ASN:ND2  | 1:G:346:ALA:O    | 2.42                     | 0.51              |
| 1:K:203:ASN:OD1  | 1:K:206:ASN:N    | 2.44                     | 0.51              |
| 1:M:291:THR:HG22 | 1:M:291:THR:O    | 2.09                     | 0.51              |
| 1:K:149:ASP:OD1  | 1:K:149:ASP:N    | 2.44                     | 0.51              |
| 1:S:250:GLU:OE2  | 1:W:256:ARG:NH1  | 2.44                     | 0.51              |
| 1:A:315:LEU:HD22 | 1:A:323:LYS:O    | 2.11                     | 0.51              |
| 1:C:27:SER:OG    | 1:C:29:GLN:OE1   | 2.06                     | 0.51              |
| 1:E:88:ARG:NE    | 1:E:327:GLU:OE1  | 2.38                     | 0.51              |
| 1:F:305:MET:HE2  | 1:F:333:ARG:HH11 | 1.76                     | 0.51              |
| 1:X:172:ALA:O    | 1:X:198:VAL:HG21 | 2.11                     | 0.51              |
| 1:c:8:VAL:HG13   | 1:c:9:SER:N      | 2.26                     | 0.51              |
| 1:C:315:LEU:HG   | 1:C:316:ALA:H    | 1.75                     | 0.51              |
| 1:a:237:ILE:HD11 | 1:a:241:HIS:HB3  | 1.92                     | 0.51              |
| 1:E:74:MET:N     | 1:E:74:MET:SD    | 2.84                     | 0.50              |
| 1:J:58:ASP:OD1   | 1:J:59:GLY:N     | 2.45                     | 0.50              |
| 1:L:52:ASP:OD1   | 1:L:53:ALA:N     | 2.45                     | 0.50              |
| 1:A:291:THR:HG22 | 1:A:291:THR:O    | 2.11                     | 0.50              |
| 1:K:180:VAL:HG22 | 1:K:181:VAL:N    | 2.26                     | 0.50              |
| 1:L:253:GLN:NE2  | 1:b:251:ASN:OD1  | 2.44                     | 0.50              |
| 1:Y:275:ASP:OD1  | 1:Y:279:GLN:N    | 2.44                     | 0.50              |
| 1:A:184:THR:HG23 | 1:A:185:LYS:H    | 1.75                     | 0.50              |
| 1:C:57:VAL:HG11  | 1:G:126:LYS:HD3  | 1.93                     | 0.50              |
| 1:U:25:VAL:HG23  | 1:U:25:VAL:O     | 2.11                     | 0.50              |
| 1:a:214:ASP:O    | 1:a:215:GLU:HG2  | 2.11                     | 0.50              |
| 1:c:64:VAL:HG21  | 1:c:67:SER:OG    | 2.12                     | 0.50              |
| 1:d:131:GLY:O    | 1:d:181:VAL:HG21 | 2.12                     | 0.50              |
| 1:A:71:ASP:OD1   | 1:A:72:GLY:N     | 2.43                     | 0.50              |
| 1:B:54:LEU:HD22  | 1:F:27:SER:OG    | 2.11                     | 0.50              |
| 1:I:135:THR:HG22 | 1:I:163:LYS:HB2  | 1.93                     | 0.50              |
| 1:P:240:ALA:O    | 1:P:243:LYS:NZ   | 2.44                     | 0.50              |
| 1:S:192:ASP:OD1  | 1:S:193:THR:N    | 2.44                     | 0.50              |
| 1:U:286:ASN:OD1  | 1:U:287:ARG:N    | 2.44                     | 0.50              |
| 1:Z:96:THR:O     | 1:Z:100:THR:HG23 | 2.10                     | 0.50              |
| 1:O:180:VAL:HG22 | 1:O:181:VAL:H    | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:96:THR:HG22  | 1:P:96:THR:O     | 2.12                     | 0.50              |
| 1:R:88:ARG:NH2   | 1:V:67:SER:O     | 2.44                     | 0.50              |
| 1:S:116:LYS:NZ   | 1:W:73:GLU:O     | 2.39                     | 0.50              |
| 1:W:197:THR:HG23 | 1:W:198:VAL:HG23 | 1.93                     | 0.50              |
| 1:N:73:GLU:O     | 1:c:116:LYS:NZ   | 2.45                     | 0.50              |
| 1:N:275:ASP:OD1  | 1:N:279:GLN:N    | 2.43                     | 0.50              |
| 1:P:224:GLN:O    | 1:P:227:THR:OG1  | 2.30                     | 0.50              |
| 1:U:255:SER:O    | 1:U:274:THR:HG21 | 2.11                     | 0.50              |
| 1:C:64:VAL:HG12  | 1:C:64:VAL:O     | 2.12                     | 0.50              |
| 1:G:143:LEU:C    | 1:G:144:THR:HG1  | 2.12                     | 0.50              |
| 1:G:304:GLN:OE1  | 1:G:304:GLN:N    | 2.41                     | 0.50              |
| 1:K:98:ASN:O     | 1:K:99:THR:OG1   | 2.26                     | 0.50              |
| 1:Q:291:THR:O    | 1:Q:291:THR:HG22 | 2.12                     | 0.50              |
| 1:U:291:THR:HG22 | 1:U:291:THR:O    | 2.11                     | 0.50              |
| 1:Z:25:VAL:O     | 1:Z:25:VAL:HG13  | 2.12                     | 0.50              |
| 1:a:158:THR:O    | 1:a:158:THR:HG22 | 2.12                     | 0.50              |
| 1:a:233:ASP:OD1  | 1:a:234:ILE:N    | 2.44                     | 0.50              |
| 1:B:171:CYS:SG   | 1:B:172:ALA:N    | 2.83                     | 0.50              |
| 1:C:23:ILE:HG22  | 1:D:50:GLN:HG3   | 1.92                     | 0.50              |
| 1:F:164:THR:HG21 | 1:F:331:GLY:HA2  | 1.93                     | 0.50              |
| 1:I:25:VAL:HG23  | 1:I:25:VAL:O     | 2.12                     | 0.50              |
| 1:L:50:GLN:NE2   | 1:L:77:THR:OG1   | 2.44                     | 0.50              |
| 1:Q:90:VAL:HG11  | 1:U:70:GLU:O     | 2.12                     | 0.50              |
| 1:B:172:ALA:O    | 1:B:198:VAL:HG21 | 2.12                     | 0.50              |
| 1:E:149:ASP:N    | 1:E:150:PRO:HD3  | 2.27                     | 0.50              |
| 1:F:105:ARG:NH2  | 1:Q:13:ASN:O     | 2.44                     | 0.50              |
| 1:K:200:VAL:HG21 | 1:K:343:LEU:HA   | 1.94                     | 0.50              |
| 1:L:215:GLU:HB2  | 1:L:248:LEU:HD21 | 1.94                     | 0.50              |
| 1:N:339:ALA:HB2  | 1:c:26:LEU:HD12  | 1.93                     | 0.50              |
| 1:V:33:PHE:O     | 1:V:37:THR:HG23  | 2.11                     | 0.50              |
| 1:H:134:ARG:NE   | 1:H:136:ASP:OD2  | 2.44                     | 0.49              |
| 1:V:25:VAL:HG13  | 1:V:25:VAL:O     | 2.11                     | 0.49              |
| 1:b:140:ASP:OD1  | 1:b:140:ASP:C    | 2.55                     | 0.49              |
| 1:G:167:PHE:CD2  | 1:G:181:VAL:HG23 | 2.48                     | 0.49              |
| 1:J:87:LEU:CB    | 1:J:120:ILE:HD11 | 2.41                     | 0.49              |
| 1:O:96:THR:O     | 1:O:97:ALA:HB3   | 2.13                     | 0.49              |
| 1:P:52:ASP:OD1   | 1:P:53:ALA:N     | 2.45                     | 0.49              |
| 1:Q:136:ASP:OD1  | 1:Q:137:VAL:N    | 2.46                     | 0.49              |
| 1:W:123:ASP:O    | 1:W:127:ILE:HD12 | 2.12                     | 0.49              |
| 1:A:144:THR:O    | 1:A:146:SER:N    | 2.45                     | 0.49              |
| 1:C:317:LYS:HG2  | 1:C:318:ASP:H    | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:137:VAL:C    | 1:H:138:LEU:HD12 | 2.37                     | 0.49              |
| 1:M:322:GLU:OE2  | 1:M:324:TRP:NE1  | 2.45                     | 0.49              |
| 1:Q:206:ASN:ND2  | 1:Q:214:ASP:OD1  | 2.45                     | 0.49              |
| 1:S:103:TYR:O    | 1:W:50:GLN:NE2   | 2.45                     | 0.49              |
| 1:F:46:ILE:HD13  | 1:F:142:TYR:HD1  | 1.77                     | 0.49              |
| 1:I:218:ILE:HD12 | 1:I:218:ILE:H    | 1.77                     | 0.49              |
| 1:P:315:LEU:HD11 | 1:P:325:MET:HB2  | 1.93                     | 0.49              |
| 1:Y:49:TRP:NE1   | 1:Y:334:HIS:O    | 2.46                     | 0.49              |
| 1:O:30:ASP:OD1   | 1:O:30:ASP:N     | 2.45                     | 0.49              |
| 1:Q:248:LEU:HD23 | 1:Q:248:LEU:C    | 2.37                     | 0.49              |
| 1:T:16:LYS:C     | 1:T:17:LEU:HD12  | 2.36                     | 0.49              |
| 1:W:269:GLU:OE2  | 1:a:278:GLY:N    | 2.43                     | 0.49              |
| 1:c:85:GLN:HB2   | 1:c:164:THR:HG23 | 1.94                     | 0.49              |
| 1:K:144:THR:HG1  | 1:K:146:SER:HG   | 1.54                     | 0.49              |
| 1:L:129:LEU:HD13 | 1:L:289:MET:HG2  | 1.94                     | 0.49              |
| 1:S:136:ASP:OD1  | 1:S:137:VAL:N    | 2.43                     | 0.49              |
| 1:S:314:GLU:C    | 1:S:315:LEU:HD12 | 2.38                     | 0.49              |
| 1:I:105:ARG:NH2  | 1:I:108:GLU:OE1  | 2.46                     | 0.49              |
| 1:S:125:GLU:OE2  | 1:S:129:LEU:HD12 | 2.13                     | 0.49              |
| 1:T:122:ARG:NH1  | 1:X:55:ALA:O     | 2.39                     | 0.49              |
| 1:a:211:ILE:HG23 | 1:a:211:ILE:O    | 2.13                     | 0.49              |
| 1:d:157:ASP:O    | 1:d:158:THR:OG1  | 2.22                     | 0.49              |
| 1:B:131:GLY:HA2  | 1:B:180:VAL:HG13 | 1.95                     | 0.49              |
| 1:B:152:VAL:HG23 | 1:B:152:VAL:O    | 2.13                     | 0.49              |
| 1:G:166:ALA:C    | 1:G:167:PHE:CG   | 2.91                     | 0.49              |
| 1:W:240:ALA:O    | 1:W:243:LYS:NZ   | 2.45                     | 0.49              |
| 1:D:334:HIS:NE2  | 1:D:336:ASN:O    | 2.46                     | 0.49              |
| 1:E:44:GLN:O     | 1:E:46:ILE:N     | 2.45                     | 0.49              |
| 1:E:135:THR:HG22 | 1:E:135:THR:O    | 2.12                     | 0.49              |
| 1:N:190:ASP:O    | 1:N:194:GLY:N    | 2.41                     | 0.49              |
| 1:U:8:VAL:O      | 1:U:8:VAL:HG13   | 2.12                     | 0.49              |
| 1:D:180:VAL:HG22 | 1:D:181:VAL:N    | 2.28                     | 0.48              |
| 1:G:176:LEU:H    | 1:G:176:LEU:HD23 | 1.78                     | 0.48              |
| 1:H:132:GLN:NE2  | 1:H:164:THR:O    | 2.46                     | 0.48              |
| 1:I:224:GLN:O    | 1:I:227:THR:OG1  | 2.29                     | 0.48              |
| 1:N:336:ASN:O    | 1:N:339:ALA:N    | 2.46                     | 0.48              |
| 1:R:275:ASP:OD1  | 1:R:279:GLN:N    | 2.46                     | 0.48              |
| 1:U:213:PHE:CD1  | 1:U:345:THR:HG22 | 2.48                     | 0.48              |
| 1:Y:42:ILE:HD13  | 1:Y:305:MET:SD   | 2.52                     | 0.48              |
| 1:Z:213:PHE:CZ   | 1:Z:294:VAL:HG21 | 2.48                     | 0.48              |
| 1:R:33:PHE:O     | 1:R:37:THR:HG23  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:98:ASN:ND2   | 1:Y:108:GLU:OE1  | 2.42                     | 0.48              |
| 1:d:172:ALA:HB3  | 1:d:198:VAL:HG23 | 1.95                     | 0.48              |
| 1:A:52:ASP:N     | 1:A:52:ASP:OD1   | 2.46                     | 0.48              |
| 1:D:33:PHE:O     | 1:D:37:THR:HG23  | 2.13                     | 0.48              |
| 1:J:77:THR:O     | 1:P:13:ASN:ND2   | 2.41                     | 0.48              |
| 1:M:203:ASN:OD1  | 1:M:348:GLY:N    | 2.45                     | 0.48              |
| 1:d:93:VAL:HG21  | 1:d:109:LEU:HD13 | 1.95                     | 0.48              |
| 1:B:132:GLN:NE2  | 1:B:164:THR:OG1  | 2.46                     | 0.48              |
| 1:H:137:VAL:HG22 | 1:H:162:ARG:NH1  | 2.28                     | 0.48              |
| 1:V:33:PHE:CD2   | 1:V:129:LEU:HD21 | 2.48                     | 0.48              |
| 1:Z:213:PHE:HE1  | 1:Z:343:LEU:HD23 | 1.77                     | 0.48              |
| 1:D:196:VAL:HG22 | 1:D:196:VAL:O    | 2.13                     | 0.48              |
| 1:E:64:VAL:HG12  | 1:E:65:GLU:N     | 2.28                     | 0.48              |
| 1:H:91:VAL:HG12  | 1:H:324:TRP:HB2  | 1.95                     | 0.48              |
| 1:H:206:ASN:O    | 1:H:349:LYS:N    | 2.45                     | 0.48              |
| 1:V:259:ILE:HD11 | 1:Z:259:ILE:HB   | 1.95                     | 0.48              |
| 1:W:45:THR:HG21  | 1:W:162:ARG:HH12 | 1.79                     | 0.48              |
| 1:d:88:ARG:NE    | 1:d:327:GLU:OE2  | 2.47                     | 0.48              |
| 1:R:190:ASP:O    | 1:R:194:GLY:N    | 2.41                     | 0.48              |
| 1:U:92:ARG:NE    | 1:Y:71:ASP:OD1   | 2.46                     | 0.48              |
| 1:V:87:LEU:CB    | 1:V:120:ILE:HD11 | 2.43                     | 0.48              |
| 1:Z:97:ALA:O     | 1:Z:100:THR:OG1  | 2.26                     | 0.48              |
| 1:Z:250:GLU:OE2  | 1:c:256:ARG:NE   | 2.47                     | 0.48              |
| 1:B:182:ASP:OD1  | 1:B:183:LYS:N    | 2.46                     | 0.48              |
| 1:E:118:LYS:CB   | 1:F:54:LEU:HD21  | 2.44                     | 0.48              |
| 1:I:157:ASP:C    | 1:I:158:THR:HG1  | 2.15                     | 0.48              |
| 1:Y:199:LYS:NZ   | 1:Y:220:ASP:OD2  | 2.25                     | 0.48              |
| 1:D:213:PHE:CD2  | 1:D:244:ILE:HG21 | 2.48                     | 0.48              |
| 1:H:319:GLY:HA2  | 1:O:325:MET:HE1  | 1.94                     | 0.48              |
| 1:J:8:VAL:HG11   | 1:a:108:GLU:OE2  | 2.12                     | 0.48              |
| 1:K:91:VAL:HG12  | 1:K:91:VAL:O     | 2.13                     | 0.48              |
| 1:O:308:ARG:NH2  | 1:O:327:GLU:OE1  | 2.46                     | 0.48              |
| 1:C:156:ASN:OD1  | 1:G:3:ASN:ND2    | 2.47                     | 0.48              |
| 1:P:102:ASN:N    | 1:P:108:GLU:OE1  | 2.46                     | 0.48              |
| 1:Q:171:CYS:SG   | 1:Q:340:SER:OG   | 2.72                     | 0.48              |
| 1:T:295:TYR:CD1  | 1:T:342:VAL:HG22 | 2.49                     | 0.48              |
| 1:d:8:VAL:HG12   | 1:d:9:SER:N      | 2.28                     | 0.48              |
| 1:A:199:LYS:NZ   | 1:A:220:ASP:OD1  | 2.47                     | 0.48              |
| 1:B:10:TYR:OH    | 1:G:162:ARG:NH2  | 2.47                     | 0.48              |
| 1:B:73:GLU:O     | 1:F:116:LYS:NZ   | 2.41                     | 0.48              |
| 1:F:182:ASP:OD1  | 1:F:183:LYS:N    | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:97:ALA:O     | 1:J:100:THR:OG1  | 2.25                     | 0.48              |
| 1:c:289:MET:HE1  | 1:c:295:TYR:CD2  | 2.49                     | 0.48              |
| 1:K:231:GLU:O    | 1:K:232:ALA:HB3  | 2.14                     | 0.47              |
| 1:U:316:ALA:HB1  | 1:X:316:ALA:HB2  | 1.94                     | 0.47              |
| 1:V:122:ARG:NH1  | 1:Z:57:VAL:HG13  | 2.29                     | 0.47              |
| 1:A:176:LEU:HD23 | 1:A:176:LEU:O    | 2.14                     | 0.47              |
| 1:C:235:ILE:HG23 | 1:C:296:PHE:CE1  | 2.49                     | 0.47              |
| 1:D:275:ASP:OD1  | 1:D:279:GLN:N    | 2.47                     | 0.47              |
| 1:H:152:VAL:O    | 1:H:152:VAL:HG22 | 2.14                     | 0.47              |
| 1:J:152:VAL:HG12 | 1:J:152:VAL:O    | 2.14                     | 0.47              |
| 1:B:342:VAL:HG11 | 1:B:344:PHE:CE1  | 2.50                     | 0.47              |
| 1:G:30:ASP:O     | 1:G:31:THR:OG1   | 2.27                     | 0.47              |
| 1:M:82:ASN:ND2   | 1:M:332:LEU:O    | 2.41                     | 0.47              |
| 1:B:262:ASN:O    | 1:B:263:THR:OG1  | 2.32                     | 0.47              |
| 1:B:334:HIS:NE2  | 1:B:336:ASN:O    | 2.47                     | 0.47              |
| 1:C:171:CYS:SG   | 1:C:342:VAL:HG23 | 2.55                     | 0.47              |
| 1:b:85:GLN:HB2   | 1:b:164:THR:HG23 | 1.96                     | 0.47              |
| 1:A:208:THR:HG22 | 1:A:208:THR:O    | 2.15                     | 0.47              |
| 1:A:213:PHE:CD1  | 1:A:343:LEU:HD23 | 2.49                     | 0.47              |
| 1:K:275:ASP:OD1  | 1:K:279:GLN:N    | 2.48                     | 0.47              |
| 1:O:112:GLN:OE1  | 1:O:112:GLN:N    | 2.41                     | 0.47              |
| 1:d:152:VAL:HG23 | 1:d:152:VAL:O    | 2.14                     | 0.47              |
| 1:B:93:VAL:HG21  | 1:B:109:LEU:HD23 | 1.95                     | 0.47              |
| 1:E:142:TYR:HA   | 1:E:146:SER:HA   | 1.97                     | 0.47              |
| 1:G:90:VAL:HG12  | 1:G:325:MET:SD   | 2.55                     | 0.47              |
| 1:G:97:ALA:O     | 1:G:100:THR:OG1  | 2.32                     | 0.47              |
| 1:I:213:PHE:HD1  | 1:I:218:ILE:HD11 | 1.78                     | 0.47              |
| 1:K:42:ILE:O     | 1:K:307:LEU:HD12 | 2.15                     | 0.47              |
| 1:O:25:VAL:HG12  | 1:O:26:LEU:N     | 2.30                     | 0.47              |
| 1:W:180:VAL:HG22 | 1:W:181:VAL:N    | 2.30                     | 0.47              |
| 1:X:156:ASN:C    | 1:X:156:ASN:OD1  | 2.57                     | 0.47              |
| 1:E:112:GLN:NE2  | 1:F:74:MET:SD    | 2.85                     | 0.47              |
| 1:K:30:ASP:N     | 1:K:30:ASP:OD2   | 2.47                     | 0.47              |
| 1:W:64:VAL:HG12  | 1:W:65:GLU:N     | 2.30                     | 0.47              |
| 1:X:315:LEU:HD11 | 1:X:325:MET:HB2  | 1.96                     | 0.47              |
| 1:Z:85:GLN:NE2   | 1:c:61:ASN:O     | 2.48                     | 0.47              |
| 1:d:273:ILE:HG22 | 1:d:274:THR:N    | 2.30                     | 0.47              |
| 1:F:83:VAL:O     | 1:F:164:THR:HG22 | 2.14                     | 0.47              |
| 1:M:235:ILE:HG23 | 1:M:296:PHE:HE1  | 1.80                     | 0.47              |
| 1:Z:318:ASP:OD1  | 1:Z:318:ASP:N    | 2.48                     | 0.47              |
| 1:d:176:LEU:HD23 | 1:d:181:VAL:HG13 | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:184:THR:HG23 | 1:A:185:LYS:N    | 2.30                     | 0.47              |
| 1:F:91:VAL:HG11  | 1:F:113:LEU:HD12 | 1.96                     | 0.47              |
| 1:I:170:LEU:HD23 | 1:I:334:HIS:HB2  | 1.96                     | 0.47              |
| 1:N:231:GLU:N    | 1:N:231:GLU:OE1  | 2.48                     | 0.47              |
| 1:P:131:GLY:O    | 1:P:181:VAL:HG23 | 2.15                     | 0.47              |
| 1:R:82:ASN:ND2   | 1:R:332:LEU:O    | 2.43                     | 0.47              |
| 1:S:290:PRO:O    | 1:S:291:THR:HG22 | 2.15                     | 0.47              |
| 1:U:95:ASP:OD2   | 1:X:308:ARG:NH2  | 2.48                     | 0.47              |
| 1:V:152:VAL:HG22 | 1:V:152:VAL:O    | 2.14                     | 0.47              |
| 1:a:57:VAL:O     | 1:a:57:VAL:HG23  | 2.15                     | 0.47              |
| 1:c:289:MET:HE1  | 1:c:295:TYR:CE2  | 2.50                     | 0.47              |
| 1:B:95:ASP:OD1   | 1:B:96:THR:N     | 2.45                     | 0.46              |
| 1:L:53:ALA:HA    | 1:b:25:VAL:HG23  | 1.97                     | 0.46              |
| 1:M:200:VAL:HG13 | 1:M:200:VAL:O    | 2.14                     | 0.46              |
| 1:R:9:SER:N      | 1:Z:65:GLU:OE1   | 2.48                     | 0.46              |
| 1:X:30:ASP:N     | 1:X:30:ASP:OD1   | 2.46                     | 0.46              |
| 1:Z:308:ARG:NH2  | 1:Z:327:GLU:OE2  | 2.48                     | 0.46              |
| 1:I:313:THR:OG1  | 1:I:325:MET:O    | 2.32                     | 0.46              |
| 1:M:141:GLN:O    | 1:M:144:THR:HG22 | 2.16                     | 0.46              |
| 1:Z:64:VAL:HG12  | 1:Z:65:GLU:N     | 2.30                     | 0.46              |
| 1:Z:136:ASP:OD2  | 1:Z:136:ASP:N    | 2.48                     | 0.46              |
| 1:B:54:LEU:HD22  | 1:F:27:SER:CB    | 2.45                     | 0.46              |
| 1:Q:328:MET:HG2  | 1:Q:330:VAL:HG13 | 1.96                     | 0.46              |
| 1:U:45:THR:OG1   | 1:U:84:THR:OG1   | 2.31                     | 0.46              |
| 1:Y:113:LEU:HD22 | 1:Y:312:ARG:HG2  | 1.96                     | 0.46              |
| 1:Y:235:ILE:HG23 | 1:Y:296:PHE:CE1  | 2.49                     | 0.46              |
| 1:Z:336:ASN:O    | 1:Z:339:ALA:N    | 2.43                     | 0.46              |
| 1:B:66:GLY:O     | 1:F:88:ARG:NH2   | 2.45                     | 0.46              |
| 1:D:124:LEU:HD13 | 1:D:330:VAL:HG21 | 1.97                     | 0.46              |
| 1:F:213:PHE:CD1  | 1:F:345:THR:HG22 | 2.50                     | 0.46              |
| 1:T:172:ALA:O    | 1:T:198:VAL:HG21 | 2.14                     | 0.46              |
| 1:C:105:ARG:NH1  | 1:D:50:GLN:OE1   | 2.49                     | 0.46              |
| 1:D:131:GLY:O    | 1:D:180:VAL:HG23 | 2.16                     | 0.46              |
| 1:I:298:ARG:O    | 1:I:299:SER:OG   | 2.28                     | 0.46              |
| 1:S:177:ALA:N    | 1:S:180:VAL:O    | 2.40                     | 0.46              |
| 1:D:162:ARG:NH1  | 1:D:329:GLU:OE2  | 2.48                     | 0.46              |
| 1:F:85:GLN:HB2   | 1:F:164:THR:HG23 | 1.98                     | 0.46              |
| 1:F:143:LEU:O    | 1:F:144:THR:CG2  | 2.60                     | 0.46              |
| 1:M:203:ASN:OD1  | 1:M:204:ALA:N    | 2.46                     | 0.46              |
| 1:P:32:PRO:O     | 1:P:35:SER:N     | 2.46                     | 0.46              |
| 1:S:93:VAL:HG21  | 1:S:109:LEU:HD12 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:315:LEU:HD21 | 1:U:325:MET:HE3  | 1.98                     | 0.46              |
| 1:V:149:ASP:OD2  | 1:V:149:ASP:N    | 2.49                     | 0.46              |
| 1:W:259:ILE:HD12 | 1:a:259:ILE:HD11 | 1.97                     | 0.46              |
| 1:O:25:VAL:HG12  | 1:O:26:LEU:H     | 1.80                     | 0.46              |
| 1:U:52:ASP:OD1   | 1:U:53:ALA:N     | 2.41                     | 0.46              |
| 1:U:303:THR:OG1  | 1:U:333:ARG:NH1  | 2.49                     | 0.46              |
| 1:Y:136:ASP:OD1  | 1:Y:137:VAL:N    | 2.49                     | 0.46              |
| 1:c:213:PHE:O    | 1:c:214:ASP:C    | 2.59                     | 0.46              |
| 1:A:237:ILE:HG13 | 1:A:285:VAL:HG12 | 1.97                     | 0.46              |
| 1:E:215:GLU:O    | 1:E:217:ASP:N    | 2.49                     | 0.46              |
| 1:I:263:THR:O    | 1:I:264:LYS:HB3  | 2.15                     | 0.46              |
| 1:M:298:ARG:O    | 1:M:299:SER:OG   | 2.30                     | 0.46              |
| 1:R:318:ASP:N    | 1:R:318:ASP:OD1  | 2.49                     | 0.46              |
| 1:W:240:ALA:HA   | 1:a:223:LEU:HD11 | 1.97                     | 0.46              |
| 1:Y:197:THR:HG21 | 1:Y:338:TYR:HA   | 1.97                     | 0.46              |
| 1:Z:58:ASP:OD1   | 1:Z:59:GLY:N     | 2.48                     | 0.46              |
| 1:E:259:ILE:HD12 | 1:F:259:ILE:HD11 | 1.96                     | 0.46              |
| 1:J:43:ASN:OD1   | 1:P:100:THR:OG1  | 2.30                     | 0.46              |
| 1:O:238:ASN:ND2  | 1:O:293:ALA:O    | 2.49                     | 0.46              |
| 1:Q:294:VAL:HG22 | 1:Q:343:LEU:HB2  | 1.98                     | 0.46              |
| 1:R:88:ARG:NE    | 1:R:327:GLU:OE2  | 2.49                     | 0.46              |
| 1:W:200:VAL:HG12 | 1:W:200:VAL:O    | 2.16                     | 0.46              |
| 1:c:214:ASP:O    | 1:c:215:GLU:C    | 2.58                     | 0.46              |
| 1:U:263:THR:O    | 1:U:263:THR:HG22 | 2.16                     | 0.46              |
| 1:E:332:LEU:HD23 | 1:E:332:LEU:H    | 1.81                     | 0.45              |
| 1:W:83:VAL:HG12  | 1:W:84:THR:N     | 2.31                     | 0.45              |
| 1:W:180:VAL:HG22 | 1:W:181:VAL:H    | 1.81                     | 0.45              |
| 1:B:158:THR:HG23 | 1:B:158:THR:O    | 2.15                     | 0.45              |
| 1:E:12:GLN:NE2   | 1:X:108:GLU:OE2  | 2.49                     | 0.45              |
| 1:E:136:ASP:OD1  | 1:E:137:VAL:N    | 2.49                     | 0.45              |
| 1:J:237:ILE:HD11 | 1:J:241:HIS:HB2  | 1.98                     | 0.45              |
| 1:M:170:LEU:HD23 | 1:M:334:HIS:HB2  | 1.98                     | 0.45              |
| 1:N:70:GLU:N     | 1:N:70:GLU:OE2   | 2.49                     | 0.45              |
| 1:T:14:GLY:O     | 1:U:105:ARG:NH1  | 2.50                     | 0.45              |
| 1:W:172:ALA:HB2  | 1:W:198:VAL:HG21 | 1.97                     | 0.45              |
| 1:C:235:ILE:HD12 | 1:C:281:TYR:HB3  | 1.99                     | 0.45              |
| 1:F:124:LEU:HD13 | 1:F:330:VAL:HG21 | 1.97                     | 0.45              |
| 1:F:306:VAL:HG23 | 1:F:306:VAL:O    | 2.16                     | 0.45              |
| 1:T:113:LEU:HD21 | 1:T:312:ARG:CD   | 2.46                     | 0.45              |
| 1:Y:307:LEU:HD23 | 1:Y:329:GLU:OE1  | 2.16                     | 0.45              |
| 1:C:57:VAL:HG11  | 1:G:126:LYS:CD   | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:136:ASP:OD1  | 1:I:137:VAL:N    | 2.49                     | 0.45              |
| 1:K:65:GLU:CD    | 1:O:325:MET:HE2  | 2.42                     | 0.45              |
| 1:K:223:LEU:C    | 1:K:223:LEU:HD23 | 2.40                     | 0.45              |
| 1:L:30:ASP:O     | 1:L:31:THR:OG1   | 2.27                     | 0.45              |
| 1:M:8:VAL:O      | 1:M:8:VAL:HG13   | 2.16                     | 0.45              |
| 1:N:173:HIS:O    | 1:N:173:HIS:ND1  | 2.49                     | 0.45              |
| 1:S:180:VAL:HG12 | 1:S:181:VAL:N    | 2.32                     | 0.45              |
| 1:S:220:ASP:OD1  | 1:S:221:MET:N    | 2.50                     | 0.45              |
| 1:E:334:HIS:CD2  | 1:E:337:PRO:HA   | 2.51                     | 0.45              |
| 1:J:253:GLN:OE1  | 1:J:253:GLN:N    | 2.44                     | 0.45              |
| 1:L:275:ASP:OD1  | 1:L:279:GLN:N    | 2.38                     | 0.45              |
| 1:P:205:SER:O    | 1:P:206:ASN:ND2  | 2.49                     | 0.45              |
| 1:R:265:GLN:OE1  | 1:R:265:GLN:N    | 2.48                     | 0.45              |
| 1:S:117:GLY:O    | 1:S:120:ILE:HG22 | 2.16                     | 0.45              |
| 1:E:238:ASN:O    | 1:E:239:PRO:C    | 2.60                     | 0.45              |
| 1:K:58:ASP:OD2   | 1:O:122:ARG:NH1  | 2.44                     | 0.45              |
| 1:N:236:MET:HE2  | 1:N:297:PHE:HZ   | 1.81                     | 0.45              |
| 1:T:27:SER:CB    | 1:X:54:LEU:HD12  | 2.47                     | 0.45              |
| 1:B:213:PHE:HD2  | 1:B:244:ILE:HG21 | 1.82                     | 0.45              |
| 1:K:184:THR:HG22 | 1:K:184:THR:O    | 2.17                     | 0.45              |
| 1:U:10:TYR:OH    | 1:Y:162:ARG:NH1  | 2.49                     | 0.45              |
| 1:F:102:ASN:ND2  | 1:Q:12:GLN:OE1   | 2.47                     | 0.45              |
| 1:G:198:VAL:O    | 1:G:198:VAL:HG13 | 2.17                     | 0.45              |
| 1:T:152:VAL:O    | 1:T:152:VAL:HG22 | 2.17                     | 0.45              |
| 1:Y:291:THR:HG22 | 1:Y:291:THR:O    | 2.17                     | 0.45              |
| 1:c:82:ASN:ND2   | 1:c:332:LEU:O    | 2.50                     | 0.45              |
| 1:c:131:GLY:O    | 1:c:180:VAL:HG23 | 2.16                     | 0.45              |
| 1:H:190:ASP:O    | 1:H:194:GLY:N    | 2.48                     | 0.45              |
| 1:M:157:ASP:O    | 1:M:158:THR:OG1  | 2.26                     | 0.45              |
| 1:S:225:LEU:O    | 1:S:230:SER:OG   | 2.34                     | 0.45              |
| 1:V:55:ALA:O     | 1:V:56:SER:OG    | 2.25                     | 0.45              |
| 1:a:224:GLN:O    | 1:a:227:THR:HG22 | 2.17                     | 0.45              |
| 1:d:238:ASN:OD1  | 1:d:239:PRO:HD2  | 2.17                     | 0.45              |
| 1:D:182:ASP:OD1  | 1:D:183:LYS:N    | 2.50                     | 0.45              |
| 1:D:231:GLU:OE1  | 1:D:231:GLU:N    | 2.49                     | 0.45              |
| 1:H:40:GLU:OE1   | 1:H:305:MET:HE1  | 2.17                     | 0.45              |
| 1:J:117:GLY:O    | 1:J:120:ILE:HG22 | 2.17                     | 0.45              |
| 1:P:101:ALA:O    | 1:P:102:ASN:HB2  | 2.17                     | 0.45              |
| 1:d:162:ARG:O    | 1:d:163:LYS:C    | 2.60                     | 0.45              |
| 1:B:50:GLN:NE2   | 1:F:103:TYR:O    | 2.49                     | 0.44              |
| 1:B:122:ARG:NH1  | 1:G:192:ASP:OD1  | 2.49                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:91:VAL:HG22  | 1:P:74:MET:HE2   | 1.99                     | 0.44              |
| 1:K:102:ASN:OD1  | 1:K:105:ARG:NH2  | 2.49                     | 0.44              |
| 1:c:250:GLU:OE1  | 1:c:258:ARG:NH2  | 2.49                     | 0.44              |
| 1:I:294:VAL:HG22 | 1:I:343:LEU:HB2  | 1.98                     | 0.44              |
| 1:V:318:ASP:OD2  | 1:V:318:ASP:N    | 2.48                     | 0.44              |
| 1:H:214:ASP:OD1  | 1:H:244:ILE:HG22 | 2.17                     | 0.44              |
| 1:K:65:GLU:OE2   | 1:O:325:MET:HE2  | 2.18                     | 0.44              |
| 1:O:273:ILE:HG22 | 1:O:274:THR:N    | 2.31                     | 0.44              |
| 1:d:52:ASP:OD1   | 1:d:53:ALA:N     | 2.50                     | 0.44              |
| 1:C:52:ASP:OD2   | 1:C:53:ALA:N     | 2.46                     | 0.44              |
| 1:E:241:HIS:NE2  | 1:E:291:THR:O    | 2.48                     | 0.44              |
| 1:P:56:SER:OG    | 1:P:191:PRO:O    | 2.30                     | 0.44              |
| 1:c:71:ASP:OD1   | 1:c:71:ASP:N     | 2.49                     | 0.44              |
| 1:C:259:ILE:HD12 | 1:D:259:ILE:HD11 | 1.98                     | 0.44              |
| 1:I:162:ARG:NE   | 1:Y:10:TYR:OH    | 2.51                     | 0.44              |
| 1:J:180:VAL:HG12 | 1:J:181:VAL:N    | 2.33                     | 0.44              |
| 1:U:275:ASP:OD1  | 1:U:279:GLN:N    | 2.51                     | 0.44              |
| 1:Z:302:TRP:CE3  | 1:Z:332:LEU:HD21 | 2.52                     | 0.44              |
| 1:a:96:THR:O     | 1:a:100:THR:HG23 | 2.18                     | 0.44              |
| 1:d:157:ASP:OD2  | 1:d:157:ASP:N    | 2.49                     | 0.44              |
| 1:B:314:GLU:OE1  | 1:B:324:TRP:NE1  | 2.50                     | 0.44              |
| 1:C:207:PRO:HG2  | 1:C:209:THR:HG22 | 2.00                     | 0.44              |
| 1:D:30:ASP:OD1   | 1:D:30:ASP:N     | 2.50                     | 0.44              |
| 1:E:132:GLN:O    | 1:E:166:ALA:N    | 2.48                     | 0.44              |
| 1:H:93:VAL:HG21  | 1:H:108:GLU:O    | 2.18                     | 0.44              |
| 1:H:214:ASP:O    | 1:H:215:GLU:HG2  | 2.17                     | 0.44              |
| 1:H:302:TRP:O    | 1:H:303:THR:HG23 | 2.16                     | 0.44              |
| 1:T:237:ILE:HD11 | 1:T:241:HIS:HB2  | 2.00                     | 0.44              |
| 1:d:290:PRO:O    | 1:d:291:THR:HG22 | 2.17                     | 0.44              |
| 1:B:101:ALA:HB2  | 1:B:107:ARG:HB2  | 1.99                     | 0.44              |
| 1:E:81:SER:OG    | 1:E:82:ASN:N     | 2.51                     | 0.44              |
| 1:H:65:GLU:OE1   | 1:L:162:ARG:NH1  | 2.51                     | 0.44              |
| 1:N:252:THR:OG1  | 1:N:256:ARG:O    | 2.36                     | 0.44              |
| 1:P:67:SER:O     | 1:P:67:SER:OG    | 2.34                     | 0.44              |
| 1:U:202:GLN:O    | 1:U:203:ASN:OD1  | 2.35                     | 0.44              |
| 1:U:292:ASP:O    | 1:U:345:THR:HG23 | 2.18                     | 0.44              |
| 1:W:171:CYS:SG   | 1:W:340:SER:OG   | 2.76                     | 0.44              |
| 1:W:237:ILE:HG23 | 1:W:238:ASN:N    | 2.30                     | 0.44              |
| 1:W:273:ILE:HG22 | 1:W:274:THR:N    | 2.32                     | 0.44              |
| 1:X:220:ASP:OD1  | 1:X:221:MET:N    | 2.51                     | 0.44              |
| 1:A:197:THR:O    | 1:A:198:VAL:HG13 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:199:LYS:NZ   | 1:L:220:ASP:OD2  | 2.39                     | 0.44              |
| 1:P:222:THR:HG21 | 1:P:275:ASP:OD2  | 2.17                     | 0.44              |
| 1:R:143:LEU:HD23 | 1:R:143:LEU:H    | 1.82                     | 0.44              |
| 1:S:180:VAL:HG12 | 1:S:181:VAL:H    | 1.82                     | 0.44              |
| 1:X:328:MET:HE3  | 1:X:330:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:213:PHE:HE1  | 1:D:294:VAL:HG21 | 1.82                     | 0.44              |
| 1:L:149:ASP:OD1  | 1:L:149:ASP:N    | 2.51                     | 0.44              |
| 1:T:315:LEU:HG   | 1:T:316:ALA:H    | 1.83                     | 0.44              |
| 1:A:137:VAL:O    | 1:A:137:VAL:HG23 | 2.18                     | 0.43              |
| 1:L:36:MET:O     | 1:L:37:THR:C     | 2.60                     | 0.43              |
| 1:Y:279:GLN:CD   | 1:Y:281:TYR:HH   | 2.25                     | 0.43              |
| 1:a:317:LYS:NZ   | 1:a:322:GLU:OE1  | 2.46                     | 0.43              |
| 1:C:223:LEU:C    | 1:C:223:LEU:HD23 | 2.43                     | 0.43              |
| 1:E:237:ILE:HG21 | 1:E:285:VAL:HG22 | 1.99                     | 0.43              |
| 1:U:200:VAL:HG13 | 1:U:200:VAL:O    | 2.18                     | 0.43              |
| 1:W:45:THR:OG1   | 1:W:84:THR:OG1   | 2.25                     | 0.43              |
| 1:b:164:THR:HG21 | 1:b:331:GLY:HA2  | 1.99                     | 0.43              |
| 1:c:105:ARG:NH2  | 1:c:108:GLU:OE1  | 2.51                     | 0.43              |
| 1:c:136:ASP:OD2  | 1:c:142:TYR:OH   | 2.34                     | 0.43              |
| 1:P:11:ASP:O     | 1:P:12:GLN:C     | 2.62                     | 0.43              |
| 1:X:236:MET:HB3  | 1:X:289:MET:HE2  | 2.00                     | 0.43              |
| 1:a:147:ALA:HB1  | 1:a:150:PRO:HG3  | 2.00                     | 0.43              |
| 1:a:237:ILE:HD11 | 1:a:241:HIS:CB   | 2.48                     | 0.43              |
| 1:b:52:ASP:OD1   | 1:b:53:ALA:N     | 2.51                     | 0.43              |
| 1:d:30:ASP:OD1   | 1:d:31:THR:N     | 2.48                     | 0.43              |
| 1:C:156:ASN:O    | 1:C:159:HIS:NE2  | 2.51                     | 0.43              |
| 1:J:273:ILE:HG22 | 1:J:274:THR:N    | 2.32                     | 0.43              |
| 1:N:17:LEU:HG    | 1:N:18:SER:N     | 2.33                     | 0.43              |
| 1:S:262:ASN:ND2  | 1:W:265:GLN:O    | 2.47                     | 0.43              |
| 1:V:117:GLY:O    | 1:V:120:ILE:HG22 | 2.19                     | 0.43              |
| 1:C:143:LEU:O    | 1:C:144:THR:C    | 2.61                     | 0.43              |
| 1:H:96:THR:HG21  | 1:H:108:GLU:OE2  | 2.18                     | 0.43              |
| 1:J:25:VAL:O     | 1:J:25:VAL:HG13  | 2.17                     | 0.43              |
| 1:Q:125:GLU:OE2  | 1:Q:286:ASN:ND2  | 2.48                     | 0.43              |
| 1:R:83:VAL:HG12  | 1:R:84:THR:N     | 2.34                     | 0.43              |
| 1:V:87:LEU:HB3   | 1:V:120:ILE:HD11 | 2.00                     | 0.43              |
| 1:W:290:PRO:O    | 1:W:291:THR:HG22 | 2.18                     | 0.43              |
| 1:Z:87:LEU:CB    | 1:Z:120:ILE:HD11 | 2.48                     | 0.43              |
| 1:C:33:PHE:CZ    | 1:C:37:THR:HG21  | 2.53                     | 0.43              |
| 1:D:25:VAL:O     | 1:D:26:LEU:HD12  | 2.19                     | 0.43              |
| 1:D:91:VAL:HG13  | 1:D:91:VAL:O     | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:213:PHE:HB2  | 1:E:244:ILE:HG21 | 2.00                     | 0.43              |
| 1:J:51:THR:HG23  | 1:J:51:THR:O     | 2.19                     | 0.43              |
| 1:N:96:THR:O     | 1:N:100:THR:HG23 | 2.18                     | 0.43              |
| 1:W:92:ARG:O     | 1:W:93:VAL:C     | 2.61                     | 0.43              |
| 1:X:164:THR:O    | 1:X:164:THR:HG22 | 2.19                     | 0.43              |
| 1:B:79:ILE:HD11  | 1:Q:13:ASN:HB3   | 2.00                     | 0.43              |
| 1:D:43:ASN:OD1   | 1:D:44:GLN:N     | 2.50                     | 0.43              |
| 1:G:165:GLY:C    | 1:G:169:PHE:HB2  | 2.44                     | 0.43              |
| 1:L:30:ASP:OD1   | 1:L:30:ASP:N     | 2.49                     | 0.43              |
| 1:O:154:GLY:O    | 1:O:155:LEU:C    | 2.61                     | 0.43              |
| 1:R:52:ASP:OD1   | 1:R:53:ALA:N     | 2.49                     | 0.43              |
| 1:S:88:ARG:NH2   | 1:W:68:ARG:O     | 2.52                     | 0.43              |
| 1:T:96:THR:O     | 1:T:100:THR:OG1  | 2.34                     | 0.43              |
| 1:U:136:ASP:OD1  | 1:U:137:VAL:N    | 2.51                     | 0.43              |
| 1:c:152:VAL:HG12 | 1:c:152:VAL:O    | 2.19                     | 0.43              |
| 1:J:81:SER:OG    | 1:J:134:ARG:NH2  | 2.52                     | 0.43              |
| 1:L:267:ILE:HD13 | 1:b:262:ASN:HA   | 2.01                     | 0.43              |
| 1:M:262:ASN:OD1  | 1:M:263:THR:N    | 2.52                     | 0.43              |
| 1:T:290:PRO:O    | 1:T:291:THR:HG22 | 2.18                     | 0.43              |
| 1:U:213:PHE:HE1  | 1:U:345:THR:HG22 | 1.78                     | 0.43              |
| 1:Y:97:ALA:O     | 1:Y:100:THR:OG1  | 2.34                     | 0.43              |
| 1:Z:87:LEU:HB2   | 1:Z:120:ILE:HD11 | 2.01                     | 0.43              |
| 1:A:42:ILE:HG23  | 1:A:42:ILE:O     | 2.19                     | 0.43              |
| 1:A:326:ILE:O    | 1:A:326:ILE:HG23 | 2.19                     | 0.43              |
| 1:C:83:VAL:HG12  | 1:C:84:THR:N     | 2.34                     | 0.43              |
| 1:J:96:THR:O     | 1:J:100:THR:HG23 | 2.19                     | 0.43              |
| 1:L:88:ARG:NE    | 1:L:327:GLU:OE2  | 2.50                     | 0.43              |
| 1:X:190:ASP:O    | 1:X:194:GLY:N    | 2.45                     | 0.43              |
| 1:Z:162:ARG:NH1  | 1:Z:329:GLU:OE2  | 2.51                     | 0.43              |
| 1:b:85:GLN:CB    | 1:b:164:THR:HG23 | 2.49                     | 0.43              |
| 1:A:95:ASP:OD1   | 1:A:96:THR:N     | 2.51                     | 0.43              |
| 1:B:141:GLN:HG3  | 1:B:144:THR:HG23 | 2.01                     | 0.43              |
| 1:F:271:ASN:OD1  | 1:F:272:SER:N    | 2.52                     | 0.43              |
| 1:G:64:VAL:HG12  | 1:G:65:GLU:N     | 2.33                     | 0.43              |
| 1:I:87:LEU:H     | 1:I:87:LEU:HD23  | 1.84                     | 0.43              |
| 1:I:143:LEU:HD13 | 1:Y:17:LEU:HD22  | 1.99                     | 0.43              |
| 1:I:205:SER:OG   | 1:I:214:ASP:OD2  | 2.37                     | 0.43              |
| 1:P:8:VAL:O      | 1:P:9:SER:OG     | 2.31                     | 0.43              |
| 1:W:275:ASP:OD1  | 1:W:279:GLN:N    | 2.52                     | 0.43              |
| 1:Y:25:VAL:HG23  | 1:Y:25:VAL:O     | 2.19                     | 0.43              |
| 1:Y:309:ALA:O    | 1:Y:310:PRO:C    | 2.62                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:315:LEU:HD12 | 1:d:315:LEU:N    | 2.34                     | 0.43              |
| 1:R:336:ASN:O    | 1:R:339:ALA:N    | 2.42                     | 0.42              |
| 1:U:148:ALA:O    | 1:U:152:VAL:HG22 | 2.19                     | 0.42              |
| 1:W:253:GLN:OE1  | 1:W:253:GLN:N    | 2.42                     | 0.42              |
| 1:Y:263:THR:O    | 1:Y:264:LYS:HB3  | 2.19                     | 0.42              |
| 1:Z:211:ILE:O    | 1:Z:211:ILE:HG23 | 2.19                     | 0.42              |
| 1:M:202:GLN:N    | 1:M:217:ASP:OD2  | 2.47                     | 0.42              |
| 1:U:310:PRO:HB3  | 1:U:326:ILE:HD11 | 2.01                     | 0.42              |
| 1:W:25:VAL:HG13  | 1:W:25:VAL:O     | 2.18                     | 0.42              |
| 1:a:45:THR:HG22  | 1:a:307:LEU:HD13 | 2.01                     | 0.42              |
| 1:b:30:ASP:N     | 1:b:30:ASP:OD1   | 2.52                     | 0.42              |
| 1:d:143:LEU:C    | 1:d:144:THR:HG22 | 2.44                     | 0.42              |
| 1:d:275:ASP:OD1  | 1:d:279:GLN:N    | 2.48                     | 0.42              |
| 1:B:107:ARG:NH1  | 1:B:108:GLU:O    | 2.52                     | 0.42              |
| 1:B:132:GLN:O    | 1:B:166:ALA:N    | 2.51                     | 0.42              |
| 1:E:117:GLY:O    | 1:E:120:ILE:HG22 | 2.20                     | 0.42              |
| 1:I:241:HIS:NE2  | 1:I:291:THR:O    | 2.52                     | 0.42              |
| 1:J:250:GLU:OE2  | 1:R:256:ARG:NE   | 2.52                     | 0.42              |
| 1:Q:309:ALA:O    | 1:Q:310:PRO:C    | 2.62                     | 0.42              |
| 1:R:231:GLU:OE1  | 1:R:298:ARG:NH2  | 2.52                     | 0.42              |
| 1:V:307:LEU:HD23 | 1:V:329:GLU:OE1  | 2.19                     | 0.42              |
| 1:Y:34:VAL:HG13  | 1:Y:304:GLN:HE22 | 1.84                     | 0.42              |
| 1:A:343:LEU:O    | 1:A:344:PHE:C    | 2.62                     | 0.42              |
| 1:K:177:ALA:HB2  | 1:K:182:ASP:HB2  | 2.00                     | 0.42              |
| 1:K:320:SER:O    | 1:K:320:SER:OG   | 2.30                     | 0.42              |
| 1:T:64:VAL:O     | 1:T:65:GLU:HG3   | 2.18                     | 0.42              |
| 1:X:238:ASN:O    | 1:X:239:PRO:C    | 2.63                     | 0.42              |
| 1:A:181:VAL:HG23 | 1:A:181:VAL:O    | 2.20                     | 0.42              |
| 1:D:58:ASP:OD1   | 1:D:59:GLY:N     | 2.52                     | 0.42              |
| 1:G:167:PHE:HA   | 1:G:170:LEU:HA   | 2.01                     | 0.42              |
| 1:H:57:VAL:HG23  | 1:L:123:ASP:OD1  | 2.19                     | 0.42              |
| 1:H:305:MET:HE3  | 1:H:333:ARG:NE   | 2.34                     | 0.42              |
| 1:I:69:ALA:HB1   | 1:Y:90:VAL:HG11  | 2.02                     | 0.42              |
| 1:I:339:ALA:HA   | 1:Y:26:LEU:HD21  | 2.01                     | 0.42              |
| 1:J:11:ASP:N     | 1:J:11:ASP:OD1   | 2.52                     | 0.42              |
| 1:O:290:PRO:O    | 1:O:291:THR:HG22 | 2.19                     | 0.42              |
| 1:P:171:CYS:HG   | 1:P:340:SER:CB   | 2.26                     | 0.42              |
| 1:U:308:ARG:HG2  | 1:U:329:GLU:HB2  | 2.02                     | 0.42              |
| 1:X:138:LEU:N    | 1:X:138:LEU:HD12 | 2.33                     | 0.42              |
| 1:Z:33:PHE:O     | 1:Z:37:THR:HG23  | 2.19                     | 0.42              |
| 1:b:96:THR:O     | 1:b:100:THR:HG23 | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:4:PRO:O      | 1:d:5:THR:OG1    | 2.32                     | 0.42              |
| 1:A:144:THR:O    | 1:A:145:ASN:C    | 2.62                     | 0.42              |
| 1:A:168:GLN:CB   | 1:A:180:VAL:HG21 | 2.49                     | 0.42              |
| 1:A:248:LEU:O    | 1:A:252:THR:HG22 | 2.20                     | 0.42              |
| 1:B:117:GLY:O    | 1:B:120:ILE:HG22 | 2.20                     | 0.42              |
| 1:L:180:VAL:HG12 | 1:L:181:VAL:N    | 2.35                     | 0.42              |
| 1:N:298:ARG:O    | 1:N:299:SER:OG   | 2.34                     | 0.42              |
| 1:T:117:GLY:O    | 1:T:120:ILE:HG22 | 2.19                     | 0.42              |
| 1:W:139:ALA:O    | 1:W:141:GLN:NE2  | 2.51                     | 0.42              |
| 1:C:235:ILE:HG12 | 1:C:296:PHE:CD1  | 2.54                     | 0.42              |
| 1:E:83:VAL:HG21  | 1:E:164:THR:HA   | 2.00                     | 0.42              |
| 1:K:76:PRO:O     | 1:K:77:THR:HG22  | 2.20                     | 0.42              |
| 1:O:155:LEU:O    | 1:O:156:ASN:C    | 2.61                     | 0.42              |
| 1:E:83:VAL:HG11  | 1:E:164:THR:CA   | 2.47                     | 0.42              |
| 1:K:5:THR:O      | 1:K:5:THR:HG22   | 2.19                     | 0.42              |
| 1:O:180:VAL:HG22 | 1:O:181:VAL:N    | 2.35                     | 0.42              |
| 1:T:134:ARG:NH1  | 1:T:137:VAL:HG22 | 2.34                     | 0.42              |
| 1:a:157:ASP:O    | 1:a:158:THR:C    | 2.63                     | 0.42              |
| 1:d:223:LEU:HD23 | 1:d:223:LEU:C    | 2.45                     | 0.42              |
| 1:C:221:MET:HG3  | 1:C:296:PHE:CE2  | 2.54                     | 0.42              |
| 1:I:135:THR:HG23 | 1:I:135:THR:O    | 2.19                     | 0.42              |
| 1:N:293:ALA:HB2  | 1:N:344:PHE:HD1  | 1.84                     | 0.42              |
| 1:R:180:VAL:HG12 | 1:R:181:VAL:N    | 2.34                     | 0.42              |
| 1:b:90:VAL:HG12  | 1:b:91:VAL:N     | 2.35                     | 0.42              |
| 1:d:145:ASN:O    | 1:d:146:SER:CB   | 2.68                     | 0.42              |
| 1:K:136:ASP:OD1  | 1:K:137:VAL:N    | 2.49                     | 0.42              |
| 1:P:186:ASN:OD1  | 1:P:200:VAL:HG23 | 2.20                     | 0.42              |
| 1:P:213:PHE:CE1  | 1:P:244:ILE:HG21 | 2.55                     | 0.42              |
| 1:P:248:LEU:O    | 1:P:256:ARG:NH2  | 2.53                     | 0.42              |
| 1:R:230:SER:OG   | 1:R:231:GLU:N    | 2.52                     | 0.42              |
| 1:V:336:ASN:O    | 1:V:339:ALA:N    | 2.47                     | 0.42              |
| 1:C:90:VAL:HG12  | 1:C:91:VAL:N     | 2.35                     | 0.41              |
| 1:W:233:ASP:OD2  | 1:W:234:ILE:N    | 2.52                     | 0.41              |
| 1:X:124:LEU:HD22 | 1:X:328:MET:HE1  | 2.02                     | 0.41              |
| 1:Z:117:GLY:O    | 1:Z:120:ILE:HG22 | 2.20                     | 0.41              |
| 1:b:86:ILE:HG22  | 1:b:87:LEU:N     | 2.35                     | 0.41              |
| 1:C:134:ARG:NE   | 1:C:142:TYR:OH   | 2.53                     | 0.41              |
| 1:E:336:ASN:O    | 1:E:337:PRO:C    | 2.63                     | 0.41              |
| 1:K:264:LYS:NZ   | 1:S:269:GLU:OE1  | 2.43                     | 0.41              |
| 1:M:92:ARG:NE    | 1:Q:71:ASP:OD2   | 2.53                     | 0.41              |
| 1:Q:45:THR:HG1   | 1:Q:84:THR:HG1   | 1.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:236:MET:HG3  | 1:R:289:MET:SD   | 2.61                     | 0.41              |
| 1:c:57:VAL:HG23  | 1:c:57:VAL:O     | 2.19                     | 0.41              |
| 1:B:198:VAL:HG12 | 1:B:198:VAL:O    | 2.20                     | 0.41              |
| 1:C:8:VAL:HG22   | 1:C:9:SER:H      | 1.85                     | 0.41              |
| 1:E:33:PHE:O     | 1:E:37:THR:HG23  | 2.20                     | 0.41              |
| 1:F:93:VAL:HG22  | 1:Q:7:PHE:CD2    | 2.54                     | 0.41              |
| 1:I:18:SER:O     | 1:I:18:SER:OG    | 2.35                     | 0.41              |
| 1:I:74:MET:HE1   | 1:Y:92:ARG:O     | 2.19                     | 0.41              |
| 1:K:273:ILE:HG22 | 1:K:274:THR:N    | 2.35                     | 0.41              |
| 1:b:253:GLN:OE1  | 1:b:253:GLN:N    | 2.50                     | 0.41              |
| 1:c:215:GLU:O    | 1:c:216:ALA:HB3  | 2.20                     | 0.41              |
| 1:F:91:VAL:HG11  | 1:F:113:LEU:CD1  | 2.51                     | 0.41              |
| 1:G:88:ARG:CZ    | 1:G:325:MET:HE2  | 2.51                     | 0.41              |
| 1:H:83:VAL:HG22  | 1:H:84:THR:H     | 1.86                     | 0.41              |
| 1:L:303:THR:HG22 | 1:L:304:GLN:N    | 2.35                     | 0.41              |
| 1:Q:3:ASN:N      | 1:Q:4:PRO:CD     | 2.83                     | 0.41              |
| 1:Q:263:THR:O    | 1:Q:264:LYS:HB3  | 2.19                     | 0.41              |
| 1:a:88:ARG:NH1   | 1:d:64:VAL:O     | 2.47                     | 0.41              |
| 1:d:321:TYR:O    | 1:d:322:GLU:C    | 2.63                     | 0.41              |
| 1:d:322:GLU:OE2  | 1:d:324:TRP:NE1  | 2.48                     | 0.41              |
| 1:A:309:ALA:O    | 1:A:310:PRO:C    | 2.64                     | 0.41              |
| 1:B:54:LEU:HD22  | 1:F:27:SER:HB3   | 2.02                     | 0.41              |
| 1:C:241:HIS:NE2  | 1:C:291:THR:O    | 2.52                     | 0.41              |
| 1:Y:234:ILE:HD12 | 1:Y:299:SER:HB3  | 2.02                     | 0.41              |
| 1:B:131:GLY:HA3  | 1:B:180:VAL:HG13 | 2.01                     | 0.41              |
| 1:C:266:PHE:O    | 1:C:266:PHE:CG   | 2.72                     | 0.41              |
| 1:M:70:GLU:N     | 1:M:70:GLU:OE1   | 2.54                     | 0.41              |
| 1:N:286:ASN:OD1  | 1:N:288:TRP:N    | 2.53                     | 0.41              |
| 1:O:211:ILE:HG13 | 1:O:212:GLY:N    | 2.35                     | 0.41              |
| 1:O:263:THR:HG21 | 1:d:262:ASN:OD1  | 2.21                     | 0.41              |
| 1:V:82:ASN:ND2   | 1:V:332:LEU:O    | 2.50                     | 0.41              |
| 1:O:137:VAL:HG22 | 1:O:137:VAL:O    | 2.21                     | 0.41              |
| 1:P:73:GLU:O     | 1:P:73:GLU:HG3   | 2.20                     | 0.41              |
| 1:P:223:LEU:C    | 1:P:223:LEU:HD23 | 2.45                     | 0.41              |
| 1:Q:141:GLN:O    | 1:Q:144:THR:HG22 | 2.21                     | 0.41              |
| 1:S:64:VAL:CG1   | 1:S:65:GLU:H     | 2.29                     | 0.41              |
| 1:U:17:LEU:O     | 1:U:18:SER:C     | 2.63                     | 0.41              |
| 1:W:335:ARG:O    | 1:W:336:ASN:C    | 2.64                     | 0.41              |
| 1:Z:237:ILE:HD11 | 1:Z:241:HIS:CB   | 2.49                     | 0.41              |
| 1:a:127:ILE:HD11 | 1:d:60:ASN:HB3   | 2.03                     | 0.41              |
| 1:B:40:GLU:OE1   | 1:B:333:ARG:NH1  | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:273:ILE:HD12 | 1:C:283:ILE:HD11 | 2.03                     | 0.41              |
| 1:F:144:THR:O    | 1:F:145:ASN:CG   | 2.64                     | 0.41              |
| 1:N:146:SER:O    | 1:N:147:ALA:C    | 2.64                     | 0.41              |
| 1:O:125:GLU:OE2  | 1:O:286:ASN:ND2  | 2.53                     | 0.41              |
| 1:X:210:ASN:OD1  | 1:X:211:ILE:N    | 2.53                     | 0.41              |
| 1:a:70:GLU:HA    | 1:a:70:GLU:OE2   | 2.21                     | 0.41              |
| 1:d:239:PRO:O    | 1:d:240:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:168:GLN:NE2  | 1:A:344:PHE:CZ   | 2.88                     | 0.41              |
| 1:A:213:PHE:HD1  | 1:A:343:LEU:HD23 | 1.85                     | 0.41              |
| 1:B:66:GLY:O     | 1:F:88:ARG:NH1   | 2.51                     | 0.41              |
| 1:E:316:ALA:HB1  | 1:b:316:ALA:HB2  | 2.02                     | 0.41              |
| 1:F:237:ILE:HD11 | 1:F:241:HIS:HB2  | 2.01                     | 0.41              |
| 1:H:96:THR:O     | 1:H:96:THR:HG22  | 2.21                     | 0.41              |
| 1:H:305:MET:HE3  | 1:H:333:ARG:CZ   | 2.51                     | 0.41              |
| 1:I:256:ARG:HA   | 1:I:274:THR:HG22 | 2.02                     | 0.41              |
| 1:K:314:GLU:CG   | 1:K:314:GLU:O    | 2.68                     | 0.41              |
| 1:M:17:LEU:O     | 1:M:18:SER:C     | 2.64                     | 0.41              |
| 1:M:90:VAL:HG12  | 1:M:91:VAL:N     | 2.36                     | 0.41              |
| 1:M:208:THR:HG22 | 1:M:208:THR:O    | 2.20                     | 0.41              |
| 1:O:215:GLU:CG   | 1:O:248:LEU:HD13 | 2.50                     | 0.41              |
| 1:O:335:ARG:O    | 1:O:336:ASN:C    | 2.63                     | 0.41              |
| 1:P:263:THR:HG22 | 1:P:265:GLN:H    | 1.85                     | 0.41              |
| 1:R:85:GLN:HB2   | 1:R:164:THR:HG23 | 2.02                     | 0.41              |
| 1:S:137:VAL:O    | 1:S:137:VAL:HG22 | 2.20                     | 0.41              |
| 1:V:82:ASN:OD1   | 1:V:165:GLY:N    | 2.54                     | 0.41              |
| 1:V:290:PRO:O    | 1:V:291:THR:HG22 | 2.21                     | 0.41              |
| 1:W:18:SER:OG    | 1:a:46:ILE:O     | 2.39                     | 0.41              |
| 1:W:21:ASN:OD1   | 1:W:22:TRP:N     | 2.53                     | 0.41              |
| 1:W:30:ASP:N     | 1:W:30:ASP:OD1   | 2.53                     | 0.41              |
| 1:Y:91:VAL:HG13  | 1:Y:91:VAL:O     | 2.20                     | 0.41              |
| 1:Y:141:GLN:O    | 1:Y:144:THR:HG22 | 2.20                     | 0.41              |
| 1:Y:310:PRO:HG2  | 1:Y:328:MET:HE3  | 2.02                     | 0.41              |
| 1:Z:259:ILE:HD11 | 1:c:259:ILE:HB   | 2.02                     | 0.41              |
| 1:d:9:SER:O      | 1:d:9:SER:OG     | 2.36                     | 0.41              |
| 1:d:293:ALA:HB2  | 1:d:344:PHE:HD1  | 1.85                     | 0.41              |
| 1:C:326:ILE:HG22 | 1:C:327:GLU:N    | 2.35                     | 0.41              |
| 1:H:90:VAL:HG11  | 1:P:69:ALA:HB2   | 2.01                     | 0.41              |
| 1:H:108:GLU:OE2  | 1:d:12:GLN:NE2   | 2.54                     | 0.41              |
| 1:H:213:PHE:O    | 1:H:213:PHE:CG   | 2.74                     | 0.41              |
| 1:J:203:ASN:ND2  | 1:J:210:ASN:OD1  | 2.53                     | 0.41              |
| 1:O:70:GLU:O     | 1:d:90:VAL:HG11  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:105:ARG:NH2  | 1:T:108:GLU:OE2  | 2.54                     | 0.41              |
| 1:F:40:GLU:OE1   | 1:F:333:ARG:NH1  | 2.54                     | 0.40              |
| 1:F:64:VAL:HG12  | 1:F:65:GLU:N     | 2.36                     | 0.40              |
| 1:H:83:VAL:HG22  | 1:H:84:THR:N     | 2.36                     | 0.40              |
| 1:I:286:ASN:OD1  | 1:I:287:ARG:N    | 2.54                     | 0.40              |
| 1:Q:45:THR:OG1   | 1:Q:84:THR:OG1   | 2.29                     | 0.40              |
| 1:R:12:GLN:O     | 1:R:13:ASN:C     | 2.64                     | 0.40              |
| 1:X:298:ARG:NH1  | 1:X:301:ASP:OD1  | 2.52                     | 0.40              |
| 1:c:273:ILE:HG22 | 1:c:274:THR:N    | 2.36                     | 0.40              |
| 1:c:336:ASN:O    | 1:c:339:ALA:N    | 2.48                     | 0.40              |
| 1:d:298:ARG:O    | 1:d:299:SER:HB3  | 2.21                     | 0.40              |
| 1:G:40:GLU:O     | 1:G:41:SER:C     | 2.64                     | 0.40              |
| 1:H:237:ILE:O    | 1:H:285:VAL:HA   | 2.21                     | 0.40              |
| 1:S:105:ARG:O    | 1:S:106:GLY:C    | 2.64                     | 0.40              |
| 1:U:315:LEU:CD2  | 1:U:325:MET:HE3  | 2.51                     | 0.40              |
| 1:X:81:SER:O     | 1:X:134:ARG:NH2  | 2.54                     | 0.40              |
| 1:Y:87:LEU:HD23  | 1:Y:87:LEU:H     | 1.85                     | 0.40              |
| 1:d:231:GLU:O    | 1:d:232:ALA:HB3  | 2.21                     | 0.40              |
| 1:E:42:ILE:O     | 1:E:43:ASN:CB    | 2.70                     | 0.40              |
| 1:F:317:LYS:O    | 1:F:318:ASP:OD1  | 2.39                     | 0.40              |
| 1:K:88:ARG:NH1   | 1:S:64:VAL:O     | 2.48                     | 0.40              |
| 1:K:336:ASN:O    | 1:K:337:PRO:C    | 2.63                     | 0.40              |
| 1:S:321:TYR:O    | 1:S:322:GLU:C    | 2.63                     | 0.40              |
| 1:U:95:ASP:N     | 1:U:95:ASP:OD1   | 2.54                     | 0.40              |
| 1:V:87:LEU:HB2   | 1:V:120:ILE:HD11 | 2.03                     | 0.40              |
| 1:A:200:VAL:HG22 | 1:A:200:VAL:O    | 2.21                     | 0.40              |
| 1:E:144:THR:N    | 1:E:146:SER:OG   | 2.55                     | 0.40              |
| 1:F:95:ASP:O     | 1:U:308:ARG:NH2  | 2.54                     | 0.40              |
| 1:G:57:VAL:HG22  | 1:G:58:ASP:N     | 2.37                     | 0.40              |
| 1:O:200:VAL:O    | 1:O:200:VAL:HG13 | 2.20                     | 0.40              |
| 1:R:31:THR:HB    | 1:R:34:VAL:HG22  | 2.03                     | 0.40              |
| 1:R:78:VAL:HG12  | 1:R:79:ILE:N     | 2.36                     | 0.40              |
| 1:T:113:LEU:HD21 | 1:T:312:ARG:HD3  | 2.03                     | 0.40              |
| 1:W:47:PHE:HB2   | 1:W:305:MET:HE1  | 2.03                     | 0.40              |
| 1:d:162:ARG:O    | 1:d:164:THR:HG23 | 2.22                     | 0.40              |
| 1:C:57:VAL:HG13  | 1:G:123:ASP:CG   | 2.46                     | 0.40              |
| 1:J:61:ASN:HB3   | 1:N:87:LEU:HD22  | 2.04                     | 0.40              |
| 1:S:335:ARG:O    | 1:S:336:ASN:C    | 2.64                     | 0.40              |
| 1:T:88:ARG:NH1   | 1:X:65:GLU:O     | 2.54                     | 0.40              |
| 1:Z:302:TRP:CZ3  | 1:Z:332:LEU:HD21 | 2.56                     | 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     | 343/352 (97%) | 286 (83%) | 57 (17%) | 0        | 100         | 100 |
| 1   | B     | 344/352 (98%) | 284 (83%) | 59 (17%) | 1 (0%)   | 36          | 65  |
| 1   | C     | 345/352 (98%) | 309 (90%) | 36 (10%) | 0        | 100         | 100 |
| 1   | D     | 343/352 (97%) | 308 (90%) | 35 (10%) | 0        | 100         | 100 |
| 1   | E     | 344/352 (98%) | 272 (79%) | 68 (20%) | 4 (1%)   | 10          | 35  |
| 1   | F     | 344/352 (98%) | 298 (87%) | 46 (13%) | 0        | 100         | 100 |
| 1   | G     | 345/352 (98%) | 288 (84%) | 56 (16%) | 1 (0%)   | 36          | 65  |
| 1   | H     | 339/352 (96%) | 303 (89%) | 36 (11%) | 0        | 100         | 100 |
| 1   | I     | 344/352 (98%) | 322 (94%) | 22 (6%)  | 0        | 100         | 100 |
| 1   | J     | 340/352 (97%) | 308 (91%) | 32 (9%)  | 0        | 100         | 100 |
| 1   | K     | 345/352 (98%) | 276 (80%) | 68 (20%) | 1 (0%)   | 36          | 65  |
| 1   | L     | 345/352 (98%) | 314 (91%) | 31 (9%)  | 0        | 100         | 100 |
| 1   | M     | 344/352 (98%) | 318 (92%) | 26 (8%)  | 0        | 100         | 100 |
| 1   | N     | 345/352 (98%) | 314 (91%) | 31 (9%)  | 0        | 100         | 100 |
| 1   | O     | 345/352 (98%) | 264 (76%) | 81 (24%) | 0        | 100         | 100 |
| 1   | P     | 341/352 (97%) | 294 (86%) | 47 (14%) | 0        | 100         | 100 |
| 1   | Q     | 344/352 (98%) | 324 (94%) | 20 (6%)  | 0        | 100         | 100 |
| 1   | R     | 340/352 (97%) | 310 (91%) | 30 (9%)  | 0        | 100         | 100 |
| 1   | S     | 339/352 (96%) | 287 (85%) | 52 (15%) | 0        | 100         | 100 |
| 1   | T     | 343/352 (97%) | 306 (89%) | 37 (11%) | 0        | 100         | 100 |
| 1   | U     | 344/352 (98%) | 313 (91%) | 31 (9%)  | 0        | 100         | 100 |
| 1   | V     | 343/352 (97%) | 307 (90%) | 36 (10%) | 0        | 100         | 100 |
| 1   | W     | 345/352 (98%) | 298 (86%) | 47 (14%) | 0        | 100         | 100 |
| 1   | X     | 344/352 (98%) | 312 (91%) | 32 (9%)  | 0        | 100         | 100 |
| 1   | Y     | 344/352 (98%) | 319 (93%) | 25 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 1   | Z     | 345/352 (98%)     | 323 (94%)  | 22 (6%)    | 0        | 100         | 100 |
| 1   | a     | 344/352 (98%)     | 284 (83%)  | 60 (17%)   | 0        | 100         | 100 |
| 1   | b     | 344/352 (98%)     | 328 (95%)  | 16 (5%)    | 0        | 100         | 100 |
| 1   | c     | 345/352 (98%)     | 311 (90%)  | 34 (10%)   | 0        | 100         | 100 |
| 1   | d     | 345/352 (98%)     | 286 (83%)  | 59 (17%)   | 0        | 100         | 100 |
| All | All   | 10305/10560 (98%) | 9066 (88%) | 1232 (12%) | 7 (0%)   | 49          | 78  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 44  | GLN  |
| 1   | G     | 168 | GLN  |
| 1   | B     | 20  | ALA  |
| 1   | E     | 45  | THR  |
| 1   | E     | 145 | ASN  |
| 1   | K     | 204 | ALA  |
| 1   | E     | 42  | ILE  |

### 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     | 285/287 (99%)  | 285 (100%) | 0        | 100         | 100 |
| 1   | B     | 285/287 (99%)  | 285 (100%) | 0        | 100         | 100 |
| 1   | C     | 286/287 (100%) | 286 (100%) | 0        | 100         | 100 |
| 1   | D     | 284/287 (99%)  | 284 (100%) | 0        | 100         | 100 |
| 1   | E     | 285/287 (99%)  | 285 (100%) | 0        | 100         | 100 |
| 1   | F     | 285/287 (99%)  | 285 (100%) | 0        | 100         | 100 |
| 1   | G     | 286/287 (100%) | 286 (100%) | 0        | 100         | 100 |
| 1   | H     | 283/287 (99%)  | 283 (100%) | 0        | 100         | 100 |
| 1   | I     | 285/287 (99%)  | 285 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | J     | 281/287 (98%)   | 281 (100%)  | 0        | 100         | 100 |
| 1   | K     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | L     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | M     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | N     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | O     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | P     | 282/287 (98%)   | 282 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | R     | 281/287 (98%)   | 281 (100%)  | 0        | 100         | 100 |
| 1   | S     | 280/287 (98%)   | 280 (100%)  | 0        | 100         | 100 |
| 1   | T     | 284/287 (99%)   | 284 (100%)  | 0        | 100         | 100 |
| 1   | U     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | V     | 284/287 (99%)   | 284 (100%)  | 0        | 100         | 100 |
| 1   | W     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | X     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | Y     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | Z     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | a     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | b     | 285/287 (99%)   | 285 (100%)  | 0        | 100         | 100 |
| 1   | c     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| 1   | d     | 286/287 (100%)  | 286 (100%)  | 0        | 100         | 100 |
| All | All   | 8539/8610 (99%) | 8539 (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 (71) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | GLN  |
| 1   | A     | 203 | ASN  |
| 1   | A     | 241 | HIS  |
| 1   | A     | 249 | GLN  |
| 1   | B     | 271 | ASN  |
| 1   | B     | 279 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 112 | GLN  |
| 1   | C     | 141 | GLN  |
| 1   | C     | 253 | GLN  |
| 1   | D     | 63  | HIS  |
| 1   | E     | 12  | GLN  |
| 1   | E     | 202 | GLN  |
| 1   | F     | 29  | GLN  |
| 1   | F     | 159 | HIS  |
| 1   | F     | 206 | ASN  |
| 1   | G     | 61  | ASN  |
| 1   | G     | 238 | ASN  |
| 1   | G     | 279 | GLN  |
| 1   | H     | 202 | GLN  |
| 1   | H     | 203 | ASN  |
| 1   | H     | 279 | GLN  |
| 1   | I     | 168 | GLN  |
| 1   | I     | 249 | GLN  |
| 1   | I     | 279 | GLN  |
| 1   | I     | 304 | GLN  |
| 1   | J     | 145 | ASN  |
| 1   | J     | 251 | ASN  |
| 1   | K     | 186 | ASN  |
| 1   | L     | 50  | GLN  |
| 1   | L     | 279 | GLN  |
| 1   | M     | 249 | GLN  |
| 1   | M     | 251 | ASN  |
| 1   | M     | 279 | GLN  |
| 1   | N     | 206 | ASN  |
| 1   | O     | 3   | ASN  |
| 1   | O     | 43  | ASN  |
| 1   | O     | 145 | ASN  |
| 1   | O     | 173 | HIS  |
| 1   | O     | 336 | ASN  |
| 1   | Q     | 85  | GLN  |
| 1   | R     | 238 | ASN  |
| 1   | R     | 241 | HIS  |
| 1   | S     | 12  | GLN  |
| 1   | S     | 206 | ASN  |
| 1   | S     | 210 | ASN  |
| 1   | T     | 132 | GLN  |
| 1   | T     | 336 | ASN  |
| 1   | W     | 262 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 12  | GLN  |
| 1   | X     | 13  | ASN  |
| 1   | X     | 60  | ASN  |
| 1   | X     | 202 | GLN  |
| 1   | Y     | 102 | ASN  |
| 1   | Y     | 206 | ASN  |
| 1   | Z     | 44  | GLN  |
| 1   | Z     | 60  | ASN  |
| 1   | Z     | 102 | ASN  |
| 1   | Z     | 206 | ASN  |
| 1   | a     | 141 | GLN  |
| 1   | a     | 168 | GLN  |
| 1   | a     | 241 | HIS  |
| 1   | a     | 262 | ASN  |
| 1   | c     | 44  | GLN  |
| 1   | c     | 85  | GLN  |
| 1   | c     | 102 | ASN  |
| 1   | c     | 241 | HIS  |
| 1   | c     | 279 | GLN  |
| 1   | d     | 43  | ASN  |
| 1   | d     | 63  | HIS  |
| 1   | d     | 210 | ASN  |
| 1   | d     | 251 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

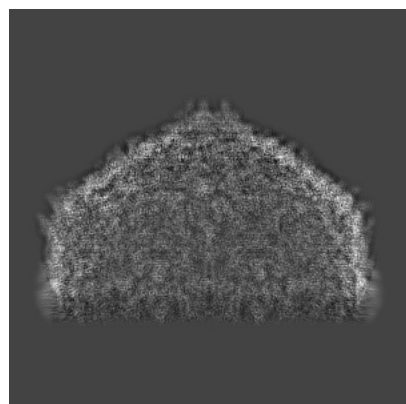
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14485. These allow visual inspection of the internal detail of the map and identification of artifacts.

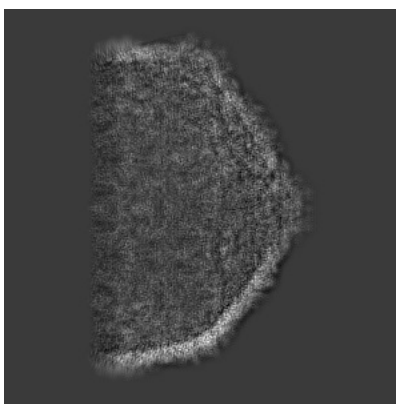
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

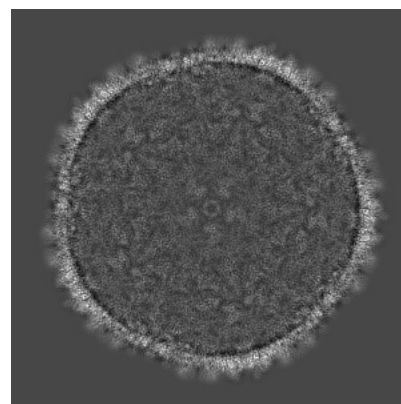
#### 6.1.1 Primary map



X

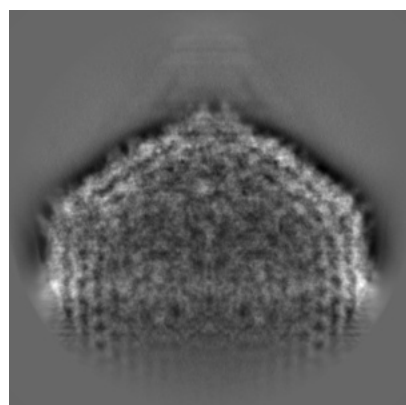


Y

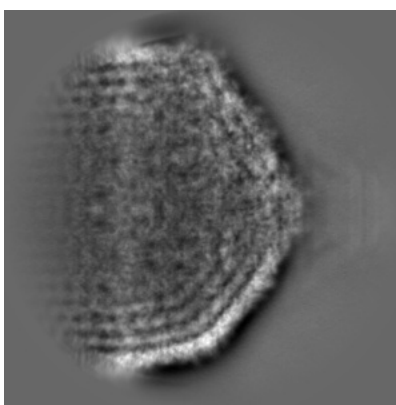


Z

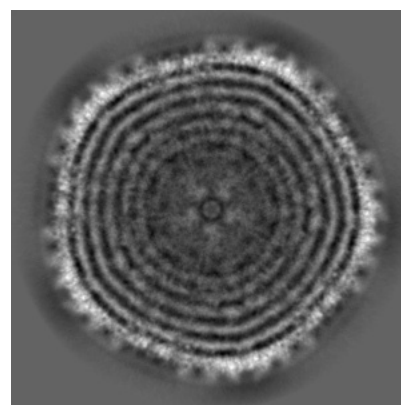
#### 6.1.2 Raw map



X



Y



Z

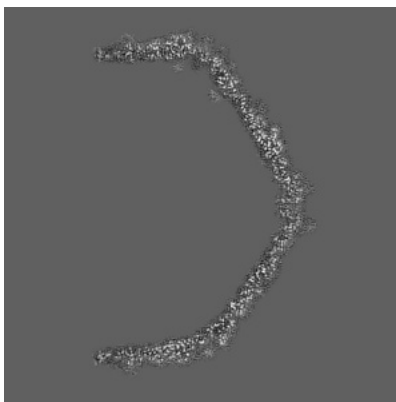
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

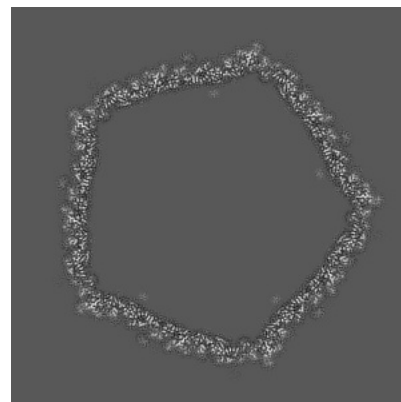
### 6.2.1 Primary map



X Index: 200

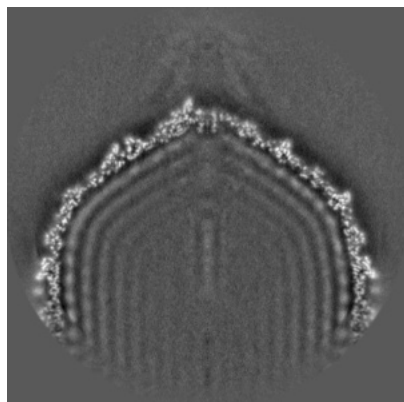


Y Index: 200

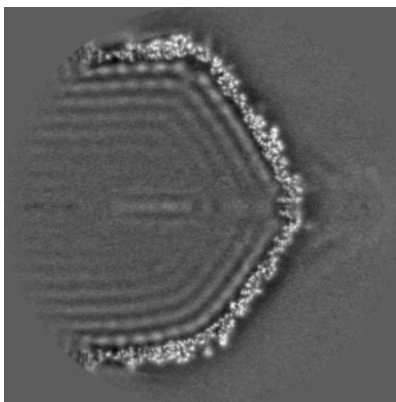


Z Index: 200

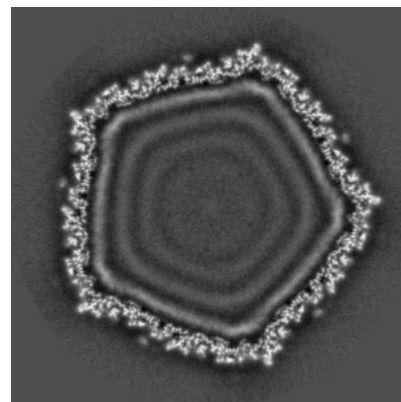
### 6.2.2 Raw map



X Index: 200



Y Index: 200

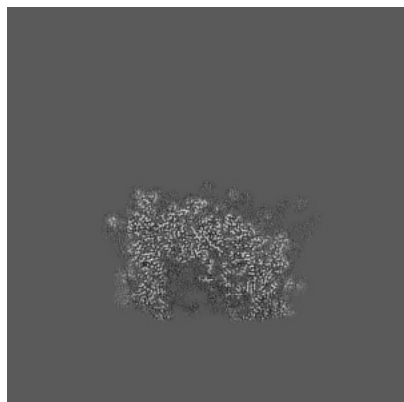


Z Index: 200

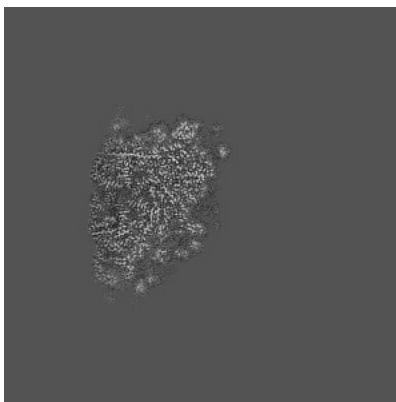
The images above show central slices of the map in three orthogonal directions.

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

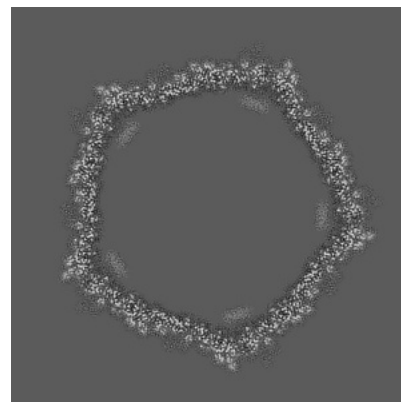
### 6.3.1 Primary map



X Index: 58

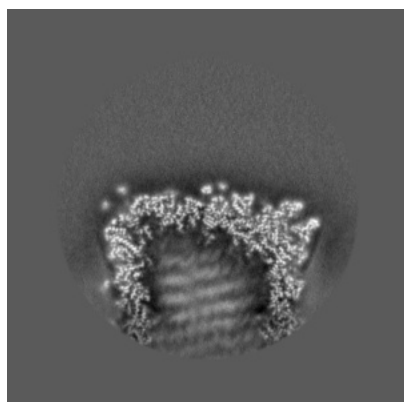


Y Index: 347

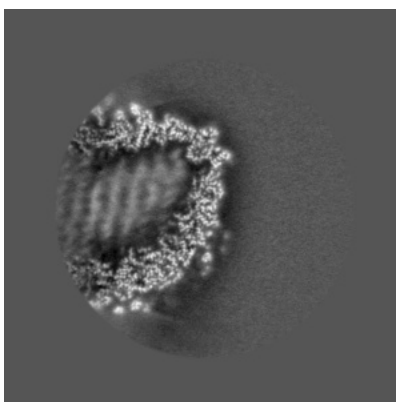


Z Index: 210

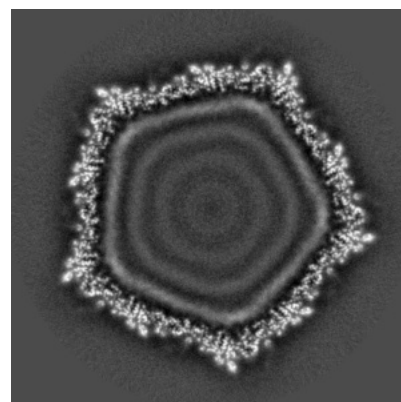
### 6.3.2 Raw map



X Index: 66



Y Index: 335

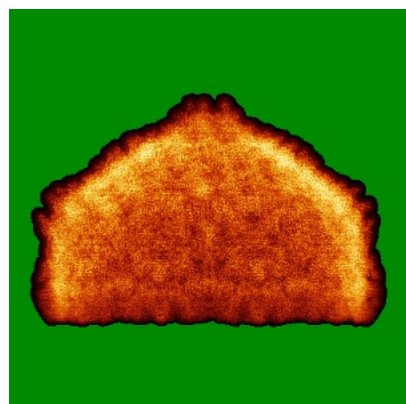


Z Index: 211

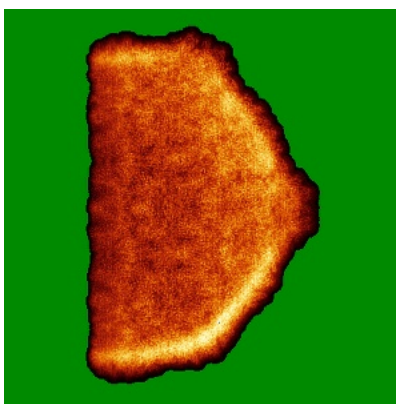
The images above show the largest variance slices of the map in three orthogonal directions.

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

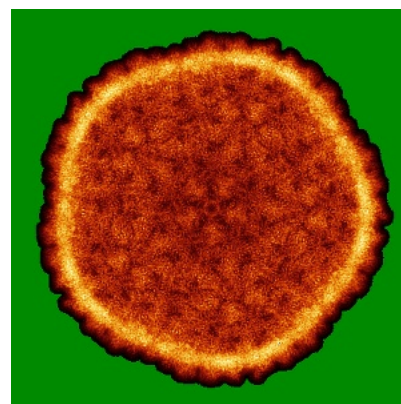
### 6.4.1 Primary map



X

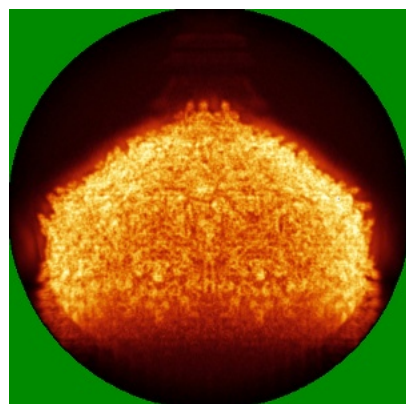


Y

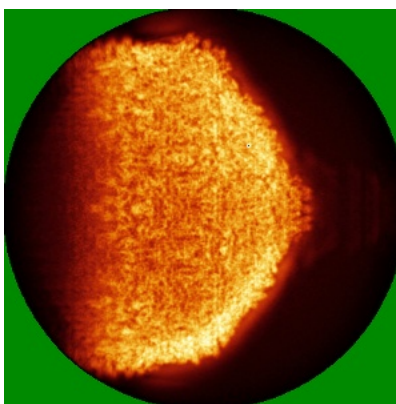


Z

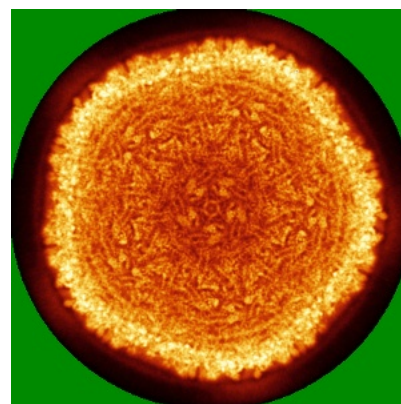
### 6.4.2 Raw map



X



Y

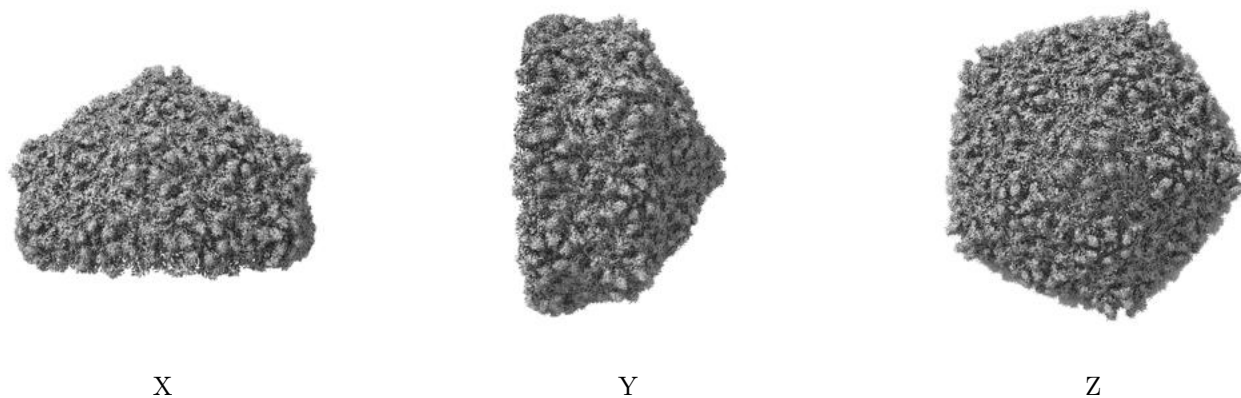


Z

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.

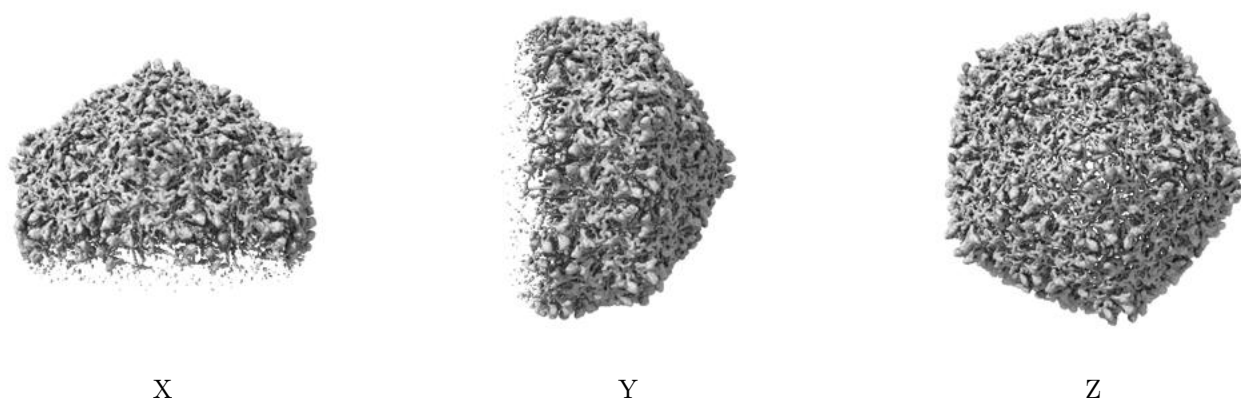
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

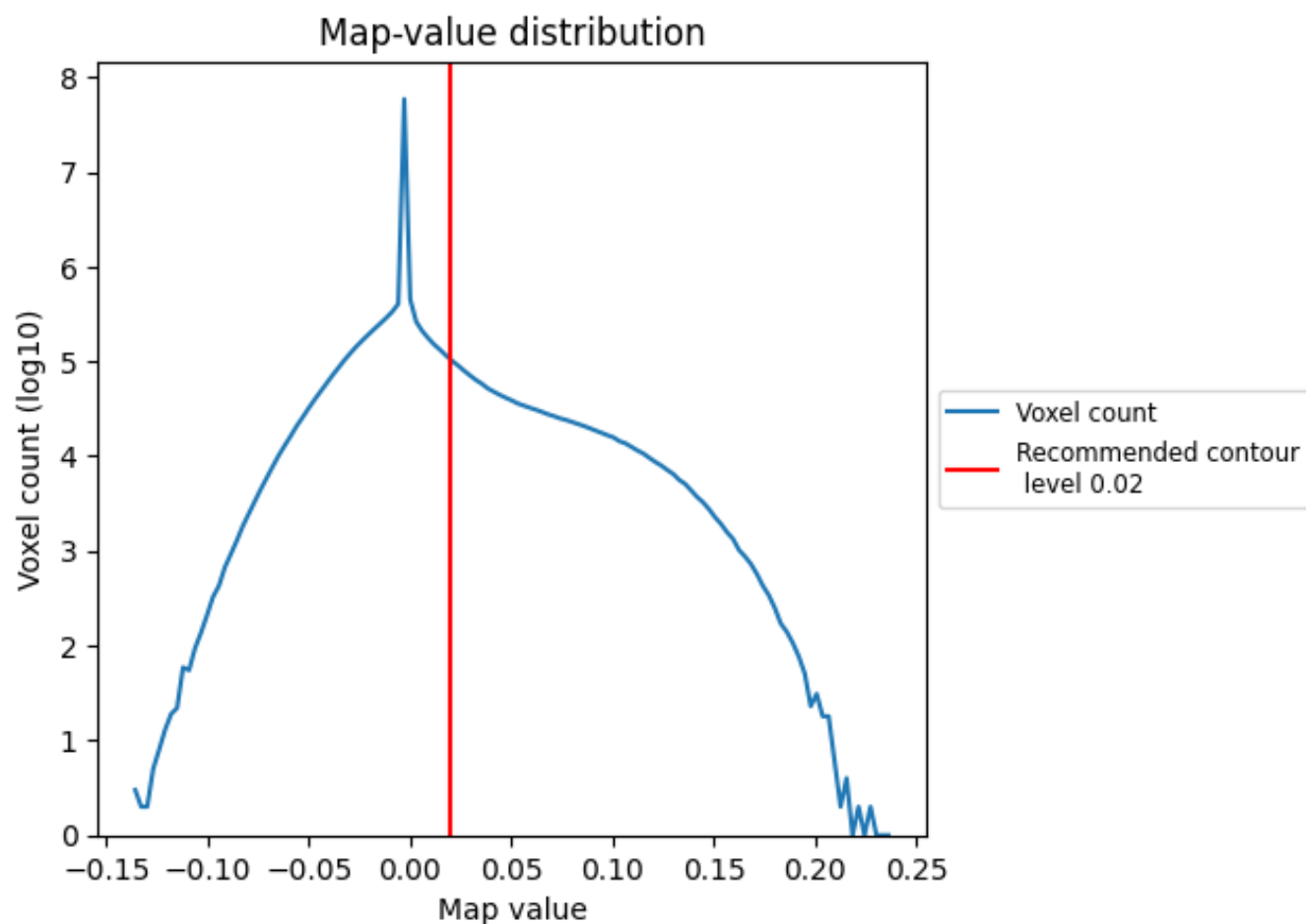
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

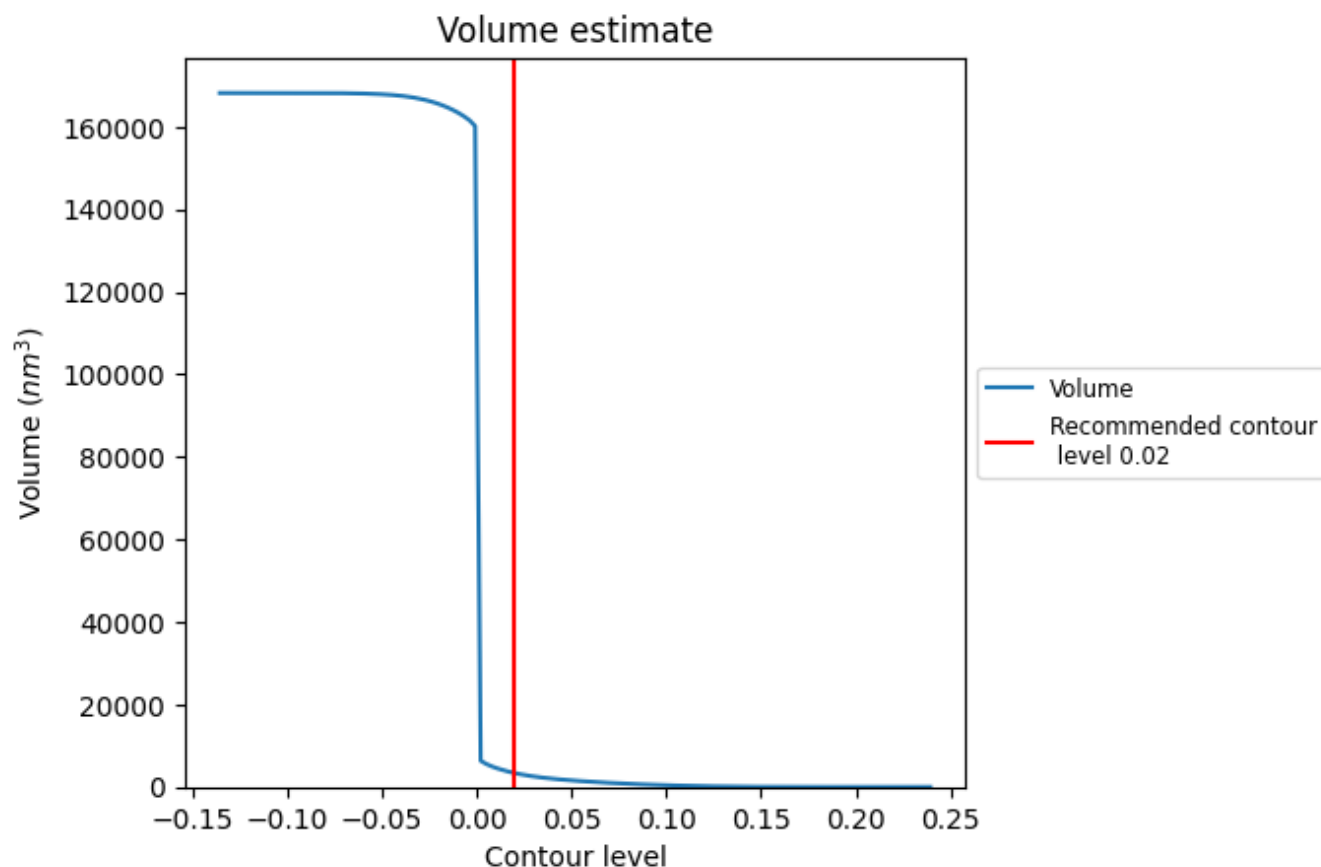
This section contains the results of statistical analysis of the map.

### 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.

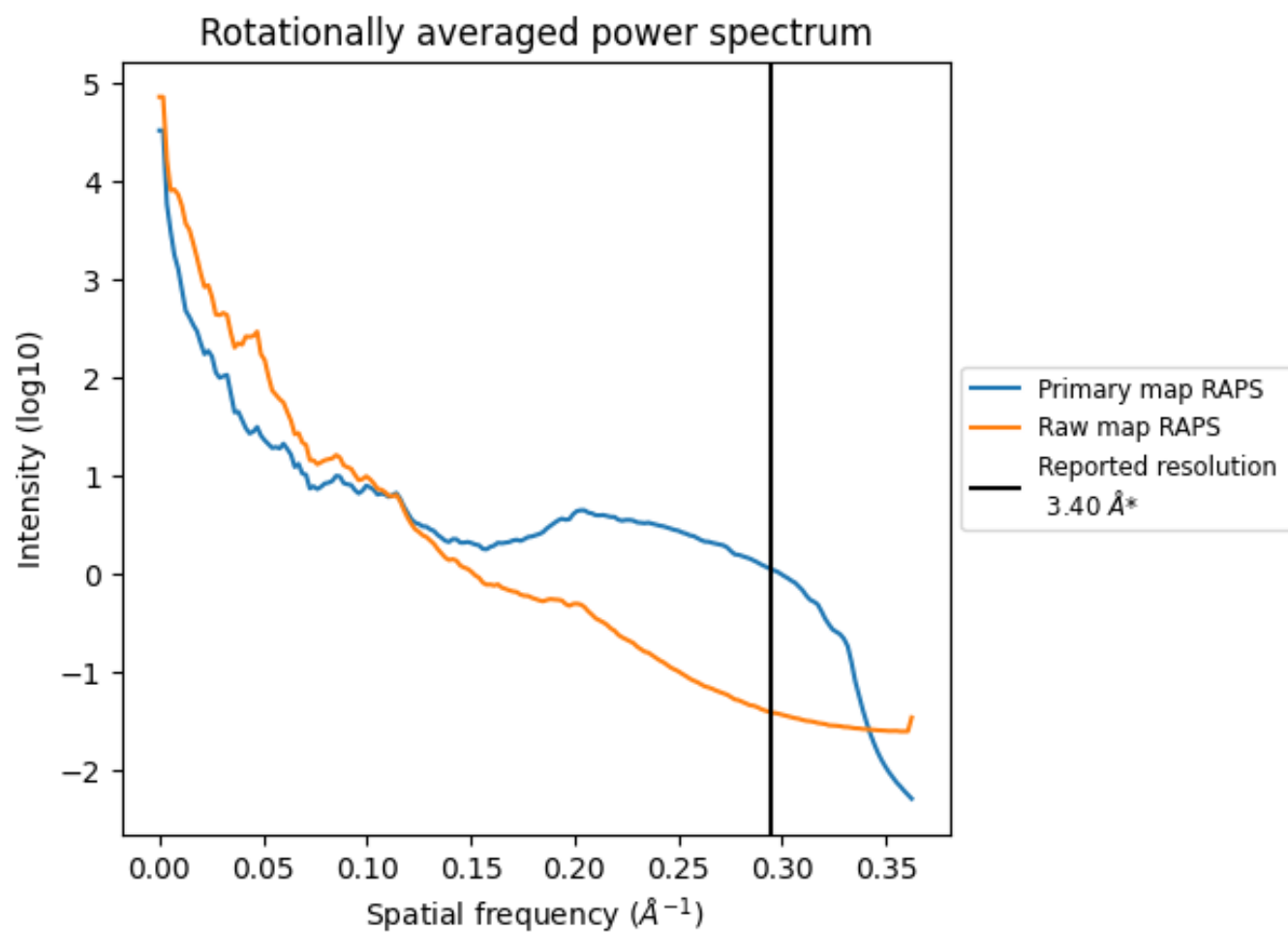
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3366 nm<sup>3</sup>; this corresponds to an approximate mass of 3040 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 ⓘ

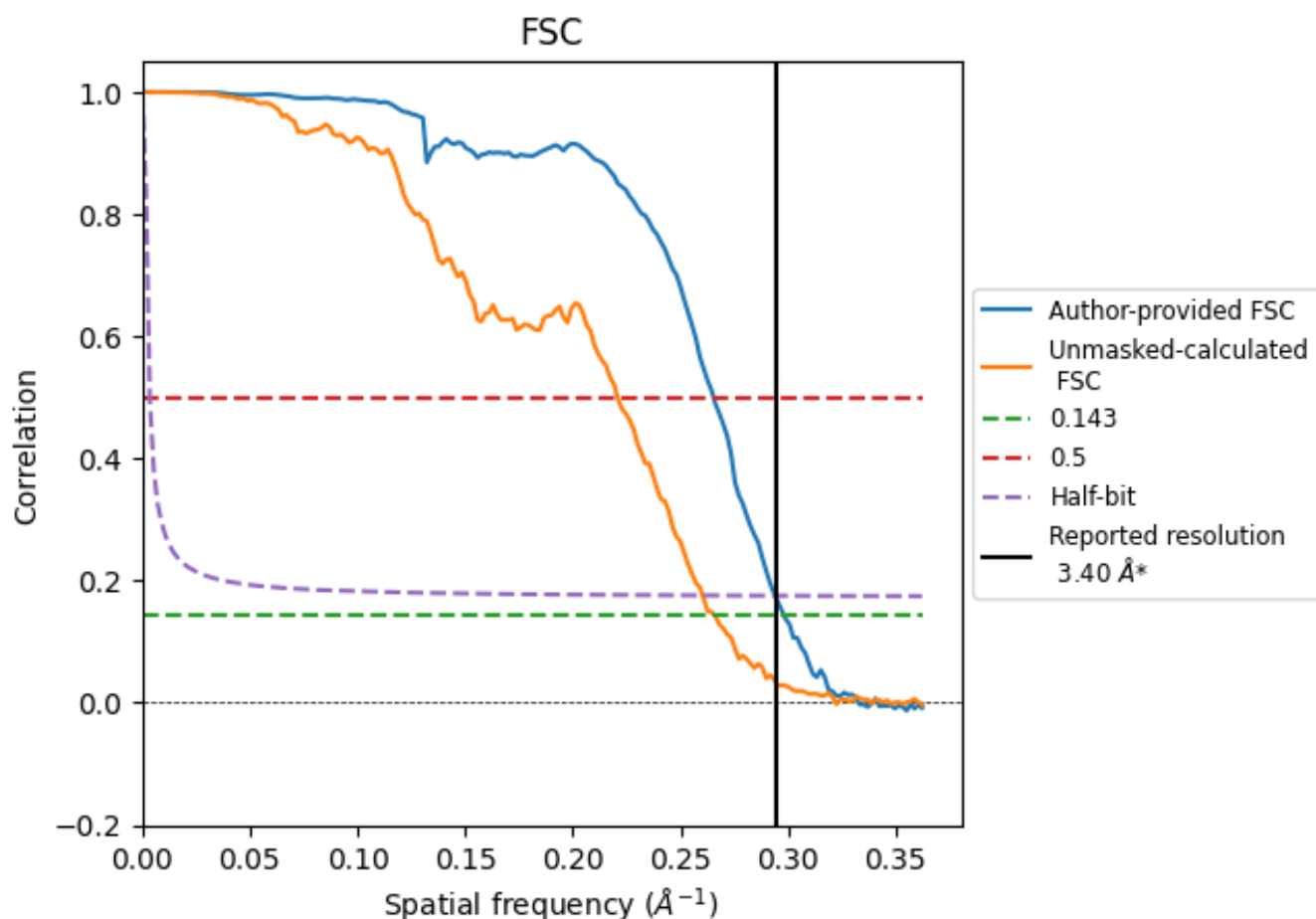


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.40                               | -    | -        |
| Author-provided FSC curve | 3.35                               | 3.77 | 3.40     |
| Unmasked-calculated*      | 3.76                               | 4.53 | 3.84     |

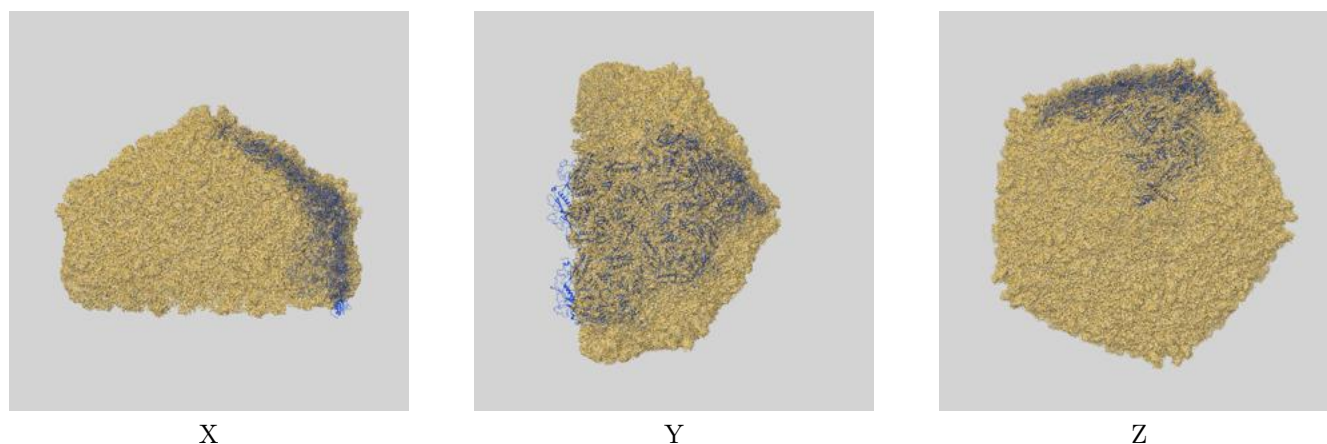
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.4 by more than 10 %

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

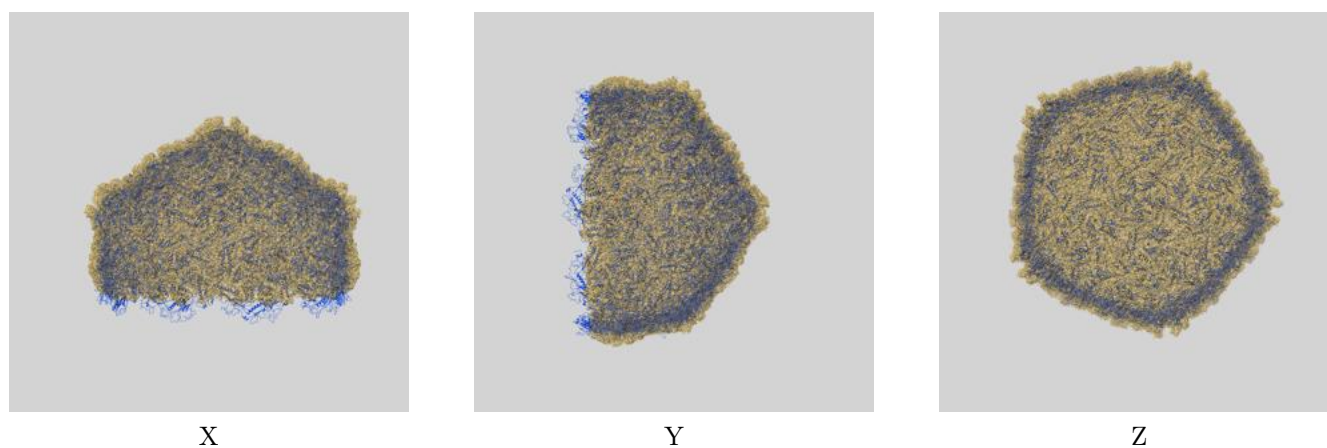
This section contains information regarding the fit between EMDB map EMD-14485 and PDB model 7Z46. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlays

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

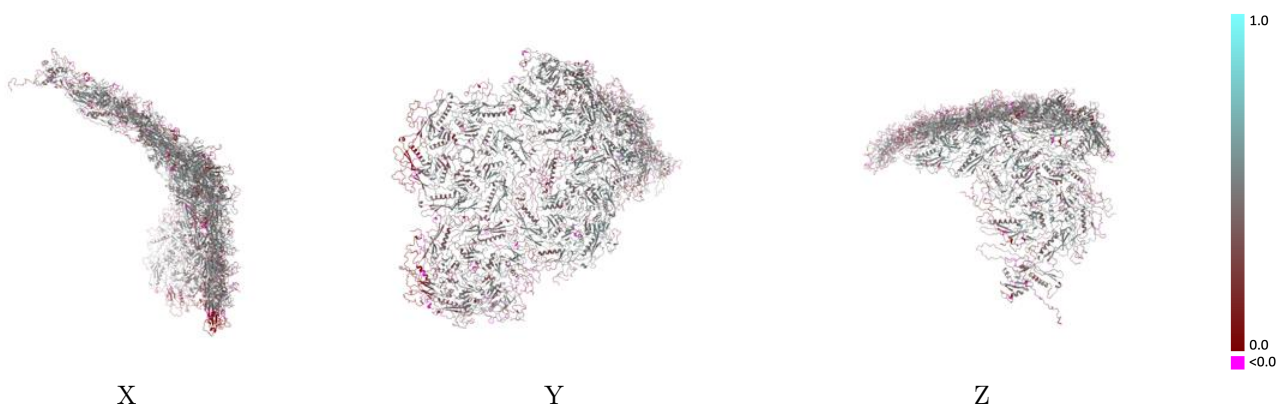


#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)

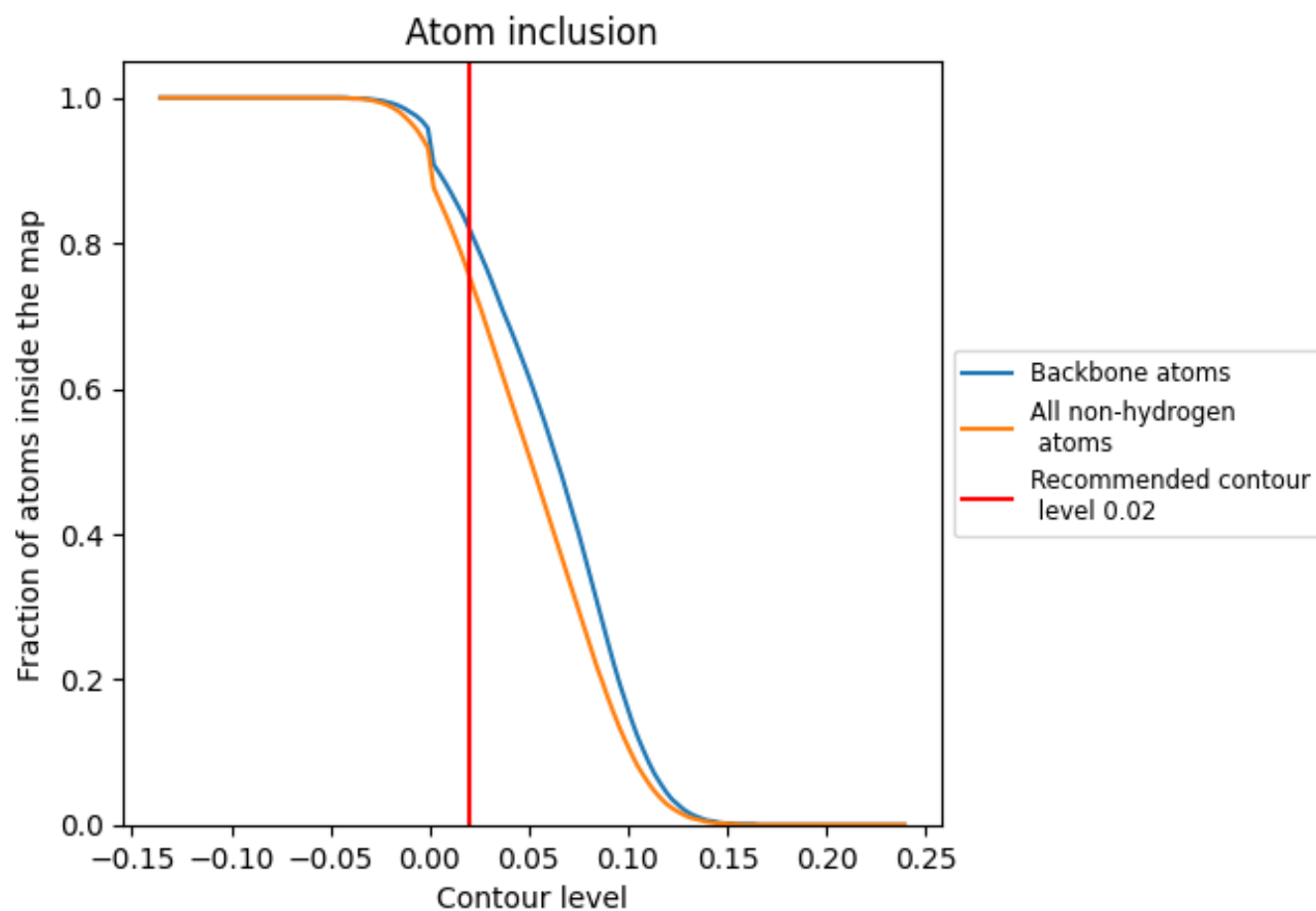


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7550   |  0.3830   |
| A     |  0.7270   |  0.3210   |
| B     |  0.8090   |  0.3980   |
| C     |  0.8090   |  0.4110   |
| D     |  0.7960   |  0.4000   |
| E     |  0.7960   |  0.3920   |
| F     |  0.8220   |  0.4260   |
| G     |  0.7820   |  0.3770   |
| H     |  0.8290   |  0.4230   |
| I     |  0.8190   |  0.4010   |
| J     |  0.8260   |  0.4230   |
| K     |  0.7560   |  0.3360   |
| L     |  0.8420   |  0.4430   |
| M     |  0.8570   |  0.4390   |
| N     |  0.8410  |  0.4280  |
| O     |  0.7550 |  0.3370 |
| P     |  0.7790 |  0.3900 |
| Q     |  0.8390 |  0.4240 |
| R     |  0.7170 |  0.3890 |
| S     |  0.6790 |  0.3420 |
| T     |  0.7480 |  0.3530 |
| U     |  0.8420 |  0.4290 |
| V     |  0.4040 |  0.2520 |
| W     |  0.3530 |  0.2210 |
| X     |  0.8380 |  0.4440 |
| Y     |  0.8440 |  0.4330 |
| Z     |  0.5790 |  0.3330 |
| a     |  0.5760 |  0.3170 |
| b     |  0.8450 |  0.4540 |
| c     |  0.7990 |  0.4040 |
| d     |  0.7530 |  0.3560 |

