



## Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:07 AM UTC

PDB ID : 9LH7 / pdb\_00009lh7  
EMDB ID : EMD-63088  
Title : Pore-like heptameric T201A Vibrio cholerae cytolysin mutant  
Authors : Chatterjee, A.; Dutta, S.; Chattopadhyay, K.; Naskar, P.; Singh, M.  
Deposited on : 2025-01-11  
Resolution : 3.76 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

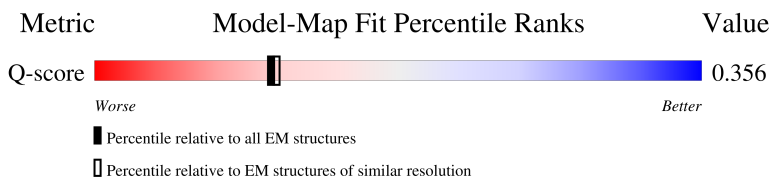
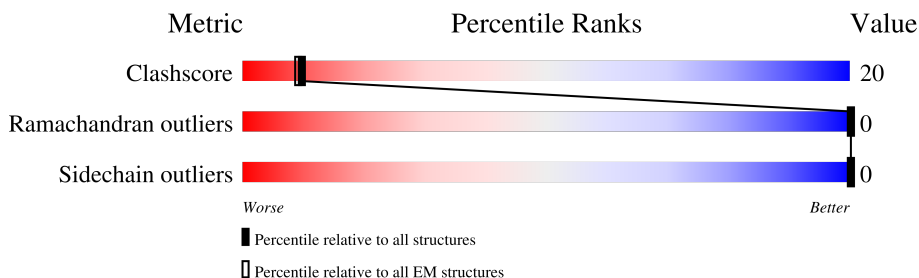
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.76 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                       | 10214 ( 3.26 - 4.26 )                                    |

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     | 581    | <div> <div>5%</div> <div>64%</div> <div>35%</div> <div>.</div> </div> |
| 1   | B     | 581    | <div> <div>6%</div> <div>64%</div> <div>35%</div> <div>.</div> </div> |
| 1   | C     | 581    | <div> <div>6%</div> <div>65%</div> <div>34%</div> <div>.</div> </div> |
| 1   | D     | 581    | <div> <div>6%</div> <div>64%</div> <div>34%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                           |
|-----|-------|--------|----------------------------------------------------------------------------|
| 1   | E     | 581    | <div><div></div><div>6%</div><div>65%</div><div>34%</div><div></div></div> |
| 1   | F     | 581    | <div><div></div><div>5%</div><div>64%</div><div>35%</div><div></div></div> |
| 1   | N     | 581    | <div><div></div><div>5%</div><div>64%</div><div>35%</div><div></div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30555 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 Cytolysin VCC.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4371  | 2735 | 755 | 873 | 8 |         |       |
| 1   | B     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4364  | 2729 | 755 | 872 | 8 |         |       |
| 1   | C     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4364  | 2729 | 755 | 872 | 8 |         |       |
| 1   | D     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4364  | 2729 | 755 | 872 | 8 |         |       |
| 1   | E     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4364  | 2729 | 755 | 872 | 8 |         |       |
| 1   | F     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4364  | 2729 | 755 | 872 | 8 |         |       |
| 1   | N     | 575      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4364  | 2729 | 755 | 872 | 8 |         |       |

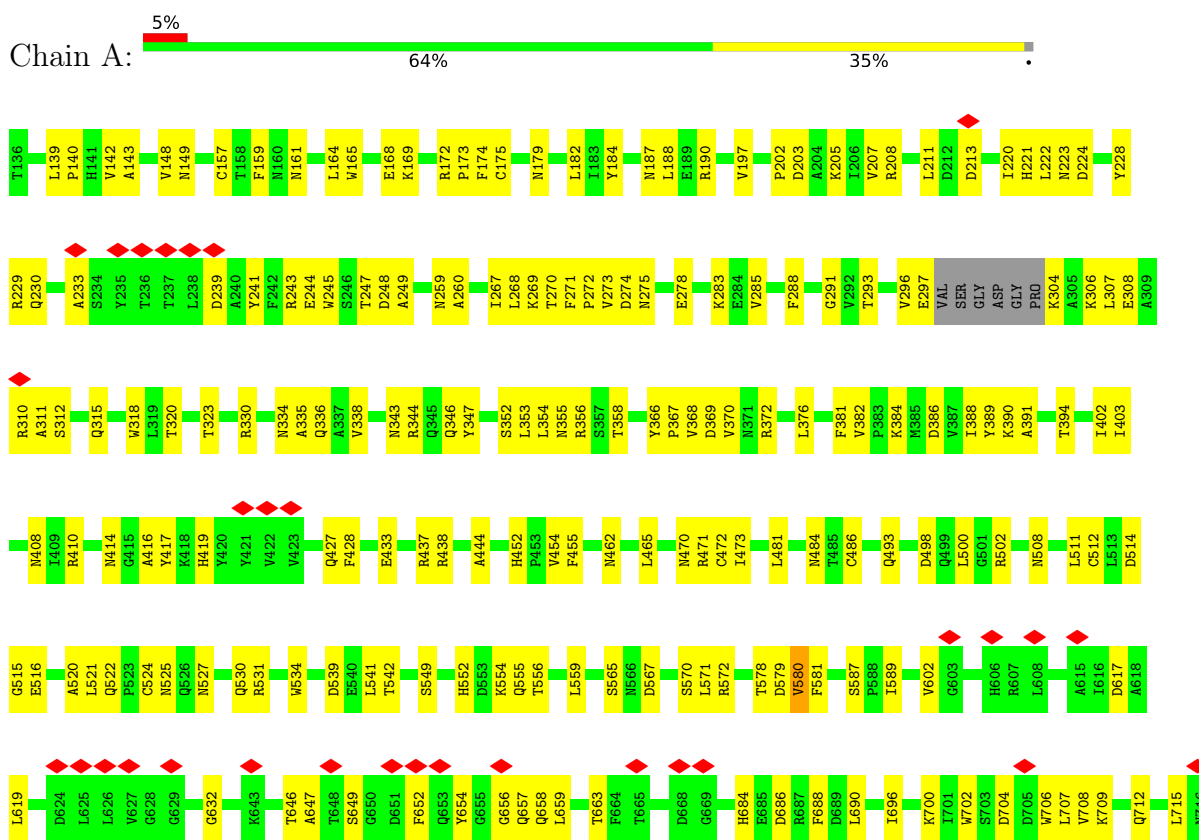
There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| A     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| A     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |
| B     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| B     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |
| C     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| C     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |
| D     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| D     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |
| E     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| E     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |
| F     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| F     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |
| N     | 201     | ALA      | THR    | engineered mutation | UNP A0A0H6SZL4 |
| N     | 289     | ALA      | GLU    | conflict            | UNP A0A0H6SZL4 |

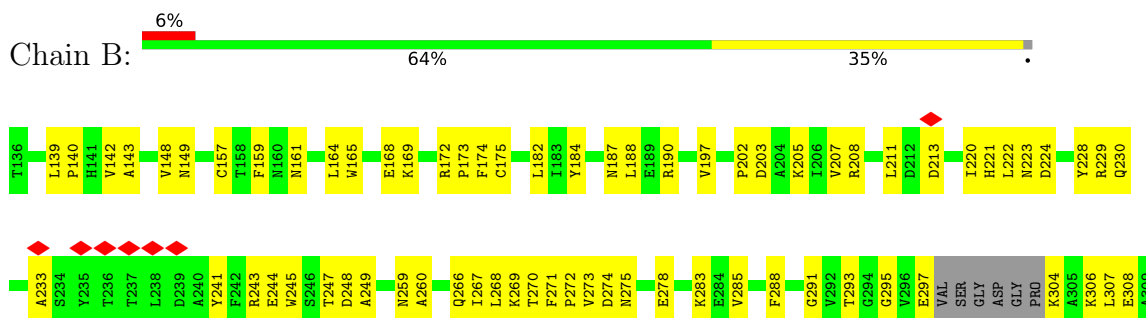
### 3 Residue-property plots

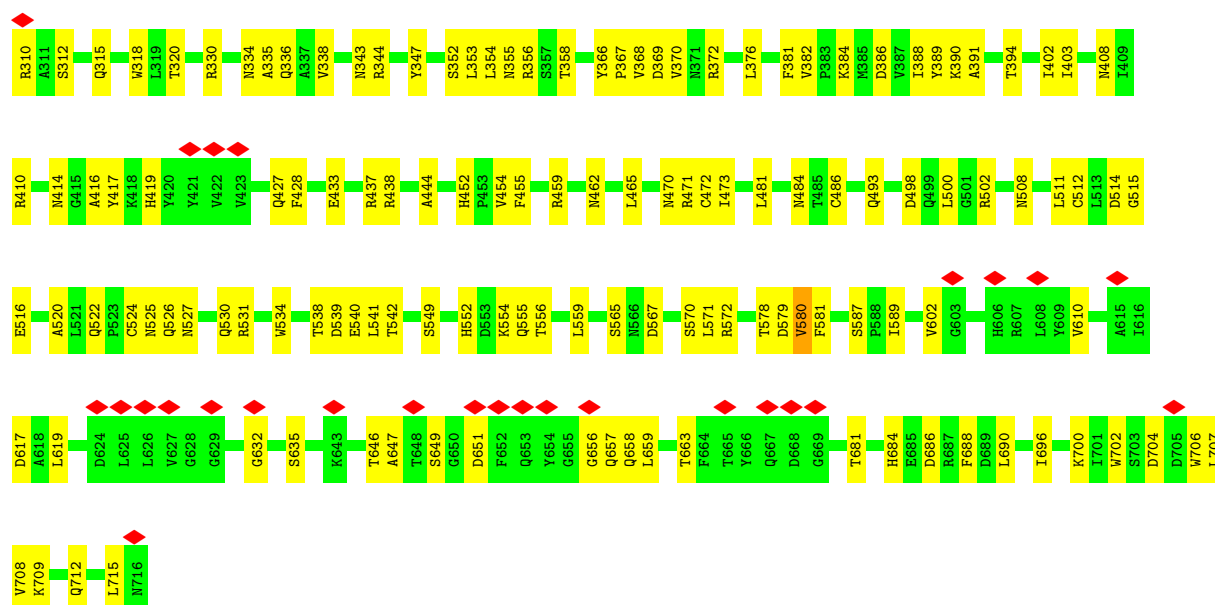
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Cytolysin VCC

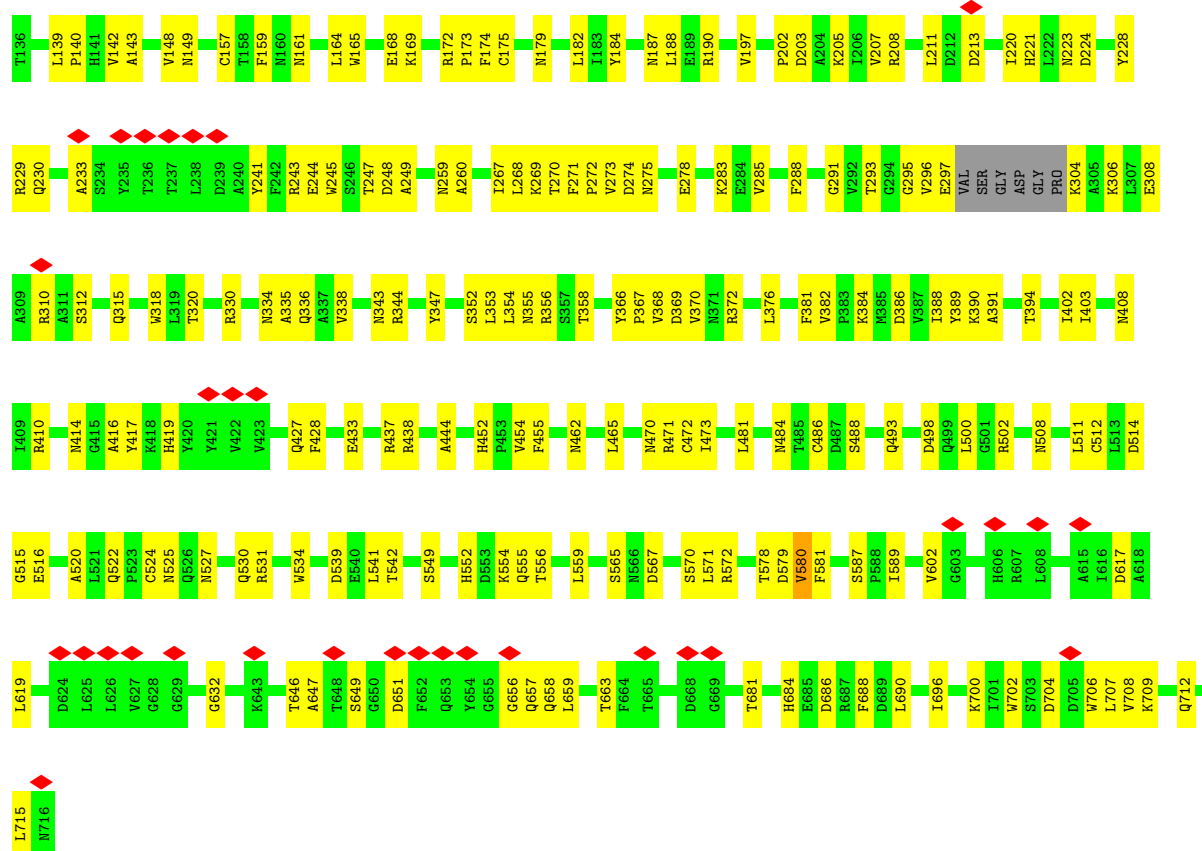


#### • Molecule 1: Cytolysin VCC

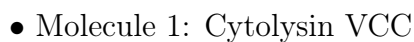




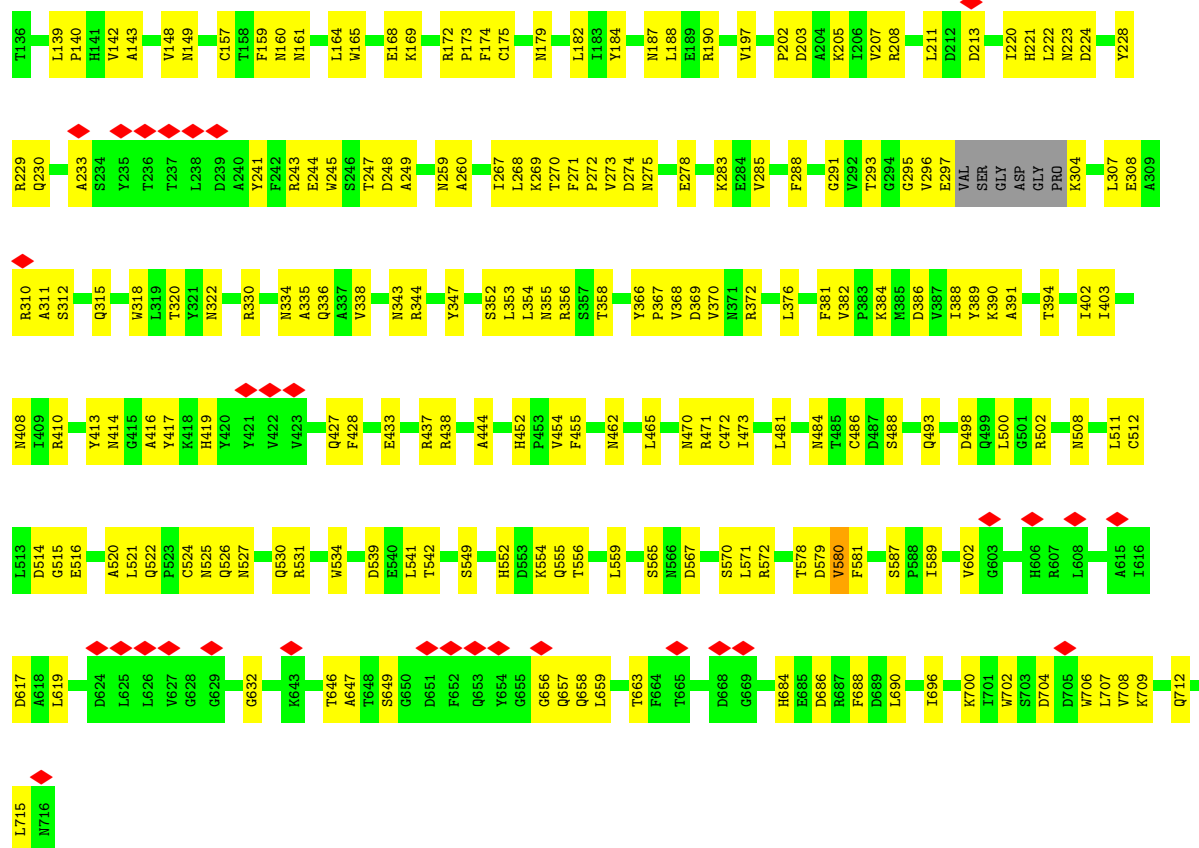
• Molecule 1: Cytolysin VCC



• Molecule 1: Cytolysin VCC

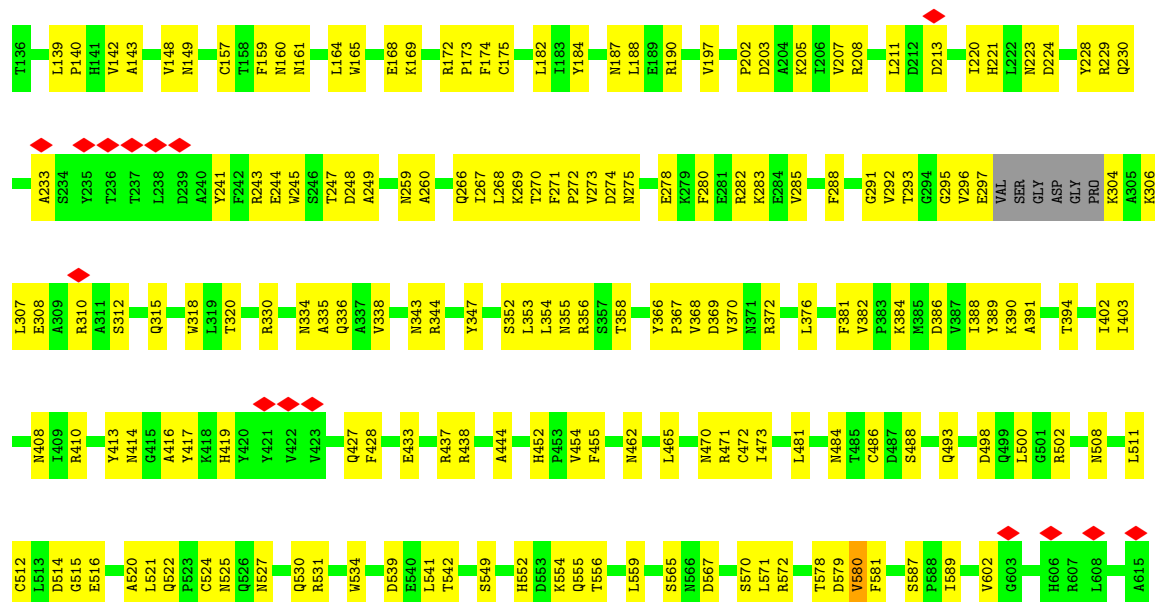


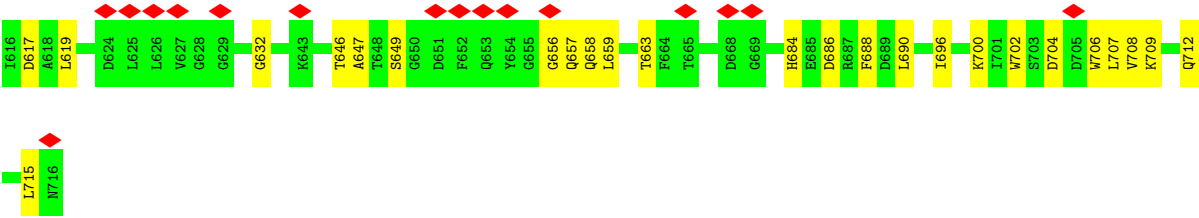
Chain F: 



• Molecule 1: Cytolysin VCC

Chain N: 





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 136870                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 47.0                                    | Depositor |
| Minimum defocus (nm)                 | 750                                     | Depositor |
| Maximum defocus (nm)                 | 2250                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 1.254                                   | Depositor |
| Minimum map value                    | -0.804                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.033                                   | Depositor |
| Recommended contour level            | 0.0663                                  | Depositor |
| Map size (Å)                         | 294.4, 294.4, 294.4                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.91999996, 0.91999996, 0.91999996      | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.18         | 0/4465      | 0.41        | 1/6091 (0.0%)  |
| 1   | B     | 0.17         | 0/4457      | 0.41        | 1/6080 (0.0%)  |
| 1   | C     | 0.17         | 0/4457      | 0.41        | 1/6080 (0.0%)  |
| 1   | D     | 0.17         | 0/4457      | 0.41        | 1/6080 (0.0%)  |
| 1   | E     | 0.17         | 0/4457      | 0.41        | 1/6080 (0.0%)  |
| 1   | F     | 0.17         | 0/4457      | 0.41        | 1/6080 (0.0%)  |
| 1   | N     | 0.18         | 0/4457      | 0.41        | 1/6080 (0.0%)  |
| All | All   | 0.17         | 0/31207     | 0.41        | 7/42571 (0.0%) |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | B     | 580 | VAL  | N-CA-C | -5.47 | 106.08                 | 111.77              |
| 1   | A     | 580 | VAL  | N-CA-C | -5.46 | 106.09                 | 111.77              |
| 1   | N     | 580 | VAL  | N-CA-C | -5.41 | 106.14                 | 111.77              |
| 1   | F     | 580 | VAL  | N-CA-C | -5.41 | 106.14                 | 111.77              |
| 1   | D     | 580 | VAL  | N-CA-C | -5.41 | 106.15                 | 111.77              |
| 1   | E     | 580 | VAL  | N-CA-C | -5.39 | 106.17                 | 111.77              |
| 1   | C     | 580 | VAL  | N-CA-C | -5.34 | 106.21                 | 111.77              |

There are no chirality outliers.

There are no planarity outliers.

### 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     | 4371  | 0        | 4021     | 200     | 0            |
| 1   | B     | 4364  | 0        | 4014     | 193     | 0            |
| 1   | C     | 4364  | 0        | 4014     | 189     | 0            |
| 1   | D     | 4364  | 0        | 4014     | 190     | 0            |
| 1   | E     | 4364  | 0        | 4014     | 189     | 0            |
| 1   | F     | 4364  | 0        | 4014     | 195     | 0            |
| 1   | N     | 4364  | 0        | 4014     | 200     | 0            |
| All | All   | 30555 | 0        | 28105    | 1150    | 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 20.

All (1150) 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:E:288:PHE:CZ  | 1:F:315:GLN:HB3 | 1.45                     | 1.50              |
| 1:A:315:GLN:HB3 | 1:N:288:PHE:CZ  | 1.52                     | 1.41              |
| 1:C:288:PHE:CZ  | 1:D:315:GLN:HB3 | 1.56                     | 1.40              |
| 1:B:288:PHE:CZ  | 1:C:315:GLN:HB3 | 1.57                     | 1.39              |
| 1:F:288:PHE:CZ  | 1:N:315:GLN:HB3 | 1.58                     | 1.37              |
| 1:D:288:PHE:CZ  | 1:E:315:GLN:HB3 | 1.58                     | 1.36              |
| 1:A:288:PHE:CZ  | 1:B:315:GLN:HB3 | 1.60                     | 1.34              |
| 1:A:283:LYS:HG2 | 1:B:320:THR:OG1 | 1.50                     | 1.11              |
| 1:D:283:LYS:HG2 | 1:E:320:THR:OG1 | 1.53                     | 1.08              |
| 1:E:288:PHE:CZ  | 1:F:315:GLN:CB  | 2.35                     | 1.08              |
| 1:A:320:THR:OG1 | 1:N:283:LYS:HG2 | 1.54                     | 1.06              |
| 1:D:288:PHE:CE1 | 1:E:315:GLN:HB3 | 1.94                     | 1.02              |
| 1:A:315:GLN:HB3 | 1:N:288:PHE:CE1 | 1.93                     | 1.02              |
| 1:A:315:GLN:CB  | 1:N:288:PHE:CZ  | 2.42                     | 1.01              |
| 1:C:283:LYS:HG2 | 1:D:320:THR:OG1 | 1.61                     | 1.01              |
| 1:E:288:PHE:CE1 | 1:F:315:GLN:HB3 | 1.95                     | 1.00              |
| 1:A:288:PHE:CE1 | 1:B:315:GLN:HB3 | 1.96                     | 1.00              |
| 1:B:283:LYS:HG2 | 1:C:320:THR:OG1 | 1.62                     | 1.00              |
| 1:E:283:LYS:HG2 | 1:F:320:THR:OG1 | 1.63                     | 0.98              |
| 1:C:288:PHE:CE1 | 1:D:315:GLN:HB3 | 1.98                     | 0.98              |
| 1:D:288:PHE:CZ  | 1:E:315:GLN:CB  | 2.47                     | 0.97              |
| 1:F:283:LYS:HG2 | 1:N:320:THR:OG1 | 1.62                     | 0.96              |
| 1:B:288:PHE:CZ  | 1:C:315:GLN:CB  | 2.47                     | 0.96              |
| 1:C:288:PHE:CZ  | 1:D:315:GLN:CB  | 2.47                     | 0.95              |
| 1:B:288:PHE:CE1 | 1:C:315:GLN:HB3 | 2.02                     | 0.95              |
| 1:A:288:PHE:CZ  | 1:B:315:GLN:CB  | 2.52                     | 0.93              |
| 1:F:512:CYS:HB3 | 1:F:524:CYS:HB3 | 1.50                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:512:CYS:HB3  | 1:N:524:CYS:HB3  | 1.50                     | 0.93              |
| 1:F:288:PHE:CZ   | 1:N:315:GLN:CB   | 2.51                     | 0.93              |
| 1:F:288:PHE:CE1  | 1:N:315:GLN:HB3  | 2.04                     | 0.92              |
| 1:A:512:CYS:HB3  | 1:A:524:CYS:HB3  | 1.50                     | 0.92              |
| 1:E:512:CYS:HB3  | 1:E:524:CYS:HB3  | 1.50                     | 0.91              |
| 1:C:512:CYS:HB3  | 1:C:524:CYS:HB3  | 1.50                     | 0.91              |
| 1:D:512:CYS:HB3  | 1:D:524:CYS:HB3  | 1.51                     | 0.90              |
| 1:A:306:LYS:CB   | 1:N:297:GLU:OE1  | 2.20                     | 0.90              |
| 1:B:512:CYS:HB3  | 1:B:524:CYS:HB3  | 1.50                     | 0.90              |
| 1:A:274:ASP:HB2  | 1:B:382:VAL:HG12 | 1.57                     | 0.84              |
| 1:A:382:VAL:HG12 | 1:N:274:ASP:HB2  | 1.57                     | 0.83              |
| 1:D:274:ASP:HB2  | 1:E:382:VAL:HG12 | 1.62                     | 0.81              |
| 1:C:274:ASP:HB2  | 1:D:382:VAL:HG12 | 1.61                     | 0.81              |
| 1:F:274:ASP:HB2  | 1:N:382:VAL:HG12 | 1.60                     | 0.81              |
| 1:F:512:CYS:HB3  | 1:F:524:CYS:CB   | 2.12                     | 0.79              |
| 1:C:297:GLU:OE1  | 1:D:306:LYS:CB   | 2.29                     | 0.79              |
| 1:B:297:GLU:OE1  | 1:C:306:LYS:CB   | 2.31                     | 0.79              |
| 1:C:512:CYS:HB3  | 1:C:524:CYS:CB   | 2.12                     | 0.79              |
| 1:N:512:CYS:HB3  | 1:N:524:CYS:CB   | 2.12                     | 0.79              |
| 1:D:297:GLU:OE1  | 1:E:306:LYS:CB   | 2.30                     | 0.79              |
| 1:E:512:CYS:HB3  | 1:E:524:CYS:CB   | 2.12                     | 0.79              |
| 1:B:512:CYS:HB3  | 1:B:524:CYS:CB   | 2.12                     | 0.79              |
| 1:D:512:CYS:HB3  | 1:D:524:CYS:CB   | 2.12                     | 0.78              |
| 1:A:512:CYS:HB3  | 1:A:524:CYS:CB   | 2.12                     | 0.78              |
| 1:B:274:ASP:HB2  | 1:C:382:VAL:HG12 | 1.65                     | 0.77              |
| 1:E:274:ASP:HB2  | 1:F:382:VAL:HG12 | 1.66                     | 0.77              |
| 1:D:172:ARG:NH1  | 1:D:173:PRO:O    | 2.18                     | 0.77              |
| 1:A:172:ARG:NH1  | 1:A:173:PRO:O    | 2.18                     | 0.76              |
| 1:C:172:ARG:NH1  | 1:C:173:PRO:O    | 2.18                     | 0.76              |
| 1:A:306:LYS:CB   | 1:N:297:GLU:CD   | 2.58                     | 0.76              |
| 1:C:408:ASN:HD21 | 1:C:437:ARG:HD3  | 1.51                     | 0.76              |
| 1:E:408:ASN:HD21 | 1:E:437:ARG:HD3  | 1.50                     | 0.76              |
| 1:B:525:ASN:H    | 1:B:530:GLN:HE22 | 1.34                     | 0.76              |
| 1:F:172:ARG:NH1  | 1:F:173:PRO:O    | 2.18                     | 0.76              |
| 1:N:408:ASN:HD21 | 1:N:437:ARG:HD3  | 1.51                     | 0.76              |
| 1:A:525:ASN:H    | 1:A:530:GLN:HE22 | 1.34                     | 0.76              |
| 1:F:408:ASN:HD21 | 1:F:437:ARG:HD3  | 1.51                     | 0.76              |
| 1:A:408:ASN:HD21 | 1:A:437:ARG:HD3  | 1.51                     | 0.76              |
| 1:C:525:ASN:H    | 1:C:530:GLN:HE22 | 1.34                     | 0.76              |
| 1:E:172:ARG:NH1  | 1:E:173:PRO:O    | 2.18                     | 0.76              |
| 1:D:525:ASN:H    | 1:D:530:GLN:HE22 | 1.34                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:172:ARG:NH1  | 1:N:173:PRO:O    | 2.18                     | 0.75              |
| 1:B:172:ARG:NH1  | 1:B:173:PRO:O    | 2.18                     | 0.75              |
| 1:A:297:GLU:OE1  | 1:B:306:LYS:CB   | 2.35                     | 0.75              |
| 1:B:408:ASN:HD21 | 1:B:437:ARG:HD3  | 1.51                     | 0.75              |
| 1:D:408:ASN:HD21 | 1:D:437:ARG:HD3  | 1.51                     | 0.75              |
| 1:N:525:ASN:H    | 1:N:530:GLN:HE22 | 1.34                     | 0.75              |
| 1:E:525:ASN:H    | 1:E:530:GLN:HE22 | 1.34                     | 0.74              |
| 1:E:291:GLY:HA2  | 1:F:312:SER:HA   | 1.69                     | 0.74              |
| 1:F:525:ASN:H    | 1:F:530:GLN:HE22 | 1.34                     | 0.74              |
| 1:N:690:LEU:HD21 | 1:N:715:LEU:HD22 | 1.70                     | 0.74              |
| 1:E:690:LEU:HD21 | 1:E:715:LEU:HD22 | 1.70                     | 0.74              |
| 1:F:690:LEU:HD21 | 1:F:715:LEU:HD22 | 1.70                     | 0.74              |
| 1:D:656:GLY:HA3  | 1:D:658:GLN:HE22 | 1.53                     | 0.74              |
| 1:N:656:GLY:HA3  | 1:N:658:GLN:HE22 | 1.53                     | 0.74              |
| 1:A:690:LEU:HD21 | 1:A:715:LEU:HD22 | 1.70                     | 0.73              |
| 1:D:690:LEU:HD21 | 1:D:715:LEU:HD22 | 1.70                     | 0.73              |
| 1:C:656:GLY:HA3  | 1:C:658:GLN:HE22 | 1.53                     | 0.73              |
| 1:F:656:GLY:HA3  | 1:F:658:GLN:HE22 | 1.53                     | 0.73              |
| 1:A:656:GLY:HA3  | 1:A:658:GLN:HE22 | 1.53                     | 0.73              |
| 1:E:656:GLY:HA3  | 1:E:658:GLN:HE22 | 1.53                     | 0.73              |
| 1:B:690:LEU:HD21 | 1:B:715:LEU:HD22 | 1.70                     | 0.73              |
| 1:C:690:LEU:HD21 | 1:C:715:LEU:HD22 | 1.70                     | 0.73              |
| 1:F:297:GLU:OE1  | 1:N:306:LYS:CB   | 2.37                     | 0.72              |
| 1:A:306:LYS:CB   | 1:N:297:GLU:OE2  | 2.38                     | 0.72              |
| 1:E:293:THR:OG1  | 1:F:310:ARG:HG2  | 1.90                     | 0.72              |
| 1:B:656:GLY:HA3  | 1:B:658:GLN:HE22 | 1.53                     | 0.71              |
| 1:A:172:ARG:HE   | 1:A:229:ARG:HH22 | 1.39                     | 0.71              |
| 1:A:403:ILE:HD11 | 1:A:444:ALA:HB3  | 1.72                     | 0.71              |
| 1:D:403:ILE:HD11 | 1:D:444:ALA:HB3  | 1.72                     | 0.70              |
| 1:E:403:ILE:HD11 | 1:E:444:ALA:HB3  | 1.72                     | 0.70              |
| 1:B:403:ILE:HD11 | 1:B:444:ALA:HB3  | 1.72                     | 0.70              |
| 1:B:172:ARG:HE   | 1:B:229:ARG:HH22 | 1.39                     | 0.70              |
| 1:N:172:ARG:HE   | 1:N:229:ARG:HH22 | 1.40                     | 0.70              |
| 1:N:403:ILE:HD11 | 1:N:444:ALA:HB3  | 1.72                     | 0.70              |
| 1:F:403:ILE:HD11 | 1:F:444:ALA:HB3  | 1.72                     | 0.70              |
| 1:C:403:ILE:HD11 | 1:C:444:ALA:HB3  | 1.72                     | 0.70              |
| 1:B:285:VAL:HG22 | 1:C:318:TRP:CD1  | 2.27                     | 0.69              |
| 1:D:283:LYS:HG2  | 1:E:320:THR:CB   | 2.21                     | 0.69              |
| 1:E:472:CYS:HB3  | 1:E:486:CYS:SG   | 2.33                     | 0.69              |
| 1:C:297:GLU:CD   | 1:D:306:LYS:CB   | 2.66                     | 0.69              |
| 1:N:472:CYS:HB3  | 1:N:486:CYS:SG   | 2.33                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:323:THR:OG1  | 1:A:346:GLN:NE2  | 2.25                     | 0.69              |
| 1:A:472:CYS:HB3  | 1:A:486:CYS:SG   | 2.33                     | 0.69              |
| 1:B:472:CYS:HB3  | 1:B:486:CYS:SG   | 2.33                     | 0.69              |
| 1:E:288:PHE:HZ   | 1:F:315:GLN:HB3  | 1.45                     | 0.69              |
| 1:D:587:SER:O    | 1:D:712:GLN:NE2  | 2.26                     | 0.69              |
| 1:B:587:SER:O    | 1:B:712:GLN:NE2  | 2.26                     | 0.68              |
| 1:C:472:CYS:HB3  | 1:C:486:CYS:SG   | 2.33                     | 0.68              |
| 1:D:172:ARG:HE   | 1:D:229:ARG:HH22 | 1.39                     | 0.68              |
| 1:A:312:SER:HA   | 1:N:291:GLY:HA2  | 1.74                     | 0.68              |
| 1:A:652:PHE:CE2  | 1:A:654:TYR:HB2  | 2.29                     | 0.68              |
| 1:A:587:SER:O    | 1:A:712:GLN:NE2  | 2.26                     | 0.68              |
| 1:E:172:ARG:HE   | 1:E:229:ARG:HH22 | 1.39                     | 0.68              |
| 1:F:472:CYS:HB3  | 1:F:486:CYS:SG   | 2.33                     | 0.68              |
| 1:F:587:SER:O    | 1:F:712:GLN:NE2  | 2.26                     | 0.68              |
| 1:N:587:SER:O    | 1:N:712:GLN:NE2  | 2.26                     | 0.68              |
| 1:B:297:GLU:OE2  | 1:C:306:LYS:CB   | 2.42                     | 0.68              |
| 1:E:587:SER:O    | 1:E:712:GLN:NE2  | 2.26                     | 0.68              |
| 1:B:297:GLU:CD   | 1:C:306:LYS:CB   | 2.67                     | 0.68              |
| 1:C:587:SER:O    | 1:C:712:GLN:NE2  | 2.26                     | 0.68              |
| 1:D:472:CYS:HB3  | 1:D:486:CYS:SG   | 2.33                     | 0.68              |
| 1:F:172:ARG:HE   | 1:F:229:ARG:HH22 | 1.39                     | 0.68              |
| 1:C:205:LYS:HB2  | 1:C:391:ALA:HB3  | 1.77                     | 0.67              |
| 1:D:285:VAL:HG22 | 1:E:318:TRP:CD1  | 2.29                     | 0.67              |
| 1:B:205:LYS:HB2  | 1:B:391:ALA:HB3  | 1.77                     | 0.67              |
| 1:C:161:ASN:ND2  | 1:C:169:LYS:O    | 2.27                     | 0.67              |
| 1:F:161:ASN:ND2  | 1:F:169:LYS:O    | 2.27                     | 0.67              |
| 1:F:205:LYS:HB2  | 1:F:391:ALA:HB3  | 1.77                     | 0.67              |
| 1:A:334:ASN:OD1  | 1:A:335:ALA:N    | 2.24                     | 0.67              |
| 1:C:172:ARG:HE   | 1:C:229:ARG:HH22 | 1.39                     | 0.67              |
| 1:D:205:LYS:HB2  | 1:D:391:ALA:HB3  | 1.77                     | 0.67              |
| 1:E:205:LYS:HB2  | 1:E:391:ALA:HB3  | 1.77                     | 0.67              |
| 1:N:205:LYS:HB2  | 1:N:391:ALA:HB3  | 1.77                     | 0.67              |
| 1:E:285:VAL:HG22 | 1:F:318:TRP:CD1  | 2.30                     | 0.67              |
| 1:B:516:GLU:N    | 1:B:516:GLU:OE2  | 2.28                     | 0.67              |
| 1:A:205:LYS:HB2  | 1:A:391:ALA:HB3  | 1.77                     | 0.66              |
| 1:A:516:GLU:OE2  | 1:A:516:GLU:N    | 2.28                     | 0.66              |
| 1:N:161:ASN:ND2  | 1:N:169:LYS:O    | 2.27                     | 0.66              |
| 1:C:516:GLU:OE2  | 1:C:516:GLU:N    | 2.28                     | 0.66              |
| 1:A:274:ASP:HB2  | 1:B:382:VAL:CG1  | 2.24                     | 0.66              |
| 1:E:248:ASP:OD1  | 1:E:249:ALA:N    | 2.29                     | 0.66              |
| 1:A:248:ASP:OD1  | 1:A:249:ALA:N    | 2.29                     | 0.66              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:288:PHE:CE1 | 1:E:315:GLN:CB   | 2.77                     | 0.66              |
| 1:E:161:ASN:ND2 | 1:E:169:LYS:O    | 2.27                     | 0.66              |
| 1:D:248:ASP:OD1 | 1:D:249:ALA:N    | 2.29                     | 0.66              |
| 1:F:516:GLU:OE2 | 1:F:516:GLU:N    | 2.28                     | 0.66              |
| 1:A:320:THR:CB  | 1:N:283:LYS:HG2  | 2.25                     | 0.66              |
| 1:B:161:ASN:ND2 | 1:B:169:LYS:O    | 2.27                     | 0.66              |
| 1:F:288:PHE:HZ  | 1:N:315:GLN:HB3  | 1.50                     | 0.66              |
| 1:B:248:ASP:OD1 | 1:B:249:ALA:N    | 2.29                     | 0.66              |
| 1:D:516:GLU:N   | 1:D:516:GLU:OE2  | 2.28                     | 0.66              |
| 1:A:161:ASN:ND2 | 1:A:169:LYS:O    | 2.27                     | 0.66              |
| 1:C:297:GLU:OE2 | 1:D:306:LYS:CB   | 2.43                     | 0.66              |
| 1:C:248:ASP:OD1 | 1:C:249:ALA:N    | 2.29                     | 0.65              |
| 1:N:248:ASP:OD1 | 1:N:249:ALA:N    | 2.29                     | 0.65              |
| 1:A:508:ASN:HB3 | 1:A:511:LEU:HD23 | 1.79                     | 0.65              |
| 1:N:508:ASN:HB3 | 1:N:511:LEU:HD23 | 1.78                     | 0.65              |
| 1:F:248:ASP:OD1 | 1:F:249:ALA:N    | 2.29                     | 0.65              |
| 1:F:508:ASN:HB3 | 1:F:511:LEU:HD23 | 1.79                     | 0.65              |
| 1:A:283:LYS:HG2 | 1:B:320:THR:CB   | 2.26                     | 0.65              |
| 1:B:172:ARG:NH2 | 1:B:229:ARG:HH12 | 1.95                     | 0.65              |
| 1:B:291:GLY:HA2 | 1:C:312:SER:HA   | 1.79                     | 0.65              |
| 1:C:334:ASN:OD1 | 1:C:335:ALA:N    | 2.24                     | 0.65              |
| 1:A:382:VAL:CG1 | 1:N:274:ASP:HB2  | 2.27                     | 0.65              |
| 1:A:470:ASN:HB2 | 1:N:527:ASN:OD1  | 1.96                     | 0.65              |
| 1:D:291:GLY:HA2 | 1:E:312:SER:HA   | 1.78                     | 0.65              |
| 1:D:334:ASN:OD1 | 1:D:335:ALA:N    | 2.24                     | 0.65              |
| 1:D:508:ASN:HB3 | 1:D:511:LEU:HD23 | 1.78                     | 0.65              |
| 1:E:508:ASN:HB3 | 1:E:511:LEU:HD23 | 1.79                     | 0.65              |
| 1:B:508:ASN:HB3 | 1:B:511:LEU:HD23 | 1.78                     | 0.65              |
| 1:C:554:LYS:HE3 | 1:C:570:SER:HB3  | 1.79                     | 0.65              |
| 1:F:297:GLU:OE2 | 1:N:306:LYS:CB   | 2.45                     | 0.65              |
| 1:B:334:ASN:OD1 | 1:B:335:ALA:N    | 2.24                     | 0.64              |
| 1:C:283:LYS:HG2 | 1:D:320:THR:CB   | 2.27                     | 0.64              |
| 1:E:554:LYS:HE3 | 1:E:570:SER:HB3  | 1.79                     | 0.64              |
| 1:F:554:LYS:HE3 | 1:F:570:SER:HB3  | 1.79                     | 0.64              |
| 1:A:172:ARG:NH2 | 1:A:229:ARG:HH12 | 1.95                     | 0.64              |
| 1:B:554:LYS:HE3 | 1:B:570:SER:HB3  | 1.80                     | 0.64              |
| 1:D:172:ARG:NH2 | 1:D:229:ARG:HH12 | 1.95                     | 0.64              |
| 1:D:554:LYS:HE3 | 1:D:570:SER:HB3  | 1.79                     | 0.64              |
| 1:E:172:ARG:NH2 | 1:E:229:ARG:HH12 | 1.95                     | 0.64              |
| 1:N:554:LYS:HE3 | 1:N:570:SER:HB3  | 1.80                     | 0.64              |
| 1:A:554:LYS:HE3 | 1:A:570:SER:HB3  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:508:ASN:HB3  | 1:C:511:LEU:HD23 | 1.79                     | 0.64              |
| 1:C:172:ARG:NH2  | 1:C:229:ARG:HH12 | 1.95                     | 0.64              |
| 1:A:315:GLN:HB3  | 1:N:288:PHE:HZ   | 1.53                     | 0.64              |
| 1:N:516:GLU:N    | 1:N:516:GLU:OE2  | 2.28                     | 0.64              |
| 1:N:172:ARG:NH2  | 1:N:229:ARG:HH12 | 1.95                     | 0.64              |
| 1:B:283:LYS:HG2  | 1:C:320:THR:CB   | 2.27                     | 0.64              |
| 1:D:161:ASN:ND2  | 1:D:169:LYS:O    | 2.27                     | 0.64              |
| 1:F:172:ARG:NH2  | 1:F:229:ARG:HH12 | 1.95                     | 0.64              |
| 1:N:700:LYS:HB2  | 1:N:712:GLN:HB3  | 1.80                     | 0.64              |
| 1:E:700:LYS:HB2  | 1:E:712:GLN:HB3  | 1.80                     | 0.63              |
| 1:F:297:GLU:CD   | 1:N:306:LYS:CB   | 2.71                     | 0.63              |
| 1:E:516:GLU:OE2  | 1:E:516:GLU:N    | 2.28                     | 0.63              |
| 1:A:318:TRP:CD1  | 1:N:285:VAL:HG22 | 2.33                     | 0.63              |
| 1:A:700:LYS:HB2  | 1:A:712:GLN:HB3  | 1.80                     | 0.63              |
| 1:A:657:GLN:OE1  | 1:A:657:GLN:N    | 2.32                     | 0.63              |
| 1:F:700:LYS:HB2  | 1:F:712:GLN:HB3  | 1.80                     | 0.63              |
| 1:B:223:ASN:OD1  | 1:B:224:ASP:N    | 2.32                     | 0.63              |
| 1:A:315:GLN:CB   | 1:N:288:PHE:CE1  | 2.76                     | 0.63              |
| 1:D:657:GLN:N    | 1:D:657:GLN:OE1  | 2.32                     | 0.63              |
| 1:D:700:LYS:HB2  | 1:D:712:GLN:HB3  | 1.80                     | 0.63              |
| 1:E:657:GLN:N    | 1:E:657:GLN:OE1  | 2.32                     | 0.63              |
| 1:F:657:GLN:OE1  | 1:F:657:GLN:N    | 2.32                     | 0.63              |
| 1:N:657:GLN:N    | 1:N:657:GLN:OE1  | 2.32                     | 0.63              |
| 1:E:182:LEU:HD21 | 1:E:220:ILE:HG23 | 1.81                     | 0.63              |
| 1:E:285:VAL:HG22 | 1:F:318:TRP:CG   | 2.34                     | 0.63              |
| 1:N:223:ASN:OD1  | 1:N:224:ASP:N    | 2.32                     | 0.63              |
| 1:C:555:GLN:HG3  | 1:C:556:THR:HG23 | 1.81                     | 0.63              |
| 1:B:657:GLN:N    | 1:B:657:GLN:OE1  | 2.32                     | 0.62              |
| 1:N:555:GLN:HG3  | 1:N:556:THR:HG23 | 1.81                     | 0.62              |
| 1:C:308:GLU:N    | 1:C:308:GLU:OE1  | 2.33                     | 0.62              |
| 1:D:555:GLN:HG3  | 1:D:556:THR:HG23 | 1.81                     | 0.62              |
| 1:F:555:GLN:HG3  | 1:F:556:THR:HG23 | 1.81                     | 0.62              |
| 1:D:182:LEU:HD21 | 1:D:220:ILE:HG23 | 1.81                     | 0.62              |
| 1:A:182:LEU:HD21 | 1:A:220:ILE:HG23 | 1.81                     | 0.62              |
| 1:B:308:GLU:N    | 1:B:308:GLU:OE1  | 2.33                     | 0.62              |
| 1:E:527:ASN:OD1  | 1:F:470:ASN:HB2  | 1.99                     | 0.62              |
| 1:N:580:VAL:HG12 | 1:N:580:VAL:O    | 2.00                     | 0.62              |
| 1:B:354:LEU:HD21 | 1:B:414:ASN:HD21 | 1.65                     | 0.62              |
| 1:B:700:LYS:HB2  | 1:B:712:GLN:HB3  | 1.81                     | 0.62              |
| 1:A:555:GLN:HG3  | 1:A:556:THR:HG23 | 1.81                     | 0.62              |
| 1:C:657:GLN:OE1  | 1:C:657:GLN:N    | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:223:ASN:OD1  | 1:E:224:ASP:N    | 2.32                     | 0.62              |
| 1:F:182:LEU:HD21 | 1:F:220:ILE:HG23 | 1.81                     | 0.62              |
| 1:B:182:LEU:HD21 | 1:B:220:ILE:HG23 | 1.81                     | 0.62              |
| 1:C:410:ARG:HH21 | 1:C:437:ARG:HH21 | 1.47                     | 0.62              |
| 1:C:700:LYS:HB2  | 1:C:712:GLN:HB3  | 1.80                     | 0.62              |
| 1:D:308:GLU:N    | 1:D:308:GLU:OE1  | 2.33                     | 0.62              |
| 1:F:172:ARG:HE   | 1:F:229:ARG:NH2  | 1.98                     | 0.62              |
| 1:A:354:LEU:HD21 | 1:A:414:ASN:HD21 | 1.65                     | 0.62              |
| 1:B:410:ARG:HH21 | 1:B:437:ARG:HH21 | 1.47                     | 0.62              |
| 1:C:172:ARG:HE   | 1:C:229:ARG:NH2  | 1.98                     | 0.62              |
| 1:D:223:ASN:OD1  | 1:D:224:ASP:N    | 2.32                     | 0.62              |
| 1:D:297:GLU:CD   | 1:E:306:LYS:CB   | 2.73                     | 0.62              |
| 1:F:308:GLU:N    | 1:F:308:GLU:OE1  | 2.32                     | 0.62              |
| 1:A:308:GLU:N    | 1:A:308:GLU:OE1  | 2.33                     | 0.61              |
| 1:B:555:GLN:HG3  | 1:B:556:THR:HG23 | 1.81                     | 0.61              |
| 1:B:580:VAL:HG12 | 1:B:580:VAL:O    | 2.00                     | 0.61              |
| 1:C:354:LEU:HD21 | 1:C:414:ASN:HD21 | 1.65                     | 0.61              |
| 1:E:308:GLU:OE1  | 1:E:308:GLU:N    | 2.32                     | 0.61              |
| 1:E:555:GLN:HG3  | 1:E:556:THR:HG23 | 1.81                     | 0.61              |
| 1:F:527:ASN:OD1  | 1:N:470:ASN:HB2  | 2.00                     | 0.61              |
| 1:A:410:ARG:HH21 | 1:A:437:ARG:HH21 | 1.47                     | 0.61              |
| 1:D:285:VAL:HG22 | 1:E:318:TRP:CG   | 2.35                     | 0.61              |
| 1:E:172:ARG:HE   | 1:E:229:ARG:NH2  | 1.98                     | 0.61              |
| 1:F:274:ASP:HB2  | 1:N:382:VAL:CG1  | 2.31                     | 0.61              |
| 1:F:580:VAL:HG12 | 1:F:580:VAL:O    | 2.00                     | 0.61              |
| 1:B:172:ARG:HE   | 1:B:229:ARG:NH2  | 1.98                     | 0.61              |
| 1:C:182:LEU:HD21 | 1:C:220:ILE:HG23 | 1.81                     | 0.61              |
| 1:A:346:GLN:OE1  | 1:N:280:PHE:CG   | 2.53                     | 0.61              |
| 1:C:580:VAL:HG12 | 1:C:580:VAL:O    | 2.00                     | 0.61              |
| 1:D:354:LEU:HD21 | 1:D:414:ASN:HD21 | 1.65                     | 0.61              |
| 1:D:580:VAL:HG12 | 1:D:580:VAL:O    | 2.00                     | 0.61              |
| 1:N:172:ARG:HE   | 1:N:229:ARG:NH2  | 1.98                     | 0.61              |
| 1:C:291:GLY:HA2  | 1:D:312:SER:HA   | 1.83                     | 0.61              |
| 1:E:580:VAL:HG12 | 1:E:580:VAL:O    | 2.00                     | 0.61              |
| 1:C:223:ASN:OD1  | 1:C:224:ASP:N    | 2.32                     | 0.61              |
| 1:D:410:ARG:HH21 | 1:D:437:ARG:HH21 | 1.47                     | 0.61              |
| 1:N:182:LEU:HD21 | 1:N:220:ILE:HG23 | 1.81                     | 0.61              |
| 1:E:354:LEU:HD21 | 1:E:414:ASN:HD21 | 1.65                     | 0.61              |
| 1:A:223:ASN:OD1  | 1:A:224:ASP:N    | 2.32                     | 0.61              |
| 1:A:310:ARG:HG2  | 1:N:293:THR:OG1  | 2.01                     | 0.61              |
| 1:E:334:ASN:OD1  | 1:E:335:ALA:N    | 2.24                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:354:LEU:HD21 | 1:F:414:ASN:HD21 | 1.65                     | 0.61              |
| 1:A:172:ARG:HE   | 1:A:229:ARG:NH2  | 1.98                     | 0.60              |
| 1:A:580:VAL:HG12 | 1:A:580:VAL:O    | 2.00                     | 0.60              |
| 1:F:334:ASN:OD1  | 1:F:335:ALA:N    | 2.24                     | 0.60              |
| 1:N:308:GLU:N    | 1:N:308:GLU:OE1  | 2.32                     | 0.60              |
| 1:B:275:ASN:HB2  | 1:C:376:LEU:HB2  | 1.83                     | 0.60              |
| 1:N:410:ARG:HH21 | 1:N:437:ARG:HH21 | 1.47                     | 0.60              |
| 1:C:527:ASN:OD1  | 1:D:470:ASN:HB2  | 2.01                     | 0.60              |
| 1:A:288:PHE:CE1  | 1:B:315:GLN:CB   | 2.81                     | 0.60              |
| 1:B:285:VAL:HG22 | 1:C:318:TRP:CG   | 2.37                     | 0.60              |
| 1:D:706:TRP:HE3  | 1:D:707:LEU:HD22 | 1.67                     | 0.60              |
| 1:C:288:PHE:HZ   | 1:D:315:GLN:HB3  | 1.52                     | 0.60              |
| 1:D:172:ARG:HE   | 1:D:229:ARG:NH2  | 1.98                     | 0.60              |
| 1:F:223:ASN:OD1  | 1:F:224:ASP:N    | 2.32                     | 0.60              |
| 1:F:514:ASP:OD1  | 1:F:515:GLY:N    | 2.35                     | 0.60              |
| 1:N:354:LEU:HD21 | 1:N:414:ASN:HD21 | 1.65                     | 0.60              |
| 1:N:498:ASP:OD2  | 1:N:502:ARG:NE   | 2.32                     | 0.60              |
| 1:A:346:GLN:HE21 | 1:N:282:ARG:HD2  | 1.67                     | 0.60              |
| 1:D:283:LYS:CG   | 1:E:320:THR:OG1  | 2.39                     | 0.60              |
| 1:E:142:VAL:HG22 | 1:E:581:PHE:HB3  | 1.84                     | 0.60              |
| 1:E:283:LYS:HG2  | 1:F:320:THR:CB   | 2.31                     | 0.60              |
| 1:E:285:VAL:HG13 | 1:F:318:TRP:NE1  | 2.17                     | 0.60              |
| 1:N:514:ASP:OD1  | 1:N:515:GLY:N    | 2.35                     | 0.60              |
| 1:A:142:VAL:HG22 | 1:A:581:PHE:HB3  | 1.84                     | 0.60              |
| 1:A:318:TRP:CG   | 1:N:285:VAL:HG22 | 2.37                     | 0.60              |
| 1:A:706:TRP:HE3  | 1:A:707:LEU:HD22 | 1.66                     | 0.60              |
| 1:B:706:TRP:HE3  | 1:B:707:LEU:HD22 | 1.67                     | 0.60              |
| 1:C:285:VAL:HG22 | 1:D:318:TRP:CD1  | 2.37                     | 0.60              |
| 1:E:410:ARG:HH21 | 1:E:437:ARG:HH21 | 1.47                     | 0.59              |
| 1:F:410:ARG:HH21 | 1:F:437:ARG:HH21 | 1.47                     | 0.59              |
| 1:N:706:TRP:HE3  | 1:N:707:LEU:HD22 | 1.66                     | 0.59              |
| 1:C:706:TRP:HE3  | 1:C:707:LEU:HD22 | 1.67                     | 0.59              |
| 1:D:514:ASP:OD1  | 1:D:515:GLY:N    | 2.35                     | 0.59              |
| 1:E:706:TRP:HE3  | 1:E:707:LEU:HD22 | 1.66                     | 0.59              |
| 1:A:283:LYS:CG   | 1:B:320:THR:OG1  | 2.39                     | 0.59              |
| 1:B:498:ASP:OD2  | 1:B:502:ARG:NE   | 2.31                     | 0.59              |
| 1:C:271:PHE:HB2  | 1:C:386:ASP:HB2  | 1.84                     | 0.59              |
| 1:C:274:ASP:HB2  | 1:D:382:VAL:CG1  | 2.30                     | 0.59              |
| 1:F:706:TRP:HE3  | 1:F:707:LEU:HD22 | 1.66                     | 0.59              |
| 1:B:228:TYR:C    | 1:B:229:ARG:HD3  | 2.28                     | 0.59              |
| 1:C:228:TYR:C    | 1:C:229:ARG:HD3  | 2.28                     | 0.59              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:283:LYS:CG   | 1:D:320:THR:OG1 | 2.43                     | 0.59              |
| 1:D:271:PHE:HB2  | 1:D:386:ASP:HB2 | 1.84                     | 0.59              |
| 1:F:228:TYR:C    | 1:F:229:ARG:HD3 | 2.28                     | 0.59              |
| 1:N:142:VAL:HG22 | 1:N:581:PHE:HB3 | 1.84                     | 0.59              |
| 1:A:228:TYR:C    | 1:A:229:ARG:HD3 | 2.28                     | 0.59              |
| 1:D:142:VAL:HG22 | 1:D:581:PHE:HB3 | 1.84                     | 0.59              |
| 1:D:228:TYR:C    | 1:D:229:ARG:HD3 | 2.28                     | 0.59              |
| 1:N:228:TYR:C    | 1:N:229:ARG:HD3 | 2.28                     | 0.59              |
| 1:E:228:TYR:C    | 1:E:229:ARG:HD3 | 2.28                     | 0.59              |
| 1:A:297:GLU:CD   | 1:B:306:LYS:CB  | 2.76                     | 0.59              |
| 1:B:142:VAL:HG22 | 1:B:581:PHE:HB3 | 1.84                     | 0.59              |
| 1:E:271:PHE:HB2  | 1:E:386:ASP:HB2 | 1.84                     | 0.59              |
| 1:C:402:ILE:HG12 | 1:C:702:TRP:HZ2 | 1.68                     | 0.59              |
| 1:D:274:ASP:HB2  | 1:E:382:VAL:CG1 | 2.31                     | 0.59              |
| 1:E:402:ILE:HG12 | 1:E:702:TRP:HZ2 | 1.68                     | 0.59              |
| 1:E:514:ASP:OD1  | 1:E:515:GLY:N   | 2.35                     | 0.59              |
| 1:N:334:ASN:OD1  | 1:N:335:ALA:N   | 2.24                     | 0.59              |
| 1:B:271:PHE:HB2  | 1:B:386:ASP:HB2 | 1.84                     | 0.59              |
| 1:B:514:ASP:OD1  | 1:B:515:GLY:N   | 2.35                     | 0.59              |
| 1:C:514:ASP:OD1  | 1:C:515:GLY:N   | 2.35                     | 0.59              |
| 1:F:271:PHE:HB2  | 1:F:386:ASP:HB2 | 1.84                     | 0.59              |
| 1:F:402:ILE:HG12 | 1:F:702:TRP:HZ2 | 1.68                     | 0.59              |
| 1:C:498:ASP:OD2  | 1:C:502:ARG:NE  | 2.32                     | 0.58              |
| 1:F:500:LEU:HD22 | 1:F:531:ARG:HE  | 1.68                     | 0.58              |
| 1:C:500:LEU:HD22 | 1:C:531:ARG:HE  | 1.68                     | 0.58              |
| 1:N:500:LEU:HD22 | 1:N:531:ARG:HE  | 1.68                     | 0.58              |
| 1:C:142:VAL:HG22 | 1:C:581:PHE:HB3 | 1.84                     | 0.58              |
| 1:N:402:ILE:HG12 | 1:N:702:TRP:HZ2 | 1.68                     | 0.58              |
| 1:A:271:PHE:HB2  | 1:A:386:ASP:HB2 | 1.84                     | 0.58              |
| 1:E:295:GLY:HA2  | 1:F:308:GLU:HA  | 1.83                     | 0.58              |
| 1:F:142:VAL:HG22 | 1:F:581:PHE:HB3 | 1.84                     | 0.58              |
| 1:N:271:PHE:HB2  | 1:N:386:ASP:HB2 | 1.84                     | 0.58              |
| 1:A:514:ASP:OD1  | 1:A:515:GLY:N   | 2.35                     | 0.58              |
| 1:B:500:LEU:HD22 | 1:B:531:ARG:HE  | 1.68                     | 0.58              |
| 1:D:500:LEU:HD22 | 1:D:531:ARG:HE  | 1.68                     | 0.58              |
| 1:B:288:PHE:CE1  | 1:C:315:GLN:CB  | 2.83                     | 0.58              |
| 1:B:402:ILE:HG12 | 1:B:702:TRP:HZ2 | 1.68                     | 0.58              |
| 1:E:525:ASN:H    | 1:E:530:GLN:NE2 | 2.02                     | 0.58              |
| 1:A:498:ASP:OD2  | 1:A:502:ARG:NE  | 2.32                     | 0.58              |
| 1:N:165:TRP:HH2  | 1:N:233:ALA:HA  | 1.69                     | 0.58              |
| 1:A:500:LEU:HD22 | 1:A:531:ARG:HE  | 1.69                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:165:TRP:HH2  | 1:B:233:ALA:HA   | 1.69                     | 0.57              |
| 1:D:402:ILE:HG12 | 1:D:702:TRP:HZ2  | 1.68                     | 0.57              |
| 1:E:221:HIS:NE2  | 1:E:223:ASN:O    | 2.37                     | 0.57              |
| 1:D:165:TRP:HH2  | 1:D:233:ALA:HA   | 1.69                     | 0.57              |
| 1:A:402:ILE:HG12 | 1:A:702:TRP:HZ2  | 1.68                     | 0.57              |
| 1:C:165:TRP:HH2  | 1:C:233:ALA:HA   | 1.69                     | 0.57              |
| 1:D:221:HIS:NE2  | 1:D:223:ASN:O    | 2.37                     | 0.57              |
| 1:E:288:PHE:CE1  | 1:F:315:GLN:CB   | 2.75                     | 0.57              |
| 1:A:283:LYS:HB2  | 1:A:318:TRP:HB2  | 1.87                     | 0.57              |
| 1:B:283:LYS:CG   | 1:C:320:THR:OG1  | 2.47                     | 0.57              |
| 1:B:527:ASN:OD1  | 1:C:470:ASN:HB2  | 2.05                     | 0.57              |
| 1:E:520:ALA:O    | 1:E:522:GLN:NE2  | 2.38                     | 0.57              |
| 1:E:165:TRP:HH2  | 1:E:233:ALA:HA   | 1.69                     | 0.57              |
| 1:A:527:ASN:OD1  | 1:B:470:ASN:HB2  | 2.04                     | 0.57              |
| 1:C:221:HIS:NE2  | 1:C:223:ASN:O    | 2.37                     | 0.57              |
| 1:B:283:LYS:HB2  | 1:B:318:TRP:HB2  | 1.87                     | 0.57              |
| 1:N:221:HIS:NE2  | 1:N:223:ASN:O    | 2.37                     | 0.57              |
| 1:A:320:THR:OG1  | 1:N:283:LYS:CG   | 2.41                     | 0.57              |
| 1:E:500:LEU:HD22 | 1:E:531:ARG:HE   | 1.69                     | 0.57              |
| 1:F:525:ASN:H    | 1:F:530:GLN:NE2  | 2.02                     | 0.57              |
| 1:A:579:ASP:HA   | 1:N:197:VAL:HG21 | 1.87                     | 0.57              |
| 1:D:297:GLU:OE2  | 1:E:306:LYS:CB   | 2.53                     | 0.57              |
| 1:D:498:ASP:OD2  | 1:D:502:ARG:NE   | 2.32                     | 0.57              |
| 1:N:283:LYS:HB2  | 1:N:318:TRP:HB2  | 1.87                     | 0.57              |
| 1:F:520:ALA:O    | 1:F:522:GLN:NE2  | 2.38                     | 0.57              |
| 1:A:472:CYS:SG   | 1:A:486:CYS:HA   | 2.45                     | 0.56              |
| 1:C:472:CYS:SG   | 1:C:486:CYS:HA   | 2.45                     | 0.56              |
| 1:E:472:CYS:SG   | 1:E:486:CYS:HA   | 2.45                     | 0.56              |
| 1:N:472:CYS:SG   | 1:N:486:CYS:HA   | 2.45                     | 0.56              |
| 1:F:221:HIS:NE2  | 1:F:223:ASN:O    | 2.37                     | 0.56              |
| 1:F:472:CYS:SG   | 1:F:486:CYS:HA   | 2.45                     | 0.56              |
| 1:A:346:GLN:OE1  | 1:N:280:PHE:CD2  | 2.58                     | 0.56              |
| 1:D:283:LYS:HB2  | 1:D:318:TRP:HB2  | 1.87                     | 0.56              |
| 1:A:165:TRP:HH2  | 1:A:233:ALA:HA   | 1.69                     | 0.56              |
| 1:A:221:HIS:NE2  | 1:A:223:ASN:O    | 2.37                     | 0.56              |
| 1:B:221:HIS:NE2  | 1:B:223:ASN:O    | 2.37                     | 0.56              |
| 1:C:283:LYS:HB2  | 1:C:318:TRP:HB2  | 1.87                     | 0.56              |
| 1:F:283:LYS:HG2  | 1:N:320:THR:CB   | 2.35                     | 0.56              |
| 1:N:520:ALA:O    | 1:N:522:GLN:NE2  | 2.38                     | 0.56              |
| 1:C:293:THR:OG1  | 1:D:310:ARG:HG2  | 2.05                     | 0.56              |
| 1:F:165:TRP:HH2  | 1:F:233:ALA:HA   | 1.69                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:275:ASN:HB2  | 1:E:376:LEU:HB2  | 1.87                     | 0.56              |
| 1:D:472:CYS:SG   | 1:D:486:CYS:HA   | 2.46                     | 0.56              |
| 1:E:274:ASP:HB2  | 1:F:382:VAL:CG1  | 2.35                     | 0.56              |
| 1:A:285:VAL:HG22 | 1:B:318:TRP:CD1  | 2.41                     | 0.56              |
| 1:B:472:CYS:SG   | 1:B:486:CYS:HA   | 2.46                     | 0.56              |
| 1:B:525:ASN:H    | 1:B:530:GLN:NE2  | 2.02                     | 0.56              |
| 1:D:706:TRP:CE3  | 1:D:707:LEU:HD22 | 2.41                     | 0.56              |
| 1:E:288:PHE:HZ   | 1:F:315:GLN:CB   | 2.07                     | 0.56              |
| 1:A:288:PHE:HZ   | 1:B:315:GLN:HB3  | 1.57                     | 0.55              |
| 1:B:658:GLN:OE1  | 1:B:709:LYS:NZ   | 2.39                     | 0.55              |
| 1:C:706:TRP:CE3  | 1:C:707:LEU:HD22 | 2.41                     | 0.55              |
| 1:C:658:GLN:OE1  | 1:C:709:LYS:NZ   | 2.39                     | 0.55              |
| 1:D:525:ASN:H    | 1:D:530:GLN:NE2  | 2.02                     | 0.55              |
| 1:B:706:TRP:CE3  | 1:B:707:LEU:HD22 | 2.41                     | 0.55              |
| 1:E:274:ASP:HA   | 1:E:330:ARG:HD3  | 1.89                     | 0.55              |
| 1:F:293:THR:OG1  | 1:N:310:ARG:HG2  | 2.06                     | 0.55              |
| 1:A:291:GLY:HA2  | 1:B:312:SER:HA   | 1.88                     | 0.55              |
| 1:E:706:TRP:CE3  | 1:E:707:LEU:HD22 | 2.41                     | 0.55              |
| 1:F:283:LYS:HB2  | 1:F:318:TRP:HB2  | 1.87                     | 0.55              |
| 1:B:293:THR:OG1  | 1:C:310:ARG:HG2  | 2.06                     | 0.55              |
| 1:N:706:TRP:CE3  | 1:N:707:LEU:HD22 | 2.41                     | 0.55              |
| 1:E:283:LYS:HB2  | 1:E:318:TRP:HB2  | 1.87                     | 0.55              |
| 1:A:520:ALA:O    | 1:A:522:GLN:NE2  | 2.38                     | 0.55              |
| 1:D:274:ASP:HA   | 1:D:330:ARG:HD3  | 1.89                     | 0.55              |
| 1:C:274:ASP:HA   | 1:C:330:ARG:HD3  | 1.89                     | 0.55              |
| 1:F:658:GLN:OE1  | 1:F:709:LYS:NZ   | 2.39                     | 0.55              |
| 1:N:525:ASN:H    | 1:N:530:GLN:NE2  | 2.02                     | 0.55              |
| 1:E:498:ASP:OD2  | 1:E:502:ARG:NE   | 2.32                     | 0.54              |
| 1:N:658:GLN:OE1  | 1:N:709:LYS:NZ   | 2.39                     | 0.54              |
| 1:B:274:ASP:HA   | 1:B:330:ARG:HD3  | 1.89                     | 0.54              |
| 1:C:285:VAL:HG22 | 1:D:318:TRP:CG   | 2.42                     | 0.54              |
| 1:F:274:ASP:HA   | 1:F:330:ARG:HD3  | 1.89                     | 0.54              |
| 1:C:520:ALA:O    | 1:C:522:GLN:NE2  | 2.38                     | 0.54              |
| 1:F:285:VAL:HG22 | 1:N:318:TRP:CD1  | 2.41                     | 0.54              |
| 1:A:297:GLU:OE2  | 1:B:306:LYS:CB   | 2.56                     | 0.54              |
| 1:B:275:ASN:HD22 | 1:C:376:LEU:HA   | 1.71                     | 0.54              |
| 1:D:520:ALA:O    | 1:D:522:GLN:NE2  | 2.38                     | 0.54              |
| 1:A:706:TRP:CE3  | 1:A:707:LEU:HD22 | 2.41                     | 0.54              |
| 1:D:658:GLN:OE1  | 1:D:709:LYS:NZ   | 2.39                     | 0.54              |
| 1:F:706:TRP:CE3  | 1:F:707:LEU:HD22 | 2.41                     | 0.54              |
| 1:A:164:LEU:HD22 | 1:A:241:TYR:HB2  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:382:VAL:HG11 | 1:N:273:VAL:O    | 2.08                     | 0.53              |
| 1:B:520:ALA:O    | 1:B:522:GLN:NE2  | 2.38                     | 0.53              |
| 1:E:658:GLN:OE1  | 1:E:709:LYS:NZ   | 2.40                     | 0.53              |
| 1:A:274:ASP:HA   | 1:A:330:ARG:HD3  | 1.89                     | 0.53              |
| 1:N:188:LEU:HD12 | 1:N:455:PHE:HZ   | 1.73                     | 0.53              |
| 1:A:376:LEU:HB2  | 1:N:275:ASN:HB2  | 1.89                     | 0.53              |
| 1:B:259:ASN:OD1  | 1:B:260:ALA:N    | 2.42                     | 0.53              |
| 1:B:274:ASP:HB2  | 1:C:382:VAL:CG1  | 2.36                     | 0.53              |
| 1:N:274:ASP:HA   | 1:N:330:ARG:HD3  | 1.89                     | 0.53              |
| 1:B:358:THR:HB   | 1:B:428:PHE:HD1  | 1.74                     | 0.53              |
| 1:F:188:LEU:HD12 | 1:F:455:PHE:HZ   | 1.73                     | 0.53              |
| 1:E:259:ASN:OD1  | 1:E:260:ALA:N    | 2.42                     | 0.53              |
| 1:N:164:LEU:HD22 | 1:N:241:TYR:HB2  | 1.90                     | 0.53              |
| 1:C:270:THR:HG21 | 1:C:330:ARG:HH22 | 1.74                     | 0.53              |
| 1:C:525:ASN:H    | 1:C:530:GLN:NE2  | 2.02                     | 0.53              |
| 1:E:270:THR:HG21 | 1:E:330:ARG:HH22 | 1.74                     | 0.53              |
| 1:F:259:ASN:OD1  | 1:F:260:ALA:N    | 2.42                     | 0.53              |
| 1:A:318:TRP:NE1  | 1:N:285:VAL:HG13 | 2.24                     | 0.53              |
| 1:B:275:ASN:ND2  | 1:C:376:LEU:HA   | 2.24                     | 0.53              |
| 1:C:188:LEU:HD12 | 1:C:455:PHE:HZ   | 1.74                     | 0.53              |
| 1:N:358:THR:HB   | 1:N:428:PHE:HD1  | 1.74                     | 0.53              |
| 1:N:416:ALA:HB1  | 1:N:427:GLN:HB3  | 1.90                     | 0.53              |
| 1:A:416:ALA:HB1  | 1:A:427:GLN:HB3  | 1.90                     | 0.53              |
| 1:B:164:LEU:HD22 | 1:B:241:TYR:HB2  | 1.90                     | 0.53              |
| 1:B:336:GLN:OE1  | 1:B:336:GLN:N    | 2.42                     | 0.53              |
| 1:E:336:GLN:N    | 1:E:336:GLN:OE1  | 2.42                     | 0.53              |
| 1:E:358:THR:HB   | 1:E:428:PHE:HD1  | 1.74                     | 0.53              |
| 1:A:270:THR:HG21 | 1:A:330:ARG:HH22 | 1.74                     | 0.53              |
| 1:C:259:ASN:OD1  | 1:C:260:ALA:N    | 2.42                     | 0.53              |
| 1:D:188:LEU:HD12 | 1:D:455:PHE:HZ   | 1.74                     | 0.53              |
| 1:F:416:ALA:HB1  | 1:F:427:GLN:HB3  | 1.90                     | 0.53              |
| 1:D:358:THR:HB   | 1:D:428:PHE:HD1  | 1.74                     | 0.53              |
| 1:N:259:ASN:OD1  | 1:N:260:ALA:N    | 2.42                     | 0.53              |
| 1:N:270:THR:HG21 | 1:N:330:ARG:HH22 | 1.74                     | 0.53              |
| 1:A:278:GLU:OE2  | 1:A:278:GLU:N    | 2.39                     | 0.52              |
| 1:A:525:ASN:H    | 1:A:530:GLN:NE2  | 2.02                     | 0.52              |
| 1:F:336:GLN:N    | 1:F:336:GLN:OE1  | 2.42                     | 0.52              |
| 1:F:358:THR:HB   | 1:F:428:PHE:HD1  | 1.74                     | 0.52              |
| 1:A:285:VAL:HG22 | 1:B:318:TRP:CG   | 2.45                     | 0.52              |
| 1:A:308:GLU:HA   | 1:N:295:GLY:HA2  | 1.90                     | 0.52              |
| 1:A:336:GLN:N    | 1:A:336:GLN:OE1  | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:336:GLN:N    | 1:C:336:GLN:OE1  | 2.42                     | 0.52              |
| 1:D:416:ALA:HB1  | 1:D:427:GLN:HB3  | 1.90                     | 0.52              |
| 1:A:259:ASN:OD1  | 1:A:260:ALA:N    | 2.42                     | 0.52              |
| 1:A:512:CYS:HB2  | 1:A:524:CYS:SG   | 2.50                     | 0.52              |
| 1:N:512:CYS:HB2  | 1:N:524:CYS:SG   | 2.50                     | 0.52              |
| 1:A:188:LEU:HD12 | 1:A:455:PHE:HZ   | 1.73                     | 0.52              |
| 1:B:188:LEU:HD12 | 1:B:455:PHE:HZ   | 1.73                     | 0.52              |
| 1:B:230:GLN:CD   | 1:B:243:ARG:HE   | 2.18                     | 0.52              |
| 1:B:512:CYS:HB2  | 1:B:524:CYS:SG   | 2.50                     | 0.52              |
| 1:C:416:ALA:HB1  | 1:C:427:GLN:HB3  | 1.90                     | 0.52              |
| 1:C:512:CYS:HB2  | 1:C:524:CYS:SG   | 2.50                     | 0.52              |
| 1:D:164:LEU:HD22 | 1:D:241:TYR:HB2  | 1.90                     | 0.52              |
| 1:D:230:GLN:CD   | 1:D:243:ARG:HE   | 2.18                     | 0.52              |
| 1:D:512:CYS:HB2  | 1:D:524:CYS:SG   | 2.50                     | 0.52              |
| 1:E:164:LEU:HD22 | 1:E:241:TYR:HB2  | 1.90                     | 0.52              |
| 1:E:512:CYS:HB2  | 1:E:524:CYS:SG   | 2.50                     | 0.52              |
| 1:N:336:GLN:OE1  | 1:N:336:GLN:N    | 2.42                     | 0.52              |
| 1:A:197:VAL:HG21 | 1:B:579:ASP:HA   | 1.92                     | 0.52              |
| 1:C:213:ASP:OD1  | 1:C:213:ASP:N    | 2.43                     | 0.52              |
| 1:C:358:THR:HB   | 1:C:428:PHE:HD1  | 1.74                     | 0.52              |
| 1:D:270:THR:HG21 | 1:D:330:ARG:HH22 | 1.74                     | 0.52              |
| 1:D:336:GLN:OE1  | 1:D:336:GLN:N    | 2.42                     | 0.52              |
| 1:D:465:LEU:HD12 | 1:D:552:HIS:CG   | 2.45                     | 0.52              |
| 1:F:213:ASP:N    | 1:F:213:ASP:OD1  | 2.43                     | 0.52              |
| 1:A:358:THR:HB   | 1:A:428:PHE:HD1  | 1.74                     | 0.52              |
| 1:B:270:THR:HG21 | 1:B:330:ARG:HH22 | 1.74                     | 0.52              |
| 1:B:416:ALA:HB1  | 1:B:427:GLN:HB3  | 1.90                     | 0.52              |
| 1:B:465:LEU:HD12 | 1:B:552:HIS:CG   | 2.45                     | 0.52              |
| 1:C:230:GLN:CD   | 1:C:243:ARG:HE   | 2.18                     | 0.52              |
| 1:E:473:ILE:HD11 | 1:E:481:LEU:HD22 | 1.92                     | 0.52              |
| 1:F:164:LEU:HD22 | 1:F:241:TYR:HB2  | 1.90                     | 0.52              |
| 1:F:512:CYS:HB2  | 1:F:524:CYS:SG   | 2.50                     | 0.52              |
| 1:N:473:ILE:HD11 | 1:N:481:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:315:GLN:CB   | 1:N:288:PHE:HZ   | 2.15                     | 0.52              |
| 1:B:285:VAL:HG13 | 1:C:318:TRP:NE1  | 2.25                     | 0.52              |
| 1:C:288:PHE:CE1  | 1:D:315:GLN:CB   | 2.82                     | 0.52              |
| 1:D:267:ILE:HD13 | 1:D:338:VAL:HB   | 1.93                     | 0.52              |
| 1:D:285:VAL:HG13 | 1:E:318:TRP:NE1  | 2.25                     | 0.52              |
| 1:B:278:GLU:OE2  | 1:B:278:GLU:N    | 2.39                     | 0.51              |
| 1:D:259:ASN:OD1  | 1:D:260:ALA:N    | 2.42                     | 0.51              |
| 1:E:188:LEU:HD12 | 1:E:455:PHE:HZ   | 1.73                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:275:ASN:HB2  | 1:F:376:LEU:HB2  | 1.91                     | 0.51              |
| 1:B:267:ILE:HD13 | 1:B:338:VAL:HB   | 1.92                     | 0.51              |
| 1:C:267:ILE:HD13 | 1:C:338:VAL:HB   | 1.92                     | 0.51              |
| 1:E:267:ILE:HD13 | 1:E:338:VAL:HB   | 1.92                     | 0.51              |
| 1:E:292:VAL:N    | 1:F:311:ALA:O    | 2.24                     | 0.51              |
| 1:E:416:ALA:HB1  | 1:E:427:GLN:HB3  | 1.90                     | 0.51              |
| 1:A:267:ILE:HD13 | 1:A:338:VAL:HB   | 1.92                     | 0.51              |
| 1:A:473:ILE:HD11 | 1:A:481:LEU:HD22 | 1.92                     | 0.51              |
| 1:F:275:ASN:HB2  | 1:N:376:LEU:HB2  | 1.90                     | 0.51              |
| 1:F:291:GLY:HA2  | 1:N:312:SER:HA   | 1.90                     | 0.51              |
| 1:F:473:ILE:HD11 | 1:F:481:LEU:HD22 | 1.93                     | 0.51              |
| 1:F:498:ASP:OD2  | 1:F:502:ARG:NE   | 2.32                     | 0.51              |
| 1:B:213:ASP:OD1  | 1:B:213:ASP:N    | 2.43                     | 0.51              |
| 1:D:473:ILE:HD11 | 1:D:481:LEU:HD22 | 1.92                     | 0.51              |
| 1:D:688:PHE:HZ   | 1:D:715:LEU:HD21 | 1.76                     | 0.51              |
| 1:F:270:THR:HG21 | 1:F:330:ARG:HH22 | 1.74                     | 0.51              |
| 1:C:164:LEU:HD22 | 1:C:241:TYR:HB2  | 1.90                     | 0.51              |
| 1:D:527:ASN:OD1  | 1:E:470:ASN:HB2  | 2.11                     | 0.51              |
| 1:E:213:ASP:OD1  | 1:E:213:ASP:N    | 2.43                     | 0.51              |
| 1:E:465:LEU:HD12 | 1:E:552:HIS:CG   | 2.45                     | 0.51              |
| 1:N:465:LEU:HD12 | 1:N:552:HIS:CG   | 2.45                     | 0.51              |
| 1:B:207:VAL:HB   | 1:B:389:TYR:HB2  | 1.93                     | 0.51              |
| 1:E:230:GLN:CD   | 1:E:243:ARG:HE   | 2.18                     | 0.51              |
| 1:F:157:CYS:CB   | 1:F:175:CYS:SG   | 2.99                     | 0.51              |
| 1:F:465:LEU:HD12 | 1:F:552:HIS:CG   | 2.45                     | 0.51              |
| 1:N:157:CYS:CB   | 1:N:175:CYS:SG   | 2.99                     | 0.51              |
| 1:A:230:GLN:CD   | 1:A:243:ARG:HE   | 2.18                     | 0.51              |
| 1:A:465:LEU:HD12 | 1:A:552:HIS:CG   | 2.45                     | 0.51              |
| 1:C:207:VAL:HB   | 1:C:389:TYR:HB2  | 1.93                     | 0.51              |
| 1:F:288:PHE:CE1  | 1:N:315:GLN:CB   | 2.87                     | 0.51              |
| 1:N:472:CYS:CB   | 1:N:486:CYS:HG   | 2.24                     | 0.51              |
| 1:N:688:PHE:HZ   | 1:N:715:LEU:HD21 | 1.76                     | 0.51              |
| 1:A:207:VAL:HB   | 1:A:389:TYR:HB2  | 1.93                     | 0.51              |
| 1:D:207:VAL:HB   | 1:D:389:TYR:HB2  | 1.93                     | 0.51              |
| 1:F:230:GLN:CD   | 1:F:243:ARG:HE   | 2.18                     | 0.51              |
| 1:N:230:GLN:CD   | 1:N:243:ARG:HE   | 2.18                     | 0.51              |
| 1:A:157:CYS:CB   | 1:A:175:CYS:SG   | 2.99                     | 0.51              |
| 1:N:207:VAL:HB   | 1:N:389:TYR:HB2  | 1.93                     | 0.51              |
| 1:N:268:LEU:HB2  | 1:N:390:LYS:HB2  | 1.93                     | 0.51              |
| 1:N:278:GLU:OE2  | 1:N:278:GLU:N    | 2.40                     | 0.51              |
| 1:A:688:PHE:HZ   | 1:A:715:LEU:HD21 | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:157:CYS:CB   | 1:B:175:CYS:SG   | 2.99                     | 0.50              |
| 1:C:465:LEU:HD12 | 1:C:552:HIS:CG   | 2.45                     | 0.50              |
| 1:N:394:THR:O    | 1:N:394:THR:HG22 | 2.12                     | 0.50              |
| 1:A:213:ASP:N    | 1:A:213:ASP:OD1  | 2.43                     | 0.50              |
| 1:A:268:LEU:HB2  | 1:A:390:LYS:HB2  | 1.93                     | 0.50              |
| 1:C:275:ASN:HB2  | 1:D:376:LEU:HB2  | 1.93                     | 0.50              |
| 1:F:267:ILE:HD13 | 1:F:338:VAL:HB   | 1.92                     | 0.50              |
| 1:F:268:LEU:HB2  | 1:F:390:LYS:HB2  | 1.93                     | 0.50              |
| 1:A:243:ARG:HG3  | 1:A:245:TRP:HE1  | 1.77                     | 0.50              |
| 1:A:296:VAL:HG12 | 1:B:307:LEU:O    | 2.11                     | 0.50              |
| 1:B:394:THR:O    | 1:B:394:THR:HG22 | 2.12                     | 0.50              |
| 1:C:278:GLU:OE2  | 1:C:278:GLU:N    | 2.40                     | 0.50              |
| 1:C:688:PHE:HZ   | 1:C:715:LEU:HD21 | 1.76                     | 0.50              |
| 1:F:688:PHE:HZ   | 1:F:715:LEU:HD21 | 1.76                     | 0.50              |
| 1:N:267:ILE:HD13 | 1:N:338:VAL:HB   | 1.92                     | 0.50              |
| 1:B:473:ILE:HD11 | 1:B:481:LEU:HD22 | 1.93                     | 0.50              |
| 1:B:688:PHE:HZ   | 1:B:715:LEU:HD21 | 1.76                     | 0.50              |
| 1:C:197:VAL:HG21 | 1:D:579:ASP:HA   | 1.93                     | 0.50              |
| 1:C:473:ILE:HD11 | 1:C:481:LEU:HD22 | 1.92                     | 0.50              |
| 1:D:278:GLU:OE2  | 1:D:278:GLU:N    | 2.39                     | 0.50              |
| 1:E:207:VAL:HB   | 1:E:389:TYR:HB2  | 1.93                     | 0.50              |
| 1:F:190:ARG:NH2  | 1:F:203:ASP:OD2  | 2.45                     | 0.50              |
| 1:F:273:VAL:O    | 1:N:382:VAL:HG11 | 2.11                     | 0.50              |
| 1:C:243:ARG:HG3  | 1:C:245:TRP:HE1  | 1.77                     | 0.50              |
| 1:E:157:CYS:CB   | 1:E:175:CYS:SG   | 2.99                     | 0.50              |
| 1:E:688:PHE:HZ   | 1:E:715:LEU:HD21 | 1.76                     | 0.50              |
| 1:F:243:ARG:HG3  | 1:F:245:TRP:HE1  | 1.77                     | 0.50              |
| 1:B:243:ARG:HG3  | 1:B:245:TRP:HE1  | 1.77                     | 0.50              |
| 1:D:275:ASN:HD22 | 1:E:376:LEU:HA   | 1.76                     | 0.50              |
| 1:D:472:CYS:CB   | 1:D:486:CYS:HG   | 2.24                     | 0.50              |
| 1:E:190:ARG:NH2  | 1:E:203:ASP:OD2  | 2.45                     | 0.50              |
| 1:B:472:CYS:CB   | 1:B:486:CYS:HG   | 2.24                     | 0.50              |
| 1:C:157:CYS:CB   | 1:C:175:CYS:SG   | 2.99                     | 0.50              |
| 1:E:278:GLU:OE2  | 1:E:278:GLU:N    | 2.39                     | 0.50              |
| 1:F:602:VAL:HG21 | 1:F:696:ILE:HG13 | 1.94                     | 0.50              |
| 1:D:243:ARG:HG3  | 1:D:245:TRP:HE1  | 1.77                     | 0.50              |
| 1:B:268:LEU:HB2  | 1:B:390:LYS:HB2  | 1.93                     | 0.49              |
| 1:D:172:ARG:NH1  | 1:D:174:PHE:HA   | 2.27                     | 0.49              |
| 1:F:207:VAL:HB   | 1:F:389:TYR:HB2  | 1.93                     | 0.49              |
| 1:B:168:GLU:OE1  | 1:B:168:GLU:N    | 2.45                     | 0.49              |
| 1:B:172:ARG:NH1  | 1:B:174:PHE:HA   | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:394:THR:HG22 | 1:C:394:THR:O    | 2.11                     | 0.49              |
| 1:N:213:ASP:OD1  | 1:N:213:ASP:N    | 2.43                     | 0.49              |
| 1:N:602:VAL:HG21 | 1:N:696:ILE:HG13 | 1.94                     | 0.49              |
| 1:B:433:GLU:OE1  | 1:B:433:GLU:N    | 2.41                     | 0.49              |
| 1:D:157:CYS:CB   | 1:D:175:CYS:SG   | 2.99                     | 0.49              |
| 1:E:243:ARG:HG3  | 1:E:245:TRP:HE1  | 1.77                     | 0.49              |
| 1:A:353:LEU:O    | 1:A:372:ARG:NH2  | 2.45                     | 0.49              |
| 1:B:271:PHE:HB3  | 1:B:272:PRO:HD3  | 1.94                     | 0.49              |
| 1:B:602:VAL:HG21 | 1:B:696:ILE:HG13 | 1.94                     | 0.49              |
| 1:D:190:ARG:NH2  | 1:D:203:ASP:OD2  | 2.45                     | 0.49              |
| 1:E:602:VAL:HG21 | 1:E:696:ILE:HG13 | 1.94                     | 0.49              |
| 1:N:241:TYR:CE1  | 1:N:417:TYR:HB2  | 2.48                     | 0.49              |
| 1:N:343:ASN:OD1  | 1:N:344:ARG:N    | 2.45                     | 0.49              |
| 1:A:143:ALA:HB1  | 1:N:202:PRO:HG3  | 1.93                     | 0.49              |
| 1:A:172:ARG:NH1  | 1:A:174:PHE:HA   | 2.27                     | 0.49              |
| 1:C:268:LEU:HB2  | 1:C:390:LYS:HB2  | 1.93                     | 0.49              |
| 1:C:271:PHE:HB3  | 1:C:272:PRO:HD3  | 1.94                     | 0.49              |
| 1:C:602:VAL:HG21 | 1:C:696:ILE:HG13 | 1.94                     | 0.49              |
| 1:D:353:LEU:O    | 1:D:372:ARG:NH2  | 2.46                     | 0.49              |
| 1:F:394:THR:HG22 | 1:F:394:THR:O    | 2.12                     | 0.49              |
| 1:F:427:GLN:OE1  | 1:F:427:GLN:N    | 2.46                     | 0.49              |
| 1:A:343:ASN:OD1  | 1:A:344:ARG:N    | 2.45                     | 0.49              |
| 1:E:268:LEU:HB2  | 1:E:390:LYS:HB2  | 1.93                     | 0.49              |
| 1:F:241:TYR:CE1  | 1:F:417:TYR:HB2  | 2.48                     | 0.49              |
| 1:F:271:PHE:HB3  | 1:F:272:PRO:HD3  | 1.94                     | 0.49              |
| 1:F:343:ASN:OD1  | 1:F:344:ARG:N    | 2.45                     | 0.49              |
| 1:A:452:HIS:HB3  | 1:A:454:VAL:HG12 | 1.95                     | 0.49              |
| 1:B:241:TYR:CE1  | 1:B:417:TYR:HB2  | 2.48                     | 0.49              |
| 1:C:343:ASN:OD1  | 1:C:344:ARG:N    | 2.45                     | 0.49              |
| 1:E:241:TYR:CE1  | 1:E:417:TYR:HB2  | 2.48                     | 0.49              |
| 1:N:353:LEU:O    | 1:N:372:ARG:NH2  | 2.45                     | 0.49              |
| 1:A:394:THR:HG22 | 1:A:394:THR:O    | 2.12                     | 0.49              |
| 1:B:343:ASN:OD1  | 1:B:344:ARG:N    | 2.45                     | 0.49              |
| 1:C:353:LEU:O    | 1:C:372:ARG:NH2  | 2.45                     | 0.49              |
| 1:D:268:LEU:HB2  | 1:D:390:LYS:HB2  | 1.93                     | 0.49              |
| 1:N:243:ARG:HG3  | 1:N:245:TRP:HE1  | 1.77                     | 0.49              |
| 1:N:427:GLN:N    | 1:N:427:GLN:OE1  | 2.46                     | 0.49              |
| 1:N:452:HIS:HB3  | 1:N:454:VAL:HG12 | 1.95                     | 0.49              |
| 1:A:427:GLN:OE1  | 1:A:427:GLN:N    | 2.46                     | 0.49              |
| 1:B:353:LEU:O    | 1:B:372:ARG:NH2  | 2.45                     | 0.49              |
| 1:B:417:TYR:HD2  | 1:B:419:HIS:CE1  | 2.31                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:159:PHE:HE1  | 1:C:438:ARG:HD2  | 1.78                     | 0.49              |
| 1:C:285:VAL:HG13 | 1:D:318:TRP:NE1  | 2.28                     | 0.49              |
| 1:C:417:TYR:HD2  | 1:C:419:HIS:CE1  | 2.31                     | 0.49              |
| 1:D:241:TYR:CE1  | 1:D:417:TYR:HB2  | 2.48                     | 0.49              |
| 1:D:275:ASN:ND2  | 1:E:376:LEU:HA   | 2.27                     | 0.49              |
| 1:E:159:PHE:HE1  | 1:E:438:ARG:HD2  | 1.78                     | 0.49              |
| 1:F:172:ARG:NH1  | 1:F:174:PHE:HA   | 2.27                     | 0.49              |
| 1:N:271:PHE:HB3  | 1:N:272:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:602:VAL:HG21 | 1:A:696:ILE:HG13 | 1.94                     | 0.49              |
| 1:D:273:VAL:O    | 1:E:382:VAL:HG11 | 2.12                     | 0.49              |
| 1:E:172:ARG:NH1  | 1:E:174:PHE:HA   | 2.27                     | 0.49              |
| 1:E:343:ASN:OD1  | 1:E:344:ARG:N    | 2.45                     | 0.49              |
| 1:E:353:LEU:O    | 1:E:372:ARG:NH2  | 2.45                     | 0.49              |
| 1:B:159:PHE:HE1  | 1:B:438:ARG:HD2  | 1.78                     | 0.48              |
| 1:C:168:GLU:OE1  | 1:C:168:GLU:N    | 2.45                     | 0.48              |
| 1:C:190:ARG:NH2  | 1:C:203:ASP:OD2  | 2.45                     | 0.48              |
| 1:C:241:TYR:CE1  | 1:C:417:TYR:HB2  | 2.48                     | 0.48              |
| 1:D:293:THR:OG1  | 1:E:310:ARG:HG2  | 2.13                     | 0.48              |
| 1:D:651:ASP:O    | 1:D:681:THR:OG1  | 2.26                     | 0.48              |
| 1:E:427:GLN:N    | 1:E:427:GLN:OE1  | 2.46                     | 0.48              |
| 1:N:159:PHE:HE1  | 1:N:438:ARG:HD2  | 1.78                     | 0.48              |
| 1:N:243:ARG:HG3  | 1:N:245:TRP:NE1  | 2.28                     | 0.48              |
| 1:A:417:TYR:HD2  | 1:A:419:HIS:CE1  | 2.31                     | 0.48              |
| 1:D:159:PHE:HE1  | 1:D:438:ARG:HD2  | 1.78                     | 0.48              |
| 1:D:271:PHE:HB3  | 1:D:272:PRO:HD3  | 1.95                     | 0.48              |
| 1:D:343:ASN:OD1  | 1:D:344:ARG:N    | 2.45                     | 0.48              |
| 1:D:602:VAL:HG21 | 1:D:696:ILE:HG13 | 1.93                     | 0.48              |
| 1:A:159:PHE:HE1  | 1:A:438:ARG:HD2  | 1.78                     | 0.48              |
| 1:A:243:ARG:HG3  | 1:A:245:TRP:NE1  | 2.28                     | 0.48              |
| 1:B:190:ARG:NH2  | 1:B:203:ASP:OD2  | 2.45                     | 0.48              |
| 1:B:274:ASP:OD2  | 1:C:376:LEU:HD13 | 2.13                     | 0.48              |
| 1:D:213:ASP:N    | 1:D:213:ASP:OD1  | 2.43                     | 0.48              |
| 1:D:524:CYS:HB2  | 1:D:530:GLN:OE1  | 2.13                     | 0.48              |
| 1:E:394:THR:HG22 | 1:E:394:THR:O    | 2.12                     | 0.48              |
| 1:A:190:ARG:NH2  | 1:A:203:ASP:OD2  | 2.45                     | 0.48              |
| 1:A:376:LEU:HA   | 1:N:275:ASN:HD22 | 1.78                     | 0.48              |
| 1:B:273:VAL:O    | 1:C:382:VAL:HG11 | 2.13                     | 0.48              |
| 1:B:427:GLN:N    | 1:B:427:GLN:OE1  | 2.46                     | 0.48              |
| 1:B:452:HIS:HB3  | 1:B:454:VAL:HG12 | 1.95                     | 0.48              |
| 1:D:394:THR:HG22 | 1:D:394:THR:O    | 2.12                     | 0.48              |
| 1:D:417:TYR:HD2  | 1:D:419:HIS:CE1  | 2.31                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:278:GLU:OE2  | 1:F:278:GLU:N    | 2.39                     | 0.48              |
| 1:A:241:TYR:CE1  | 1:A:417:TYR:HB2  | 2.48                     | 0.48              |
| 1:B:651:ASP:O    | 1:B:681:THR:OG1  | 2.26                     | 0.48              |
| 1:C:172:ARG:NH1  | 1:C:174:PHE:HA   | 2.27                     | 0.48              |
| 1:E:271:PHE:HB3  | 1:E:272:PRO:HD3  | 1.94                     | 0.48              |
| 1:E:417:TYR:HD2  | 1:E:419:HIS:CE1  | 2.31                     | 0.48              |
| 1:D:427:GLN:N    | 1:D:427:GLN:OE1  | 2.46                     | 0.48              |
| 1:E:524:CYS:HB2  | 1:E:530:GLN:OE1  | 2.13                     | 0.48              |
| 1:F:184:TYR:CE1  | 1:F:211:LEU:HD21 | 2.49                     | 0.48              |
| 1:N:433:GLU:OE1  | 1:N:433:GLU:N    | 2.41                     | 0.48              |
| 1:B:524:CYS:HB2  | 1:B:530:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:184:TYR:CE1  | 1:C:211:LEU:HD21 | 2.49                     | 0.48              |
| 1:C:427:GLN:OE1  | 1:C:427:GLN:N    | 2.46                     | 0.48              |
| 1:F:243:ARG:HG3  | 1:F:245:TRP:NE1  | 2.29                     | 0.48              |
| 1:A:202:PRO:HG3  | 1:B:143:ALA:HB1  | 1.96                     | 0.48              |
| 1:C:452:HIS:HB3  | 1:C:454:VAL:HG12 | 1.95                     | 0.48              |
| 1:E:243:ARG:HG3  | 1:E:245:TRP:NE1  | 2.28                     | 0.48              |
| 1:E:275:ASN:HD22 | 1:F:376:LEU:HA   | 1.79                     | 0.48              |
| 1:F:452:HIS:HB3  | 1:F:454:VAL:HG12 | 1.95                     | 0.48              |
| 1:N:172:ARG:NH1  | 1:N:174:PHE:HA   | 2.27                     | 0.48              |
| 1:B:184:TYR:CE1  | 1:B:211:LEU:HD21 | 2.49                     | 0.48              |
| 1:C:369:ASP:OD1  | 1:C:370:VAL:N    | 2.47                     | 0.48              |
| 1:E:184:TYR:CE1  | 1:E:211:LEU:HD21 | 2.49                     | 0.48              |
| 1:F:285:VAL:HG22 | 1:N:318:TRP:CG   | 2.49                     | 0.48              |
| 1:F:417:TYR:HD2  | 1:F:419:HIS:CE1  | 2.31                     | 0.48              |
| 1:F:617:ASP:OD2  | 1:F:632:GLY:N    | 2.47                     | 0.48              |
| 1:B:243:ARG:HG3  | 1:B:245:TRP:NE1  | 2.28                     | 0.48              |
| 1:C:524:CYS:HB2  | 1:C:530:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:617:ASP:OD2  | 1:C:632:GLY:N    | 2.47                     | 0.48              |
| 1:D:184:TYR:CE1  | 1:D:211:LEU:HD21 | 2.49                     | 0.48              |
| 1:F:159:PHE:HE1  | 1:F:438:ARG:HD2  | 1.78                     | 0.48              |
| 1:N:417:TYR:HD2  | 1:N:419:HIS:CE1  | 2.31                     | 0.48              |
| 1:A:617:ASP:OD2  | 1:A:632:GLY:N    | 2.47                     | 0.47              |
| 1:B:369:ASP:OD1  | 1:B:370:VAL:N    | 2.47                     | 0.47              |
| 1:D:243:ARG:HG3  | 1:D:245:TRP:NE1  | 2.28                     | 0.47              |
| 1:E:283:LYS:CG   | 1:F:320:THR:OG1  | 2.49                     | 0.47              |
| 1:N:184:TYR:CE1  | 1:N:211:LEU:HD21 | 2.49                     | 0.47              |
| 1:N:369:ASP:OD1  | 1:N:370:VAL:N    | 2.47                     | 0.47              |
| 1:A:273:VAL:O    | 1:B:382:VAL:HG11 | 2.12                     | 0.47              |
| 1:A:524:CYS:HB2  | 1:A:530:GLN:OE1  | 2.13                     | 0.47              |
| 1:E:617:ASP:OD2  | 1:E:632:GLY:N    | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:353:LEU:O    | 1:F:372:ARG:NH2  | 2.45                     | 0.47              |
| 1:D:369:ASP:OD1  | 1:D:370:VAL:N    | 2.47                     | 0.47              |
| 1:N:524:CYS:HB2  | 1:N:530:GLN:OE1  | 2.13                     | 0.47              |
| 1:B:617:ASP:OD2  | 1:B:632:GLY:N    | 2.47                     | 0.47              |
| 1:A:271:PHE:HB3  | 1:A:272:PRO:HD3  | 1.94                     | 0.47              |
| 1:D:452:HIS:HB3  | 1:D:454:VAL:HG12 | 1.95                     | 0.47              |
| 1:F:275:ASN:HD22 | 1:N:376:LEU:HA   | 1.79                     | 0.47              |
| 1:N:190:ARG:NH2  | 1:N:203:ASP:OD2  | 2.45                     | 0.47              |
| 1:C:243:ARG:HG3  | 1:C:245:TRP:NE1  | 2.28                     | 0.47              |
| 1:C:244:GLU:C    | 1:C:245:TRP:CD1  | 2.93                     | 0.47              |
| 1:D:244:GLU:C    | 1:D:245:TRP:CD1  | 2.93                     | 0.47              |
| 1:E:433:GLU:OE1  | 1:E:433:GLU:N    | 2.41                     | 0.47              |
| 1:E:452:HIS:HB3  | 1:E:454:VAL:HG12 | 1.95                     | 0.47              |
| 1:F:524:CYS:HB2  | 1:F:530:GLN:OE1  | 2.13                     | 0.47              |
| 1:N:244:GLU:C    | 1:N:245:TRP:CD1  | 2.93                     | 0.47              |
| 1:A:369:ASP:OD1  | 1:A:370:VAL:N    | 2.47                     | 0.47              |
| 1:C:202:PRO:HG3  | 1:D:143:ALA:HB1  | 1.97                     | 0.47              |
| 1:C:273:VAL:O    | 1:D:382:VAL:HG11 | 2.14                     | 0.47              |
| 1:E:244:GLU:C    | 1:E:245:TRP:CD1  | 2.93                     | 0.47              |
| 1:E:472:CYS:CB   | 1:E:486:CYS:SG   | 3.03                     | 0.47              |
| 1:F:197:VAL:HG21 | 1:N:579:ASP:HA   | 1.96                     | 0.47              |
| 1:F:433:GLU:OE1  | 1:F:433:GLU:N    | 2.41                     | 0.47              |
| 1:F:565:SER:HB3  | 1:F:571:LEU:HG   | 1.97                     | 0.47              |
| 1:N:617:ASP:OD2  | 1:N:632:GLY:N    | 2.47                     | 0.47              |
| 1:A:184:TYR:CE1  | 1:A:211:LEU:HD21 | 2.49                     | 0.47              |
| 1:B:244:GLU:C    | 1:B:245:TRP:CD1  | 2.93                     | 0.47              |
| 1:D:433:GLU:OE1  | 1:D:433:GLU:N    | 2.41                     | 0.47              |
| 1:F:369:ASP:OD1  | 1:F:370:VAL:N    | 2.47                     | 0.47              |
| 1:A:376:LEU:HA   | 1:N:275:ASN:ND2  | 2.28                     | 0.47              |
| 1:C:651:ASP:O    | 1:C:681:THR:OG1  | 2.26                     | 0.47              |
| 1:E:369:ASP:OD1  | 1:E:370:VAL:N    | 2.47                     | 0.47              |
| 1:N:565:SER:HB3  | 1:N:571:LEU:HG   | 1.97                     | 0.47              |
| 1:D:197:VAL:HG21 | 1:E:579:ASP:HA   | 1.97                     | 0.47              |
| 1:E:197:VAL:HG21 | 1:F:579:ASP:HA   | 1.95                     | 0.47              |
| 1:A:307:LEU:O    | 1:N:296:VAL:HG12 | 2.15                     | 0.46              |
| 1:A:658:GLN:OE1  | 1:A:709:LYS:NZ   | 2.39                     | 0.46              |
| 1:D:617:ASP:OD2  | 1:D:632:GLY:N    | 2.47                     | 0.46              |
| 1:A:293:THR:OG1  | 1:B:310:ARG:HG2  | 2.15                     | 0.46              |
| 1:B:472:CYS:CB   | 1:B:486:CYS:SG   | 3.03                     | 0.46              |
| 1:E:188:LEU:HD12 | 1:E:455:PHE:CZ   | 2.50                     | 0.46              |
| 1:A:244:GLU:C    | 1:A:245:TRP:CD1  | 2.93                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:565:SER:HB3  | 1:A:571:LEU:HG   | 1.97                     | 0.46              |
| 1:N:269:LYS:O    | 1:N:388:ILE:HG22 | 2.16                     | 0.46              |
| 1:C:565:SER:HB3  | 1:C:571:LEU:HG   | 1.97                     | 0.46              |
| 1:F:188:LEU:HD12 | 1:F:455:PHE:CZ   | 2.50                     | 0.46              |
| 1:A:275:ASN:HB2  | 1:B:376:LEU:HB2  | 1.98                     | 0.46              |
| 1:B:241:TYR:HE1  | 1:B:417:TYR:HB2  | 1.81                     | 0.46              |
| 1:D:454:VAL:HG13 | 1:D:455:PHE:CD1  | 2.51                     | 0.46              |
| 1:A:454:VAL:HG13 | 1:A:455:PHE:CD1  | 2.51                     | 0.46              |
| 1:A:472:CYS:CB   | 1:A:486:CYS:SG   | 3.03                     | 0.46              |
| 1:B:559:LEU:HD23 | 1:B:559:LEU:H    | 1.81                     | 0.46              |
| 1:B:565:SER:HB3  | 1:B:571:LEU:HG   | 1.97                     | 0.46              |
| 1:C:472:CYS:SG   | 1:C:493:GLN:OE1  | 2.73                     | 0.46              |
| 1:C:472:CYS:CB   | 1:C:486:CYS:HG   | 2.29                     | 0.46              |
| 1:D:565:SER:HB3  | 1:D:571:LEU:HG   | 1.97                     | 0.46              |
| 1:E:168:GLU:OE1  | 1:E:168:GLU:N    | 2.45                     | 0.46              |
| 1:F:244:GLU:C    | 1:F:245:TRP:CD1  | 2.93                     | 0.46              |
| 1:A:188:LEU:HD12 | 1:A:455:PHE:CZ   | 2.51                     | 0.46              |
| 1:A:472:CYS:CB   | 1:A:486:CYS:HG   | 2.29                     | 0.46              |
| 1:C:241:TYR:HE1  | 1:C:417:TYR:HB2  | 1.81                     | 0.46              |
| 1:C:472:CYS:CB   | 1:C:486:CYS:SG   | 3.03                     | 0.46              |
| 1:D:512:CYS:CB   | 1:D:524:CYS:SG   | 3.04                     | 0.46              |
| 1:E:269:LYS:O    | 1:E:388:ILE:HG22 | 2.16                     | 0.46              |
| 1:E:273:VAL:O    | 1:F:382:VAL:HG11 | 2.16                     | 0.46              |
| 1:E:565:SER:HB3  | 1:E:571:LEU:HG   | 1.97                     | 0.46              |
| 1:N:559:LEU:HD23 | 1:N:559:LEU:H    | 1.81                     | 0.46              |
| 1:A:269:LYS:O    | 1:A:388:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:274:ASP:CB   | 1:B:382:VAL:HG12 | 2.38                     | 0.46              |
| 1:B:454:VAL:HG13 | 1:B:455:PHE:CD1  | 2.51                     | 0.46              |
| 1:D:188:LEU:HD12 | 1:D:455:PHE:CZ   | 2.51                     | 0.46              |
| 1:D:269:LYS:O    | 1:D:388:ILE:HG22 | 2.16                     | 0.46              |
| 1:E:559:LEU:HD23 | 1:E:559:LEU:H    | 1.81                     | 0.46              |
| 1:F:168:GLU:OE1  | 1:F:168:GLU:N    | 2.45                     | 0.46              |
| 1:F:454:VAL:HG13 | 1:F:455:PHE:CD1  | 2.51                     | 0.46              |
| 1:F:472:CYS:CB   | 1:F:486:CYS:SG   | 3.03                     | 0.46              |
| 1:A:512:CYS:CB   | 1:A:524:CYS:SG   | 3.04                     | 0.46              |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:H    | 1.81                     | 0.46              |
| 1:B:356:ARG:NH2  | 1:B:367:PRO:HB3  | 2.31                     | 0.46              |
| 1:C:296:VAL:HG12 | 1:D:307:LEU:O    | 2.15                     | 0.46              |
| 1:C:534:TRP:CE2  | 1:C:541:LEU:HD12 | 2.51                     | 0.46              |
| 1:D:534:TRP:CE2  | 1:D:541:LEU:HD12 | 2.52                     | 0.46              |
| 1:E:241:TYR:HE1  | 1:E:417:TYR:HB2  | 1.81                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:347:TYR:HA   | 1:A:352:SER:OG   | 2.17                     | 0.45              |
| 1:E:534:TRP:CE2  | 1:E:541:LEU:HD12 | 2.51                     | 0.45              |
| 1:N:356:ARG:NH2  | 1:N:367:PRO:HB3  | 2.31                     | 0.45              |
| 1:N:657:GLN:O    | 1:N:657:GLN:HG2  | 2.16                     | 0.45              |
| 1:B:188:LEU:HD12 | 1:B:455:PHE:CZ   | 2.51                     | 0.45              |
| 1:B:334:ASN:ND2  | 1:C:179:ASN:ND2  | 2.64                     | 0.45              |
| 1:B:525:ASN:N    | 1:B:530:GLN:HE22 | 2.09                     | 0.45              |
| 1:C:559:LEU:H    | 1:C:559:LEU:HD23 | 1.81                     | 0.45              |
| 1:D:241:TYR:HE1  | 1:D:417:TYR:HB2  | 1.81                     | 0.45              |
| 1:E:512:CYS:CB   | 1:E:524:CYS:SG   | 3.04                     | 0.45              |
| 1:F:275:ASN:ND2  | 1:N:376:LEU:HA   | 2.31                     | 0.45              |
| 1:F:512:CYS:CB   | 1:F:524:CYS:SG   | 3.04                     | 0.45              |
| 1:A:205:LYS:HD3  | 1:A:455:PHE:CD2  | 2.51                     | 0.45              |
| 1:A:657:GLN:HG2  | 1:A:657:GLN:O    | 2.17                     | 0.45              |
| 1:B:534:TRP:CE2  | 1:B:541:LEU:HD12 | 2.51                     | 0.45              |
| 1:F:296:VAL:HG12 | 1:N:307:LEU:O    | 2.15                     | 0.45              |
| 1:N:512:CYS:CB   | 1:N:524:CYS:SG   | 3.04                     | 0.45              |
| 1:A:356:ARG:NH2  | 1:A:367:PRO:HB3  | 2.31                     | 0.45              |
| 1:C:454:VAL:HG13 | 1:C:455:PHE:CD1  | 2.51                     | 0.45              |
| 1:C:512:CYS:CB   | 1:C:524:CYS:SG   | 3.04                     | 0.45              |
| 1:C:525:ASN:N    | 1:C:530:GLN:HE22 | 2.09                     | 0.45              |
| 1:D:500:LEU:HD22 | 1:D:531:ARG:HH21 | 1.81                     | 0.45              |
| 1:E:567:ASP:OD1  | 1:E:567:ASP:N    | 2.49                     | 0.45              |
| 1:N:188:LEU:HD12 | 1:N:455:PHE:CZ   | 2.51                     | 0.45              |
| 1:A:239:ASP:OD2  | 1:A:417:TYR:OH   | 2.26                     | 0.45              |
| 1:C:188:LEU:HD12 | 1:C:455:PHE:CZ   | 2.51                     | 0.45              |
| 1:E:356:ARG:NH2  | 1:E:367:PRO:HB3  | 2.31                     | 0.45              |
| 1:E:657:GLN:O    | 1:E:657:GLN:HG2  | 2.17                     | 0.45              |
| 1:F:269:LYS:O    | 1:F:388:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:472:CYS:SG   | 1:A:493:GLN:OE1  | 2.73                     | 0.45              |
| 1:B:269:LYS:O    | 1:B:388:ILE:HG22 | 2.16                     | 0.45              |
| 1:B:500:LEU:HD22 | 1:B:531:ARG:HH21 | 1.81                     | 0.45              |
| 1:B:512:CYS:CB   | 1:B:524:CYS:SG   | 3.04                     | 0.45              |
| 1:C:269:LYS:O    | 1:C:388:ILE:HG22 | 2.16                     | 0.45              |
| 1:C:295:GLY:HA2  | 1:D:308:GLU:HA   | 1.98                     | 0.45              |
| 1:C:500:LEU:HD22 | 1:C:531:ARG:HH21 | 1.81                     | 0.45              |
| 1:D:559:LEU:HD23 | 1:D:559:LEU:H    | 1.81                     | 0.45              |
| 1:E:454:VAL:HG13 | 1:E:455:PHE:CD1  | 2.51                     | 0.45              |
| 1:F:657:GLN:O    | 1:F:657:GLN:HG2  | 2.17                     | 0.45              |
| 1:A:168:GLU:OE1  | 1:A:168:GLU:N    | 2.45                     | 0.45              |
| 1:C:347:TYR:HA   | 1:C:352:SER:OG   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:356:ARG:NH2  | 1:C:367:PRO:HB3  | 2.31                     | 0.45              |
| 1:E:205:LYS:HD3  | 1:E:455:PHE:CD2  | 2.51                     | 0.45              |
| 1:F:356:ARG:NH2  | 1:F:367:PRO:HB3  | 2.31                     | 0.45              |
| 1:F:534:TRP:CE2  | 1:F:541:LEU:HD12 | 2.52                     | 0.45              |
| 1:F:649:SER:HB3  | 1:F:659:LEU:HB2  | 1.99                     | 0.45              |
| 1:N:205:LYS:HD3  | 1:N:455:PHE:CD2  | 2.52                     | 0.45              |
| 1:A:649:SER:HB3  | 1:A:659:LEU:HB2  | 1.99                     | 0.45              |
| 1:B:205:LYS:HD3  | 1:B:455:PHE:CD2  | 2.52                     | 0.45              |
| 1:B:347:TYR:HA   | 1:B:352:SER:OG   | 2.17                     | 0.45              |
| 1:F:205:LYS:HD3  | 1:F:455:PHE:CD2  | 2.51                     | 0.45              |
| 1:F:347:TYR:HA   | 1:F:352:SER:OG   | 2.17                     | 0.45              |
| 1:N:384:LYS:HE2  | 1:N:384:LYS:HB2  | 1.75                     | 0.45              |
| 1:A:433:GLU:OE1  | 1:A:433:GLU:N    | 2.41                     | 0.45              |
| 1:B:657:GLN:O    | 1:B:657:GLN:HG2  | 2.17                     | 0.45              |
| 1:C:205:LYS:HD3  | 1:C:455:PHE:CD2  | 2.51                     | 0.45              |
| 1:D:205:LYS:HD3  | 1:D:455:PHE:CD2  | 2.51                     | 0.45              |
| 1:D:356:ARG:NH2  | 1:D:367:PRO:HB3  | 2.31                     | 0.45              |
| 1:D:684:HIS:NE2  | 1:D:686:ASP:OD2  | 2.50                     | 0.45              |
| 1:E:275:ASN:ND2  | 1:F:376:LEU:HA   | 2.31                     | 0.45              |
| 1:E:472:CYS:SG   | 1:E:493:GLN:OE1  | 2.73                     | 0.45              |
| 1:F:559:LEU:HD23 | 1:F:559:LEU:H    | 1.81                     | 0.45              |
| 1:N:454:VAL:HG13 | 1:N:455:PHE:CD1  | 2.51                     | 0.45              |
| 1:N:649:SER:HB3  | 1:N:659:LEU:HB2  | 1.99                     | 0.45              |
| 1:A:285:VAL:HG13 | 1:B:318:TRP:NE1  | 2.32                     | 0.45              |
| 1:A:346:GLN:HE21 | 1:N:282:ARG:CD   | 2.30                     | 0.45              |
| 1:B:202:PRO:HG3  | 1:C:143:ALA:HB1  | 1.99                     | 0.45              |
| 1:E:647:ALA:HB1  | 1:E:659:LEU:HD11 | 1.99                     | 0.45              |
| 1:F:500:LEU:HD22 | 1:F:531:ARG:HH21 | 1.81                     | 0.45              |
| 1:N:472:CYS:SG   | 1:N:493:GLN:OE1  | 2.73                     | 0.45              |
| 1:D:168:GLU:OE1  | 1:D:168:GLU:N    | 2.45                     | 0.44              |
| 1:E:649:SER:HB3  | 1:E:659:LEU:HB2  | 1.99                     | 0.44              |
| 1:N:500:LEU:HD22 | 1:N:531:ARG:HH21 | 1.81                     | 0.44              |
| 1:N:567:ASP:OD1  | 1:N:567:ASP:N    | 2.49                     | 0.44              |
| 1:A:220:ILE:HD11 | 1:A:381:PHE:HD2  | 1.82                     | 0.44              |
| 1:A:534:TRP:CE2  | 1:A:541:LEU:HD12 | 2.51                     | 0.44              |
| 1:B:567:ASP:OD1  | 1:B:567:ASP:N    | 2.49                     | 0.44              |
| 1:B:647:ALA:HB1  | 1:B:659:LEU:HD11 | 1.99                     | 0.44              |
| 1:B:649:SER:HB3  | 1:B:659:LEU:HB2  | 1.99                     | 0.44              |
| 1:D:657:GLN:O    | 1:D:657:GLN:HG2  | 2.17                     | 0.44              |
| 1:E:172:ARG:HD2  | 1:E:172:ARG:C    | 2.42                     | 0.44              |
| 1:E:202:PRO:HG3  | 1:F:143:ALA:HB1  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:647:ALA:HB1  | 1:F:659:LEU:HD11 | 1.99                     | 0.44              |
| 1:N:534:TRP:CE2  | 1:N:541:LEU:HD12 | 2.51                     | 0.44              |
| 1:C:647:ALA:HB1  | 1:C:659:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:647:ALA:HB1  | 1:A:659:LEU:HD11 | 2.00                     | 0.44              |
| 1:C:275:ASN:HD22 | 1:D:376:LEU:HA   | 1.82                     | 0.44              |
| 1:C:657:GLN:O    | 1:C:657:GLN:HG2  | 2.17                     | 0.44              |
| 1:D:347:TYR:HA   | 1:D:352:SER:OG   | 2.17                     | 0.44              |
| 1:D:567:ASP:N    | 1:D:567:ASP:OD1  | 2.49                     | 0.44              |
| 1:D:647:ALA:HB1  | 1:D:659:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:649:SER:HB3  | 1:D:659:LEU:HB2  | 1.99                     | 0.44              |
| 1:F:202:PRO:HG3  | 1:N:143:ALA:HB1  | 1.98                     | 0.44              |
| 1:B:684:HIS:NE2  | 1:B:686:ASP:OD2  | 2.50                     | 0.44              |
| 1:B:688:PHE:CZ   | 1:B:690:LEU:HD11 | 2.53                     | 0.44              |
| 1:C:649:SER:HB3  | 1:C:659:LEU:HB2  | 1.99                     | 0.44              |
| 1:N:347:TYR:HA   | 1:N:352:SER:OG   | 2.16                     | 0.44              |
| 1:N:647:ALA:HB1  | 1:N:659:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:202:PRO:HG3  | 1:E:143:ALA:HB1  | 2.00                     | 0.44              |
| 1:E:472:CYS:CB   | 1:E:486:CYS:HG   | 2.31                     | 0.44              |
| 1:F:688:PHE:CZ   | 1:F:690:LEU:HD11 | 2.53                     | 0.44              |
| 1:A:408:ASN:ND2  | 1:A:437:ARG:HH11 | 2.16                     | 0.44              |
| 1:B:366:TYR:CE1  | 1:B:368:VAL:HB   | 2.53                     | 0.44              |
| 1:C:148:VAL:O    | 1:C:149:ASN:ND2  | 2.51                     | 0.44              |
| 1:C:366:TYR:CE1  | 1:C:368:VAL:HB   | 2.53                     | 0.44              |
| 1:D:148:VAL:O    | 1:D:149:ASN:ND2  | 2.51                     | 0.44              |
| 1:E:220:ILE:HD11 | 1:E:381:PHE:HD2  | 1.82                     | 0.44              |
| 1:E:500:LEU:HD22 | 1:E:531:ARG:HH21 | 1.81                     | 0.44              |
| 1:N:168:GLU:OE1  | 1:N:168:GLU:N    | 2.45                     | 0.44              |
| 1:N:241:TYR:HE1  | 1:N:417:TYR:HB2  | 1.81                     | 0.44              |
| 1:A:172:ARG:HD2  | 1:A:172:ARG:C    | 2.42                     | 0.44              |
| 1:C:172:ARG:HD2  | 1:C:172:ARG:C    | 2.42                     | 0.44              |
| 1:E:347:TYR:HA   | 1:E:352:SER:OG   | 2.16                     | 0.44              |
| 1:E:688:PHE:CZ   | 1:E:690:LEU:HD11 | 2.53                     | 0.44              |
| 1:A:500:LEU:HD22 | 1:A:531:ARG:HH21 | 1.81                     | 0.44              |
| 1:B:148:VAL:O    | 1:B:149:ASN:ND2  | 2.51                     | 0.44              |
| 1:B:408:ASN:ND2  | 1:B:437:ARG:HH11 | 2.16                     | 0.44              |
| 1:D:172:ARG:C    | 1:D:172:ARG:HD2  | 2.43                     | 0.44              |
| 1:D:220:ILE:HD11 | 1:D:381:PHE:HD2  | 1.82                     | 0.44              |
| 1:D:688:PHE:CZ   | 1:D:690:LEU:HD11 | 2.53                     | 0.44              |
| 1:E:704:ASP:OD1  | 1:E:707:LEU:HD23 | 2.18                     | 0.44              |
| 1:B:172:ARG:HD2  | 1:B:172:ARG:C    | 2.42                     | 0.43              |
| 1:B:197:VAL:HG21 | 1:C:579:ASP:HA   | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:275:ASN:ND2  | 1:D:376:LEU:HA   | 2.33                     | 0.43              |
| 1:N:684:HIS:NE2  | 1:N:686:ASP:OD2  | 2.50                     | 0.43              |
| 1:A:241:TYR:HE1  | 1:A:417:TYR:HB2  | 1.81                     | 0.43              |
| 1:C:220:ILE:HD11 | 1:C:381:PHE:HD2  | 1.82                     | 0.43              |
| 1:C:433:GLU:OE1  | 1:C:433:GLU:N    | 2.41                     | 0.43              |
| 1:C:684:HIS:NE2  | 1:C:686:ASP:OD2  | 2.50                     | 0.43              |
| 1:D:384:LYS:HB2  | 1:D:384:LYS:HE2  | 1.75                     | 0.43              |
| 1:E:148:VAL:O    | 1:E:149:ASN:ND2  | 2.51                     | 0.43              |
| 1:F:684:HIS:NE2  | 1:F:686:ASP:OD2  | 2.50                     | 0.43              |
| 1:N:688:PHE:CZ   | 1:N:690:LEU:HD11 | 2.53                     | 0.43              |
| 1:A:366:TYR:CE1  | 1:A:368:VAL:HB   | 2.53                     | 0.43              |
| 1:A:384:LYS:HE2  | 1:A:384:LYS:HB2  | 1.76                     | 0.43              |
| 1:B:472:CYS:SG   | 1:B:493:GLN:OE1  | 2.73                     | 0.43              |
| 1:F:160:ASN:O    | 1:F:413:TYR:OH   | 2.36                     | 0.43              |
| 1:A:179:ASN:ND2  | 1:N:334:ASN:ND2  | 2.66                     | 0.43              |
| 1:A:525:ASN:N    | 1:A:530:GLN:HE22 | 2.09                     | 0.43              |
| 1:A:684:HIS:NE2  | 1:A:686:ASP:OD2  | 2.50                     | 0.43              |
| 1:B:526:GLN:NE2  | 1:C:488:SER:OG   | 2.51                     | 0.43              |
| 1:B:704:ASP:OD1  | 1:B:707:LEU:HD23 | 2.18                     | 0.43              |
| 1:C:646:THR:HB   | 1:C:663:THR:HB   | 2.01                     | 0.43              |
| 1:D:704:ASP:OD1  | 1:D:707:LEU:HD23 | 2.18                     | 0.43              |
| 1:F:220:ILE:HD11 | 1:F:381:PHE:HD2  | 1.82                     | 0.43              |
| 1:F:472:CYS:SG   | 1:F:493:GLN:OE1  | 2.73                     | 0.43              |
| 1:N:704:ASP:OD1  | 1:N:707:LEU:HD23 | 2.18                     | 0.43              |
| 1:A:704:ASP:OD1  | 1:A:707:LEU:HD23 | 2.18                     | 0.43              |
| 1:E:684:HIS:NE2  | 1:E:686:ASP:OD2  | 2.50                     | 0.43              |
| 1:F:241:TYR:HE1  | 1:F:417:TYR:HB2  | 1.81                     | 0.43              |
| 1:N:408:ASN:ND2  | 1:N:437:ARG:HH11 | 2.16                     | 0.43              |
| 1:N:472:CYS:CB   | 1:N:486:CYS:SG   | 3.03                     | 0.43              |
| 1:A:139:LEU:HD12 | 1:A:140:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:139:LEU:HD12 | 1:C:140:PRO:HD2  | 2.01                     | 0.43              |
| 1:D:139:LEU:HD12 | 1:D:140:PRO:HD2  | 2.00                     | 0.43              |
| 1:D:274:ASP:OD2  | 1:E:376:LEU:HD13 | 2.18                     | 0.43              |
| 1:D:472:CYS:SG   | 1:D:493:GLN:OE1  | 2.73                     | 0.43              |
| 1:N:172:ARG:HD2  | 1:N:172:ARG:C    | 2.42                     | 0.43              |
| 1:A:567:ASP:N    | 1:A:567:ASP:OD1  | 2.49                     | 0.43              |
| 1:B:220:ILE:HD11 | 1:B:381:PHE:HD2  | 1.82                     | 0.43              |
| 1:C:247:THR:OG1  | 1:C:248:ASP:N    | 2.52                     | 0.43              |
| 1:C:589:ILE:HG13 | 1:C:712:GLN:NE2  | 2.34                     | 0.43              |
| 1:C:688:PHE:CZ   | 1:C:690:LEU:HD11 | 2.53                     | 0.43              |
| 1:D:247:THR:OG1  | 1:D:248:ASP:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:148:VAL:O    | 1:A:149:ASN:ND2  | 2.51                     | 0.43              |
| 1:B:295:GLY:HA2  | 1:C:308:GLU:HA   | 1.99                     | 0.43              |
| 1:D:366:TYR:CE1  | 1:D:368:VAL:HB   | 2.53                     | 0.43              |
| 1:F:704:ASP:OD1  | 1:F:707:LEU:HD23 | 2.18                     | 0.43              |
| 1:D:646:THR:HB   | 1:D:663:THR:HB   | 2.01                     | 0.43              |
| 1:F:148:VAL:O    | 1:F:149:ASN:ND2  | 2.51                     | 0.43              |
| 1:F:172:ARG:C    | 1:F:172:ARG:HD2  | 2.43                     | 0.43              |
| 1:F:646:THR:HB   | 1:F:663:THR:HB   | 2.01                     | 0.43              |
| 1:N:139:LEU:HD12 | 1:N:140:PRO:HD2  | 2.01                     | 0.43              |
| 1:N:148:VAL:O    | 1:N:149:ASN:ND2  | 2.51                     | 0.43              |
| 1:N:220:ILE:HD11 | 1:N:381:PHE:HD2  | 1.82                     | 0.43              |
| 1:A:382:VAL:HG12 | 1:N:274:ASP:CB   | 2.40                     | 0.43              |
| 1:B:471:ARG:HH11 | 1:B:484:ASN:HA   | 1.84                     | 0.43              |
| 1:B:646:THR:HB   | 1:B:663:THR:HB   | 2.01                     | 0.43              |
| 1:D:589:ILE:HG13 | 1:D:712:GLN:NE2  | 2.34                     | 0.43              |
| 1:F:366:TYR:CE1  | 1:F:368:VAL:HB   | 2.53                     | 0.43              |
| 1:N:366:TYR:CE1  | 1:N:368:VAL:HB   | 2.53                     | 0.43              |
| 1:A:688:PHE:CZ   | 1:A:690:LEU:HD11 | 2.53                     | 0.42              |
| 1:B:589:ILE:HG13 | 1:B:712:GLN:NE2  | 2.34                     | 0.42              |
| 1:C:288:PHE:HZ   | 1:D:315:GLN:CB   | 2.18                     | 0.42              |
| 1:D:408:ASN:ND2  | 1:D:437:ARG:HH11 | 2.16                     | 0.42              |
| 1:E:296:VAL:HG12 | 1:F:307:LEU:O    | 2.19                     | 0.42              |
| 1:E:366:TYR:CE1  | 1:E:368:VAL:HB   | 2.53                     | 0.42              |
| 1:E:408:ASN:ND2  | 1:E:437:ARG:HH11 | 2.16                     | 0.42              |
| 1:E:646:THR:HB   | 1:E:663:THR:HB   | 2.01                     | 0.42              |
| 1:F:285:VAL:HG13 | 1:N:318:TRP:NE1  | 2.33                     | 0.42              |
| 1:N:187:ASN:HB2  | 1:N:208:ARG:HB3  | 2.01                     | 0.42              |
| 1:B:247:THR:OG1  | 1:B:248:ASP:N    | 2.52                     | 0.42              |
| 1:D:525:ASN:N    | 1:D:530:GLN:HE22 | 2.09                     | 0.42              |
| 1:E:139:LEU:HD12 | 1:E:140:PRO:HD2  | 2.00                     | 0.42              |
| 1:F:187:ASN:HB2  | 1:F:208:ARG:HB3  | 2.01                     | 0.42              |
| 1:F:471:ARG:HH11 | 1:F:484:ASN:HA   | 1.84                     | 0.42              |
| 1:N:471:ARG:HH11 | 1:N:484:ASN:HA   | 1.84                     | 0.42              |
| 1:A:589:ILE:HG13 | 1:A:712:GLN:NE2  | 2.34                     | 0.42              |
| 1:B:139:LEU:HD12 | 1:B:140:PRO:HD2  | 2.00                     | 0.42              |
| 1:C:408:ASN:ND2  | 1:C:437:ARG:HH11 | 2.16                     | 0.42              |
| 1:E:247:THR:OG1  | 1:E:248:ASP:N    | 2.52                     | 0.42              |
| 1:E:589:ILE:HG13 | 1:E:712:GLN:NE2  | 2.34                     | 0.42              |
| 1:A:187:ASN:HB2  | 1:A:208:ARG:HB3  | 2.01                     | 0.42              |
| 1:C:187:ASN:HB2  | 1:C:208:ARG:HB3  | 2.01                     | 0.42              |
| 1:C:471:ARG:HH11 | 1:C:484:ASN:HA   | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:704:ASP:OD1  | 1:C:707:LEU:HD23 | 2.18                     | 0.42              |
| 1:D:297:GLU:O    | 1:D:304:LYS:N    | 2.53                     | 0.42              |
| 1:D:471:ARG:HH11 | 1:D:484:ASN:HA   | 1.84                     | 0.42              |
| 1:F:139:LEU:HD12 | 1:F:140:PRO:HD2  | 2.01                     | 0.42              |
| 1:N:268:LEU:HD22 | 1:N:390:LYS:HB2  | 2.01                     | 0.42              |
| 1:N:646:THR:HB   | 1:N:663:THR:HB   | 2.01                     | 0.42              |
| 1:A:376:LEU:HD13 | 1:N:274:ASP:OD2  | 2.20                     | 0.42              |
| 1:A:471:ARG:HH11 | 1:A:484:ASN:HA   | 1.84                     | 0.42              |
| 1:D:266:GLN:N    | 1:D:390:LYS:O    | 2.52                     | 0.42              |
| 1:E:462:ASN:HD22 | 1:E:578:THR:HG21 | 1.85                     | 0.42              |
| 1:E:471:ARG:HH11 | 1:E:484:ASN:HA   | 1.84                     | 0.42              |
| 1:N:589:ILE:HG13 | 1:N:712:GLN:NE2  | 2.34                     | 0.42              |
| 1:A:268:LEU:HD22 | 1:A:390:LYS:HB2  | 2.01                     | 0.42              |
| 1:A:646:THR:HB   | 1:A:663:THR:HB   | 2.01                     | 0.42              |
| 1:C:462:ASN:HD22 | 1:C:578:THR:HG21 | 1.85                     | 0.42              |
| 1:F:247:THR:OG1  | 1:F:248:ASP:N    | 2.52                     | 0.42              |
| 1:F:268:LEU:HD22 | 1:F:390:LYS:HB2  | 2.01                     | 0.42              |
| 1:F:283:LYS:CG   | 1:N:320:THR:OG1  | 2.51                     | 0.42              |
| 1:F:408:ASN:ND2  | 1:F:437:ARG:HH11 | 2.16                     | 0.42              |
| 1:F:589:ILE:HG13 | 1:F:712:GLN:NE2  | 2.34                     | 0.42              |
| 1:N:247:THR:OG1  | 1:N:248:ASP:N    | 2.52                     | 0.42              |
| 1:B:187:ASN:HB2  | 1:B:208:ARG:HB3  | 2.01                     | 0.42              |
| 1:B:512:CYS:SG   | 1:B:530:GLN:OE1  | 2.69                     | 0.42              |
| 1:C:297:GLU:O    | 1:C:304:LYS:N    | 2.53                     | 0.42              |
| 1:E:297:GLU:O    | 1:E:304:LYS:N    | 2.53                     | 0.42              |
| 1:E:526:GLN:NE2  | 1:F:488:SER:OG   | 2.53                     | 0.42              |
| 1:N:266:GLN:N    | 1:N:390:LYS:O    | 2.52                     | 0.42              |
| 1:B:297:GLU:O    | 1:B:304:LYS:N    | 2.53                     | 0.42              |
| 1:E:187:ASN:HB2  | 1:E:208:ARG:HB3  | 2.01                     | 0.42              |
| 1:E:619:LEU:HD23 | 1:E:708:VAL:HG21 | 2.02                     | 0.42              |
| 1:A:247:THR:OG1  | 1:A:248:ASP:N    | 2.52                     | 0.42              |
| 1:B:403:ILE:O    | 1:B:403:ILE:HG13 | 2.20                     | 0.42              |
| 1:B:410:ARG:HH21 | 1:B:437:ARG:NH2  | 2.16                     | 0.42              |
| 1:F:410:ARG:HH21 | 1:F:437:ARG:NH2  | 2.16                     | 0.42              |
| 1:F:472:CYS:CB   | 1:F:486:CYS:HG   | 2.33                     | 0.42              |
| 1:N:619:LEU:HD23 | 1:N:708:VAL:HG21 | 2.02                     | 0.42              |
| 1:A:297:GLU:O    | 1:A:304:LYS:N    | 2.53                     | 0.42              |
| 1:D:403:ILE:O    | 1:D:403:ILE:HG13 | 2.20                     | 0.42              |
| 1:E:403:ILE:O    | 1:E:403:ILE:HG13 | 2.20                     | 0.42              |
| 1:F:295:GLY:HA2  | 1:N:308:GLU:HA   | 2.02                     | 0.42              |
| 1:F:619:LEU:HD23 | 1:F:708:VAL:HG21 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:384:LYS:HE2  | 1:B:384:LYS:HB2  | 1.75                     | 0.41              |
| 1:E:295:GLY:HA3  | 1:F:308:GLU:HB3  | 2.02                     | 0.41              |
| 1:E:358:THR:HB   | 1:E:428:PHE:CD1  | 2.55                     | 0.41              |
| 1:E:525:ASN:N    | 1:E:530:GLN:HE22 | 2.09                     | 0.41              |
| 1:C:542:THR:HA   | 1:C:549:SER:HA   | 2.02                     | 0.41              |
| 1:C:567:ASP:OD1  | 1:C:567:ASP:N    | 2.50                     | 0.41              |
| 1:D:619:LEU:HD23 | 1:D:708:VAL:HG21 | 2.02                     | 0.41              |
| 1:E:334:ASN:ND2  | 1:F:179:ASN:ND2  | 2.68                     | 0.41              |
| 1:F:358:THR:HB   | 1:F:428:PHE:CD1  | 2.55                     | 0.41              |
| 1:N:160:ASN:O    | 1:N:413:TYR:OH   | 2.36                     | 0.41              |
| 1:A:462:ASN:HD22 | 1:A:578:THR:HG21 | 1.85                     | 0.41              |
| 1:A:539:ASP:OD2  | 1:A:572:ARG:NH1  | 2.54                     | 0.41              |
| 1:B:268:LEU:HD22 | 1:B:390:LYS:HB2  | 2.01                     | 0.41              |
| 1:B:288:PHE:HZ   | 1:C:315:GLN:CB   | 2.19                     | 0.41              |
| 1:B:539:ASP:OD2  | 1:B:572:ARG:NH1  | 2.54                     | 0.41              |
| 1:C:355:ASN:N    | 1:C:372:ARG:HH22 | 2.18                     | 0.41              |
| 1:D:334:ASN:ND2  | 1:E:179:ASN:ND2  | 2.67                     | 0.41              |
| 1:N:539:ASP:OD2  | 1:N:572:ARG:NH1  | 2.54                     | 0.41              |
| 1:N:542:THR:HA   | 1:N:549:SER:HA   | 2.02                     | 0.41              |
| 1:A:197:VAL:O    | 1:B:459:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:355:ASN:N    | 1:B:372:ARG:HH22 | 2.18                     | 0.41              |
| 1:B:462:ASN:HD22 | 1:B:578:THR:HG21 | 1.85                     | 0.41              |
| 1:D:268:LEU:HD22 | 1:D:390:LYS:HB2  | 2.01                     | 0.41              |
| 1:E:266:GLN:N    | 1:E:390:LYS:O    | 2.52                     | 0.41              |
| 1:E:268:LEU:HD22 | 1:E:390:LYS:HB2  | 2.01                     | 0.41              |
| 1:E:274:ASP:OD2  | 1:F:376:LEU:HD13 | 2.20                     | 0.41              |
| 1:E:384:LYS:HB2  | 1:E:384:LYS:HE2  | 1.75                     | 0.41              |
| 1:F:297:GLU:O    | 1:F:304:LYS:N    | 2.53                     | 0.41              |
| 1:F:511:LEU:HD12 | 1:F:521:LEU:HB2  | 2.03                     | 0.41              |
| 1:F:567:ASP:N    | 1:F:567:ASP:OD1  | 2.49                     | 0.41              |
| 1:N:462:ASN:HD22 | 1:N:578:THR:HG21 | 1.85                     | 0.41              |
| 1:B:266:GLN:N    | 1:B:390:LYS:O    | 2.52                     | 0.41              |
| 1:C:157:CYS:HB3  | 1:C:175:CYS:HG   | 1.86                     | 0.41              |
| 1:D:542:THR:HA   | 1:D:549:SER:HA   | 2.02                     | 0.41              |
| 1:E:355:ASN:N    | 1:E:372:ARG:HH22 | 2.18                     | 0.41              |
| 1:N:358:THR:HB   | 1:N:428:PHE:CD1  | 2.55                     | 0.41              |
| 1:A:346:GLN:NE2  | 1:N:282:ARG:HD2  | 2.32                     | 0.41              |
| 1:A:403:ILE:O    | 1:A:403:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:619:LEU:HD23 | 1:A:708:VAL:HG21 | 2.02                     | 0.41              |
| 1:C:472:CYS:SG   | 1:C:486:CYS:SG   | 3.19                     | 0.41              |
| 1:D:187:ASN:HB2  | 1:D:208:ARG:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:462:ASN:HD22 | 1:D:578:THR:HG21 | 1.85                     | 0.41              |
| 1:F:274:ASP:OD2  | 1:N:376:LEU:HD13 | 2.21                     | 0.41              |
| 1:F:525:ASN:N    | 1:F:530:GLN:HE22 | 2.09                     | 0.41              |
| 1:N:355:ASN:N    | 1:N:372:ARG:HH22 | 2.18                     | 0.41              |
| 1:N:511:LEU:HD12 | 1:N:521:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:358:THR:HB   | 1:A:428:PHE:CD1  | 2.55                     | 0.41              |
| 1:C:403:ILE:O    | 1:C:403:ILE:HG13 | 2.20                     | 0.41              |
| 1:C:539:ASP:OD2  | 1:C:572:ARG:NH1  | 2.54                     | 0.41              |
| 1:E:472:CYS:SG   | 1:E:486:CYS:SG   | 3.19                     | 0.41              |
| 1:F:384:LYS:HE2  | 1:F:384:LYS:HB2  | 1.76                     | 0.41              |
| 1:B:358:THR:HB   | 1:B:428:PHE:CD1  | 2.55                     | 0.41              |
| 1:B:542:THR:HA   | 1:B:549:SER:HA   | 2.02                     | 0.41              |
| 1:C:268:LEU:HD22 | 1:C:390:LYS:HB2  | 2.01                     | 0.41              |
| 1:D:355:ASN:N    | 1:D:372:ARG:HH22 | 2.18                     | 0.41              |
| 1:D:472:CYS:SG   | 1:D:486:CYS:SG   | 3.19                     | 0.41              |
| 1:F:526:GLN:NE2  | 1:N:488:SER:OG   | 2.54                     | 0.41              |
| 1:A:355:ASN:N    | 1:A:372:ARG:HH22 | 2.19                     | 0.41              |
| 1:C:384:LYS:HB2  | 1:C:384:LYS:HE2  | 1.76                     | 0.41              |
| 1:C:619:LEU:HD23 | 1:C:708:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:539:ASP:OD2  | 1:D:572:ARG:NH1  | 2.54                     | 0.41              |
| 1:E:175:CYS:HB2  | 1:E:222:LEU:O    | 2.21                     | 0.41              |
| 1:E:511:LEU:HD12 | 1:E:521:LEU:HB2  | 2.03                     | 0.41              |
| 1:F:462:ASN:HD22 | 1:F:578:THR:HG21 | 1.85                     | 0.41              |
| 1:F:539:ASP:OD2  | 1:F:572:ARG:NH1  | 2.53                     | 0.41              |
| 1:F:542:THR:HA   | 1:F:549:SER:HA   | 2.02                     | 0.41              |
| 1:N:297:GLU:O    | 1:N:304:LYS:N    | 2.53                     | 0.41              |
| 1:A:243:ARG:CG   | 1:A:245:TRP:HE1  | 2.34                     | 0.41              |
| 1:A:472:CYS:SG   | 1:A:486:CYS:SG   | 3.19                     | 0.41              |
| 1:A:542:THR:HA   | 1:A:549:SER:HA   | 2.02                     | 0.41              |
| 1:B:610:VAL:O    | 1:B:635:SER:N    | 2.54                     | 0.41              |
| 1:B:619:LEU:HD23 | 1:B:708:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:512:CYS:CB   | 1:D:524:CYS:CB   | 2.93                     | 0.41              |
| 1:F:175:CYS:HB2  | 1:F:222:LEU:O    | 2.21                     | 0.41              |
| 1:A:511:LEU:HD12 | 1:A:521:LEU:HB2  | 2.03                     | 0.40              |
| 1:B:175:CYS:HB2  | 1:B:222:LEU:O    | 2.21                     | 0.40              |
| 1:D:160:ASN:O    | 1:D:413:TYR:OH   | 2.36                     | 0.40              |
| 1:D:473:ILE:HG23 | 1:D:473:ILE:O    | 2.21                     | 0.40              |
| 1:A:175:CYS:HB2  | 1:A:222:LEU:O    | 2.21                     | 0.40              |
| 1:A:473:ILE:O    | 1:A:473:ILE:HG23 | 2.22                     | 0.40              |
| 1:D:239:ASP:OD2  | 1:D:417:TYR:OH   | 2.26                     | 0.40              |
| 1:A:311:ALA:O    | 1:N:292:VAL:N    | 2.32                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:417:TYR:CD2  | 1:B:419:HIS:CE1  | 3.10                     | 0.40              |
| 1:B:554:LYS:HE2  | 1:B:554:LYS:HA   | 2.03                     | 0.40              |
| 1:F:322:ASN:OD1  | 1:F:322:ASN:N    | 2.54                     | 0.40              |
| 1:N:403:ILE:O    | 1:N:403:ILE:HG13 | 2.20                     | 0.40              |
| 1:N:410:ARG:HH21 | 1:N:437:ARG:NH2  | 2.16                     | 0.40              |
| 1:B:538:THR:HB   | 1:B:540:GLU:OE1  | 2.22                     | 0.40              |
| 1:C:512:CYS:SG   | 1:C:530:GLN:OE1  | 2.69                     | 0.40              |
| 1:E:285:VAL:HG13 | 1:F:318:TRP:HE1  | 1.85                     | 0.40              |
| 1:D:175:CYS:HB2  | 1:D:222:LEU:O    | 2.21                     | 0.40              |
| 1:D:538:THR:HB   | 1:D:540:GLU:OE1  | 2.22                     | 0.40              |
| 1:E:322:ASN:OD1  | 1:E:322:ASN:N    | 2.54                     | 0.40              |
| 1:F:243:ARG:CG   | 1:F:245:TRP:HE1  | 2.34                     | 0.40              |
| 1:F:355:ASN:N    | 1:F:372:ARG:HH22 | 2.18                     | 0.40              |
| 1:F:473:ILE:HG23 | 1:F:473:ILE:O    | 2.22                     | 0.40              |
| 1:N:525:ASN:N    | 1:N:530:GLN:HE22 | 2.09                     | 0.40              |
| 1:N:646:THR:N    | 1:N:663:THR:O    | 2.38                     | 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     | 571/581 (98%)   | 545 (95%)  | 26 (5%)  | 0        | 100         | 100 |
| 1   | B     | 571/581 (98%)   | 544 (95%)  | 27 (5%)  | 0        | 100         | 100 |
| 1   | C     | 571/581 (98%)   | 544 (95%)  | 27 (5%)  | 0        | 100         | 100 |
| 1   | D     | 571/581 (98%)   | 542 (95%)  | 29 (5%)  | 0        | 100         | 100 |
| 1   | E     | 571/581 (98%)   | 545 (95%)  | 26 (5%)  | 0        | 100         | 100 |
| 1   | F     | 571/581 (98%)   | 544 (95%)  | 27 (5%)  | 0        | 100         | 100 |
| 1   | N     | 571/581 (98%)   | 545 (95%)  | 26 (5%)  | 0        | 100         | 100 |
| All | All   | 3997/4067 (98%) | 3809 (95%) | 188 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 444/485 (92%)   | 444 (100%)  | 0        | 100         | 100 |
| 1   | B     | 443/485 (91%)   | 443 (100%)  | 0        | 100         | 100 |
| 1   | C     | 443/485 (91%)   | 443 (100%)  | 0        | 100         | 100 |
| 1   | D     | 443/485 (91%)   | 443 (100%)  | 0        | 100         | 100 |
| 1   | E     | 443/485 (91%)   | 443 (100%)  | 0        | 100         | 100 |
| 1   | F     | 443/485 (91%)   | 443 (100%)  | 0        | 100         | 100 |
| 1   | N     | 443/485 (91%)   | 443 (100%)  | 0        | 100         | 100 |
| All | All   | 3102/3395 (91%) | 3102 (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 (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 149 | ASN  |
| 1   | A     | 179 | ASN  |
| 1   | A     | 193 | GLN  |
| 1   | A     | 275 | ASN  |
| 1   | A     | 315 | GLN  |
| 1   | A     | 346 | GLN  |
| 1   | A     | 414 | ASN  |
| 1   | A     | 419 | HIS  |
| 1   | A     | 430 | HIS  |
| 1   | A     | 490 | GLN  |
| 1   | A     | 698 | GLN  |
| 1   | A     | 712 | GLN  |
| 1   | B     | 149 | ASN  |
| 1   | B     | 179 | ASN  |
| 1   | B     | 193 | GLN  |
| 1   | B     | 275 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 315 | GLN  |
| 1   | B     | 414 | ASN  |
| 1   | B     | 419 | HIS  |
| 1   | B     | 430 | HIS  |
| 1   | B     | 490 | GLN  |
| 1   | B     | 526 | GLN  |
| 1   | B     | 698 | GLN  |
| 1   | B     | 712 | GLN  |
| 1   | C     | 149 | ASN  |
| 1   | C     | 179 | ASN  |
| 1   | C     | 193 | GLN  |
| 1   | C     | 275 | ASN  |
| 1   | C     | 315 | GLN  |
| 1   | C     | 414 | ASN  |
| 1   | C     | 419 | HIS  |
| 1   | C     | 430 | HIS  |
| 1   | C     | 490 | GLN  |
| 1   | C     | 526 | GLN  |
| 1   | C     | 698 | GLN  |
| 1   | C     | 712 | GLN  |
| 1   | D     | 149 | ASN  |
| 1   | D     | 179 | ASN  |
| 1   | D     | 193 | GLN  |
| 1   | D     | 275 | ASN  |
| 1   | D     | 315 | GLN  |
| 1   | D     | 414 | ASN  |
| 1   | D     | 419 | HIS  |
| 1   | D     | 430 | HIS  |
| 1   | D     | 490 | GLN  |
| 1   | D     | 698 | GLN  |
| 1   | D     | 712 | GLN  |
| 1   | E     | 149 | ASN  |
| 1   | E     | 179 | ASN  |
| 1   | E     | 193 | GLN  |
| 1   | E     | 275 | ASN  |
| 1   | E     | 315 | GLN  |
| 1   | E     | 414 | ASN  |
| 1   | E     | 419 | HIS  |
| 1   | E     | 430 | HIS  |
| 1   | E     | 490 | GLN  |
| 1   | E     | 526 | GLN  |
| 1   | E     | 698 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 712 | GLN  |
| 1   | F     | 149 | ASN  |
| 1   | F     | 179 | ASN  |
| 1   | F     | 193 | GLN  |
| 1   | F     | 275 | ASN  |
| 1   | F     | 315 | GLN  |
| 1   | F     | 414 | ASN  |
| 1   | F     | 419 | HIS  |
| 1   | F     | 430 | HIS  |
| 1   | F     | 490 | GLN  |
| 1   | F     | 526 | GLN  |
| 1   | F     | 698 | GLN  |
| 1   | F     | 712 | GLN  |
| 1   | N     | 149 | ASN  |
| 1   | N     | 179 | ASN  |
| 1   | N     | 193 | GLN  |
| 1   | N     | 275 | ASN  |
| 1   | N     | 315 | GLN  |
| 1   | N     | 414 | ASN  |
| 1   | N     | 419 | HIS  |
| 1   | N     | 430 | HIS  |
| 1   | N     | 490 | GLN  |
| 1   | N     | 526 | GLN  |
| 1   | N     | 698 | GLN  |
| 1   | N     | 712 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

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.

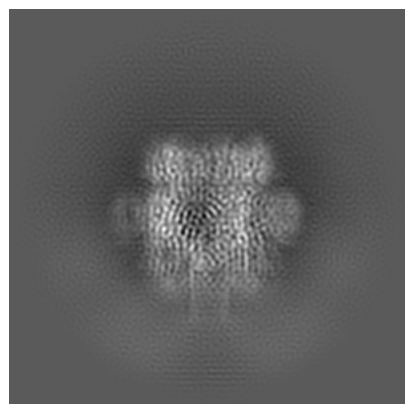
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63088. These allow visual inspection of the internal detail of the map and identification of artifacts.

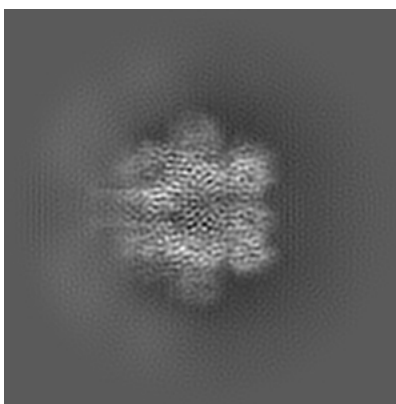
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

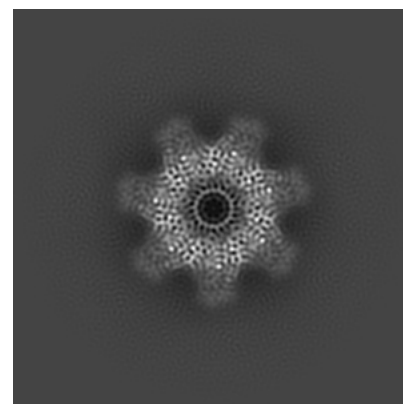
#### 6.1.1 Primary map



X

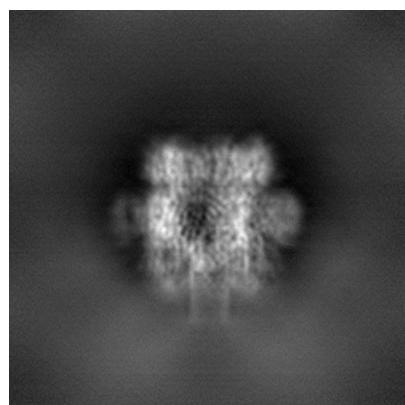


Y

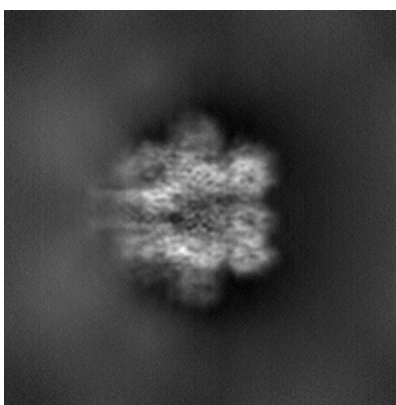


Z

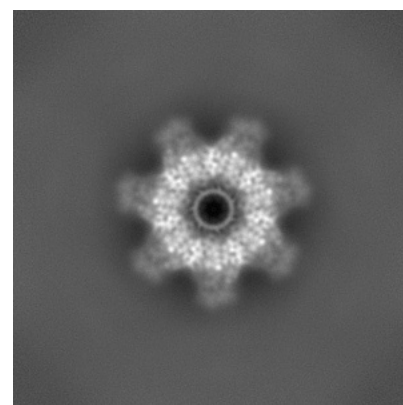
#### 6.1.2 Raw map



X



Y

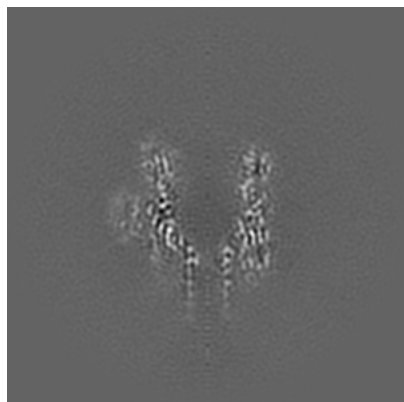


Z

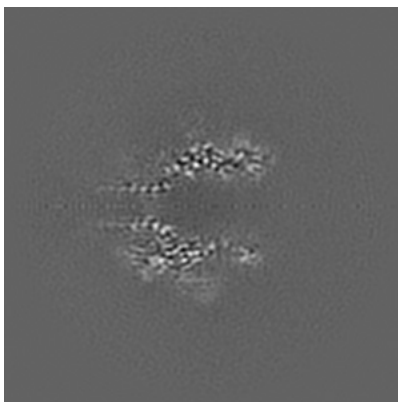
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

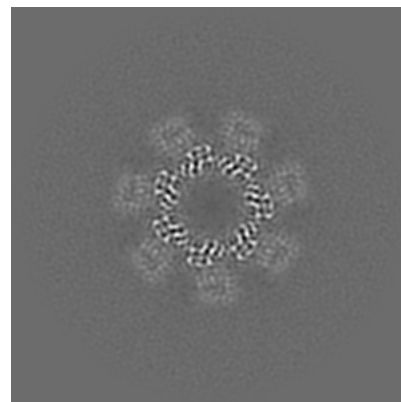
### 6.2.1 Primary map



X Index: 160

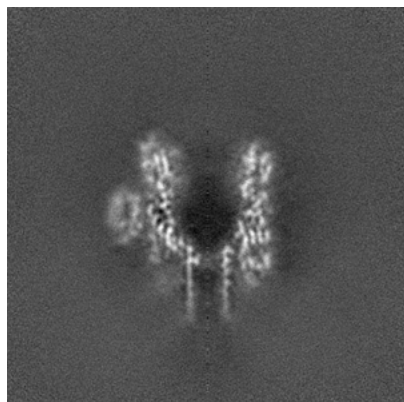


Y Index: 160

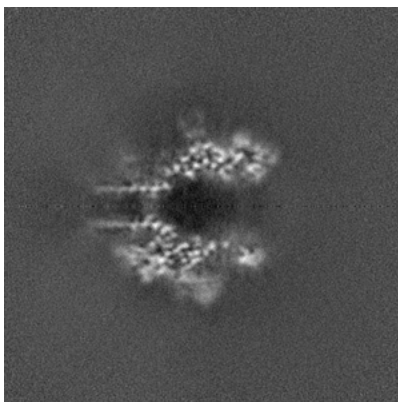


Z Index: 160

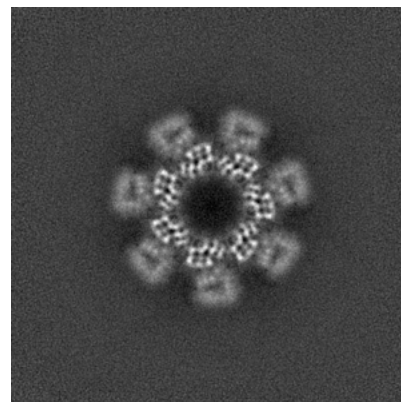
### 6.2.2 Raw map



X Index: 160



Y Index: 160

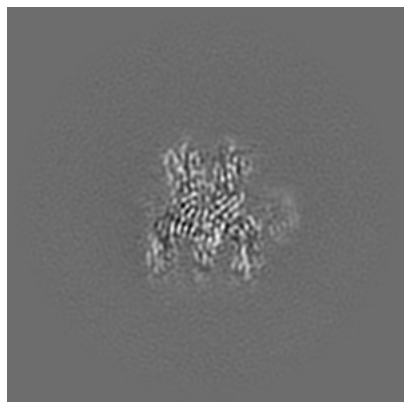


Z Index: 160

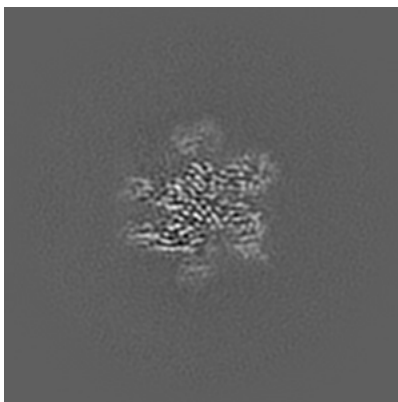
The images above show central slices of the map in three orthogonal directions.

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

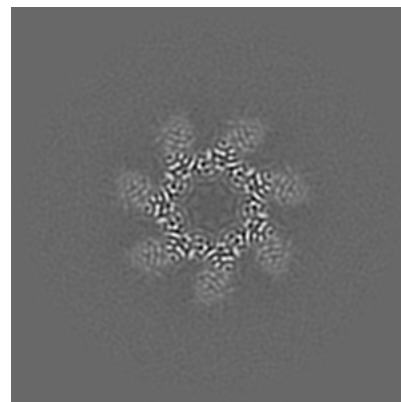
### 6.3.1 Primary map



X Index: 129

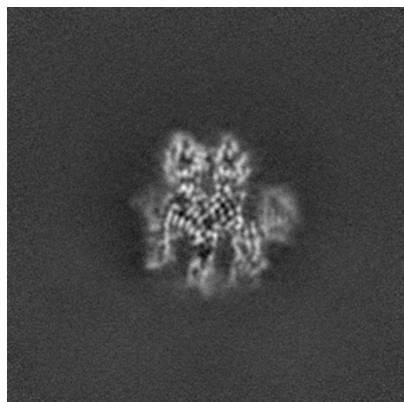


Y Index: 128

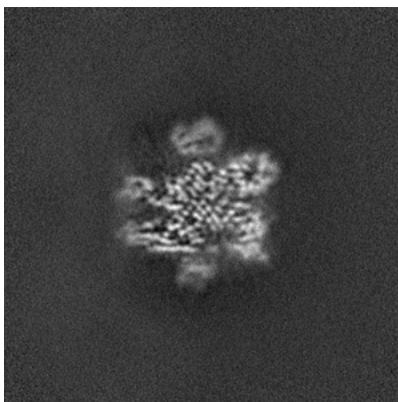


Z Index: 144

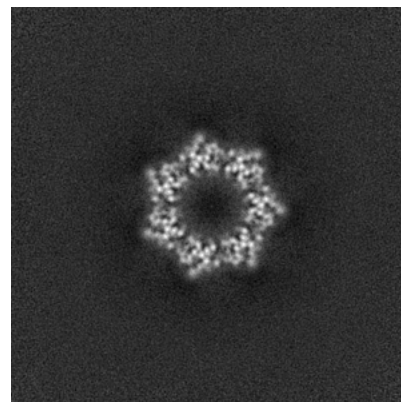
### 6.3.2 Raw map



X Index: 125



Y Index: 128

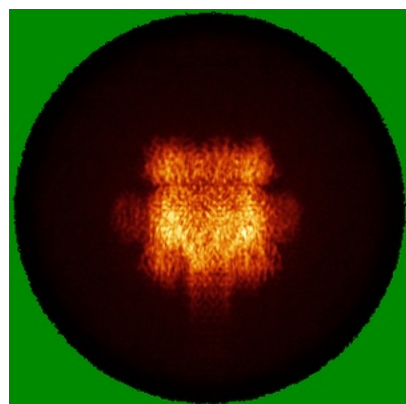


Z Index: 187

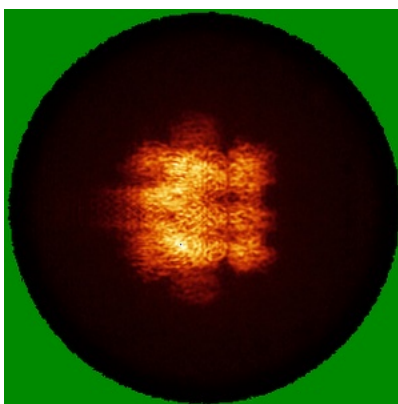
The images above show the largest variance slices of the map in three orthogonal directions.

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

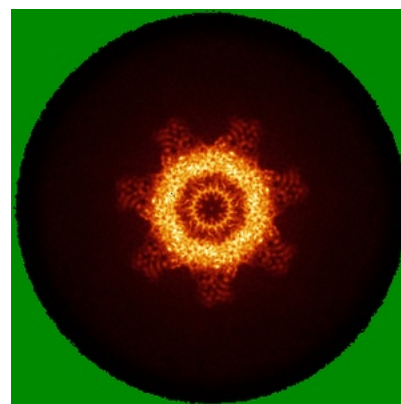
### 6.4.1 Primary map



X

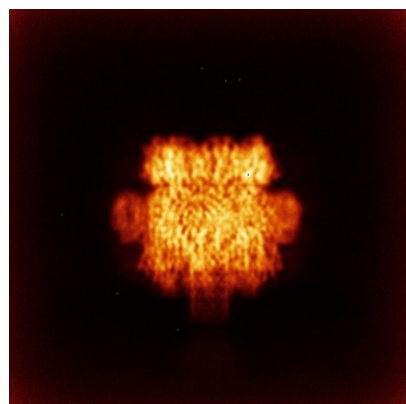


Y

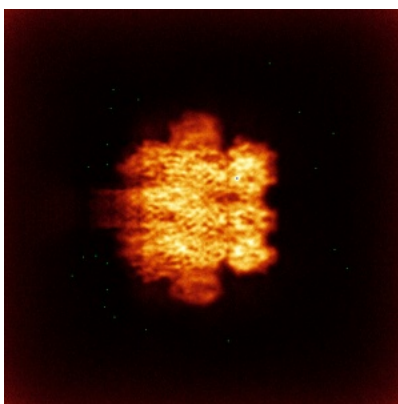


Z

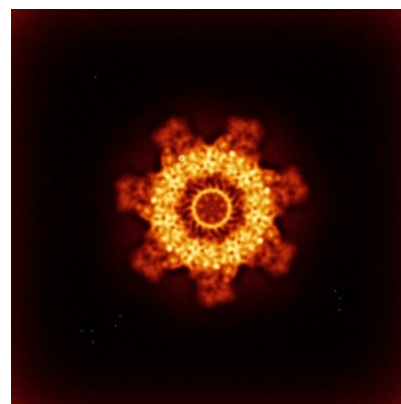
### 6.4.2 Raw map



X



Y

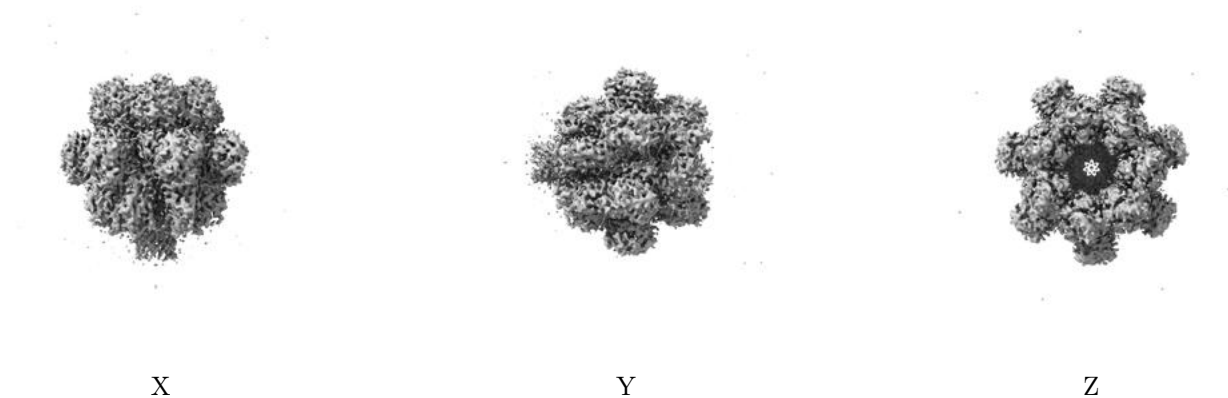


Z

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

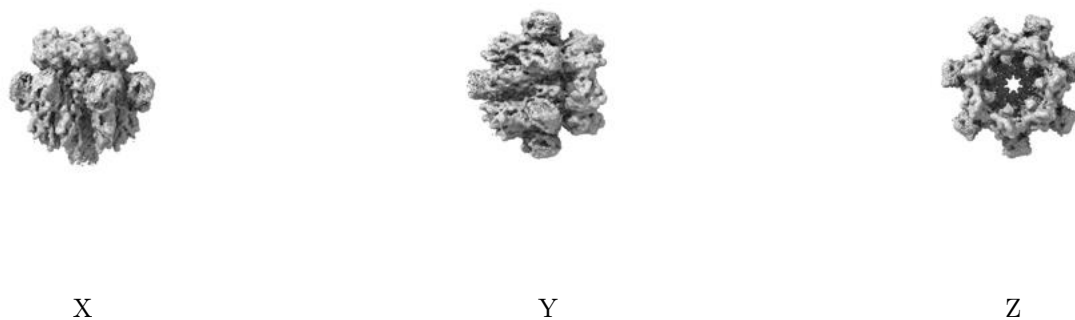
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0663. 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.

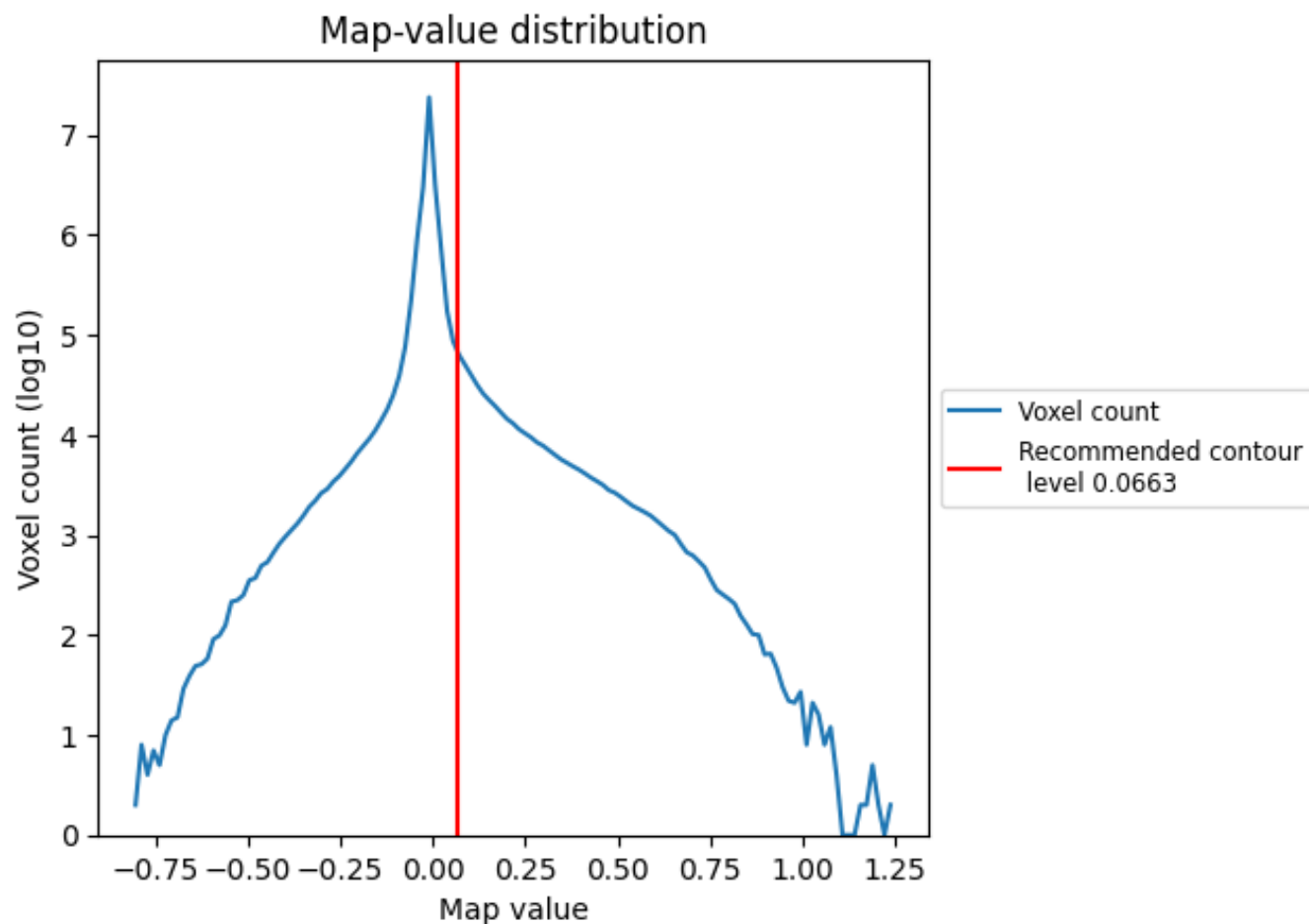
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

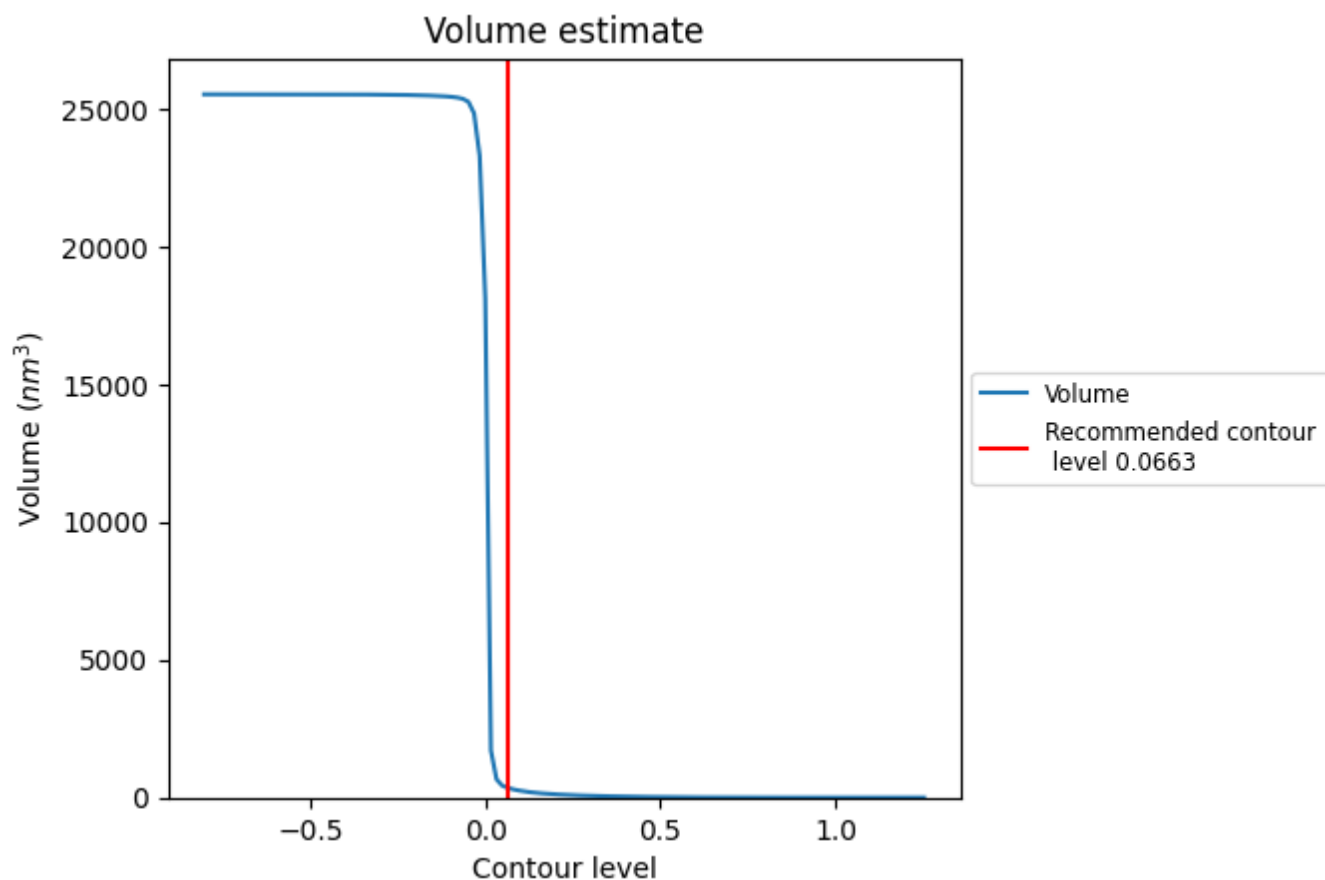
This section contains the results of statistical analysis of the map.

### 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.

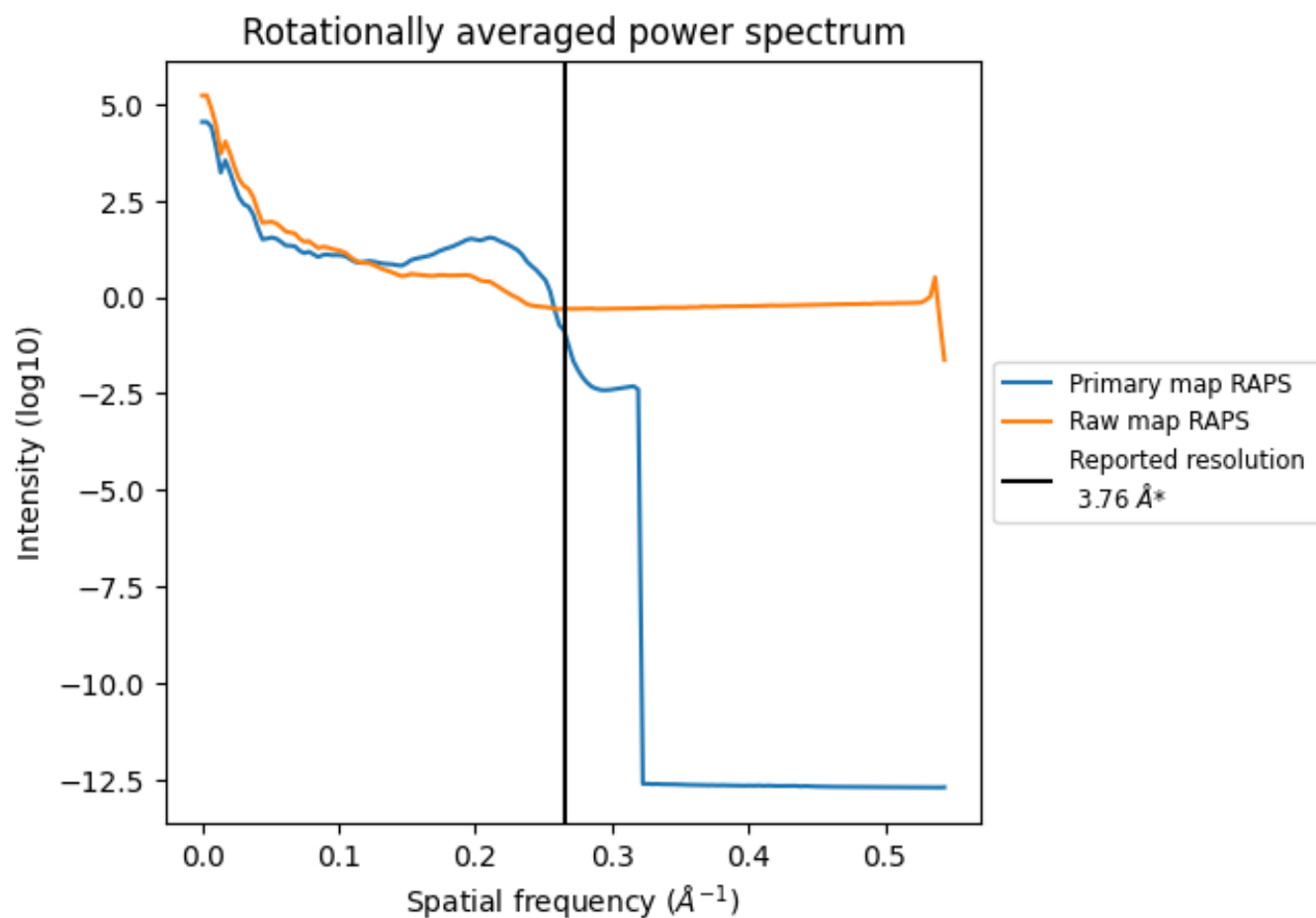
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344  $\text{nm}^3$ ; this corresponds to an approximate mass of 311 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 ⓘ

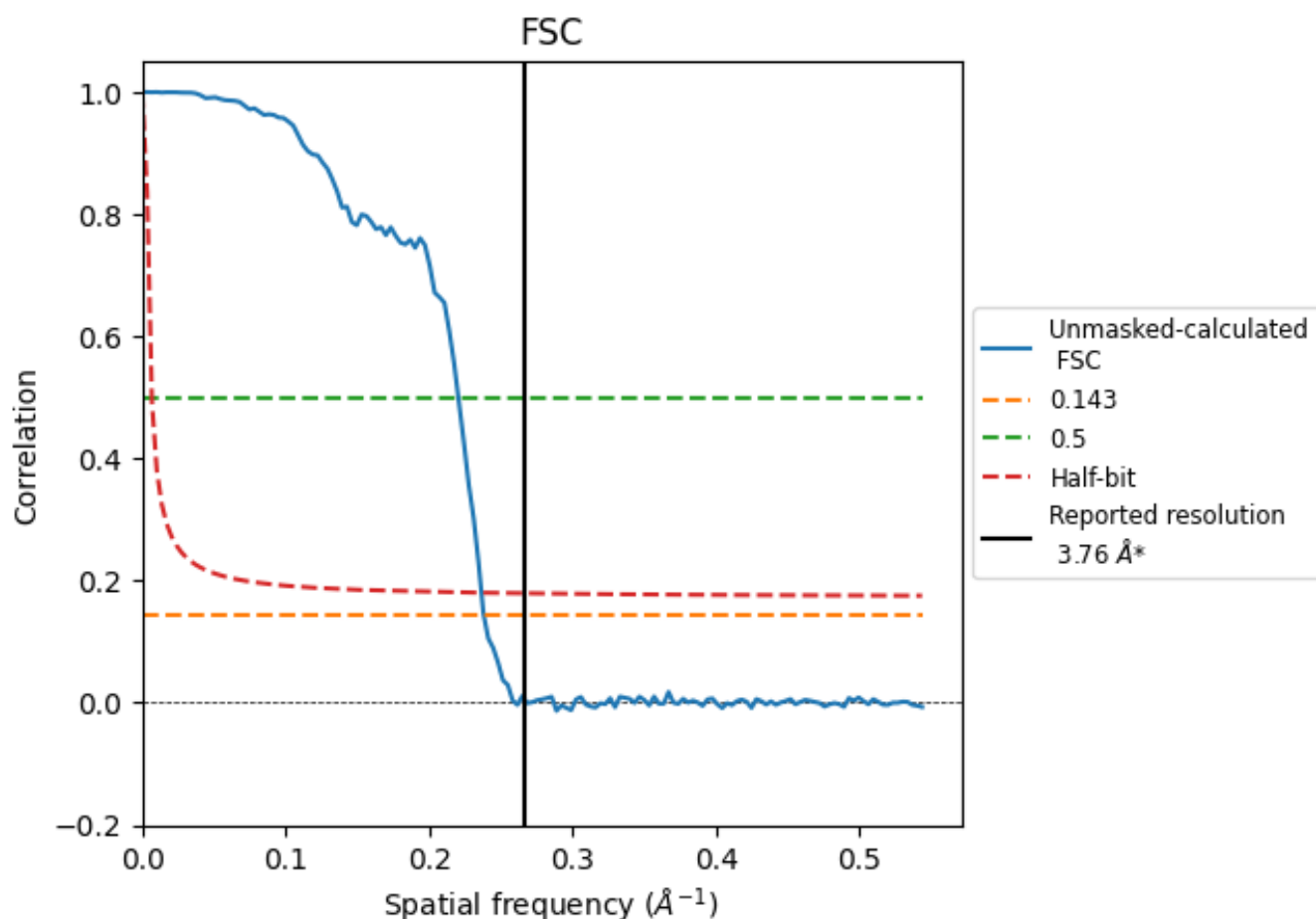


\*Reported resolution corresponds to spatial frequency of 0.266  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.266  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

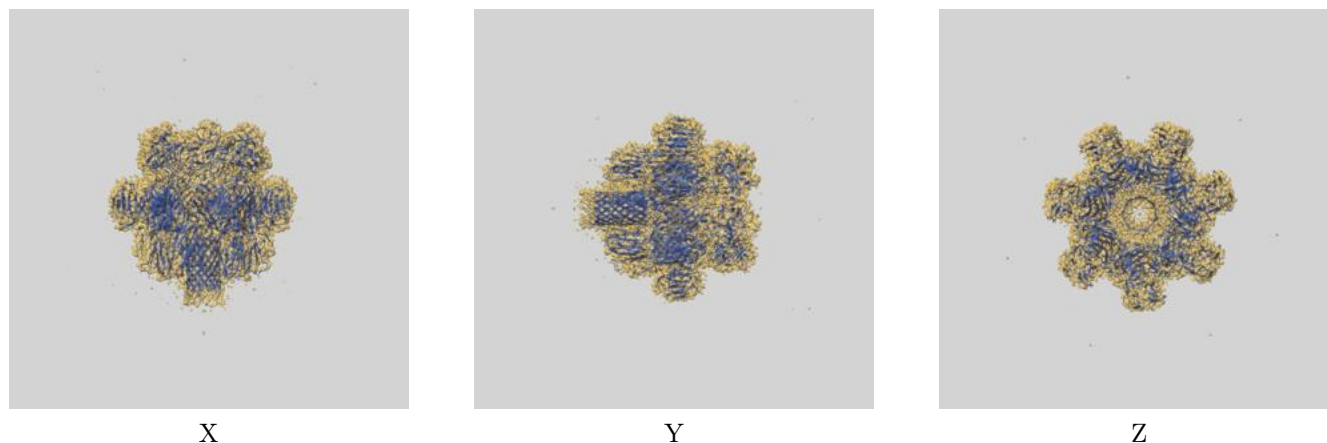
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.76                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.20                               | 4.54 | 4.23     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.76 by more than 10 %

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

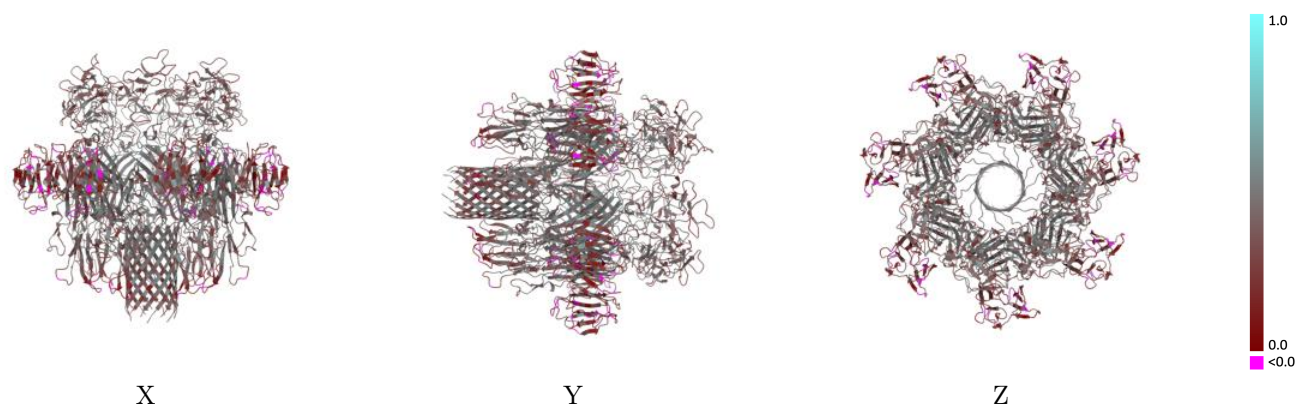
This section contains information regarding the fit between EMDB map EMD-63088 and PDB model 9LH7. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



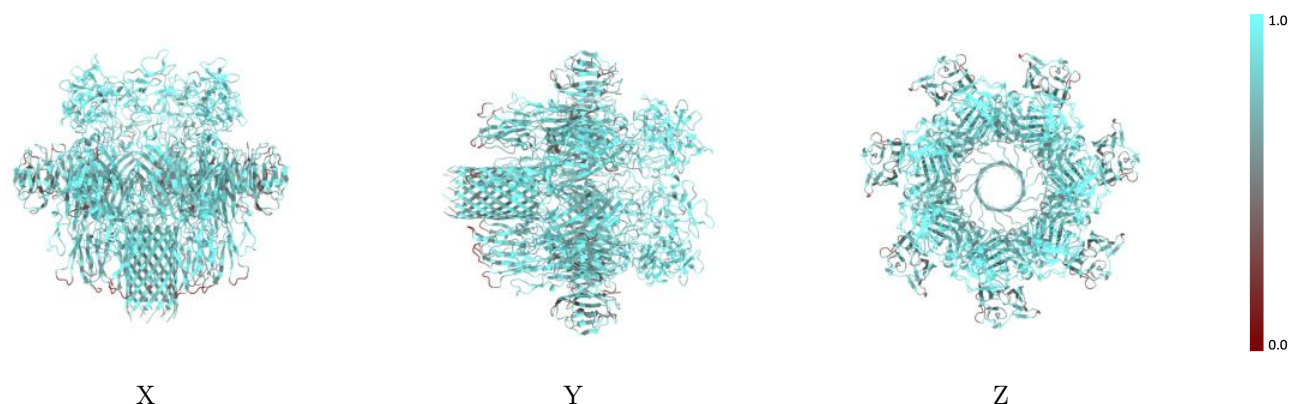
The images above show the 3D surface view of the map at the recommended contour level 0.0663 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



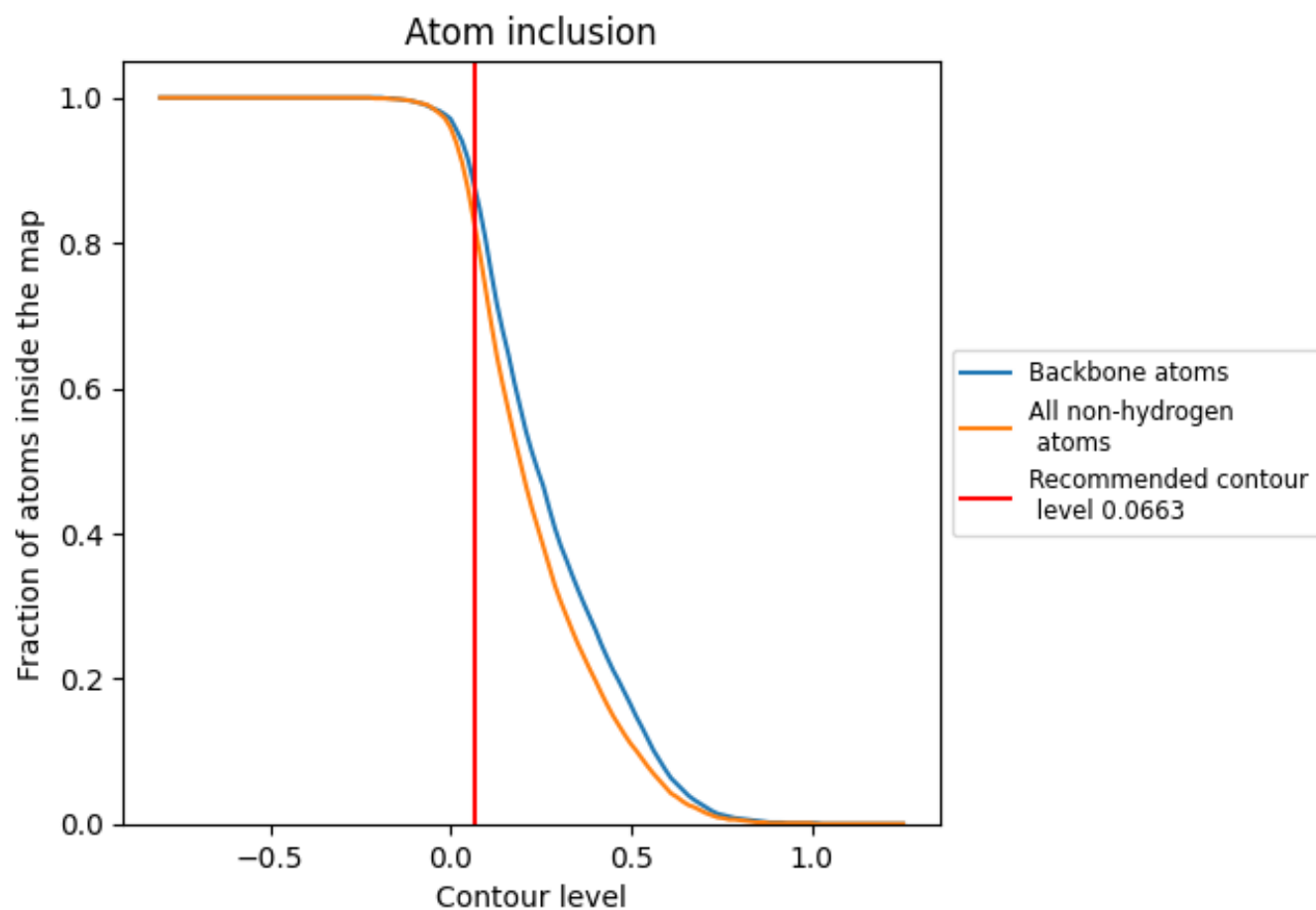
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0663).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.0663) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8260 | <div><div></div></div> 0.3560 |
| A     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.3560 |
| B     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.3550 |
| C     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.3560 |
| D     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.3570 |
| E     | <div><div></div></div> 0.8260 | <div><div></div></div> 0.3550 |
| F     | <div><div></div></div> 0.8280 | <div><div></div></div> 0.3570 |
| N     | <div><div></div></div> 0.8230 | <div><div></div></div> 0.3570 |

1.0

0.0

<0.0