



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:50 AM UTC

PDB ID : 3JAC / pdb\_00003jac  
EMDB ID : EMD-6343  
Title : Cryo-EM study of a channel  
Authors : Ge, J.; Li, W.; Zhao, Q.; Li, N.; Xiao, B.; Gao, N.; Yang, M.  
Deposited on : 2015-06-05  
Resolution : 4.80 Å(reported)  
Based on initial model : 4RAX

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

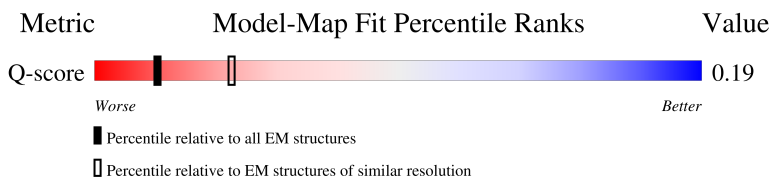
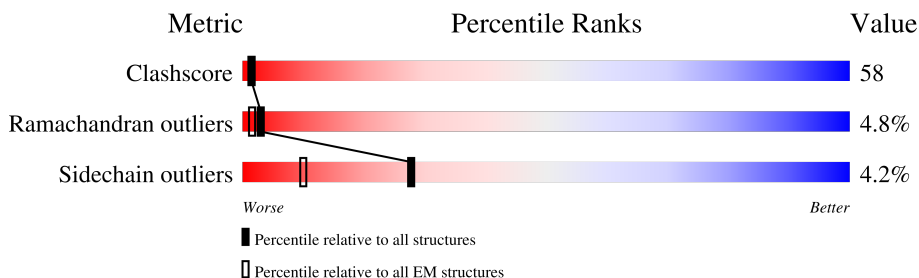
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 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                       | 1575 ( 4.30 - 5.30 )                                     |

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     | 2553   |                  |
| 1   | B     | 2553   |                  |
| 1   | C     | 2553   |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15741 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 Piezo-type mechanosensitive ion channel component 1.

| Mol | Chain | Residues | Atoms |      |     |      |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|---|---------|-------|
| 1   | A     | 918      | Total | C    | N   | O    | S | 0       | 0     |
|     |       |          | 5247  | 3208 | 995 | 1038 | 6 |         |       |
| 1   | B     | 918      | Total | C    | N   | O    | S | 0       | 0     |
|     |       |          | 5247  | 3208 | 995 | 1038 | 6 |         |       |
| 1   | C     | 918      | Total | C    | N   | O    | S | 0       | 0     |
|     |       |          | 5247  | 3208 | 995 | 1038 | 6 |         |       |

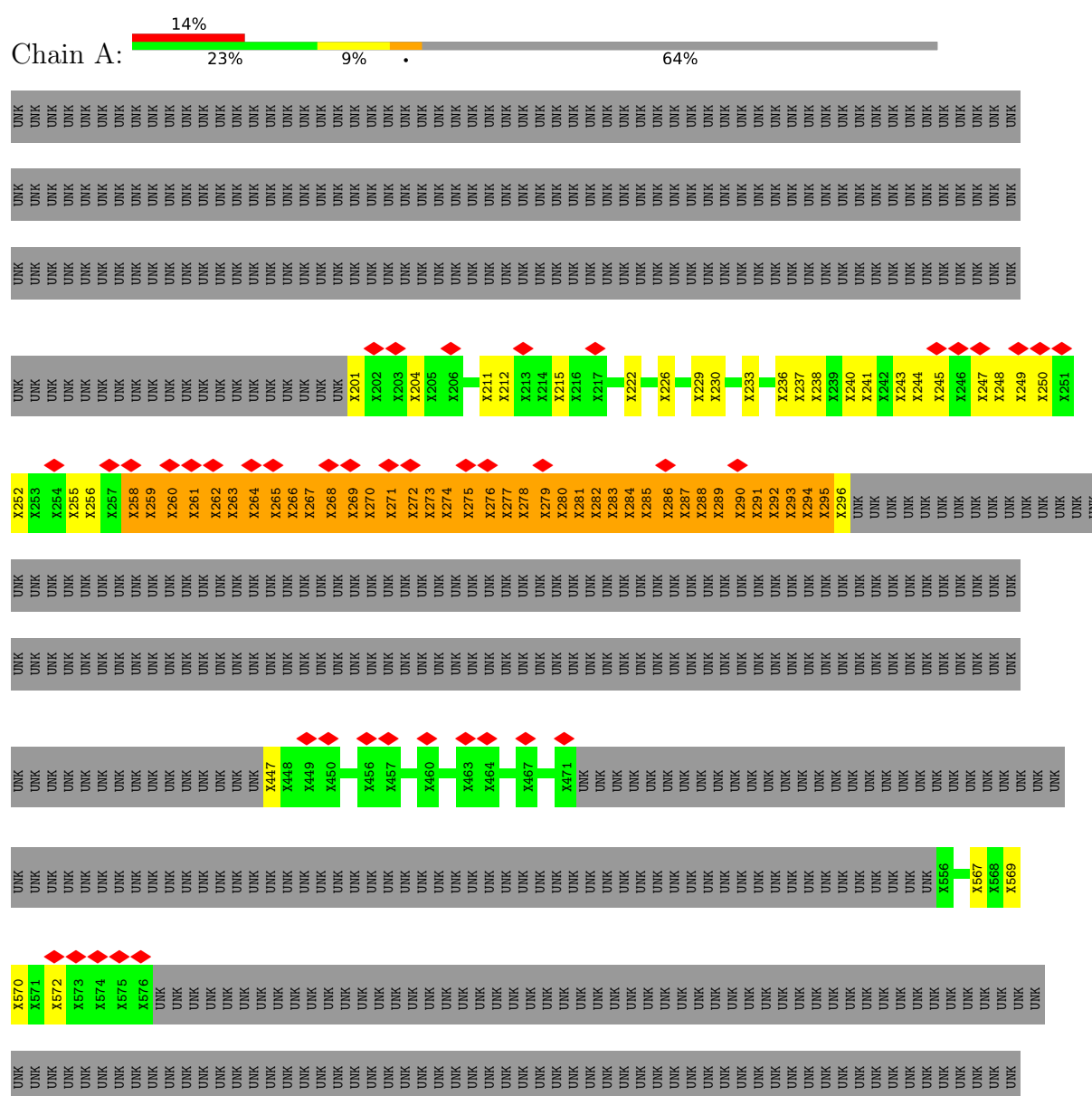
There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 2548    | LEU      | -      | expression tag | UNP E2JF22 |
| A     | 2549    | GLU      | -      | expression tag | UNP E2JF22 |
| A     | 2550    | VAL      | -      | expression tag | UNP E2JF22 |
| A     | 2551    | LEU      | -      | expression tag | UNP E2JF22 |
| A     | 2552    | PHE      | -      | expression tag | UNP E2JF22 |
| A     | 2553    | GLN      | -      | expression tag | UNP E2JF22 |
| B     | 2548    | LEU      | -      | expression tag | UNP E2JF22 |
| B     | 2549    | GLU      | -      | expression tag | UNP E2JF22 |
| B     | 2550    | VAL      | -      | expression tag | UNP E2JF22 |
| B     | 2551    | LEU      | -      | expression tag | UNP E2JF22 |
| B     | 2552    | PHE      | -      | expression tag | UNP E2JF22 |
| B     | 2553    | GLN      | -      | expression tag | UNP E2JF22 |
| C     | 2548    | LEU      | -      | expression tag | UNP E2JF22 |
| C     | 2549    | GLU      | -      | expression tag | UNP E2JF22 |
| C     | 2550    | VAL      | -      | expression tag | UNP E2JF22 |
| C     | 2551    | LEU      | -      | expression tag | UNP E2JF22 |
| C     | 2552    | PHE      | -      | expression tag | UNP E2JF22 |
| C     | 2553    | GLN      | -      | expression tag | UNP E2JF22 |

### 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: Piezo-type mechanosensitive ion channel component 1

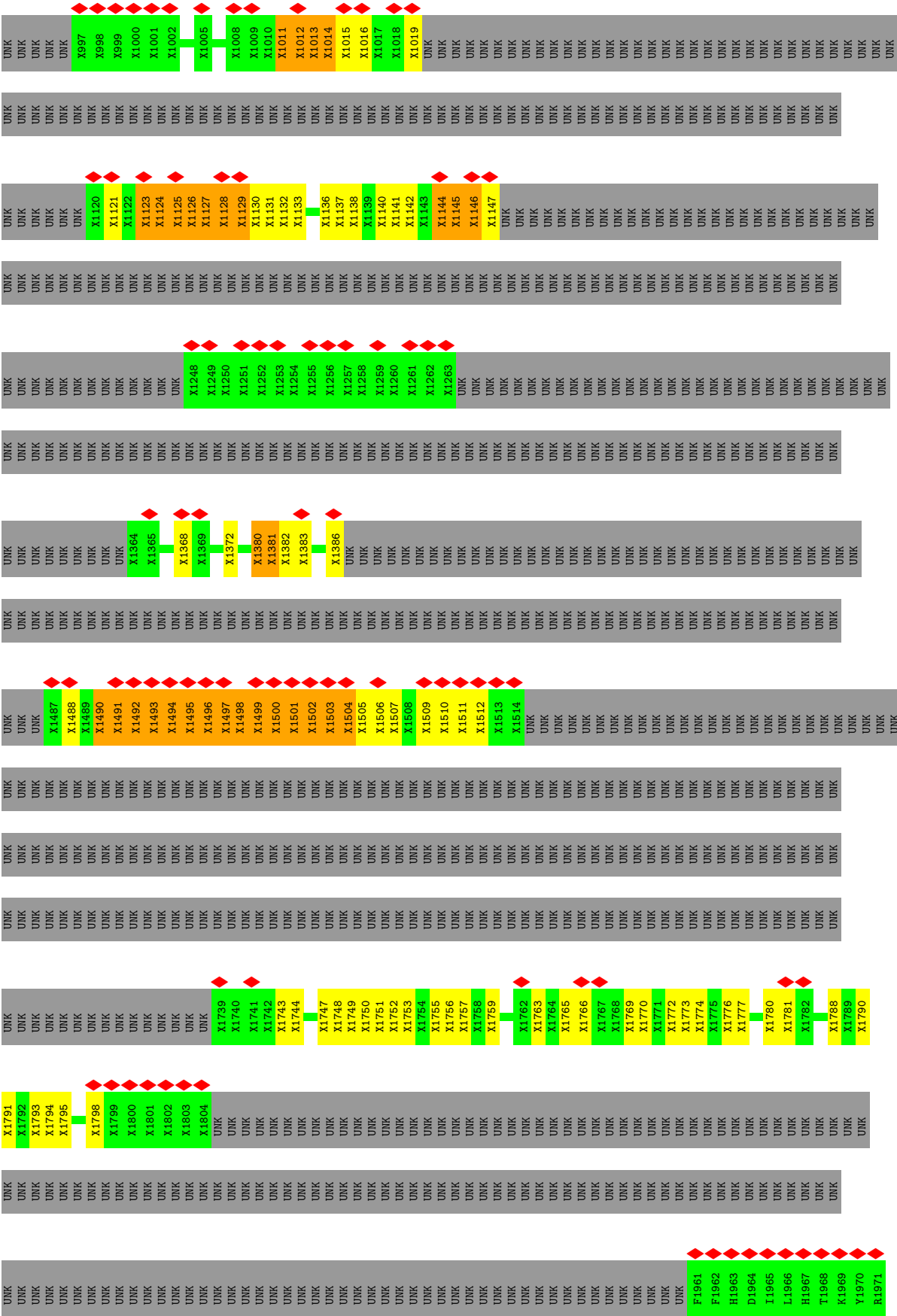


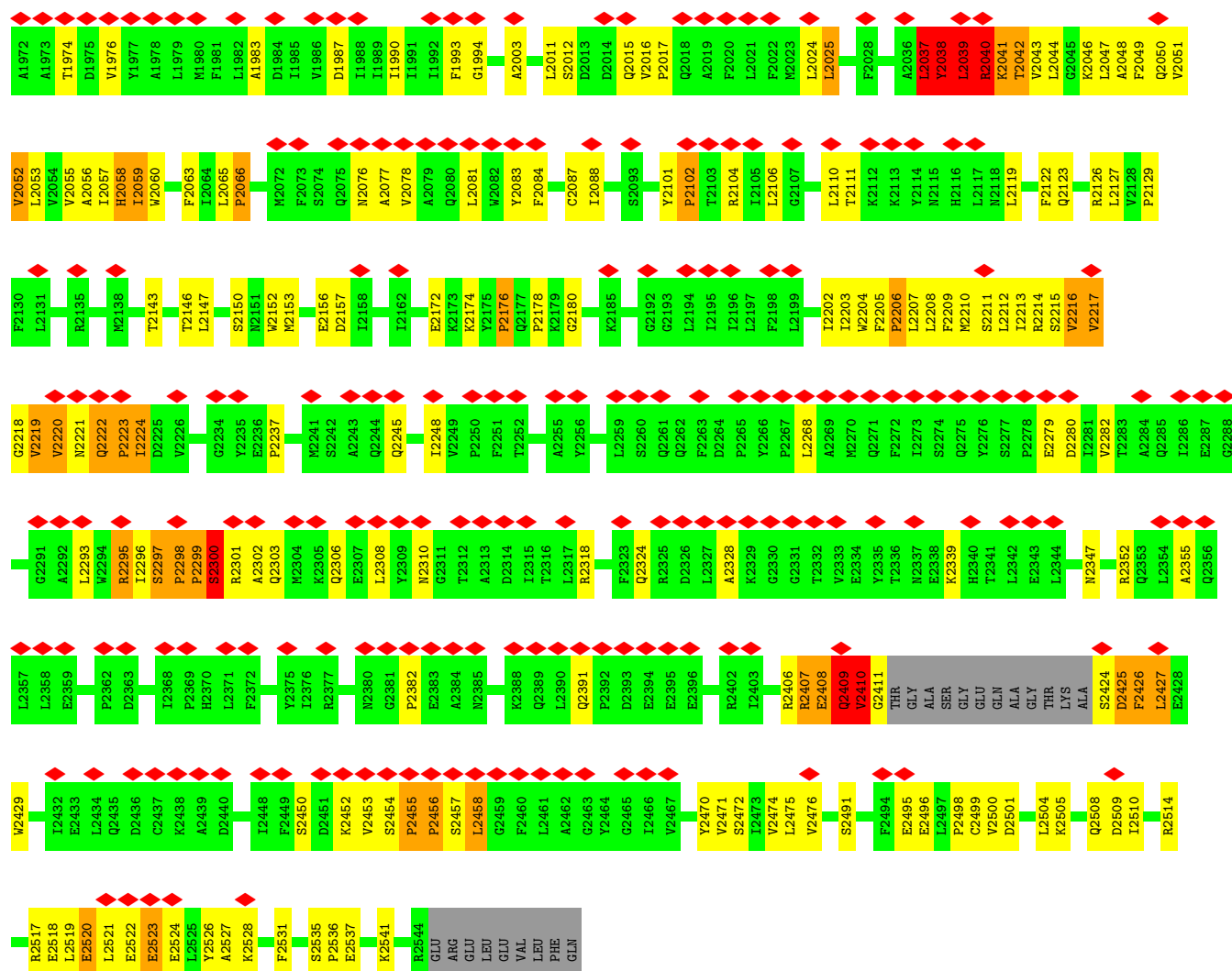




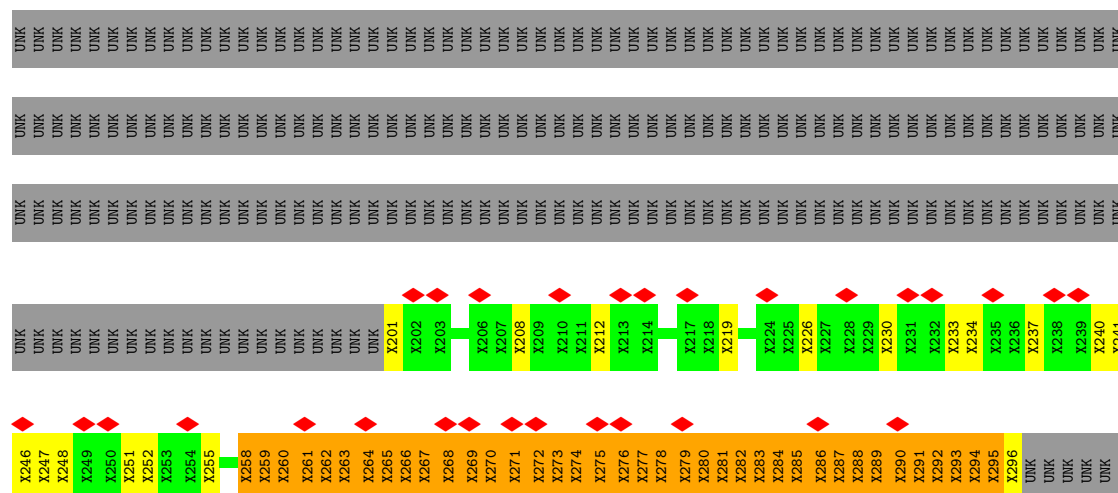
Chain B:  13% 22% 9% 56%





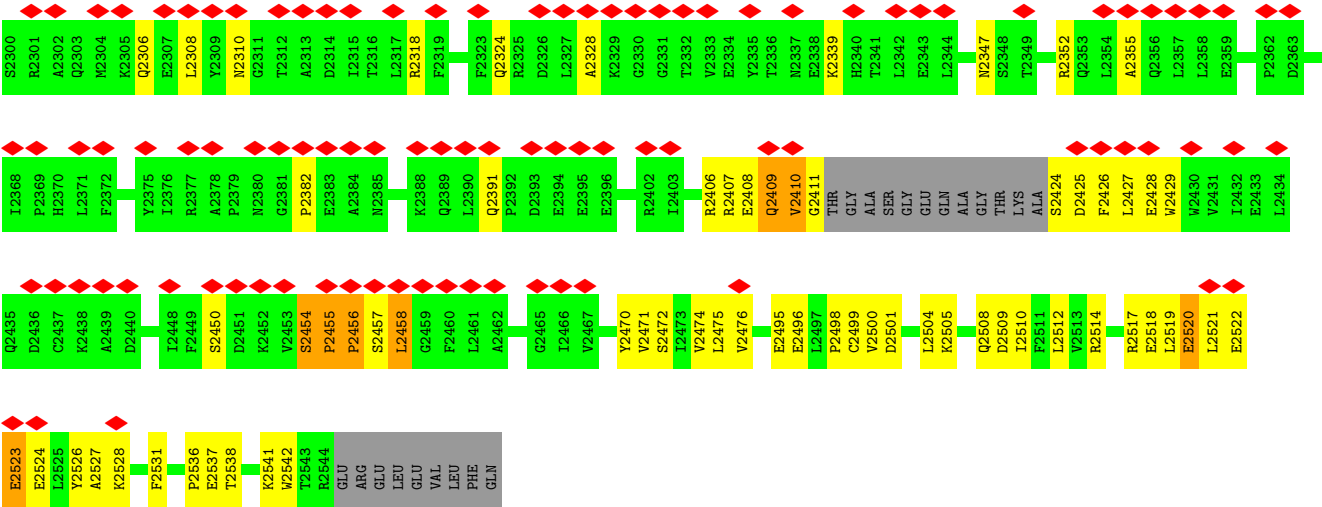


● Molecule 1: Piezo-type mechanosensitive ion channel component 1









## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C1                       | Depositor |
| Number of particles used             | 30021                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | CTFFIND                         | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 16                              | Depositor |
| Minimum defocus (nm)                 | Not provided                    |           |
| Maximum defocus (nm)                 | Not provided                    |           |
| Magnification                        | 22500                           | Depositor |
| Image detector                       | GATAN K2 (4k x 4k)              | Depositor |
| Maximum map value                    | 0.060                           | Depositor |
| Minimum map value                    | -0.026                          | Depositor |
| Average map value                    | 0.001                           | Depositor |
| Map value standard deviation         | 0.005                           | Depositor |
| Recommended contour level            | 0.0273                          | Depositor |
| Map size ( $\text{\AA}$ )            | 316.80002, 316.80002, 316.80002 | wwPDB     |
| Map dimensions                       | 240, 240, 240                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.32, 1.32, 1.32                | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.57         | 7/3562 (0.2%)   | 1.07        | 25/4908 (0.5%)  |
| 1   | B     | 0.57         | 7/3562 (0.2%)   | 1.03        | 22/4908 (0.4%)  |
| 1   | C     | 0.55         | 5/3562 (0.1%)   | 1.00        | 18/4908 (0.4%)  |
| All | All   | 0.56         | 19/10686 (0.2%) | 1.03        | 65/14724 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 80                  |
| 1   | B     | 0                   | 72                  |
| 1   | C     | 0                   | 76                  |
| All | All   | 0                   | 228                 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | C     | 2454 | SER  | C-N   | 6.65 | 1.41        | 1.33     |
| 1   | A     | 2297 | SER  | C-N   | 6.53 | 1.41        | 1.33     |
| 1   | B     | 2222 | GLN  | C-N   | 6.37 | 1.41        | 1.33     |
| 1   | C     | 2222 | GLN  | C-N   | 6.36 | 1.41        | 1.33     |
| 1   | A     | 2222 | GLN  | C-N   | 6.35 | 1.41        | 1.33     |
| 1   | B     | 2298 | PRO  | C-N   | 6.04 | 1.41        | 1.34     |
| 1   | A     | 2510 | ILE  | C-N   | 5.81 | 1.41        | 1.33     |
| 1   | C     | 2510 | ILE  | C-N   | 5.78 | 1.41        | 1.33     |
| 1   | B     | 2510 | ILE  | C-N   | 5.77 | 1.41        | 1.33     |
| 1   | A     | 2298 | PRO  | C-N   | 5.56 | 1.41        | 1.34     |
| 1   | A     | 2298 | PRO  | N-CD  | 5.30 | 1.55        | 1.47     |
| 1   | B     | 2409 | GLN  | CA-C  | 5.11 | 1.59        | 1.52     |
| 1   | C     | 2455 | PRO  | N-CD  | 5.09 | 1.54        | 1.47     |
| 1   | B     | 2455 | PRO  | N-CD  | 5.09 | 1.54        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | A     | 2455 | PRO  | N-CD  | 5.08 | 1.54        | 1.47     |
| 1   | C     | 2223 | PRO  | N-CD  | 5.07 | 1.54        | 1.47     |
| 1   | A     | 2223 | PRO  | N-CD  | 5.06 | 1.54        | 1.47     |
| 1   | B     | 2299 | PRO  | N-CD  | 5.03 | 1.54        | 1.47     |
| 1   | B     | 2223 | PRO  | N-CD  | 5.01 | 1.54        | 1.47     |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | C     | 2038 | TYR  | O-C-N   | -12.00 | 109.71      | 122.07   |
| 1   | A     | 2038 | TYR  | O-C-N   | -11.98 | 109.73      | 122.07   |
| 1   | A     | 2041 | LYS  | O-C-N   | -11.98 | 109.73      | 122.07   |
| 1   | A     | 2042 | THR  | O-C-N   | -11.96 | 109.75      | 122.07   |
| 1   | A     | 2039 | LEU  | O-C-N   | -11.96 | 109.75      | 122.07   |
| 1   | B     | 2038 | TYR  | O-C-N   | -11.94 | 109.77      | 122.07   |
| 1   | B     | 2039 | LEU  | O-C-N   | -11.94 | 109.78      | 122.07   |
| 1   | B     | 2040 | ARG  | O-C-N   | -11.92 | 109.80      | 122.07   |
| 1   | C     | 2039 | LEU  | O-C-N   | -11.91 | 109.80      | 122.07   |
| 1   | A     | 2040 | ARG  | O-C-N   | -11.90 | 109.81      | 122.07   |
| 1   | C     | 2040 | ARG  | O-C-N   | -11.90 | 109.82      | 122.07   |
| 1   | B     | 2037 | LEU  | O-C-N   | -10.84 | 109.65      | 122.11   |
| 1   | C     | 2037 | LEU  | O-C-N   | -10.83 | 109.65      | 122.11   |
| 1   | A     | 2037 | LEU  | O-C-N   | -10.82 | 109.67      | 122.11   |
| 1   | B     | 2410 | VAL  | CB-CA-C | 8.86   | 128.24      | 111.40   |
| 1   | C     | 2454 | SER  | CA-C-N  | -7.30  | 112.86      | 120.38   |
| 1   | C     | 2454 | SER  | C-N-CA  | -7.30  | 112.86      | 120.38   |
| 1   | A     | 2297 | SER  | CA-C-N  | -7.23  | 112.93      | 120.38   |
| 1   | A     | 2297 | SER  | C-N-CA  | -7.23  | 112.93      | 120.38   |
| 1   | B     | 2222 | GLN  | CA-C-N  | -6.88  | 112.40      | 119.83   |
| 1   | B     | 2222 | GLN  | C-N-CA  | -6.88  | 112.40      | 119.83   |
| 1   | A     | 2222 | GLN  | CA-C-N  | -6.83  | 112.45      | 119.83   |
| 1   | A     | 2222 | GLN  | C-N-CA  | -6.83  | 112.45      | 119.83   |
| 1   | C     | 2222 | GLN  | CA-C-N  | -6.79  | 112.49      | 119.83   |
| 1   | C     | 2222 | GLN  | C-N-CA  | -6.79  | 112.49      | 119.83   |
| 1   | B     | 2178 | PRO  | N-CA-CB | 6.79   | 110.38      | 103.25   |
| 1   | A     | 2409 | GLN  | CA-C-N  | 6.73   | 133.81      | 121.70   |
| 1   | A     | 2409 | GLN  | C-N-CA  | 6.73   | 133.81      | 121.70   |
| 1   | A     | 2456 | PRO  | N-CA-CB | 6.71   | 110.30      | 103.25   |
| 1   | A     | 2066 | PRO  | N-CA-CB | 6.71   | 110.29      | 103.25   |
| 1   | B     | 2456 | PRO  | N-CA-CB | 6.71   | 110.29      | 103.25   |
| 1   | C     | 2456 | PRO  | N-CA-CB | 6.70   | 110.28      | 103.25   |
| 1   | C     | 2178 | PRO  | N-CA-CB | 6.69   | 110.39      | 103.23   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | B     | 2066 | PRO  | N-CA-CB    | 6.67  | 110.25      | 103.25   |
| 1   | C     | 2066 | PRO  | N-CA-CB    | 6.66  | 110.25      | 103.25   |
| 1   | A     | 2178 | PRO  | N-CA-CB    | 6.66  | 110.36      | 103.23   |
| 1   | C     | 2017 | PRO  | N-CA-CB    | 6.58  | 110.27      | 103.23   |
| 1   | B     | 2017 | PRO  | N-CA-CB    | 6.57  | 110.25      | 103.23   |
| 1   | A     | 2017 | PRO  | N-CA-CB    | 6.56  | 110.25      | 103.23   |
| 1   | A     | 2102 | PRO  | N-CA-CB    | 6.44  | 110.41      | 103.33   |
| 1   | A     | 2206 | PRO  | N-CA-CB    | 6.42  | 110.39      | 103.33   |
| 1   | B     | 2102 | PRO  | N-CA-CB    | 6.41  | 110.38      | 103.33   |
| 1   | C     | 2102 | PRO  | N-CA-CB    | 6.38  | 110.34      | 103.33   |
| 1   | C     | 2206 | PRO  | N-CA-CB    | 6.37  | 110.34      | 103.33   |
| 1   | B     | 2129 | PRO  | N-CA-CB    | 6.36  | 110.33      | 103.33   |
| 1   | A     | 2498 | PRO  | N-CA-CB    | 6.35  | 110.55      | 103.44   |
| 1   | C     | 2129 | PRO  | N-CA-CB    | 6.34  | 110.31      | 103.33   |
| 1   | C     | 2536 | PRO  | N-CA-CB    | 6.34  | 110.49      | 103.26   |
| 1   | B     | 2498 | PRO  | N-CA-CB    | 6.34  | 110.54      | 103.44   |
| 1   | B     | 2536 | PRO  | N-CA-CB    | 6.32  | 110.47      | 103.26   |
| 1   | A     | 2536 | PRO  | N-CA-CB    | 6.32  | 110.46      | 103.26   |
| 1   | A     | 2129 | PRO  | N-CA-CB    | 6.32  | 110.28      | 103.33   |
| 1   | C     | 2498 | PRO  | N-CA-CB    | 6.30  | 110.50      | 103.44   |
| 1   | B     | 2300 | SER  | O-C-N      | 6.27  | 130.48      | 122.33   |
| 1   | C     | 2176 | PRO  | N-CA-CB    | 6.24  | 110.19      | 103.33   |
| 1   | B     | 2409 | GLN  | CB-CG-CD   | 6.22  | 123.17      | 112.60   |
| 1   | A     | 2176 | PRO  | N-CA-CB    | 6.21  | 110.16      | 103.33   |
| 1   | B     | 2176 | PRO  | N-CA-CB    | 6.21  | 110.16      | 103.33   |
| 1   | B     | 2410 | VAL  | CG1-CB-CG2 | -5.91 | 97.79       | 110.80   |
| 1   | A     | 2408 | GLU  | N-CA-C     | 5.63  | 118.27      | 108.76   |
| 1   | B     | 2409 | GLN  | N-CA-CB    | -5.63 | 100.98      | 110.49   |
| 1   | A     | 2298 | PRO  | CA-C-N     | -5.60 | 113.14      | 118.97   |
| 1   | A     | 2298 | PRO  | C-N-CA     | -5.60 | 113.14      | 118.97   |
| 1   | B     | 2410 | VAL  | CA-CB-CG2  | 5.08  | 119.03      | 110.40   |
| 1   | B     | 2300 | SER  | N-CA-C     | -5.07 | 105.75      | 112.34   |

There are no chirality outliers.

All (228) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1011 | UNK  | Mainchain |
| 1   | A     | 1012 | UNK  | Mainchain |
| 1   | A     | 1013 | UNK  | Mainchain |
| 1   | A     | 1014 | UNK  | Mainchain |
| 1   | A     | 1123 | UNK  | Mainchain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1124 | UNK  | Mainchain |
| 1   | A     | 1125 | UNK  | Mainchain |
| 1   | A     | 1126 | UNK  | Mainchain |
| 1   | A     | 1127 | UNK  | Mainchain |
| 1   | A     | 1128 | UNK  | Mainchain |
| 1   | A     | 1129 | UNK  | Mainchain |
| 1   | A     | 1143 | UNK  | Mainchain |
| 1   | A     | 1144 | UNK  | Mainchain |
| 1   | A     | 1145 | UNK  | Mainchain |
| 1   | A     | 1146 | UNK  | Mainchain |
| 1   | A     | 1380 | UNK  | Mainchain |
| 1   | A     | 1381 | UNK  | Mainchain |
| 1   | A     | 1490 | UNK  | Mainchain |
| 1   | A     | 1491 | UNK  | Mainchain |
| 1   | A     | 1492 | UNK  | Mainchain |
| 1   | A     | 1493 | UNK  | Mainchain |
| 1   | A     | 1494 | UNK  | Mainchain |
| 1   | A     | 1495 | UNK  | Mainchain |
| 1   | A     | 1496 | UNK  | Mainchain |
| 1   | A     | 1497 | UNK  | Mainchain |
| 1   | A     | 1498 | UNK  | Mainchain |
| 1   | A     | 1499 | UNK  | Mainchain |
| 1   | A     | 1500 | UNK  | Mainchain |
| 1   | A     | 1501 | UNK  | Mainchain |
| 1   | A     | 1502 | UNK  | Mainchain |
| 1   | A     | 1503 | UNK  | Mainchain |
| 1   | A     | 1504 | UNK  | Mainchain |
| 1   | A     | 1788 | UNK  | Mainchain |
| 1   | A     | 1789 | UNK  | Mainchain |
| 1   | A     | 1790 | UNK  | Mainchain |
| 1   | A     | 1791 | UNK  | Mainchain |
| 1   | A     | 2037 | LEU  | Mainchain |
| 1   | A     | 2038 | TYR  | Mainchain |
| 1   | A     | 2039 | LEU  | Mainchain |
| 1   | A     | 2040 | ARG  | Mainchain |
| 1   | A     | 2041 | LYS  | Mainchain |
| 1   | A     | 2042 | THR  | Mainchain |
| 1   | A     | 258  | UNK  | Mainchain |
| 1   | A     | 259  | UNK  | Mainchain |
| 1   | A     | 260  | UNK  | Mainchain |
| 1   | A     | 261  | UNK  | Mainchain |
| 1   | A     | 262  | UNK  | Mainchain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 263  | UNK  | Mainchain |
| 1   | A     | 264  | UNK  | Mainchain |
| 1   | A     | 265  | UNK  | Mainchain |
| 1   | A     | 266  | UNK  | Mainchain |
| 1   | A     | 267  | UNK  | Mainchain |
| 1   | A     | 268  | UNK  | Mainchain |
| 1   | A     | 269  | UNK  | Mainchain |
| 1   | A     | 270  | UNK  | Mainchain |
| 1   | A     | 271  | UNK  | Mainchain |
| 1   | A     | 272  | UNK  | Mainchain |
| 1   | A     | 273  | UNK  | Mainchain |
| 1   | A     | 274  | UNK  | Mainchain |
| 1   | A     | 275  | UNK  | Mainchain |
| 1   | A     | 276  | UNK  | Mainchain |
| 1   | A     | 277  | UNK  | Mainchain |
| 1   | A     | 278  | UNK  | Mainchain |
| 1   | A     | 279  | UNK  | Mainchain |
| 1   | A     | 280  | UNK  | Mainchain |
| 1   | A     | 281  | UNK  | Mainchain |
| 1   | A     | 282  | UNK  | Mainchain |
| 1   | A     | 283  | UNK  | Mainchain |
| 1   | A     | 284  | UNK  | Mainchain |
| 1   | A     | 285  | UNK  | Mainchain |
| 1   | A     | 286  | UNK  | Mainchain |
| 1   | A     | 287  | UNK  | Mainchain |
| 1   | A     | 288  | UNK  | Mainchain |
| 1   | A     | 289  | UNK  | Mainchain |
| 1   | A     | 290  | UNK  | Mainchain |
| 1   | A     | 291  | UNK  | Mainchain |
| 1   | A     | 292  | UNK  | Mainchain |
| 1   | A     | 293  | UNK  | Mainchain |
| 1   | A     | 294  | UNK  | Mainchain |
| 1   | A     | 295  | UNK  | Mainchain |
| 1   | B     | 1011 | UNK  | Mainchain |
| 1   | B     | 1012 | UNK  | Mainchain |
| 1   | B     | 1013 | UNK  | Mainchain |
| 1   | B     | 1014 | UNK  | Mainchain |
| 1   | B     | 1123 | UNK  | Mainchain |
| 1   | B     | 1124 | UNK  | Mainchain |
| 1   | B     | 1125 | UNK  | Mainchain |
| 1   | B     | 1126 | UNK  | Mainchain |
| 1   | B     | 1127 | UNK  | Mainchain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | B     | 1128 | UNK  | Mainchain |
| 1   | B     | 1129 | UNK  | Mainchain |
| 1   | B     | 1144 | UNK  | Mainchain |
| 1   | B     | 1145 | UNK  | Mainchain |
| 1   | B     | 1146 | UNK  | Mainchain |
| 1   | B     | 1380 | UNK  | Mainchain |
| 1   | B     | 1381 | UNK  | Mainchain |
| 1   | B     | 1490 | UNK  | Mainchain |
| 1   | B     | 1491 | UNK  | Mainchain |
| 1   | B     | 1492 | UNK  | Mainchain |
| 1   | B     | 1493 | UNK  | Mainchain |
| 1   | B     | 1494 | UNK  | Mainchain |
| 1   | B     | 1495 | UNK  | Mainchain |
| 1   | B     | 1496 | UNK  | Mainchain |
| 1   | B     | 1497 | UNK  | Mainchain |
| 1   | B     | 1498 | UNK  | Mainchain |
| 1   | B     | 1499 | UNK  | Mainchain |
| 1   | B     | 1500 | UNK  | Mainchain |
| 1   | B     | 1501 | UNK  | Mainchain |
| 1   | B     | 1502 | UNK  | Mainchain |
| 1   | B     | 1503 | UNK  | Mainchain |
| 1   | B     | 1504 | UNK  | Mainchain |
| 1   | B     | 2037 | LEU  | Mainchain |
| 1   | B     | 2038 | TYR  | Mainchain |
| 1   | B     | 2039 | LEU  | Mainchain |
| 1   | B     | 2040 | ARG  | Mainchain |
| 1   | B     | 2410 | VAL  | Mainchain |
| 1   | B     | 258  | UNK  | Mainchain |
| 1   | B     | 259  | UNK  | Mainchain |
| 1   | B     | 260  | UNK  | Mainchain |
| 1   | B     | 261  | UNK  | Mainchain |
| 1   | B     | 262  | UNK  | Mainchain |
| 1   | B     | 263  | UNK  | Mainchain |
| 1   | B     | 264  | UNK  | Mainchain |
| 1   | B     | 265  | UNK  | Mainchain |
| 1   | B     | 266  | UNK  | Mainchain |
| 1   | B     | 267  | UNK  | Mainchain |
| 1   | B     | 268  | UNK  | Mainchain |
| 1   | B     | 269  | UNK  | Mainchain |
| 1   | B     | 270  | UNK  | Mainchain |
| 1   | B     | 271  | UNK  | Mainchain |
| 1   | B     | 272  | UNK  | Mainchain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | B     | 273  | UNK  | Mainchain |
| 1   | B     | 274  | UNK  | Mainchain |
| 1   | B     | 275  | UNK  | Mainchain |
| 1   | B     | 276  | UNK  | Mainchain |
| 1   | B     | 277  | UNK  | Mainchain |
| 1   | B     | 278  | UNK  | Mainchain |
| 1   | B     | 279  | UNK  | Mainchain |
| 1   | B     | 280  | UNK  | Mainchain |
| 1   | B     | 281  | UNK  | Mainchain |
| 1   | B     | 284  | UNK  | Mainchain |
| 1   | B     | 285  | UNK  | Mainchain |
| 1   | B     | 286  | UNK  | Mainchain |
| 1   | B     | 287  | UNK  | Mainchain |
| 1   | B     | 288  | UNK  | Mainchain |
| 1   | B     | 289  | UNK  | Mainchain |
| 1   | B     | 290  | UNK  | Mainchain |
| 1   | B     | 291  | UNK  | Mainchain |
| 1   | B     | 292  | UNK  | Mainchain |
| 1   | B     | 293  | UNK  | Mainchain |
| 1   | B     | 294  | UNK  | Mainchain |
| 1   | B     | 295  | UNK  | Mainchain |
| 1   | C     | 1011 | UNK  | Mainchain |
| 1   | C     | 1012 | UNK  | Mainchain |
| 1   | C     | 1013 | UNK  | Mainchain |
| 1   | C     | 1014 | UNK  | Mainchain |
| 1   | C     | 1123 | UNK  | Mainchain |
| 1   | C     | 1124 | UNK  | Mainchain |
| 1   | C     | 1125 | UNK  | Mainchain |
| 1   | C     | 1126 | UNK  | Mainchain |
| 1   | C     | 1127 | UNK  | Mainchain |
| 1   | C     | 1128 | UNK  | Mainchain |
| 1   | C     | 1129 | UNK  | Mainchain |
| 1   | C     | 1130 | UNK  | Mainchain |
| 1   | C     | 1131 | UNK  | Mainchain |
| 1   | C     | 1132 | UNK  | Mainchain |
| 1   | C     | 1133 | UNK  | Mainchain |
| 1   | C     | 1145 | UNK  | Mainchain |
| 1   | C     | 1146 | UNK  | Mainchain |
| 1   | C     | 1380 | UNK  | Mainchain |
| 1   | C     | 1381 | UNK  | Mainchain |
| 1   | C     | 1490 | UNK  | Mainchain |
| 1   | C     | 1491 | UNK  | Mainchain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | C     | 1492 | UNK  | Mainchain |
| 1   | C     | 1493 | UNK  | Mainchain |
| 1   | C     | 1494 | UNK  | Mainchain |
| 1   | C     | 1495 | UNK  | Mainchain |
| 1   | C     | 1496 | UNK  | Mainchain |
| 1   | C     | 1497 | UNK  | Mainchain |
| 1   | C     | 1498 | UNK  | Mainchain |
| 1   | C     | 1499 | UNK  | Mainchain |
| 1   | C     | 1500 | UNK  | Mainchain |
| 1   | C     | 1501 | UNK  | Mainchain |
| 1   | C     | 1502 | UNK  | Mainchain |
| 1   | C     | 1503 | UNK  | Mainchain |
| 1   | C     | 1504 | UNK  | Mainchain |
| 1   | C     | 2037 | LEU  | Mainchain |
| 1   | C     | 2038 | TYR  | Mainchain |
| 1   | C     | 2039 | LEU  | Mainchain |
| 1   | C     | 2040 | ARG  | Mainchain |
| 1   | C     | 258  | UNK  | Mainchain |
| 1   | C     | 259  | UNK  | Mainchain |
| 1   | C     | 260  | UNK  | Mainchain |
| 1   | C     | 261  | UNK  | Mainchain |
| 1   | C     | 262  | UNK  | Mainchain |
| 1   | C     | 263  | UNK  | Mainchain |
| 1   | C     | 264  | UNK  | Mainchain |
| 1   | C     | 265  | UNK  | Mainchain |
| 1   | C     | 266  | UNK  | Mainchain |
| 1   | C     | 267  | UNK  | Mainchain |
| 1   | C     | 268  | UNK  | Mainchain |
| 1   | C     | 269  | UNK  | Mainchain |
| 1   | C     | 270  | UNK  | Mainchain |
| 1   | C     | 271  | UNK  | Mainchain |
| 1   | C     | 272  | UNK  | Mainchain |
| 1   | C     | 273  | UNK  | Mainchain |
| 1   | C     | 274  | UNK  | Mainchain |
| 1   | C     | 275  | UNK  | Mainchain |
| 1   | C     | 276  | UNK  | Mainchain |
| 1   | C     | 277  | UNK  | Mainchain |
| 1   | C     | 278  | UNK  | Mainchain |
| 1   | C     | 279  | UNK  | Mainchain |
| 1   | C     | 280  | UNK  | Mainchain |
| 1   | C     | 281  | UNK  | Mainchain |
| 1   | C     | 282  | UNK  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 283 | UNK  | Mainchain |
| 1   | C     | 284 | UNK  | Mainchain |
| 1   | C     | 285 | UNK  | Mainchain |
| 1   | C     | 286 | UNK  | Mainchain |
| 1   | C     | 287 | UNK  | Mainchain |
| 1   | C     | 288 | UNK  | Mainchain |
| 1   | C     | 289 | UNK  | Mainchain |
| 1   | C     | 290 | UNK  | Mainchain |
| 1   | C     | 291 | UNK  | Mainchain |
| 1   | C     | 292 | UNK  | Mainchain |
| 1   | C     | 293 | UNK  | Mainchain |
| 1   | C     | 294 | UNK  | Mainchain |
| 1   | C     | 295 | UNK  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5247  | 0        | 2895     | 505     | 0            |
| 1   | B     | 5247  | 0        | 2893     | 543     | 0            |
| 1   | C     | 5247  | 0        | 2898     | 533     | 0            |
| All | All   | 15741 | 0        | 8686     | 1408    | 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 58.

All (1408) 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:C:2410:VAL:HG21 | 1:C:2426:PHE:CD2  | 1.22                     | 1.67              |
| 1:C:2410:VAL:HG21 | 1:C:2426:PHE:CE2  | 1.16                     | 1.62              |
| 1:C:2409:GLN:CA   | 1:C:2410:VAL:HG22 | 1.28                     | 1.60              |
| 1:C:230:UNK:HA    | 1:C:259:UNK:CB    | 1.19                     | 1.58              |
| 1:B:201:UNK:HA    | 1:B:288:UNK:CB    | 1.18                     | 1.57              |
| 1:C:219:UNK:CB    | 1:C:270:UNK:CB    | 1.82                     | 1.57              |
| 1:A:201:UNK:HA    | 1:A:288:UNK:CB    | 1.16                     | 1.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:2429:TRP:CH2 | 1:C:2297:SER:HB2  | 1.35                     | 1.54              |
| 1:C:2410:VAL:CG2 | 1:C:2426:PHE:CE2  | 1.89                     | 1.53              |
| 1:B:2429:TRP:CZ2 | 1:C:2297:SER:HB2  | 1.46                     | 1.51              |
| 1:C:2409:GLN:HA  | 1:C:2410:VAL:CG2  | 1.40                     | 1.48              |
| 1:A:2491:SER:CA  | 1:C:2512:LEU:CB   | 1.89                     | 1.47              |
| 1:A:215:UNK:CB   | 1:A:274:UNK:HA    | 1.46                     | 1.45              |
| 1:A:2382:PRO:CG  | 1:C:2328:ALA:HB2  | 1.43                     | 1.43              |
| 1:C:295:UNK:HA   | 1:C:447:UNK:N     | 1.36                     | 1.40              |
| 1:A:295:UNK:HA   | 1:A:447:UNK:N     | 1.36                     | 1.40              |
| 1:B:201:UNK:CA   | 1:B:288:UNK:CB    | 1.98                     | 1.40              |
| 1:A:237:UNK:CA   | 1:A:252:UNK:HA    | 1.41                     | 1.40              |
| 1:C:2409:GLN:CB  | 1:C:2410:VAL:HG22 | 1.34                     | 1.40              |
| 1:A:237:UNK:HA   | 1:A:252:UNK:CA    | 1.33                     | 1.39              |
| 1:A:2217:VAL:O   | 1:A:2454:SER:CB   | 1.70                     | 1.38              |
| 1:C:226:UNK:CB   | 1:C:263:UNK:HA    | 1.54                     | 1.35              |
| 1:B:295:UNK:HA   | 1:B:447:UNK:N     | 1.36                     | 1.34              |
| 1:A:2491:SER:HA  | 1:C:2512:LEU:CB   | 1.47                     | 1.34              |
| 1:B:2203:ILE:O   | 1:B:2207:LEU:CB   | 1.76                     | 1.33              |
| 1:A:2491:SER:CB  | 1:C:2512:LEU:CB   | 2.05                     | 1.31              |
| 1:A:201:UNK:CA   | 1:A:288:UNK:CB    | 2.08                     | 1.31              |
| 1:B:2041:LYS:O   | 1:B:2044:LEU:N    | 1.64                     | 1.30              |
| 1:C:2410:VAL:CG2 | 1:C:2426:PHE:CD2  | 2.11                     | 1.29              |
| 1:A:233:UNK:CB   | 1:A:256:UNK:HA    | 1.62                     | 1.27              |
| 1:C:2409:GLN:CD  | 1:C:2410:VAL:O    | 1.76                     | 1.27              |
| 1:A:215:UNK:CB   | 1:A:274:UNK:CA    | 2.14                     | 1.26              |
| 1:A:2328:ALA:HB2 | 1:B:2382:PRO:CG   | 1.65                     | 1.26              |
| 1:C:2409:GLN:HA  | 1:C:2410:VAL:CB   | 1.65                     | 1.26              |
| 1:C:208:UNK:CB   | 1:C:281:UNK:CB    | 2.14                     | 1.25              |
| 1:C:295:UNK:CA   | 1:C:447:UNK:N     | 2.01                     | 1.24              |
| 1:C:230:UNK:CA   | 1:C:259:UNK:CB    | 2.15                     | 1.23              |
| 1:B:295:UNK:CA   | 1:B:447:UNK:N     | 2.01                     | 1.22              |
| 1:B:2429:TRP:CZ3 | 1:C:2298:PRO:HD2  | 1.73                     | 1.22              |
| 1:A:295:UNK:CA   | 1:A:447:UNK:N     | 2.01                     | 1.22              |
| 1:B:2429:TRP:CZ2 | 1:C:2297:SER:CB   | 2.25                     | 1.20              |
| 1:B:2172:GLU:O   | 1:B:2176:PRO:CB   | 1.90                     | 1.20              |
| 1:C:2409:GLN:HA  | 1:C:2410:VAL:CG1  | 1.70                     | 1.20              |
| 1:C:2409:GLN:CD  | 1:C:2410:VAL:C    | 1.97                     | 1.19              |
| 1:A:2172:GLU:O   | 1:A:2176:PRO:CB   | 1.90                     | 1.18              |
| 1:C:2408:GLU:O   | 1:C:2410:VAL:CG1  | 1.89                     | 1.18              |
| 1:C:1994:GLY:O   | 1:C:1996:TRP:N    | 1.76                     | 1.18              |
| 1:B:2218:GLY:HA2 | 1:B:2453:VAL:O    | 1.39                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2408:GLU:O    | 1:C:2410:VAL:HG11 | 1.41                     | 1.17              |
| 1:C:2172:GLU:O    | 1:C:2176:PRO:CB   | 1.90                     | 1.17              |
| 1:B:2429:TRP:CH2  | 1:C:2299:PRO:HD2  | 1.79                     | 1.17              |
| 1:B:295:UNK:CA    | 1:B:447:UNK:H2    | 1.56                     | 1.16              |
| 1:B:2409:GLN:HA   | 1:B:2410:VAL:HG13 | 1.25                     | 1.15              |
| 1:B:2429:TRP:CH2  | 1:C:2298:PRO:HD2  | 1.80                     | 1.15              |
| 1:A:2407:ARG:HG2  | 1:A:2426:PHE:HB2  | 1.26                     | 1.14              |
| 1:C:295:UNK:CA    | 1:C:447:UNK:H2    | 1.56                     | 1.14              |
| 1:B:2429:TRP:CH2  | 1:C:2297:SER:CB   | 2.30                     | 1.14              |
| 1:A:2293:LEU:HG   | 1:B:2295:ARG:O    | 1.45                     | 1.14              |
| 1:B:2406:ARG:NH1  | 1:C:2299:PRO:HG3  | 1.60                     | 1.13              |
| 1:C:240:UNK:CB    | 1:C:251:UNK:CB    | 2.26                     | 1.13              |
| 1:B:1509:UNK:O    | 1:B:1511:UNK:N    | 1.80                     | 1.13              |
| 1:A:295:UNK:CA    | 1:A:447:UNK:H2    | 1.56                     | 1.12              |
| 1:B:2219:VAL:O    | 1:B:2452:LYS:HE3  | 1.49                     | 1.12              |
| 1:A:2382:PRO:HG3  | 1:C:2328:ALA:HB2  | 1.21                     | 1.12              |
| 1:C:219:UNK:CA    | 1:C:270:UNK:CB    | 2.27                     | 1.12              |
| 1:C:2410:VAL:HG21 | 1:C:2426:PHE:CZ   | 1.84                     | 1.11              |
| 1:C:2409:GLN:CG   | 1:C:2410:VAL:O    | 1.98                     | 1.11              |
| 1:C:2410:VAL:CG2  | 1:C:2426:PHE:CZ   | 2.33                     | 1.11              |
| 1:B:295:UNK:C     | 1:B:447:UNK:H2    | 1.64                     | 1.11              |
| 1:B:2217:VAL:CB   | 1:B:2455:PRO:HD2  | 1.80                     | 1.10              |
| 1:A:2217:VAL:O    | 1:A:2454:SER:HB2  | 1.47                     | 1.10              |
| 1:A:2410:VAL:HG21 | 1:A:2426:PHE:HA   | 1.14                     | 1.10              |
| 1:A:2382:PRO:HG2  | 1:C:2328:ALA:HB2  | 1.21                     | 1.10              |
| 1:C:295:UNK:C     | 1:C:447:UNK:H2    | 1.64                     | 1.10              |
| 1:A:295:UNK:C     | 1:A:447:UNK:H2    | 1.64                     | 1.10              |
| 1:B:212:UNK:HA    | 1:B:277:UNK:CB    | 1.82                     | 1.09              |
| 1:A:2339:LYS:HE3  | 1:C:2245:GLN:NE2  | 1.67                     | 1.09              |
| 1:A:2328:ALA:HB2  | 1:B:2382:PRO:HG2  | 1.34                     | 1.09              |
| 1:C:208:UNK:CB    | 1:C:281:UNK:HA    | 1.84                     | 1.08              |
| 1:A:2328:ALA:HB2  | 1:B:2382:PRO:HG3  | 1.34                     | 1.08              |
| 1:B:2203:ILE:O    | 1:B:2207:LEU:N    | 1.85                     | 1.08              |
| 1:C:2504:LEU:O    | 1:C:2508:GLN:N    | 1.88                     | 1.07              |
| 1:A:2217:VAL:CB   | 1:A:2454:SER:HB2  | 1.84                     | 1.07              |
| 1:C:2041:LYS:O    | 1:C:2044:LEU:N    | 1.88                     | 1.07              |
| 1:B:2429:TRP:CZ3  | 1:C:2297:SER:HB2  | 1.89                     | 1.06              |
| 1:A:2429:TRP:CZ3  | 1:B:2298:PRO:HD2  | 1.90                     | 1.06              |
| 1:A:2407:ARG:NH2  | 1:A:2424:SER:O    | 1.88                     | 1.06              |
| 1:B:2429:TRP:CZ3  | 1:C:2298:PRO:CD   | 2.37                     | 1.06              |
| 1:A:2217:VAL:O    | 1:A:2454:SER:HB3  | 1.53                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2504:LEU:O    | 1:A:2508:GLN:N    | 1.88                     | 1.05              |
| 1:B:236:UNK:CB    | 1:B:255:UNK:CB    | 2.33                     | 1.05              |
| 1:C:2409:GLN:CA   | 1:C:2410:VAL:HG13 | 1.84                     | 1.05              |
| 1:B:2504:LEU:O    | 1:B:2508:GLN:N    | 1.88                     | 1.05              |
| 1:A:211:UNK:C     | 1:A:277:UNK:CB    | 2.34                     | 1.04              |
| 1:B:2406:ARG:CZ   | 1:C:2299:PRO:HG3  | 1.88                     | 1.04              |
| 1:B:1776:UNK:O    | 1:B:1781:UNK:N    | 1.91                     | 1.04              |
| 1:B:2203:ILE:O    | 1:B:2207:LEU:CA   | 2.04                     | 1.04              |
| 1:B:2041:LYS:O    | 1:B:2043:VAL:N    | 1.91                     | 1.04              |
| 1:A:204:UNK:CB    | 1:A:284:UNK:C     | 2.35                     | 1.03              |
| 1:A:2406:ARG:NH1  | 1:A:2408:GLU:OE1  | 1.91                     | 1.03              |
| 1:C:2410:VAL:HG21 | 1:C:2426:PHE:CG   | 1.92                     | 1.03              |
| 1:B:201:UNK:CB    | 1:B:288:UNK:CB    | 2.36                     | 1.03              |
| 1:C:1509:UNK:O    | 1:C:1511:UNK:N    | 1.92                     | 1.03              |
| 1:C:1776:UNK:O    | 1:C:1781:UNK:N    | 1.91                     | 1.03              |
| 1:A:1776:UNK:O    | 1:A:1781:UNK:N    | 1.91                     | 1.03              |
| 1:A:2297:SER:OG   | 1:A:2300:SER:HB2  | 1.57                     | 1.03              |
| 1:B:215:UNK:CB    | 1:B:273:UNK:C     | 2.37                     | 1.03              |
| 1:B:222:UNK:C     | 1:B:266:UNK:CB    | 2.37                     | 1.03              |
| 1:C:2052:VAL:HA   | 1:C:2056:ALA:HA   | 1.38                     | 1.03              |
| 1:C:2122:PHE:CB   | 1:C:2126:ARG:CB   | 2.37                     | 1.02              |
| 1:A:2407:ARG:HG3  | 1:A:2428:GLU:HG2  | 1.40                     | 1.02              |
| 1:A:2409:GLN:HA   | 1:A:2410:VAL:HG23 | 1.36                     | 1.02              |
| 1:B:2122:PHE:CB   | 1:B:2126:ARG:CB   | 2.37                     | 1.02              |
| 1:A:2122:PHE:CB   | 1:A:2126:ARG:CB   | 2.37                     | 1.02              |
| 1:C:208:UNK:CB    | 1:C:281:UNK:CA    | 2.37                     | 1.02              |
| 1:C:2409:GLN:HG3  | 1:C:2410:VAL:O    | 1.59                     | 1.02              |
| 1:B:1752:UNK:O    | 1:B:1756:UNK:N    | 1.93                     | 1.01              |
| 1:C:2059:ILE:O    | 1:C:2063:PHE:CB   | 2.08                     | 1.01              |
| 1:A:1752:UNK:O    | 1:A:1756:UNK:N    | 1.94                     | 1.01              |
| 1:C:1752:UNK:O    | 1:C:1756:UNK:N    | 1.94                     | 1.01              |
| 1:C:1983:ALA:O    | 1:C:1987:ASP:CB   | 2.09                     | 1.00              |
| 1:B:2218:GLY:CA   | 1:B:2453:VAL:O    | 2.10                     | 1.00              |
| 1:B:2409:GLN:HG3  | 1:B:2410:VAL:CG2  | 1.90                     | 1.00              |
| 1:B:2219:VAL:O    | 1:B:2452:LYS:HG2  | 1.61                     | 0.99              |
| 1:A:240:UNK:CB    | 1:A:248:UNK:HA    | 1.93                     | 0.99              |
| 1:B:237:UNK:HA    | 1:B:252:UNK:CB    | 1.92                     | 0.99              |
| 1:A:2382:PRO:CG   | 1:C:2328:ALA:CB   | 2.40                     | 0.99              |
| 1:A:2429:TRP:HZ3  | 1:B:2298:PRO:HD2  | 1.28                     | 0.98              |
| 1:C:2409:GLN:CA   | 1:C:2410:VAL:CG2  | 2.07                     | 0.98              |
| 1:A:215:UNK:CB    | 1:A:274:UNK:N     | 2.26                     | 0.97              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:2429:TRP:CE2  | 1:C:2297:SER:CB  | 2.48                     | 0.97              |
| 1:C:226:UNK:CB    | 1:C:263:UNK:CA   | 2.43                     | 0.97              |
| 1:A:1793:UNK:O    | 1:A:1797:UNK:N   | 1.96                     | 0.97              |
| 1:C:1748:UNK:O    | 1:C:1752:UNK:N   | 1.98                     | 0.97              |
| 1:A:1748:UNK:O    | 1:A:1752:UNK:N   | 1.98                     | 0.97              |
| 1:B:2429:TRP:CE2  | 1:C:2297:SER:HB2 | 2.00                     | 0.97              |
| 1:B:2410:VAL:HG13 | 1:B:2426:PHE:HB3 | 1.47                     | 0.96              |
| 1:C:2509:ASP:HA   | 1:C:2514:ARG:CB  | 1.95                     | 0.96              |
| 1:B:2293:LEU:HG   | 1:C:2295:ARG:O   | 1.64                     | 0.96              |
| 1:A:2509:ASP:HA   | 1:A:2514:ARG:CB  | 1.95                     | 0.96              |
| 1:A:2011:LEU:O    | 1:A:2015:GLN:N   | 1.97                     | 0.96              |
| 1:B:1748:UNK:O    | 1:B:1752:UNK:N   | 1.98                     | 0.96              |
| 1:A:2491:SER:C    | 1:C:2512:LEU:CB  | 2.39                     | 0.96              |
| 1:B:2429:TRP:HH2  | 1:C:2299:PRO:HD2 | 1.12                     | 0.95              |
| 1:B:2509:ASP:HA   | 1:B:2514:ARG:CB  | 1.96                     | 0.95              |
| 1:C:2052:VAL:HA   | 1:C:2056:ALA:CA  | 1.96                     | 0.95              |
| 1:C:219:UNK:HA    | 1:C:270:UNK:CB   | 1.94                     | 0.95              |
| 1:B:2219:VAL:O    | 1:B:2452:LYS:CE  | 2.14                     | 0.95              |
| 1:C:2409:GLN:CB   | 1:C:2410:VAL:CG2 | 2.26                     | 0.95              |
| 1:B:2406:ARG:NH1  | 1:C:2299:PRO:CG  | 2.30                     | 0.95              |
| 1:A:233:UNK:CB    | 1:A:256:UNK:CA   | 2.43                     | 0.94              |
| 1:B:2429:TRP:HZ3  | 1:C:2298:PRO:CD  | 1.79                     | 0.94              |
| 1:B:242:UNK:O     | 1:B:244:UNK:N    | 2.01                     | 0.94              |
| 1:A:229:UNK:C     | 1:A:259:UNK:CB   | 2.46                     | 0.94              |
| 1:B:233:UNK:O     | 1:B:236:UNK:CB   | 2.16                     | 0.94              |
| 1:A:2429:TRP:CD2  | 1:B:2297:SER:HB3 | 2.04                     | 0.93              |
| 1:A:2406:ARG:HH12 | 1:B:2299:PRO:HG3 | 1.30                     | 0.93              |
| 1:B:2409:GLN:HG2  | 1:B:2411:GLY:N   | 1.83                     | 0.93              |
| 1:B:212:UNK:CA    | 1:B:277:UNK:CB   | 2.46                     | 0.93              |
| 1:C:2202:ILE:O    | 1:C:2206:PRO:N   | 2.02                     | 0.93              |
| 1:C:2153:MET:HA   | 1:C:2156:GLU:CB  | 1.99                     | 0.93              |
| 1:A:2153:MET:HA   | 1:A:2156:GLU:CB  | 1.99                     | 0.92              |
| 1:B:2153:MET:HA   | 1:B:2156:GLU:CB  | 1.99                     | 0.92              |
| 1:C:2410:VAL:HG23 | 1:C:2426:PHE:CZ  | 2.05                     | 0.92              |
| 1:B:237:UNK:O     | 1:B:241:UNK:N    | 2.03                     | 0.92              |
| 1:A:2202:ILE:O    | 1:A:2206:PRO:N   | 2.02                     | 0.92              |
| 1:A:2299:PRO:HD2  | 1:C:2429:TRP:HH2 | 1.31                     | 0.92              |
| 1:B:2299:PRO:O    | 1:B:2303:GLN:N   | 2.03                     | 0.92              |
| 1:B:2202:ILE:O    | 1:B:2206:PRO:N   | 2.03                     | 0.92              |
| 1:C:2408:GLU:HG2  | 1:C:2429:TRP:CH2 | 2.04                     | 0.92              |
| 1:A:230:UNK:HA    | 1:A:259:UNK:CB   | 1.99                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1130:UNK:O    | 1:B:1132:UNK:N    | 2.04                     | 0.91              |
| 1:B:2219:VAL:O    | 1:B:2452:LYS:CG   | 2.19                     | 0.91              |
| 1:A:2245:GLN:NE2  | 1:B:2339:LYS:HE3  | 1.86                     | 0.91              |
| 1:B:2410:VAL:HG12 | 1:C:2425:ASP:OD2  | 1.70                     | 0.91              |
| 1:B:2409:GLN:CG   | 1:B:2411:GLY:N    | 2.35                     | 0.90              |
| 1:C:2011:LEU:O    | 1:C:2015:GLN:N    | 2.05                     | 0.90              |
| 1:C:2410:VAL:HG11 | 1:C:2426:PHE:CB   | 2.01                     | 0.90              |
| 1:B:211:UNK:C     | 1:B:277:UNK:CB    | 2.49                     | 0.90              |
| 1:A:1793:UNK:O    | 1:A:1797:UNK:CB   | 2.19                     | 0.89              |
| 1:B:2219:VAL:O    | 1:B:2452:LYS:CD   | 2.20                     | 0.89              |
| 1:A:2060:TRP:O    | 1:A:2063:PHE:N    | 2.05                     | 0.89              |
| 1:C:2409:GLN:CA   | 1:C:2410:VAL:CG1  | 2.45                     | 0.89              |
| 1:B:2011:LEU:O    | 1:B:2015:GLN:N    | 2.05                     | 0.89              |
| 1:A:2406:ARG:HG3  | 1:A:2406:ARG:HH21 | 1.36                     | 0.89              |
| 1:A:244:UNK:O     | 1:A:248:UNK:N     | 2.06                     | 0.89              |
| 1:A:2410:VAL:HG21 | 1:A:2426:PHE:CA   | 2.01                     | 0.89              |
| 1:B:2406:ARG:HH12 | 1:C:2299:PRO:CG   | 1.84                     | 0.88              |
| 1:C:2407:ARG:HG2  | 1:C:2428:GLU:HG2  | 1.55                     | 0.88              |
| 1:A:2382:PRO:HG2  | 1:C:2328:ALA:CB   | 2.02                     | 0.88              |
| 1:B:2409:GLN:HG3  | 1:B:2410:VAL:HG22 | 1.53                     | 0.88              |
| 1:C:201:UNK:HA    | 1:C:288:UNK:CB    | 2.02                     | 0.88              |
| 1:B:2495:GLU:O    | 1:B:2499:CYS:CB   | 2.22                     | 0.88              |
| 1:C:2495:GLU:O    | 1:C:2499:CYS:CB   | 2.22                     | 0.88              |
| 1:C:2409:GLN:HB2  | 1:C:2410:VAL:HG22 | 1.54                     | 0.88              |
| 1:A:2060:TRP:O    | 1:A:2063:PHE:CB   | 2.22                     | 0.87              |
| 1:B:241:UNK:N     | 1:B:248:UNK:HA    | 1.90                     | 0.87              |
| 1:A:2410:VAL:CG2  | 1:A:2426:PHE:HA   | 2.02                     | 0.87              |
| 1:B:2204:TRP:O    | 1:B:2208:LEU:CB   | 2.22                     | 0.87              |
| 1:B:1983:ALA:O    | 1:B:1987:ASP:N    | 2.05                     | 0.87              |
| 1:B:282:UNK:O     | 1:B:283:UNK:C     | 2.22                     | 0.87              |
| 1:C:1144:UNK:O    | 1:C:1146:UNK:N    | 2.07                     | 0.87              |
| 1:A:2495:GLU:O    | 1:A:2499:CYS:CB   | 2.22                     | 0.86              |
| 1:B:2406:ARG:HH12 | 1:C:2299:PRO:HG3  | 1.36                     | 0.86              |
| 1:C:2408:GLU:O    | 1:C:2410:VAL:HG13 | 1.73                     | 0.86              |
| 1:B:2084:PHE:O    | 1:B:2088:ILE:N    | 2.09                     | 0.86              |
| 1:B:2409:GLN:CA   | 1:B:2410:VAL:HG13 | 2.06                     | 0.86              |
| 1:A:294:UNK:C     | 1:A:447:UNK:H     | 1.89                     | 0.85              |
| 1:C:248:UNK:O     | 1:C:252:UNK:N     | 2.08                     | 0.85              |
| 1:A:2406:ARG:HH12 | 1:B:2299:PRO:CG   | 1.88                     | 0.85              |
| 1:C:1776:UNK:CB   | 1:C:1781:UNK:HA   | 2.07                     | 0.85              |
| 1:B:1776:UNK:CB   | 1:B:1781:UNK:HA   | 2.07                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2084:PHE:O   | 1:A:2088:ILE:N   | 2.09                     | 0.85              |
| 1:B:212:UNK:N    | 1:B:277:UNK:CB   | 2.40                     | 0.85              |
| 1:A:2429:TRP:CE3 | 1:B:2297:SER:HB3 | 2.10                     | 0.85              |
| 1:B:2429:TRP:CH2 | 1:C:2298:PRO:CD  | 2.58                     | 0.85              |
| 1:B:294:UNK:C    | 1:B:447:UNK:H    | 1.89                     | 0.85              |
| 1:C:295:UNK:O    | 1:C:447:UNK:N    | 2.10                     | 0.84              |
| 1:C:1753:UNK:O   | 1:C:1757:UNK:N   | 2.10                     | 0.84              |
| 1:A:2299:PRO:HD2 | 1:C:2429:TRP:CH2 | 2.11                     | 0.84              |
| 1:A:295:UNK:O    | 1:A:447:UNK:N    | 2.10                     | 0.84              |
| 1:A:2152:TRP:O   | 1:A:2156:GLU:N   | 2.10                     | 0.84              |
| 1:C:2152:TRP:O   | 1:C:2156:GLU:N   | 2.10                     | 0.84              |
| 1:A:1753:UNK:O   | 1:A:1757:UNK:N   | 2.10                     | 0.84              |
| 1:C:2084:PHE:O   | 1:C:2088:ILE:N   | 2.09                     | 0.84              |
| 1:A:2299:PRO:CD  | 1:C:2408:GLU:HG3 | 2.08                     | 0.84              |
| 1:B:295:UNK:C    | 1:B:447:UNK:N    | 2.35                     | 0.84              |
| 1:B:295:UNK:O    | 1:B:447:UNK:N    | 2.10                     | 0.84              |
| 1:C:294:UNK:C    | 1:C:447:UNK:H    | 1.89                     | 0.84              |
| 1:C:295:UNK:HA   | 1:C:447:UNK:H    | 1.42                     | 0.84              |
| 1:A:1776:UNK:CB  | 1:A:1781:UNK:HA  | 2.07                     | 0.84              |
| 1:B:2043:VAL:O   | 1:B:2047:LEU:N   | 2.10                     | 0.84              |
| 1:C:248:UNK:O    | 1:C:252:UNK:CB   | 2.26                     | 0.84              |
| 1:A:2217:VAL:O   | 1:A:2454:SER:CA  | 2.25                     | 0.84              |
| 1:C:2106:LEU:O   | 1:C:2110:LEU:N   | 2.10                     | 0.84              |
| 1:A:2106:LEU:O   | 1:A:2110:LEU:N   | 2.10                     | 0.83              |
| 1:B:1753:UNK:O   | 1:B:1757:UNK:N   | 2.10                     | 0.83              |
| 1:A:215:UNK:CB   | 1:A:273:UNK:C    | 2.56                     | 0.83              |
| 1:A:2153:MET:O   | 1:A:2157:ASP:N   | 2.11                     | 0.83              |
| 1:B:2152:TRP:O   | 1:B:2156:GLU:N   | 2.10                     | 0.83              |
| 1:B:2217:VAL:CB  | 1:B:2455:PRO:CD  | 2.55                     | 0.83              |
| 1:C:2153:MET:O   | 1:C:2157:ASP:N   | 2.11                     | 0.83              |
| 1:C:2409:GLN:HB2 | 1:C:2426:PHE:CE2 | 2.13                     | 0.83              |
| 1:B:1383:UNK:HA  | 1:B:1386:UNK:CB  | 2.09                     | 0.83              |
| 1:C:1383:UNK:HA  | 1:C:1386:UNK:CB  | 2.09                     | 0.83              |
| 1:A:241:UNK:HA   | 1:A:248:UNK:CB   | 2.09                     | 0.83              |
| 1:A:2050:GLN:CB  | 1:A:2051:VAL:HA  | 2.09                     | 0.83              |
| 1:A:1016:UNK:HA  | 1:A:1019:UNK:CB  | 2.09                     | 0.83              |
| 1:B:2106:LEU:O   | 1:B:2110:LEU:N   | 2.11                     | 0.82              |
| 1:A:1142:UNK:O   | 1:A:1144:UNK:N   | 2.13                     | 0.82              |
| 1:C:295:UNK:C    | 1:C:447:UNK:N    | 2.35                     | 0.82              |
| 1:C:2471:VAL:O   | 1:C:2475:LEU:CB  | 2.27                     | 0.82              |
| 1:A:295:UNK:C    | 1:A:447:UNK:N    | 2.35                     | 0.82              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:2298:PRO:HD2  | 1:C:2408:GLU:CG  | 2.10                     | 0.82              |
| 1:B:1016:UNK:HA   | 1:B:1019:UNK:CB  | 2.09                     | 0.82              |
| 1:A:1755:UNK:O    | 1:A:1759:UNK:N   | 2.13                     | 0.82              |
| 1:A:2409:GLN:HA   | 1:A:2410:VAL:CG2 | 2.09                     | 0.82              |
| 1:B:2471:VAL:O    | 1:B:2475:LEU:CB  | 2.27                     | 0.82              |
| 1:C:2050:GLN:CB   | 1:C:2051:VAL:HA  | 2.10                     | 0.82              |
| 1:A:2471:VAL:O    | 1:A:2475:LEU:CB  | 2.27                     | 0.82              |
| 1:B:2219:VAL:HG13 | 1:B:2220:VAL:H   | 1.45                     | 0.82              |
| 1:C:2410:VAL:HG11 | 1:C:2426:PHE:CG  | 2.14                     | 0.82              |
| 1:B:2153:MET:O    | 1:B:2157:ASP:N   | 2.11                     | 0.81              |
| 1:C:283:UNK:CB    | 1:C:1993:PHE:CB  | 2.58                     | 0.81              |
| 1:A:1383:UNK:HA   | 1:A:1386:UNK:CB  | 2.09                     | 0.81              |
| 1:B:1755:UNK:O    | 1:B:1759:UNK:N   | 2.13                     | 0.81              |
| 1:B:241:UNK:HA    | 1:B:248:UNK:CB   | 2.11                     | 0.81              |
| 1:B:295:UNK:CA    | 1:B:447:UNK:H    | 1.94                     | 0.81              |
| 1:C:1016:UNK:HA   | 1:C:1019:UNK:CB  | 2.09                     | 0.81              |
| 1:C:1755:UNK:O    | 1:C:1759:UNK:N   | 2.13                     | 0.81              |
| 1:C:1789:UNK:O    | 1:C:1793:UNK:N   | 2.13                     | 0.81              |
| 1:A:295:UNK:HA    | 1:A:447:UNK:H2   | 1.10                     | 0.81              |
| 1:A:295:UNK:HA    | 1:A:447:UNK:H    | 1.42                     | 0.80              |
| 1:B:295:UNK:HA    | 1:B:447:UNK:H2   | 1.10                     | 0.80              |
| 1:C:241:UNK:HA    | 1:C:248:UNK:CB   | 2.11                     | 0.80              |
| 1:C:2410:VAL:HG22 | 1:C:2426:PHE:CE2 | 2.16                     | 0.80              |
| 1:B:222:UNK:O     | 1:B:266:UNK:CB   | 2.29                     | 0.80              |
| 1:B:2429:TRP:CZ3  | 1:C:2297:SER:CB  | 2.62                     | 0.80              |
| 1:A:2044:LEU:O    | 1:A:2047:LEU:CB  | 2.30                     | 0.80              |
| 1:A:229:UNK:O     | 1:A:259:UNK:CB   | 2.30                     | 0.79              |
| 1:A:1506:UNK:O    | 1:A:1507:UNK:CB  | 2.29                     | 0.79              |
| 1:A:2470:TYR:O    | 1:A:2474:VAL:N   | 2.15                     | 0.79              |
| 1:B:2410:VAL:CA   | 1:C:2425:ASP:HB2 | 2.11                     | 0.79              |
| 1:A:2382:PRO:HG3  | 1:C:2328:ALA:CB  | 2.05                     | 0.79              |
| 1:B:233:UNK:O     | 1:B:255:UNK:CB   | 2.31                     | 0.79              |
| 1:A:265:UNK:CB    | 1:A:2528:LYS:CB  | 2.61                     | 0.79              |
| 1:A:2429:TRP:CH2  | 1:B:2299:PRO:HD2 | 2.17                     | 0.79              |
| 1:B:2203:ILE:C    | 1:B:2207:LEU:CB  | 2.55                     | 0.79              |
| 1:B:2408:GLU:N    | 1:B:2408:GLU:OE2 | 2.15                     | 0.79              |
| 1:C:1506:UNK:O    | 1:C:1507:UNK:CB  | 2.30                     | 0.79              |
| 1:C:295:UNK:CA    | 1:C:447:UNK:H    | 1.93                     | 0.78              |
| 1:C:1137:UNK:O    | 1:C:1138:UNK:C   | 2.30                     | 0.78              |
| 1:B:2041:LYS:O    | 1:B:2042:THR:C   | 2.24                     | 0.78              |
| 1:B:2409:GLN:HG2  | 1:B:2411:GLY:CA  | 2.12                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2426:PHE:O    | 1:B:2427:LEU:O    | 2.02                     | 0.78              |
| 1:B:265:UNK:CB    | 1:B:2528:LYS:CB   | 2.61                     | 0.78              |
| 1:B:1129:UNK:O    | 1:B:1132:UNK:CB   | 2.32                     | 0.78              |
| 1:B:1776:UNK:CA   | 1:B:1781:UNK:HA   | 2.14                     | 0.78              |
| 1:B:2058:HIS:C    | 1:B:2060:TRP:H    | 1.91                     | 0.78              |
| 1:C:265:UNK:CB    | 1:C:2528:LYS:CB   | 2.61                     | 0.78              |
| 1:B:2296:ILE:HD11 | 1:B:2300:SER:O    | 1.84                     | 0.78              |
| 1:C:1765:UNK:O    | 1:C:1769:UNK:N    | 2.16                     | 0.78              |
| 1:C:2409:GLN:HB2  | 1:C:2426:PHE:HE2  | 1.47                     | 0.78              |
| 1:C:1776:UNK:CA   | 1:C:1781:UNK:HA   | 2.14                     | 0.78              |
| 1:A:1765:UNK:O    | 1:A:1769:UNK:N    | 2.17                     | 0.78              |
| 1:A:2339:LYS:CE   | 1:C:2245:GLN:NE2  | 2.44                     | 0.78              |
| 1:A:2408:GLU:O    | 1:A:2410:VAL:HG22 | 1.83                     | 0.78              |
| 1:A:222:UNK:CB    | 1:A:266:UNK:CB    | 2.62                     | 0.78              |
| 1:B:2293:LEU:H    | 1:C:2295:ARG:HB2  | 1.49                     | 0.78              |
| 1:C:2407:ARG:CG   | 1:C:2428:GLU:HG2  | 2.15                     | 0.77              |
| 1:C:2409:GLN:C    | 1:C:2410:VAL:HG13 | 2.05                     | 0.77              |
| 1:B:1765:UNK:O    | 1:B:1769:UNK:N    | 2.16                     | 0.77              |
| 1:C:2003:ALA:CB   | 1:C:2102:PRO:HA   | 2.14                     | 0.77              |
| 1:A:2003:ALA:CB   | 1:A:2102:PRO:HA   | 2.14                     | 0.77              |
| 1:B:2409:GLN:HA   | 1:B:2410:VAL:CG1  | 2.09                     | 0.77              |
| 1:B:2470:TYR:O    | 1:B:2474:VAL:N    | 2.15                     | 0.77              |
| 1:B:1747:UNK:O    | 1:B:1751:UNK:N    | 2.19                     | 0.76              |
| 1:B:2219:VAL:HG22 | 1:B:2220:VAL:N    | 1.99                     | 0.76              |
| 1:B:2003:ALA:CB   | 1:B:2102:PRO:HA   | 2.14                     | 0.76              |
| 1:A:2409:GLN:HG3  | 1:A:2410:VAL:O    | 1.86                     | 0.76              |
| 1:A:2426:PHE:O    | 1:A:2428:GLU:HG3  | 1.86                     | 0.76              |
| 1:A:1776:UNK:CA   | 1:A:1781:UNK:HA   | 2.14                     | 0.76              |
| 1:B:1506:UNK:O    | 1:B:1507:UNK:CB   | 2.33                     | 0.76              |
| 1:C:1747:UNK:O    | 1:C:1750:UNK:N    | 2.19                     | 0.76              |
| 1:B:222:UNK:CB    | 1:B:266:UNK:CB    | 2.64                     | 0.76              |
| 1:B:2406:ARG:NH2  | 1:C:2299:PRO:HG3  | 1.99                     | 0.76              |
| 1:C:2237:PRO:O    | 1:C:2295:ARG:NH1  | 2.20                     | 0.76              |
| 1:B:1747:UNK:O    | 1:B:1750:UNK:N    | 2.19                     | 0.75              |
| 1:A:2407:ARG:HD2  | 1:A:2428:GLU:OE2  | 1.85                     | 0.75              |
| 1:B:2429:TRP:CE2  | 1:C:2297:SER:HB3  | 2.21                     | 0.75              |
| 1:A:1992:ILE:O    | 1:A:1994:GLY:N    | 2.19                     | 0.75              |
| 1:A:2407:ARG:HG3  | 1:A:2428:GLU:CG   | 2.16                     | 0.75              |
| 1:B:1137:UNK:O    | 1:B:1141:UNK:N    | 2.20                     | 0.75              |
| 1:A:1747:UNK:O    | 1:A:1751:UNK:N    | 2.19                     | 0.75              |
| 1:A:2237:PRO:O    | 1:A:2295:ARG:NH1  | 2.20                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2429:TRP:CZ2  | 1:B:2297:SER:HB2  | 2.22                     | 0.75              |
| 1:A:2512:LEU:N    | 1:B:2491:SER:CB   | 2.49                     | 0.75              |
| 1:B:2328:ALA:HB2  | 1:C:2382:PRO:CG   | 2.17                     | 0.75              |
| 1:C:1747:UNK:O    | 1:C:1751:UNK:N    | 2.19                     | 0.75              |
| 1:B:2298:PRO:O    | 1:B:2301:ARG:HB3  | 1.86                     | 0.75              |
| 1:C:2470:TYR:O    | 1:C:2474:VAL:N    | 2.14                     | 0.75              |
| 1:A:2408:GLU:HB2  | 1:B:2298:PRO:HG2  | 1.69                     | 0.74              |
| 1:C:1509:UNK:O    | 1:C:1510:UNK:C    | 2.34                     | 0.74              |
| 1:A:1747:UNK:O    | 1:A:1750:UNK:N    | 2.19                     | 0.74              |
| 1:A:2425:ASP:C    | 1:A:2426:PHE:HD1  | 1.94                     | 0.74              |
| 1:B:2299:PRO:HA   | 1:B:2302:ALA:HB3  | 1.69                     | 0.74              |
| 1:C:1144:UNK:O    | 1:C:1145:UNK:C    | 2.35                     | 0.74              |
| 1:A:2295:ARG:O    | 1:C:2293:LEU:HG   | 1.87                     | 0.74              |
| 1:A:2299:PRO:HD3  | 1:C:2408:GLU:HG3  | 1.67                     | 0.74              |
| 1:C:1133:UNK:O    | 1:C:1136:UNK:CB   | 2.36                     | 0.74              |
| 1:B:241:UNK:HA    | 1:B:248:UNK:CA    | 2.18                     | 0.74              |
| 1:B:2237:PRO:O    | 1:B:2295:ARG:NH1  | 2.20                     | 0.74              |
| 1:A:245:UNK:O     | 1:A:249:UNK:N     | 2.20                     | 0.74              |
| 1:C:233:UNK:CB    | 1:C:255:UNK:O     | 2.36                     | 0.74              |
| 1:A:204:UNK:CB    | 1:A:284:UNK:CB    | 2.65                     | 0.74              |
| 1:B:2219:VAL:HG22 | 1:B:2220:VAL:HG23 | 1.68                     | 0.74              |
| 1:C:2410:VAL:CG1  | 1:C:2426:PHE:HA   | 2.18                     | 0.74              |
| 1:B:2217:VAL:CB   | 1:B:2454:SER:HB2  | 2.13                     | 0.73              |
| 1:A:211:UNK:O     | 1:A:277:UNK:CB    | 2.36                     | 0.73              |
| 1:A:2491:SER:CB   | 1:C:2512:LEU:H    | 2.02                     | 0.73              |
| 1:C:2077:ALA:HA   | 1:C:2083:TYR:CB   | 2.18                     | 0.73              |
| 1:A:2409:GLN:HE21 | 1:A:2410:VAL:C    | 1.97                     | 0.73              |
| 1:B:1130:UNK:C    | 1:B:1132:UNK:N    | 2.48                     | 0.73              |
| 1:B:2424:SER:OG   | 1:B:2425:ASP:N    | 2.20                     | 0.73              |
| 1:A:1792:UNK:O    | 1:A:1793:UNK:C    | 2.37                     | 0.73              |
| 1:A:2339:LYS:CE   | 1:C:2245:GLN:HE22 | 2.01                     | 0.73              |
| 1:A:2408:GLU:HG3  | 1:A:2429:TRP:CZ3  | 2.24                     | 0.73              |
| 1:A:2077:ALA:HA   | 1:A:2083:TYR:CB   | 2.18                     | 0.73              |
| 1:C:246:UNK:C     | 1:C:248:UNK:H     | 2.00                     | 0.73              |
| 1:A:2426:PHE:O    | 1:A:2427:LEU:C    | 2.32                     | 0.73              |
| 1:A:1142:UNK:O    | 1:A:1143:UNK:C    | 2.37                     | 0.73              |
| 1:B:2077:ALA:HA   | 1:B:2083:TYR:CB   | 2.18                     | 0.73              |
| 1:C:2406:ARG:NH1  | 1:C:2408:GLU:OE2  | 2.22                     | 0.72              |
| 1:A:230:UNK:CA    | 1:A:259:UNK:CB    | 2.66                     | 0.72              |
| 1:B:204:UNK:CB    | 1:B:284:UNK:CB    | 2.67                     | 0.72              |
| 1:A:1142:UNK:O    | 1:A:1145:UNK:N    | 2.22                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:2491:SER:O    | 1:C:2512:LEU:CB  | 2.37                     | 0.72              |
| 1:A:2217:VAL:C    | 1:A:2454:SER:HB2 | 2.14                     | 0.72              |
| 1:A:2297:SER:HB2  | 1:C:2429:TRP:CZ2 | 2.25                     | 0.72              |
| 1:B:2410:VAL:N    | 1:C:2425:ASP:HB2 | 2.03                     | 0.72              |
| 1:B:2429:TRP:HZ3  | 1:C:2298:PRO:HD3 | 1.55                     | 0.72              |
| 1:B:2429:TRP:HH2  | 1:C:2299:PRO:CD  | 1.97                     | 0.72              |
| 1:B:2203:ILE:C    | 1:B:2207:LEU:H   | 1.96                     | 0.72              |
| 1:B:2429:TRP:HH2  | 1:C:2298:PRO:HD2 | 1.49                     | 0.72              |
| 1:C:295:UNK:HA    | 1:C:447:UNK:H2   | 1.10                     | 0.72              |
| 1:C:1772:UNK:O    | 1:C:1776:UNK:N   | 2.23                     | 0.72              |
| 1:C:1792:UNK:O    | 1:C:1796:UNK:N   | 2.21                     | 0.72              |
| 1:B:1772:UNK:O    | 1:B:1776:UNK:N   | 2.23                     | 0.71              |
| 1:C:234:UNK:O     | 1:C:237:UNK:CB   | 2.38                     | 0.71              |
| 1:A:1772:UNK:O    | 1:A:1776:UNK:N   | 2.23                     | 0.71              |
| 1:A:2299:PRO:HG3  | 1:C:2406:ARG:NH1 | 2.05                     | 0.71              |
| 1:C:2084:PHE:HA   | 1:C:2087:CYS:CB  | 2.20                     | 0.71              |
| 1:B:2298:PRO:O    | 1:B:2302:ALA:N   | 2.23                     | 0.71              |
| 1:C:1144:UNK:O    | 1:C:1147:UNK:N   | 2.22                     | 0.71              |
| 1:B:2202:ILE:O    | 1:B:2206:PRO:CB  | 2.38                     | 0.71              |
| 1:B:2406:ARG:NH1  | 1:C:2299:PRO:HD3 | 2.06                     | 0.71              |
| 1:C:1753:UNK:HA   | 1:C:1756:UNK:CB  | 2.21                     | 0.71              |
| 1:C:2408:GLU:HG2  | 1:C:2429:TRP:CZ3 | 2.25                     | 0.71              |
| 1:A:2084:PHE:HA   | 1:A:2087:CYS:CB  | 2.21                     | 0.71              |
| 1:A:2051:VAL:O    | 1:A:2056:ALA:HA  | 1.90                     | 0.71              |
| 1:A:2406:ARG:HH12 | 1:B:2299:PRO:CD  | 2.03                     | 0.71              |
| 1:A:294:UNK:C     | 1:A:447:UNK:N    | 2.54                     | 0.71              |
| 1:A:1753:UNK:HA   | 1:A:1756:UNK:CB  | 2.21                     | 0.71              |
| 1:B:1753:UNK:HA   | 1:B:1756:UNK:CB  | 2.21                     | 0.71              |
| 1:B:2347:ASN:O    | 1:B:2352:ARG:NH2 | 2.24                     | 0.71              |
| 1:B:2084:PHE:HA   | 1:B:2087:CYS:CB  | 2.21                     | 0.70              |
| 1:B:2406:ARG:NH1  | 1:C:2299:PRO:CD  | 2.54                     | 0.70              |
| 1:B:1509:UNK:O    | 1:B:1510:UNK:C   | 2.38                     | 0.70              |
| 1:C:2052:VAL:O    | 1:C:2056:ALA:N   | 2.24                     | 0.70              |
| 1:B:2407:ARG:NH2  | 1:B:2424:SER:O   | 2.24                     | 0.70              |
| 1:A:1773:UNK:O    | 1:A:1777:UNK:N   | 2.25                     | 0.70              |
| 1:B:1773:UNK:O    | 1:B:1777:UNK:N   | 2.25                     | 0.70              |
| 1:C:2347:ASN:O    | 1:C:2352:ARG:NH2 | 2.24                     | 0.70              |
| 1:C:2410:VAL:HG11 | 1:C:2426:PHE:CD2 | 2.26                     | 0.70              |
| 1:A:2298:PRO:HG2  | 1:C:2408:GLU:CB  | 2.22                     | 0.70              |
| 1:A:2537:GLU:O    | 1:A:2541:LYS:N   | 2.25                     | 0.70              |
| 1:B:2293:LEU:HG   | 1:C:2295:ARG:C   | 2.17                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2339:LYS:NZ   | 1:C:2245:GLN:HE22 | 1.88                     | 0.70              |
| 1:B:2410:VAL:CG1  | 1:B:2426:PHE:HB3  | 2.21                     | 0.70              |
| 1:A:2347:ASN:O    | 1:A:2352:ARG:NH2  | 2.24                     | 0.70              |
| 1:B:294:UNK:C     | 1:B:447:UNK:N     | 2.54                     | 0.70              |
| 1:C:1773:UNK:O    | 1:C:1777:UNK:N    | 2.25                     | 0.70              |
| 1:A:2408:GLU:HG3  | 1:B:2298:PRO:HG2  | 1.73                     | 0.69              |
| 1:B:215:UNK:CB    | 1:B:274:UNK:N     | 2.55                     | 0.69              |
| 1:B:295:UNK:HA    | 1:B:447:UNK:H     | 1.42                     | 0.69              |
| 1:B:2409:GLN:HG3  | 1:B:2411:GLY:N    | 2.04                     | 0.69              |
| 1:C:294:UNK:C     | 1:C:447:UNK:N     | 2.54                     | 0.69              |
| 1:B:2328:ALA:HB2  | 1:C:2382:PRO:HG3  | 1.73                     | 0.69              |
| 1:C:1990:ILE:O    | 1:C:1992:ILE:N    | 2.25                     | 0.69              |
| 1:C:2041:LYS:O    | 1:C:2042:THR:C    | 2.36                     | 0.69              |
| 1:B:2409:GLN:HG2  | 1:B:2411:GLY:HA3  | 1.73                     | 0.69              |
| 1:A:2429:TRP:CH2  | 1:B:2297:SER:HB2  | 2.28                     | 0.69              |
| 1:B:2408:GLU:HB2  | 1:C:2298:PRO:HG2  | 1.73                     | 0.69              |
| 1:B:2537:GLU:O    | 1:B:2541:LYS:N    | 2.25                     | 0.69              |
| 1:C:1994:GLY:O    | 1:C:1995:PHE:C    | 2.34                     | 0.69              |
| 1:A:2328:ALA:CB   | 1:B:2382:PRO:HG3  | 2.19                     | 0.68              |
| 1:B:2426:PHE:O    | 1:B:2427:LEU:C    | 2.35                     | 0.68              |
| 1:C:2202:ILE:O    | 1:C:2206:PRO:CB   | 2.41                     | 0.68              |
| 1:C:2408:GLU:C    | 1:C:2410:VAL:HG13 | 2.18                     | 0.68              |
| 1:A:2299:PRO:HD2  | 1:C:2408:GLU:HG3  | 1.75                     | 0.68              |
| 1:A:2429:TRP:CE2  | 1:B:2297:SER:HB3  | 2.29                     | 0.68              |
| 1:C:1509:UNK:O    | 1:C:1512:UNK:N    | 2.27                     | 0.68              |
| 1:A:2202:ILE:O    | 1:A:2206:PRO:CB   | 2.41                     | 0.68              |
| 1:B:2409:GLN:CG   | 1:B:2410:VAL:HG22 | 2.22                     | 0.68              |
| 1:B:2429:TRP:CZ2  | 1:C:2299:PRO:HD2  | 2.27                     | 0.68              |
| 1:C:2410:VAL:HG23 | 1:C:2426:PHE:CE2  | 2.16                     | 0.68              |
| 1:A:2406:ARG:HG3  | 1:A:2406:ARG:NH2  | 2.08                     | 0.68              |
| 1:B:1743:UNK:O    | 1:B:1747:UNK:N    | 2.27                     | 0.67              |
| 1:B:2410:VAL:HA   | 1:C:2425:ASP:HB2  | 1.75                     | 0.67              |
| 1:B:2119:LEU:O    | 1:B:2126:ARG:CB   | 2.43                     | 0.67              |
| 1:C:1743:UNK:O    | 1:C:1747:UNK:N    | 2.27                     | 0.67              |
| 1:A:2513:VAL:N    | 1:B:2491:SER:CB   | 2.57                     | 0.67              |
| 1:C:2119:LEU:O    | 1:C:2126:ARG:CB   | 2.43                     | 0.67              |
| 1:C:2407:ARG:HD2  | 1:C:2428:GLU:OE2  | 1.94                     | 0.67              |
| 1:B:2429:TRP:CZ3  | 1:C:2298:PRO:HD3  | 2.29                     | 0.67              |
| 1:B:2429:TRP:CD2  | 1:C:2297:SER:HB3  | 2.29                     | 0.67              |
| 1:C:2408:GLU:O    | 1:C:2426:PHE:HB3  | 1.94                     | 0.67              |
| 1:C:2501:ASP:O    | 1:C:2505:LYS:N    | 2.28                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1743:UNK:O    | 1:A:1747:UNK:N    | 2.27                     | 0.67              |
| 1:B:2410:VAL:H    | 1:C:2425:ASP:HB2  | 1.59                     | 0.67              |
| 1:C:2471:VAL:O    | 1:C:2475:LEU:N    | 2.28                     | 0.67              |
| 1:A:2236:GLU:OE2  | 1:C:2291:GLY:CA   | 2.42                     | 0.66              |
| 1:A:2060:TRP:O    | 1:A:2061:MET:C    | 2.38                     | 0.66              |
| 1:A:2119:LEU:O    | 1:A:2126:ARG:CB   | 2.43                     | 0.66              |
| 1:A:2339:LYS:HE3  | 1:C:2245:GLN:HE22 | 1.55                     | 0.66              |
| 1:B:215:UNK:CB    | 1:B:274:UNK:HA    | 2.26                     | 0.66              |
| 1:B:1133:UNK:O    | 1:B:1137:UNK:N    | 2.29                     | 0.66              |
| 1:B:236:UNK:C     | 1:B:252:UNK:HA    | 2.25                     | 0.66              |
| 1:C:2409:GLN:HA   | 1:C:2426:PHE:CD2  | 2.31                     | 0.66              |
| 1:B:2471:VAL:O    | 1:B:2475:LEU:N    | 2.28                     | 0.66              |
| 1:B:2057:ILE:O    | 1:B:2060:TRP:CB   | 2.43                     | 0.66              |
| 1:C:2410:VAL:HG11 | 1:C:2426:PHE:HB3  | 1.76                     | 0.66              |
| 1:B:1509:UNK:O    | 1:B:1512:UNK:N    | 2.29                     | 0.66              |
| 1:B:2410:VAL:HG22 | 1:B:2426:PHE:CD1  | 2.31                     | 0.66              |
| 1:A:1769:UNK:O    | 1:A:1773:UNK:N    | 2.30                     | 0.65              |
| 1:A:2299:PRO:CD   | 1:C:2429:TRP:HH2  | 2.05                     | 0.65              |
| 1:A:2471:VAL:O    | 1:A:2475:LEU:N    | 2.28                     | 0.65              |
| 1:C:1509:UNK:C    | 1:C:1511:UNK:N    | 2.59                     | 0.65              |
| 1:C:1994:GLY:O    | 1:C:1997:ALA:N    | 2.29                     | 0.65              |
| 1:C:1769:UNK:O    | 1:C:1773:UNK:N    | 2.29                     | 0.65              |
| 1:B:1769:UNK:O    | 1:B:1773:UNK:N    | 2.29                     | 0.65              |
| 1:B:2219:VAL:HG13 | 1:B:2220:VAL:N    | 2.10                     | 0.65              |
| 1:B:2058:HIS:O    | 1:B:2060:TRP:N    | 2.30                     | 0.65              |
| 1:B:2123:GLN:O    | 1:B:2127:LEU:N    | 2.28                     | 0.65              |
| 1:A:2024:LEU:O    | 1:A:2025:LEU:C    | 2.40                     | 0.65              |
| 1:B:2409:GLN:NE2  | 1:B:2426:PHE:CZ   | 2.65                     | 0.65              |
| 1:A:1792:UNK:O    | 1:A:1796:UNK:N    | 2.30                     | 0.64              |
| 1:B:1776:UNK:HA   | 1:B:1781:UNK:HA   | 1.79                     | 0.64              |
| 1:B:2024:LEU:O    | 1:B:2025:LEU:C    | 2.40                     | 0.64              |
| 1:B:2293:LEU:CD1  | 1:C:2295:ARG:HA   | 2.28                     | 0.64              |
| 1:B:2501:ASP:O    | 1:B:2505:LYS:N    | 2.28                     | 0.64              |
| 1:C:2052:VAL:HA   | 1:C:2056:ALA:CB   | 2.26                     | 0.64              |
| 1:C:2537:GLU:O    | 1:C:2541:LYS:N    | 2.25                     | 0.64              |
| 1:C:2024:LEU:O    | 1:C:2025:LEU:C    | 2.40                     | 0.64              |
| 1:A:233:UNK:CB    | 1:A:255:UNK:C     | 2.74                     | 0.64              |
| 1:A:1776:UNK:HA   | 1:A:1781:UNK:HA   | 1.79                     | 0.64              |
| 1:B:2410:VAL:HA   | 1:C:2425:ASP:CB   | 2.27                     | 0.64              |
| 1:B:2429:TRP:CD2  | 1:C:2297:SER:CB   | 2.80                     | 0.64              |
| 1:C:2408:GLU:HG2  | 1:C:2429:TRP:HH2  | 1.57                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:2205:PHE:O   | 1:B:2209:PHE:CB  | 2.45                     | 0.64              |
| 1:A:567:UNK:O    | 1:A:570:UNK:CB   | 2.46                     | 0.64              |
| 1:A:2501:ASP:O   | 1:A:2505:LYS:N   | 2.28                     | 0.64              |
| 1:B:2024:LEU:O   | 1:B:2025:LEU:O   | 2.16                     | 0.64              |
| 1:A:2406:ARG:NH1 | 1:B:2299:PRO:HD3 | 2.13                     | 0.64              |
| 1:B:2299:PRO:C   | 1:B:2301:ARG:N   | 2.52                     | 0.64              |
| 1:B:1509:UNK:C   | 1:B:1511:UNK:N   | 2.60                     | 0.64              |
| 1:C:567:UNK:O    | 1:C:570:UNK:CB   | 2.46                     | 0.64              |
| 1:C:2408:GLU:C   | 1:C:2426:PHE:HD2 | 2.06                     | 0.64              |
| 1:A:2024:LEU:O   | 1:A:2025:LEU:O   | 2.16                     | 0.63              |
| 1:C:2024:LEU:O   | 1:C:2025:LEU:O   | 2.16                     | 0.63              |
| 1:C:2495:GLU:O   | 1:C:2499:CYS:N   | 2.31                     | 0.63              |
| 1:A:2123:GLN:O   | 1:A:2127:LEU:N   | 2.27                     | 0.63              |
| 1:C:1994:GLY:C   | 1:C:1996:TRP:N   | 2.54                     | 0.63              |
| 1:B:2495:GLU:O   | 1:B:2499:CYS:N   | 2.31                     | 0.63              |
| 1:A:245:UNK:O    | 1:A:248:UNK:N    | 2.32                     | 0.63              |
| 1:B:567:UNK:O    | 1:B:570:UNK:CB   | 2.46                     | 0.63              |
| 1:C:237:UNK:HA   | 1:C:252:UNK:HA   | 1.80                     | 0.63              |
| 1:C:2123:GLN:O   | 1:C:2127:LEU:N   | 2.28                     | 0.63              |
| 1:A:2217:VAL:O   | 1:A:2454:SER:HA  | 1.99                     | 0.63              |
| 1:A:2424:SER:OG  | 1:C:2411:GLY:O   | 2.15                     | 0.63              |
| 1:B:2429:TRP:CH2 | 1:C:2299:PRO:CD  | 2.69                     | 0.63              |
| 1:A:1131:UNK:HA  | 1:A:1134:UNK:CB  | 2.29                     | 0.63              |
| 1:A:1749:UNK:O   | 1:A:1753:UNK:N   | 2.32                     | 0.63              |
| 1:B:2520:GLU:O   | 1:B:2523:GLU:CB  | 2.47                     | 0.63              |
| 1:C:1749:UNK:O   | 1:C:1753:UNK:N   | 2.32                     | 0.63              |
| 1:C:2519:LEU:O   | 1:C:2522:GLU:N   | 2.30                     | 0.62              |
| 1:A:230:UNK:N    | 1:A:259:UNK:CB   | 2.61                     | 0.62              |
| 1:C:2520:GLU:O   | 1:C:2523:GLU:CB  | 2.47                     | 0.62              |
| 1:A:2293:LEU:HG  | 1:B:2295:ARG:C   | 2.22                     | 0.62              |
| 1:A:2298:PRO:HD2 | 1:C:2408:GLU:CB  | 2.28                     | 0.62              |
| 1:B:2519:LEU:O   | 1:B:2522:GLU:N   | 2.30                     | 0.62              |
| 1:C:219:UNK:CB   | 1:C:270:UNK:CA   | 2.75                     | 0.62              |
| 1:C:1776:UNK:HA  | 1:C:1781:UNK:HA  | 1.79                     | 0.62              |
| 1:C:2083:TYR:O   | 1:C:2087:CYS:N   | 2.31                     | 0.62              |
| 1:C:1770:UNK:O   | 1:C:1774:UNK:N   | 2.33                     | 0.62              |
| 1:A:238:UNK:HA   | 1:A:241:UNK:CB   | 2.30                     | 0.62              |
| 1:A:1770:UNK:O   | 1:A:1774:UNK:N   | 2.33                     | 0.62              |
| 1:A:2298:PRO:HG2 | 1:C:2408:GLU:HB3 | 1.80                     | 0.62              |
| 1:A:2520:GLU:O   | 1:A:2523:GLU:CB  | 2.47                     | 0.62              |
| 1:B:1749:UNK:O   | 1:B:1753:UNK:N   | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2060:TRP:O    | 1:C:2063:PHE:N    | 2.32                     | 0.62              |
| 1:B:237:UNK:N     | 1:B:252:UNK:HA    | 2.15                     | 0.62              |
| 1:A:2083:TYR:O    | 1:A:2087:CYS:N    | 2.31                     | 0.61              |
| 1:A:2407:ARG:HG2  | 1:A:2426:PHE:CB   | 2.15                     | 0.61              |
| 1:B:1770:UNK:O    | 1:B:1774:UNK:N    | 2.33                     | 0.61              |
| 1:B:2058:HIS:C    | 1:B:2060:TRP:N    | 2.53                     | 0.61              |
| 1:B:2299:PRO:HG2  | 1:B:2300:SER:H    | 1.64                     | 0.61              |
| 1:C:201:UNK:CA    | 1:C:288:UNK:CB    | 2.78                     | 0.61              |
| 1:C:2051:VAL:O    | 1:C:2056:ALA:HA   | 2.00                     | 0.61              |
| 1:A:2245:GLN:HE22 | 1:B:2339:LYS:HE3  | 1.61                     | 0.61              |
| 1:B:2209:PHE:C    | 1:B:2211:SER:H    | 2.08                     | 0.61              |
| 1:B:2517:ARG:O    | 1:B:2520:GLU:CB   | 2.48                     | 0.61              |
| 1:A:2517:ARG:O    | 1:A:2520:GLU:CB   | 2.48                     | 0.61              |
| 1:B:2409:GLN:HA   | 1:B:2426:PHE:HB3  | 1.83                     | 0.61              |
| 1:A:1129:UNK:O    | 1:A:1132:UNK:CB   | 2.49                     | 0.61              |
| 1:A:2519:LEU:O    | 1:A:2522:GLU:N    | 2.30                     | 0.61              |
| 1:A:2408:GLU:CB   | 1:B:2298:PRO:HG2  | 2.30                     | 0.61              |
| 1:A:2217:VAL:CB   | 1:A:2455:PRO:HD2  | 2.31                     | 0.60              |
| 1:B:241:UNK:CA    | 1:B:248:UNK:HA    | 2.31                     | 0.60              |
| 1:C:2517:ARG:O    | 1:C:2520:GLU:CB   | 2.48                     | 0.60              |
| 1:A:2429:TRP:CZ2  | 1:B:2297:SER:CB   | 2.84                     | 0.60              |
| 1:B:2059:ILE:O    | 1:B:2063:PHE:CB   | 2.48                     | 0.60              |
| 1:B:2222:GLN:OE1  | 1:B:2282:VAL:HG13 | 2.02                     | 0.60              |
| 1:A:2297:SER:CB   | 1:C:2429:TRP:CZ2  | 2.84                     | 0.60              |
| 1:B:2409:GLN:HG3  | 1:B:2410:VAL:HG23 | 1.80                     | 0.60              |
| 1:C:2153:MET:O    | 1:C:2156:GLU:N    | 2.35                     | 0.60              |
| 1:C:1794:UNK:O    | 1:C:1798:UNK:N    | 2.35                     | 0.60              |
| 1:B:2041:LYS:C    | 1:B:2043:VAL:N    | 2.59                     | 0.60              |
| 1:B:2153:MET:O    | 1:B:2156:GLU:N    | 2.35                     | 0.60              |
| 1:C:1799:UNK:O    | 1:C:1800:UNK:C    | 2.49                     | 0.60              |
| 1:A:1015:UNK:O    | 1:A:1019:UNK:N    | 2.35                     | 0.60              |
| 1:A:2222:GLN:OE1  | 1:A:2282:VAL:HG13 | 2.01                     | 0.60              |
| 1:A:2407:ARG:HE   | 1:A:2426:PHE:H    | 1.49                     | 0.60              |
| 1:A:2429:TRP:CH2  | 1:B:2299:PRO:CD   | 2.85                     | 0.60              |
| 1:A:1382:UNK:O    | 1:A:1386:UNK:N    | 2.35                     | 0.59              |
| 1:A:2328:ALA:CB   | 1:B:2382:PRO:CG   | 2.61                     | 0.59              |
| 1:B:1141:UNK:O    | 1:B:1145:UNK:CB   | 2.49                     | 0.59              |
| 1:A:2328:ALA:CB   | 1:B:2382:PRO:HG2  | 2.20                     | 0.59              |
| 1:A:2429:TRP:CH2  | 1:B:2297:SER:CB   | 2.85                     | 0.59              |
| 1:C:2222:GLN:OE1  | 1:C:2282:VAL:HG13 | 2.02                     | 0.59              |
| 1:A:2406:ARG:CZ   | 1:A:2429:TRP:CZ2  | 2.85                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:2408:GLU:C    | 1:A:2426:PHE:HB3 | 2.28                     | 0.59              |
| 1:A:2429:TRP:CE2  | 1:B:2297:SER:CB  | 2.85                     | 0.59              |
| 1:B:1974:THR:O    | 1:B:1976:VAL:N   | 2.28                     | 0.59              |
| 1:A:2153:MET:O    | 1:A:2156:GLU:N   | 2.35                     | 0.59              |
| 1:B:204:UNK:CB    | 1:B:284:UNK:C    | 2.80                     | 0.59              |
| 1:C:1015:UNK:O    | 1:C:1019:UNK:N   | 2.35                     | 0.59              |
| 1:C:2410:VAL:CG1  | 1:C:2426:PHE:CG  | 2.86                     | 0.59              |
| 1:A:294:UNK:O     | 1:A:447:UNK:N    | 2.36                     | 0.59              |
| 1:A:2495:GLU:O    | 1:A:2499:CYS:N   | 2.31                     | 0.59              |
| 1:B:1382:UNK:O    | 1:B:1386:UNK:N   | 2.35                     | 0.59              |
| 1:B:2219:VAL:HG22 | 1:B:2220:VAL:H   | 1.66                     | 0.59              |
| 1:B:2505:LYS:HA   | 1:B:2508:GLN:CB  | 2.33                     | 0.59              |
| 1:C:2410:VAL:CG1  | 1:C:2426:PHE:CD2 | 2.86                     | 0.59              |
| 1:A:250:UNK:C     | 1:A:252:UNK:N    | 2.63                     | 0.59              |
| 1:C:2410:VAL:CG2  | 1:C:2426:PHE:CE1 | 2.86                     | 0.59              |
| 1:C:2410:VAL:CB   | 1:C:2426:PHE:CG  | 2.85                     | 0.59              |
| 1:C:2410:VAL:HG11 | 1:C:2426:PHE:CA  | 2.33                     | 0.59              |
| 1:A:2512:LEU:H    | 1:B:2491:SER:CB  | 2.15                     | 0.59              |
| 1:B:1015:UNK:O    | 1:B:1019:UNK:N   | 2.35                     | 0.59              |
| 1:C:2505:LYS:HA   | 1:C:2508:GLN:CB  | 2.33                     | 0.59              |
| 1:A:2491:SER:CB   | 1:C:2512:LEU:N   | 2.67                     | 0.58              |
| 1:A:1131:UNK:O    | 1:A:1134:UNK:CB  | 2.51                     | 0.58              |
| 1:A:2298:PRO:CD   | 1:C:2408:GLU:HB2 | 2.34                     | 0.58              |
| 1:B:259:UNK:O     | 1:B:260:UNK:C    | 2.51                     | 0.58              |
| 1:B:268:UNK:O     | 1:B:269:UNK:C    | 2.52                     | 0.58              |
| 1:B:1974:THR:C    | 1:B:1976:VAL:H   | 2.11                     | 0.58              |
| 1:C:1130:UNK:O    | 1:C:1131:UNK:C   | 2.51                     | 0.58              |
| 1:C:2409:GLN:OE1  | 1:C:2410:VAL:O   | 2.18                     | 0.58              |
| 1:C:2470:TYR:O    | 1:C:2474:VAL:CB  | 2.52                     | 0.58              |
| 1:A:1127:UNK:O    | 1:A:1128:UNK:C   | 2.51                     | 0.58              |
| 1:A:1144:UNK:O    | 1:A:1145:UNK:C   | 2.51                     | 0.58              |
| 1:A:1381:UNK:O    | 1:A:1382:UNK:C   | 2.52                     | 0.58              |
| 1:B:294:UNK:O     | 1:B:447:UNK:N    | 2.36                     | 0.58              |
| 1:B:2410:VAL:CA   | 1:C:2425:ASP:CB  | 2.81                     | 0.58              |
| 1:B:2457:SER:O    | 1:B:2458:LEU:CB  | 2.51                     | 0.58              |
| 1:B:2470:TYR:O    | 1:B:2474:VAL:CB  | 2.51                     | 0.58              |
| 1:C:1381:UNK:O    | 1:C:1382:UNK:C   | 2.52                     | 0.58              |
| 1:C:1501:UNK:O    | 1:C:1502:UNK:C   | 2.51                     | 0.58              |
| 1:A:201:UNK:CB    | 1:A:288:UNK:CB   | 2.82                     | 0.58              |
| 1:A:281:UNK:O     | 1:A:282:UNK:C    | 2.51                     | 0.58              |
| 1:A:1974:THR:C    | 1:A:1976:VAL:H   | 2.11                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:2296:ILE:CG1 | 1:B:2300:SER:HB3 | 2.34                     | 0.58              |
| 1:C:267:UNK:O    | 1:C:268:UNK:C    | 2.51                     | 0.58              |
| 1:C:277:UNK:O    | 1:C:278:UNK:C    | 2.52                     | 0.58              |
| 1:C:294:UNK:O    | 1:C:447:UNK:N    | 2.36                     | 0.58              |
| 1:C:1382:UNK:O   | 1:C:1386:UNK:N   | 2.35                     | 0.58              |
| 1:C:2408:GLU:CG  | 1:C:2429:TRP:HH2 | 2.16                     | 0.58              |
| 1:A:290:UNK:O    | 1:A:291:UNK:C    | 2.51                     | 0.58              |
| 1:A:1990:ILE:N   | 1:A:1991:ILE:HA  | 2.18                     | 0.58              |
| 1:B:1492:UNK:O   | 1:B:1493:UNK:C   | 2.51                     | 0.58              |
| 1:B:2424:SER:OG  | 1:B:2425:ASP:OD1 | 2.21                     | 0.58              |
| 1:C:1132:UNK:O   | 1:C:1133:UNK:C   | 2.51                     | 0.58              |
| 1:A:280:UNK:O    | 1:A:281:UNK:C    | 2.51                     | 0.58              |
| 1:A:1502:UNK:O   | 1:A:1503:UNK:C   | 2.51                     | 0.58              |
| 1:A:1790:UNK:O   | 1:A:1791:UNK:C   | 2.51                     | 0.58              |
| 1:B:261:UNK:O    | 1:B:262:UNK:C    | 2.51                     | 0.58              |
| 1:B:285:UNK:O    | 1:B:286:UNK:C    | 2.51                     | 0.58              |
| 1:B:1124:UNK:O   | 1:B:1125:UNK:C   | 2.51                     | 0.58              |
| 1:B:1495:UNK:O   | 1:B:1496:UNK:C   | 2.51                     | 0.58              |
| 1:A:264:UNK:O    | 1:A:265:UNK:C    | 2.52                     | 0.58              |
| 1:A:1011:UNK:O   | 1:A:1012:UNK:C   | 2.51                     | 0.58              |
| 1:B:2429:TRP:CE3 | 1:C:2297:SER:CB  | 2.86                     | 0.58              |
| 1:C:264:UNK:O    | 1:C:265:UNK:C    | 2.51                     | 0.58              |
| 1:C:2410:VAL:CB  | 1:C:2426:PHE:CD2 | 2.86                     | 0.58              |
| 1:A:1494:UNK:O   | 1:A:1495:UNK:C   | 2.51                     | 0.58              |
| 1:A:2298:PRO:HD2 | 1:C:2408:GLU:HB2 | 1.86                     | 0.58              |
| 1:B:262:UNK:O    | 1:B:263:UNK:C    | 2.52                     | 0.58              |
| 1:B:263:UNK:O    | 1:B:264:UNK:C    | 2.51                     | 0.58              |
| 1:B:1491:UNK:O   | 1:B:1492:UNK:C   | 2.51                     | 0.58              |
| 1:C:2408:GLU:CG  | 1:C:2429:TRP:CH2 | 2.85                     | 0.58              |
| 1:A:1496:UNK:O   | 1:A:1497:UNK:C   | 2.52                     | 0.58              |
| 1:A:2505:LYS:HA  | 1:A:2508:GLN:CB  | 2.33                     | 0.58              |
| 1:B:266:UNK:O    | 1:B:267:UNK:C    | 2.51                     | 0.58              |
| 1:B:271:UNK:O    | 1:B:272:UNK:C    | 2.51                     | 0.58              |
| 1:B:288:UNK:O    | 1:B:289:UNK:C    | 2.52                     | 0.58              |
| 1:B:295:UNK:O    | 1:B:296:UNK:C    | 2.52                     | 0.58              |
| 1:B:1127:UNK:O   | 1:B:1128:UNK:C   | 2.51                     | 0.58              |
| 1:B:1144:UNK:O   | 1:B:1145:UNK:C   | 2.51                     | 0.58              |
| 1:B:2083:TYR:O   | 1:B:2087:CYS:N   | 2.31                     | 0.58              |
| 1:B:2299:PRO:HG2 | 1:B:2300:SER:N   | 2.17                     | 0.58              |
| 1:C:1011:UNK:O   | 1:C:1012:UNK:C   | 2.52                     | 0.58              |
| 1:A:285:UNK:O    | 1:A:286:UNK:C    | 2.51                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2299:PRO:CD  | 1:C:2429:TRP:CH2 | 2.85                     | 0.58              |
| 1:B:1494:UNK:O   | 1:B:1495:UNK:C   | 2.51                     | 0.58              |
| 1:B:2051:VAL:C   | 1:B:2053:LEU:H   | 2.11                     | 0.58              |
| 1:B:2406:ARG:NH1 | 1:B:2408:GLU:OE1 | 2.37                     | 0.58              |
| 1:B:2409:GLN:CG  | 1:B:2410:VAL:C   | 2.76                     | 0.58              |
| 1:C:294:UNK:O    | 1:C:295:UNK:C    | 2.51                     | 0.58              |
| 1:C:1012:UNK:O   | 1:C:1013:UNK:C   | 2.51                     | 0.58              |
| 1:C:1503:UNK:O   | 1:C:1504:UNK:C   | 2.51                     | 0.58              |
| 1:C:1759:UNK:HA  | 1:C:1763:UNK:CB  | 2.34                     | 0.58              |
| 1:A:1503:UNK:O   | 1:A:1504:UNK:C   | 2.51                     | 0.57              |
| 1:A:1791:UNK:O   | 1:A:1792:UNK:C   | 2.52                     | 0.57              |
| 1:A:2298:PRO:HG2 | 1:C:2408:GLU:HB2 | 1.85                     | 0.57              |
| 1:B:294:UNK:O    | 1:B:295:UNK:C    | 2.52                     | 0.57              |
| 1:B:1493:UNK:O   | 1:B:1494:UNK:C   | 2.51                     | 0.57              |
| 1:C:271:UNK:O    | 1:C:272:UNK:C    | 2.51                     | 0.57              |
| 1:C:289:UNK:O    | 1:C:290:UNK:C    | 2.51                     | 0.57              |
| 1:C:1013:UNK:O   | 1:C:1014:UNK:C   | 2.52                     | 0.57              |
| 1:C:2409:GLN:CB  | 1:C:2426:PHE:CE2 | 2.85                     | 0.57              |
| 1:A:265:UNK:O    | 1:A:266:UNK:C    | 2.51                     | 0.57              |
| 1:A:2299:PRO:CG  | 1:C:2429:TRP:CZ2 | 2.87                     | 0.57              |
| 1:B:275:UNK:O    | 1:B:276:UNK:C    | 2.52                     | 0.57              |
| 1:B:1501:UNK:O   | 1:B:1502:UNK:C   | 2.51                     | 0.57              |
| 1:B:1794:UNK:O   | 1:B:1798:UNK:N   | 2.36                     | 0.57              |
| 1:C:1504:UNK:O   | 1:C:1505:UNK:C   | 2.51                     | 0.57              |
| 1:A:226:UNK:C    | 1:A:263:UNK:CB   | 2.77                     | 0.57              |
| 1:A:259:UNK:O    | 1:A:260:UNK:C    | 2.51                     | 0.57              |
| 1:A:1759:UNK:HA  | 1:A:1763:UNK:CB  | 2.34                     | 0.57              |
| 1:B:272:UNK:O    | 1:B:273:UNK:C    | 2.51                     | 0.57              |
| 1:B:1123:UNK:O   | 1:B:1124:UNK:C   | 2.51                     | 0.57              |
| 1:C:272:UNK:O    | 1:C:273:UNK:C    | 2.51                     | 0.57              |
| 1:C:274:UNK:O    | 1:C:275:UNK:C    | 2.51                     | 0.57              |
| 1:C:281:UNK:O    | 1:C:282:UNK:C    | 2.52                     | 0.57              |
| 1:C:1145:UNK:O   | 1:C:1146:UNK:C   | 2.51                     | 0.57              |
| 1:C:1498:UNK:O   | 1:C:1499:UNK:C   | 2.52                     | 0.57              |
| 1:C:1502:UNK:O   | 1:C:1503:UNK:C   | 2.51                     | 0.57              |
| 1:C:2457:SER:O   | 1:C:2458:LEU:CB  | 2.51                     | 0.57              |
| 1:A:222:UNK:CB   | 1:A:266:UNK:C    | 2.82                     | 0.57              |
| 1:A:287:UNK:O    | 1:A:288:UNK:C    | 2.51                     | 0.57              |
| 1:A:288:UNK:O    | 1:A:289:UNK:C    | 2.52                     | 0.57              |
| 1:A:2470:TYR:O   | 1:A:2474:VAL:CB  | 2.52                     | 0.57              |
| 1:C:1125:UNK:O   | 1:C:1126:UNK:C   | 2.51                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1124:UNK:O   | 1:A:1125:UNK:C   | 2.51                     | 0.57              |
| 1:A:1126:UNK:O   | 1:A:1127:UNK:C   | 2.51                     | 0.57              |
| 1:A:1145:UNK:O   | 1:A:1146:UNK:C   | 2.51                     | 0.57              |
| 1:B:1126:UNK:O   | 1:B:1127:UNK:C   | 2.51                     | 0.57              |
| 1:B:1759:UNK:HA  | 1:B:1763:UNK:CB  | 2.34                     | 0.57              |
| 1:C:258:UNK:O    | 1:C:259:UNK:C    | 2.52                     | 0.57              |
| 1:C:1380:UNK:O   | 1:C:1381:UNK:C   | 2.51                     | 0.57              |
| 1:A:263:UNK:O    | 1:A:264:UNK:C    | 2.51                     | 0.57              |
| 1:A:1123:UNK:O   | 1:A:1124:UNK:C   | 2.51                     | 0.57              |
| 1:A:2408:GLU:CG  | 1:A:2429:TRP:CZ3 | 2.87                     | 0.57              |
| 1:A:2457:SER:O   | 1:A:2458:LEU:CB  | 2.51                     | 0.57              |
| 1:B:1013:UNK:O   | 1:B:1014:UNK:C   | 2.52                     | 0.57              |
| 1:B:1145:UNK:O   | 1:B:1146:UNK:C   | 2.51                     | 0.57              |
| 1:C:268:UNK:O    | 1:C:269:UNK:C    | 2.51                     | 0.57              |
| 1:C:2408:GLU:C   | 1:C:2410:VAL:CG1 | 2.72                     | 0.57              |
| 1:A:272:UNK:O    | 1:A:273:UNK:C    | 2.52                     | 0.57              |
| 1:A:295:UNK:O    | 1:A:296:UNK:C    | 2.52                     | 0.57              |
| 1:A:1014:UNK:O   | 1:A:1015:UNK:C   | 2.51                     | 0.57              |
| 1:A:1499:UNK:O   | 1:A:1500:UNK:C   | 2.51                     | 0.57              |
| 1:A:1788:UNK:O   | 1:A:1789:UNK:C   | 2.52                     | 0.57              |
| 1:B:1129:UNK:O   | 1:B:1130:UNK:C   | 2.52                     | 0.57              |
| 1:C:262:UNK:O    | 1:C:263:UNK:C    | 2.51                     | 0.57              |
| 1:C:295:UNK:O    | 1:C:296:UNK:C    | 2.51                     | 0.57              |
| 1:C:1497:UNK:O   | 1:C:1498:UNK:C   | 2.52                     | 0.57              |
| 1:A:275:UNK:O    | 1:A:276:UNK:C    | 2.52                     | 0.57              |
| 1:A:278:UNK:O    | 1:A:279:UNK:C    | 2.51                     | 0.57              |
| 1:A:291:UNK:O    | 1:A:292:UNK:C    | 2.51                     | 0.57              |
| 1:A:1504:UNK:O   | 1:A:1505:UNK:C   | 2.51                     | 0.57              |
| 1:A:2406:ARG:NH1 | 1:A:2429:TRP:CZ2 | 2.73                     | 0.57              |
| 1:A:2408:GLU:CG  | 1:B:2298:PRO:HG2 | 2.35                     | 0.57              |
| 1:B:273:UNK:O    | 1:B:274:UNK:C    | 2.51                     | 0.57              |
| 1:B:280:UNK:O    | 1:B:281:UNK:C    | 2.51                     | 0.57              |
| 1:B:2424:SER:N   | 1:B:2426:PHE:CZ  | 2.73                     | 0.57              |
| 1:C:1134:UNK:C   | 1:C:1136:UNK:N   | 2.65                     | 0.57              |
| 1:A:266:UNK:O    | 1:A:267:UNK:C    | 2.51                     | 0.57              |
| 1:A:1143:UNK:O   | 1:A:1144:UNK:C   | 2.52                     | 0.57              |
| 1:A:1974:THR:O   | 1:A:1976:VAL:N   | 2.28                     | 0.57              |
| 1:A:2406:ARG:NH1 | 1:B:2299:PRO:HG3 | 2.09                     | 0.57              |
| 1:B:265:UNK:O    | 1:B:266:UNK:C    | 2.51                     | 0.57              |
| 1:B:276:UNK:O    | 1:B:277:UNK:C    | 2.51                     | 0.57              |
| 1:B:278:UNK:O    | 1:B:279:UNK:C    | 2.52                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1125:UNK:O    | 1:B:1126:UNK:C   | 2.51                     | 0.57              |
| 1:B:1146:UNK:O    | 1:B:1147:UNK:C   | 2.51                     | 0.57              |
| 1:C:279:UNK:O     | 1:C:280:UNK:C    | 2.51                     | 0.57              |
| 1:C:1799:UNK:O    | 1:C:1802:UNK:N   | 2.37                     | 0.57              |
| 1:C:2410:VAL:HG21 | 1:C:2426:PHE:CE1 | 2.35                     | 0.57              |
| 1:A:273:UNK:O     | 1:A:274:UNK:C    | 2.52                     | 0.57              |
| 1:A:1493:UNK:O    | 1:A:1494:UNK:C   | 2.51                     | 0.57              |
| 1:A:2297:SER:HB2  | 1:C:2429:TRP:CH2 | 2.39                     | 0.57              |
| 1:A:2429:TRP:CZ3  | 1:B:2297:SER:HB3 | 2.38                     | 0.57              |
| 1:B:292:UNK:O     | 1:B:293:UNK:C    | 2.52                     | 0.57              |
| 1:C:1144:UNK:C    | 1:C:1146:UNK:N   | 2.68                     | 0.57              |
| 1:C:1146:UNK:O    | 1:C:1147:UNK:C   | 2.51                     | 0.57              |
| 1:C:1491:UNK:O    | 1:C:1492:UNK:C   | 2.51                     | 0.57              |
| 1:C:1495:UNK:O    | 1:C:1496:UNK:C   | 2.51                     | 0.57              |
| 1:B:284:UNK:O     | 1:B:285:UNK:C    | 2.51                     | 0.56              |
| 1:C:1974:THR:C    | 1:C:1976:VAL:H   | 2.11                     | 0.56              |
| 1:A:258:UNK:O     | 1:A:259:UNK:C    | 2.51                     | 0.56              |
| 1:A:261:UNK:O     | 1:A:262:UNK:C    | 2.51                     | 0.56              |
| 1:A:267:UNK:O     | 1:A:268:UNK:C    | 2.51                     | 0.56              |
| 1:A:289:UNK:O     | 1:A:290:UNK:C    | 2.51                     | 0.56              |
| 1:A:2297:SER:HB2  | 1:A:2299:PRO:HG2 | 1.86                     | 0.56              |
| 1:B:215:UNK:CB    | 1:B:274:UNK:CA   | 2.83                     | 0.56              |
| 1:C:212:UNK:HA    | 1:C:277:UNK:CB   | 2.35                     | 0.56              |
| 1:C:288:UNK:O     | 1:C:289:UNK:C    | 2.52                     | 0.56              |
| 1:C:1492:UNK:O    | 1:C:1493:UNK:C   | 2.51                     | 0.56              |
| 1:A:282:UNK:O     | 1:A:283:UNK:C    | 2.51                     | 0.56              |
| 1:A:292:UNK:O     | 1:A:293:UNK:C    | 2.52                     | 0.56              |
| 1:A:1491:UNK:O    | 1:A:1492:UNK:C   | 2.51                     | 0.56              |
| 1:B:1014:UNK:O    | 1:B:1015:UNK:C   | 2.51                     | 0.56              |
| 1:B:1380:UNK:O    | 1:B:1381:UNK:C   | 2.51                     | 0.56              |
| 1:B:1381:UNK:O    | 1:B:1382:UNK:C   | 2.52                     | 0.56              |
| 1:C:266:UNK:O     | 1:C:267:UNK:C    | 2.51                     | 0.56              |
| 1:C:290:UNK:O     | 1:C:291:UNK:C    | 2.51                     | 0.56              |
| 1:C:1744:UNK:O    | 1:C:1748:UNK:N   | 2.38                     | 0.56              |
| 1:A:233:UNK:CB    | 1:A:255:UNK:O    | 2.54                     | 0.56              |
| 1:A:293:UNK:O     | 1:A:294:UNK:C    | 2.51                     | 0.56              |
| 1:A:1793:UNK:O    | 1:A:1797:UNK:CA  | 2.52                     | 0.56              |
| 1:B:260:UNK:O     | 1:B:261:UNK:C    | 2.51                     | 0.56              |
| 1:B:269:UNK:O     | 1:B:270:UNK:C    | 2.51                     | 0.56              |
| 1:B:1128:UNK:O    | 1:B:1129:UNK:C   | 2.51                     | 0.56              |
| 1:B:1744:UNK:O    | 1:B:1748:UNK:N   | 2.38                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:292:UNK:O     | 1:C:293:UNK:C    | 2.52                     | 0.56              |
| 1:C:1500:UNK:O    | 1:C:1501:UNK:C   | 2.52                     | 0.56              |
| 1:C:2410:VAL:HG21 | 1:C:2426:PHE:CD1 | 2.37                     | 0.56              |
| 1:A:238:UNK:O     | 1:A:241:UNK:N    | 2.39                     | 0.56              |
| 1:A:260:UNK:O     | 1:A:261:UNK:C    | 2.52                     | 0.56              |
| 1:A:1744:UNK:O    | 1:A:1748:UNK:N   | 2.39                     | 0.56              |
| 1:A:1766:UNK:O    | 1:A:1770:UNK:N   | 2.39                     | 0.56              |
| 1:B:279:UNK:O     | 1:B:280:UNK:C    | 2.52                     | 0.56              |
| 1:B:1490:UNK:O    | 1:B:1491:UNK:C   | 2.51                     | 0.56              |
| 1:B:1503:UNK:O    | 1:B:1504:UNK:C   | 2.51                     | 0.56              |
| 1:B:1766:UNK:O    | 1:B:1770:UNK:N   | 2.39                     | 0.56              |
| 1:B:2408:GLU:C    | 1:B:2426:PHE:HB2 | 2.31                     | 0.56              |
| 1:C:269:UNK:O     | 1:C:270:UNK:C    | 2.51                     | 0.56              |
| 1:C:276:UNK:O     | 1:C:277:UNK:C    | 2.52                     | 0.56              |
| 1:C:285:UNK:O     | 1:C:286:UNK:C    | 2.51                     | 0.56              |
| 1:C:1133:UNK:O    | 1:C:1134:UNK:C   | 2.51                     | 0.56              |
| 1:A:279:UNK:O     | 1:A:280:UNK:C    | 2.51                     | 0.56              |
| 1:A:1013:UNK:O    | 1:A:1014:UNK:C   | 2.52                     | 0.56              |
| 1:A:2407:ARG:NH2  | 1:A:2426:PHE:CD1 | 2.73                     | 0.56              |
| 1:B:1504:UNK:O    | 1:B:1505:UNK:C   | 2.51                     | 0.56              |
| 1:B:2293:LEU:HG   | 1:C:2295:ARG:CA  | 2.35                     | 0.56              |
| 1:B:2293:LEU:CG   | 1:C:2295:ARG:O   | 2.47                     | 0.56              |
| 1:C:273:UNK:O     | 1:C:274:UNK:C    | 2.51                     | 0.56              |
| 1:C:1134:UNK:O    | 1:C:1136:UNK:N   | 2.38                     | 0.56              |
| 1:A:262:UNK:O     | 1:A:263:UNK:C    | 2.51                     | 0.56              |
| 1:C:260:UNK:O     | 1:C:261:UNK:C    | 2.52                     | 0.56              |
| 1:C:261:UNK:O     | 1:C:262:UNK:C    | 2.51                     | 0.56              |
| 1:C:1127:UNK:O    | 1:C:1128:UNK:C   | 2.51                     | 0.56              |
| 1:A:268:UNK:O     | 1:A:269:UNK:C    | 2.52                     | 0.56              |
| 1:A:1789:UNK:O    | 1:A:1790:UNK:C   | 2.52                     | 0.56              |
| 1:B:229:UNK:O     | 1:B:259:UNK:CB   | 2.50                     | 0.56              |
| 1:B:270:UNK:O     | 1:B:271:UNK:C    | 2.52                     | 0.56              |
| 1:C:2410:VAL:HG12 | 1:C:2426:PHE:HA  | 1.88                     | 0.56              |
| 1:A:294:UNK:O     | 1:A:295:UNK:C    | 2.51                     | 0.56              |
| 1:A:1490:UNK:O    | 1:A:1491:UNK:C   | 2.51                     | 0.56              |
| 1:B:258:UNK:O     | 1:B:259:UNK:C    | 2.51                     | 0.56              |
| 1:B:277:UNK:O     | 1:B:278:UNK:C    | 2.52                     | 0.56              |
| 1:C:1123:UNK:O    | 1:C:1124:UNK:C   | 2.51                     | 0.56              |
| 1:C:1494:UNK:O    | 1:C:1495:UNK:C   | 2.51                     | 0.56              |
| 1:A:237:UNK:HA    | 1:A:252:UNK:CB   | 2.28                     | 0.56              |
| 1:A:276:UNK:O     | 1:A:277:UNK:C    | 2.51                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:286:UNK:O     | 1:A:287:UNK:C    | 2.51                     | 0.56              |
| 1:A:1495:UNK:O    | 1:A:1496:UNK:C   | 2.51                     | 0.56              |
| 1:B:1011:UNK:O    | 1:B:1012:UNK:C   | 2.51                     | 0.56              |
| 1:C:259:UNK:O     | 1:C:260:UNK:C    | 2.51                     | 0.56              |
| 1:C:1766:UNK:O    | 1:C:1770:UNK:N   | 2.39                     | 0.56              |
| 1:A:1501:UNK:O    | 1:A:1502:UNK:C   | 2.51                     | 0.55              |
| 1:A:2409:GLN:CA   | 1:A:2410:VAL:CG2 | 2.84                     | 0.55              |
| 1:B:1012:UNK:O    | 1:B:1013:UNK:C   | 2.51                     | 0.55              |
| 1:B:2429:TRP:CZ3  | 1:C:2297:SER:CA  | 2.89                     | 0.55              |
| 1:A:1128:UNK:O    | 1:A:1129:UNK:C   | 2.51                     | 0.55              |
| 1:B:1499:UNK:O    | 1:B:1500:UNK:C   | 2.52                     | 0.55              |
| 1:C:275:UNK:O     | 1:C:276:UNK:C    | 2.52                     | 0.55              |
| 1:C:1490:UNK:O    | 1:C:1491:UNK:C   | 2.51                     | 0.55              |
| 1:A:212:UNK:N     | 1:A:277:UNK:CB   | 2.68                     | 0.55              |
| 1:B:1500:UNK:O    | 1:B:1501:UNK:C   | 2.51                     | 0.55              |
| 1:B:293:UNK:O     | 1:B:294:UNK:C    | 2.52                     | 0.55              |
| 1:C:282:UNK:O     | 1:C:283:UNK:C    | 2.52                     | 0.55              |
| 1:C:291:UNK:O     | 1:C:292:UNK:C    | 2.51                     | 0.55              |
| 1:C:1131:UNK:O    | 1:C:1132:UNK:C   | 2.52                     | 0.55              |
| 1:A:1380:UNK:O    | 1:A:1381:UNK:C   | 2.52                     | 0.55              |
| 1:B:2429:TRP:CE3  | 1:C:2297:SER:HB2 | 2.39                     | 0.55              |
| 1:C:263:UNK:O     | 1:C:264:UNK:C    | 2.51                     | 0.55              |
| 1:C:1493:UNK:O    | 1:C:1494:UNK:C   | 2.51                     | 0.55              |
| 1:C:1499:UNK:O    | 1:C:1500:UNK:C   | 2.51                     | 0.55              |
| 1:A:1012:UNK:O    | 1:A:1013:UNK:C   | 2.51                     | 0.55              |
| 1:A:1129:UNK:O    | 1:A:1130:UNK:C   | 2.52                     | 0.55              |
| 1:A:2049:PHE:H    | 1:A:2051:VAL:CB  | 2.19                     | 0.55              |
| 1:B:274:UNK:O     | 1:B:275:UNK:C    | 2.51                     | 0.55              |
| 1:B:569:UNK:O     | 1:B:570:UNK:C    | 2.55                     | 0.55              |
| 1:C:278:UNK:O     | 1:C:279:UNK:C    | 2.51                     | 0.55              |
| 1:C:283:UNK:O     | 1:C:284:UNK:C    | 2.51                     | 0.55              |
| 1:C:1129:UNK:O    | 1:C:1130:UNK:C   | 2.51                     | 0.55              |
| 1:C:2406:ARG:HH11 | 1:C:2408:GLU:CD  | 2.13                     | 0.55              |
| 1:A:2299:PRO:HG3  | 1:C:2429:TRP:HZ2 | 1.71                     | 0.55              |
| 1:B:291:UNK:O     | 1:B:292:UNK:C    | 2.51                     | 0.55              |
| 1:C:1974:THR:O    | 1:C:1976:VAL:N   | 2.28                     | 0.55              |
| 1:A:283:UNK:O     | 1:A:284:UNK:C    | 2.51                     | 0.55              |
| 1:A:2522:GLU:O    | 1:A:2524:GLU:N   | 2.40                     | 0.55              |
| 1:B:286:UNK:O     | 1:B:287:UNK:C    | 2.51                     | 0.55              |
| 1:B:289:UNK:O     | 1:B:290:UNK:C    | 2.52                     | 0.55              |
| 1:B:1498:UNK:O    | 1:B:1499:UNK:C   | 2.52                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:201:UNK:CB    | 1:C:288:UNK:CB   | 2.84                     | 0.55              |
| 1:C:284:UNK:O     | 1:C:285:UNK:C    | 2.51                     | 0.55              |
| 1:A:1146:UNK:O    | 1:A:1147:UNK:C   | 2.51                     | 0.55              |
| 1:C:569:UNK:O     | 1:C:570:UNK:C    | 2.55                     | 0.55              |
| 1:A:1125:UNK:O    | 1:A:1126:UNK:C   | 2.51                     | 0.55              |
| 1:B:1502:UNK:O    | 1:B:1503:UNK:C   | 2.51                     | 0.55              |
| 1:C:265:UNK:O     | 1:C:266:UNK:C    | 2.52                     | 0.55              |
| 1:C:280:UNK:O     | 1:C:281:UNK:C    | 2.51                     | 0.55              |
| 1:C:1124:UNK:O    | 1:C:1125:UNK:C   | 2.51                     | 0.55              |
| 1:B:241:UNK:CA    | 1:B:248:UNK:CA   | 2.86                     | 0.54              |
| 1:C:240:UNK:C     | 1:C:248:UNK:CB   | 2.86                     | 0.54              |
| 1:C:270:UNK:O     | 1:C:271:UNK:C    | 2.52                     | 0.54              |
| 1:C:1126:UNK:O    | 1:C:1127:UNK:C   | 2.51                     | 0.54              |
| 1:C:1496:UNK:O    | 1:C:1497:UNK:C   | 2.51                     | 0.54              |
| 1:A:1492:UNK:O    | 1:A:1493:UNK:C   | 2.51                     | 0.54              |
| 1:A:2217:VAL:CA   | 1:A:2454:SER:HB2 | 2.37                     | 0.54              |
| 1:B:2296:ILE:HG13 | 1:B:2300:SER:HB3 | 1.88                     | 0.54              |
| 1:B:2410:VAL:HB   | 1:C:2425:ASP:HB3 | 1.89                     | 0.54              |
| 1:A:270:UNK:O     | 1:A:271:UNK:C    | 2.52                     | 0.54              |
| 1:A:274:UNK:O     | 1:A:275:UNK:C    | 2.52                     | 0.54              |
| 1:A:1498:UNK:O    | 1:A:1499:UNK:C   | 2.52                     | 0.54              |
| 1:B:264:UNK:O     | 1:B:265:UNK:C    | 2.51                     | 0.54              |
| 1:B:267:UNK:O     | 1:B:268:UNK:C    | 2.51                     | 0.54              |
| 1:B:1497:UNK:O    | 1:B:1498:UNK:C   | 2.52                     | 0.54              |
| 1:C:1014:UNK:O    | 1:C:1015:UNK:C   | 2.51                     | 0.54              |
| 1:C:2522:GLU:O    | 1:C:2524:GLU:N   | 2.40                     | 0.54              |
| 1:A:240:UNK:C     | 1:A:248:UNK:CB   | 2.86                     | 0.54              |
| 1:A:284:UNK:O     | 1:A:285:UNK:C    | 2.51                     | 0.54              |
| 1:A:569:UNK:O     | 1:A:570:UNK:C    | 2.55                     | 0.54              |
| 1:A:2426:PHE:O    | 1:A:2428:GLU:CG  | 2.55                     | 0.54              |
| 1:B:2293:LEU:HD12 | 1:C:2295:ARG:HA  | 1.88                     | 0.54              |
| 1:B:2425:ASP:C    | 1:B:2426:PHE:CD1 | 2.86                     | 0.54              |
| 1:B:2522:GLU:O    | 1:B:2524:GLU:N   | 2.40                     | 0.54              |
| 1:C:2410:VAL:CG2  | 1:C:2426:PHE:CG  | 2.70                     | 0.54              |
| 1:A:2060:TRP:O    | 1:A:2063:PHE:CA  | 2.56                     | 0.54              |
| 1:B:1130:UNK:O    | 1:B:1131:UNK:C   | 2.56                     | 0.54              |
| 1:A:2236:GLU:OE2  | 1:C:2291:GLY:HA2 | 2.07                     | 0.54              |
| 1:A:2491:SER:CB   | 1:C:2512:LEU:CA  | 2.83                     | 0.54              |
| 1:B:2077:ALA:CA   | 1:B:2083:TYR:CB  | 2.86                     | 0.54              |
| 1:C:2425:ASP:C    | 1:C:2426:PHE:HD1 | 2.15                     | 0.54              |
| 1:A:243:UNK:CB    | 1:A:247:UNK:CB   | 2.86                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1142:UNK:C    | 1:A:1144:UNK:N    | 2.70                     | 0.54              |
| 1:A:2077:ALA:CA   | 1:A:2083:TYR:CB   | 2.86                     | 0.54              |
| 1:A:2408:GLU:CD   | 1:A:2429:TRP:CH2  | 2.86                     | 0.54              |
| 1:B:281:UNK:O     | 1:B:282:UNK:C     | 2.51                     | 0.54              |
| 1:C:286:UNK:O     | 1:C:287:UNK:C     | 2.51                     | 0.54              |
| 1:C:1787:UNK:O    | 1:C:1788:UNK:C    | 2.56                     | 0.54              |
| 1:A:269:UNK:O     | 1:A:270:UNK:C     | 2.51                     | 0.54              |
| 1:A:277:UNK:O     | 1:A:278:UNK:C     | 2.51                     | 0.54              |
| 1:A:1500:UNK:O    | 1:A:1501:UNK:C    | 2.52                     | 0.54              |
| 1:A:2408:GLU:HG3  | 1:A:2429:TRP:CH2  | 2.43                     | 0.54              |
| 1:B:290:UNK:O     | 1:B:291:UNK:C     | 2.51                     | 0.54              |
| 1:B:1496:UNK:O    | 1:B:1497:UNK:C    | 2.52                     | 0.54              |
| 1:B:2012:SER:O    | 1:B:2016:VAL:N    | 2.39                     | 0.54              |
| 1:A:2298:PRO:CG   | 1:C:2408:GLU:CB   | 2.85                     | 0.54              |
| 1:B:2519:LEU:C    | 1:B:2521:LEU:N    | 2.66                     | 0.54              |
| 1:A:2050:GLN:CB   | 1:A:2055:VAL:CB   | 2.86                     | 0.54              |
| 1:B:2039:LEU:O    | 1:B:2040:ARG:C    | 2.51                     | 0.54              |
| 1:C:1128:UNK:O    | 1:C:1129:UNK:C    | 2.51                     | 0.54              |
| 1:A:1497:UNK:O    | 1:A:1498:UNK:C    | 2.52                     | 0.53              |
| 1:B:240:UNK:CB    | 1:B:252:UNK:CB    | 2.86                     | 0.53              |
| 1:B:2046:LYS:CB   | 1:B:2050:GLN:CB   | 2.86                     | 0.53              |
| 1:B:2328:ALA:HB2  | 1:C:2382:PRO:HG2  | 1.89                     | 0.53              |
| 1:C:233:UNK:CB    | 1:C:255:UNK:C     | 2.85                     | 0.53              |
| 1:C:2409:GLN:OE1  | 1:C:2410:VAL:C    | 2.46                     | 0.53              |
| 1:A:271:UNK:O     | 1:A:272:UNK:C     | 2.51                     | 0.53              |
| 1:A:2143:THR:O    | 1:A:2147:LEU:N    | 2.41                     | 0.53              |
| 1:B:295:UNK:N     | 1:B:447:UNK:N     | 2.56                     | 0.53              |
| 1:C:243:UNK:CB    | 1:C:247:UNK:CB    | 2.85                     | 0.53              |
| 1:C:1137:UNK:O    | 1:C:1141:UNK:N    | 2.42                     | 0.53              |
| 1:C:1986:VAL:O    | 1:C:1990:ILE:N    | 2.33                     | 0.53              |
| 1:A:295:UNK:CA    | 1:A:447:UNK:H     | 1.93                     | 0.53              |
| 1:B:243:UNK:CB    | 1:B:247:UNK:CB    | 2.86                     | 0.53              |
| 1:B:283:UNK:CB    | 1:B:1993:PHE:CB   | 2.86                     | 0.53              |
| 1:B:287:UNK:O     | 1:B:288:UNK:C     | 2.52                     | 0.53              |
| 1:C:2056:ALA:O    | 1:C:2060:TRP:CB   | 2.56                     | 0.53              |
| 1:A:295:UNK:O     | 1:A:447:UNK:CB    | 2.56                     | 0.53              |
| 1:A:2039:LEU:O    | 1:A:2040:ARG:C    | 2.51                     | 0.53              |
| 1:A:2101:TYR:HA   | 1:A:2104:ARG:CB   | 2.39                     | 0.53              |
| 1:A:2245:GLN:HE22 | 1:B:2339:LYS:CE   | 2.20                     | 0.53              |
| 1:B:2472:SER:O    | 1:B:2476:VAL:CB   | 2.56                     | 0.53              |
| 1:C:2409:GLN:N    | 1:C:2410:VAL:HG13 | 2.21                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:233:UNK:CB    | 1:A:256:UNK:N    | 2.70                     | 0.53              |
| 1:A:2519:LEU:C    | 1:A:2521:LEU:N   | 2.66                     | 0.53              |
| 1:B:2046:LYS:HA   | 1:B:2050:GLN:CB  | 2.38                     | 0.53              |
| 1:B:2101:TYR:HA   | 1:B:2104:ARG:CB  | 2.39                     | 0.53              |
| 1:C:295:UNK:O     | 1:C:447:UNK:CB   | 2.56                     | 0.53              |
| 1:C:2408:GLU:OE1  | 1:C:2408:GLU:HA  | 2.09                     | 0.53              |
| 1:A:2298:PRO:HD2  | 1:C:2408:GLU:HG2 | 1.90                     | 0.53              |
| 1:B:2218:GLY:HA3  | 1:B:2453:VAL:O   | 2.06                     | 0.53              |
| 1:C:2410:VAL:CG1  | 1:C:2426:PHE:CA  | 2.85                     | 0.53              |
| 1:A:2224:ILE:HG12 | 1:A:2324:GLN:O   | 2.09                     | 0.53              |
| 1:A:2512:LEU:C    | 1:B:2491:SER:CB  | 2.81                     | 0.53              |
| 1:B:2046:LYS:CA   | 1:B:2050:GLN:CB  | 2.87                     | 0.53              |
| 1:C:293:UNK:O     | 1:C:294:UNK:C    | 2.52                     | 0.53              |
| 1:B:211:UNK:O     | 1:B:277:UNK:CB   | 2.56                     | 0.53              |
| 1:A:2429:TRP:CZ3  | 1:B:2297:SER:CB  | 2.92                     | 0.53              |
| 1:B:295:UNK:O     | 1:B:447:UNK:CB   | 2.56                     | 0.53              |
| 1:C:1787:UNK:O    | 1:C:1791:UNK:N   | 2.42                     | 0.53              |
| 1:C:2039:LEU:O    | 1:C:2040:ARG:C   | 2.51                     | 0.53              |
| 1:A:240:UNK:C     | 1:A:248:UNK:HA   | 2.39                     | 0.53              |
| 1:A:2472:SER:O    | 1:A:2476:VAL:CB  | 2.57                     | 0.53              |
| 1:B:2429:TRP:CZ3  | 1:C:2297:SER:HA  | 2.43                     | 0.53              |
| 1:B:2429:TRP:CD2  | 1:C:2297:SER:HB2 | 2.43                     | 0.53              |
| 1:C:287:UNK:O     | 1:C:288:UNK:C    | 2.52                     | 0.53              |
| 1:C:2224:ILE:HG12 | 1:C:2324:GLN:O   | 2.09                     | 0.53              |
| 1:C:2472:SER:O    | 1:C:2476:VAL:CB  | 2.57                     | 0.53              |
| 1:C:2519:LEU:C    | 1:C:2521:LEU:N   | 2.66                     | 0.53              |
| 1:A:2038:TYR:O    | 1:A:2039:LEU:C   | 2.51                     | 0.52              |
| 1:B:2037:LEU:O    | 1:B:2038:TYR:C   | 2.51                     | 0.52              |
| 1:C:2038:TYR:O    | 1:C:2039:LEU:C   | 2.51                     | 0.52              |
| 1:C:2052:VAL:O    | 1:C:2056:ALA:HB2 | 2.09                     | 0.52              |
| 1:C:2077:ALA:CA   | 1:C:2083:TYR:CB  | 2.86                     | 0.52              |
| 1:A:2522:GLU:O    | 1:A:2523:GLU:C   | 2.53                     | 0.52              |
| 1:B:2518:GLU:O    | 1:B:2521:LEU:CB  | 2.57                     | 0.52              |
| 1:C:2050:GLN:CB   | 1:C:2051:VAL:CA  | 2.86                     | 0.52              |
| 1:C:2101:TYR:HA   | 1:C:2104:ARG:CB  | 2.39                     | 0.52              |
| 1:A:569:UNK:O     | 1:A:572:UNK:N    | 2.43                     | 0.52              |
| 1:A:1792:UNK:O    | 1:A:1793:UNK:O   | 2.27                     | 0.52              |
| 1:A:2299:PRO:CG   | 1:C:2429:TRP:HZ2 | 2.23                     | 0.52              |
| 1:B:2410:VAL:CG2  | 1:B:2426:PHE:CD1 | 2.93                     | 0.52              |
| 1:A:2041:LYS:O    | 1:A:2042:THR:C   | 2.52                     | 0.52              |
| 1:B:2050:GLN:N    | 1:B:2051:VAL:CA  | 2.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2143:THR:O    | 1:B:2147:LEU:N    | 2.41                     | 0.52              |
| 1:B:569:UNK:O     | 1:B:572:UNK:N     | 2.43                     | 0.52              |
| 1:B:2224:ILE:HG12 | 1:B:2324:GLN:O    | 2.09                     | 0.52              |
| 1:C:2518:GLU:O    | 1:C:2521:LEU:CB   | 2.57                     | 0.52              |
| 1:B:240:UNK:O     | 1:B:242:UNK:N     | 2.43                     | 0.52              |
| 1:B:2409:GLN:HA   | 1:B:2410:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:2518:GLU:O    | 1:A:2521:LEU:CB   | 2.57                     | 0.52              |
| 1:B:2299:PRO:O    | 1:B:2302:ALA:N    | 2.42                     | 0.52              |
| 1:C:2050:GLN:N    | 1:C:2051:VAL:CB   | 2.73                     | 0.52              |
| 1:C:2052:VAL:CA   | 1:C:2056:ALA:HB2  | 2.39                     | 0.52              |
| 1:A:2040:ARG:O    | 1:A:2041:LYS:C    | 2.52                     | 0.52              |
| 1:A:265:UNK:HA    | 1:A:2528:LYS:CB   | 2.40                     | 0.52              |
| 1:C:240:UNK:C     | 1:C:242:UNK:N     | 2.73                     | 0.52              |
| 1:C:2049:PHE:N    | 1:C:2051:VAL:CB   | 2.73                     | 0.52              |
| 1:A:2050:GLN:N    | 1:A:2051:VAL:CB   | 2.73                     | 0.51              |
| 1:B:240:UNK:C     | 1:B:242:UNK:N     | 2.73                     | 0.51              |
| 1:C:569:UNK:O     | 1:C:572:UNK:N     | 2.43                     | 0.51              |
| 1:B:238:UNK:C     | 1:B:240:UNK:N     | 2.73                     | 0.51              |
| 1:B:240:UNK:CB    | 1:B:252:UNK:N     | 2.73                     | 0.51              |
| 1:B:248:UNK:C     | 1:B:250:UNK:N     | 2.73                     | 0.51              |
| 1:B:2040:ARG:O    | 1:B:2041:LYS:C    | 2.52                     | 0.51              |
| 1:C:1140:UNK:C    | 1:C:1142:UNK:N    | 2.72                     | 0.51              |
| 1:C:2037:LEU:O    | 1:C:2038:TYR:C    | 2.51                     | 0.51              |
| 1:A:2299:PRO:CG   | 1:C:2406:ARG:NH1  | 2.73                     | 0.51              |
| 1:C:1137:UNK:O    | 1:C:1138:UNK:O    | 2.28                     | 0.51              |
| 1:C:2040:ARG:O    | 1:C:2041:LYS:C    | 2.52                     | 0.51              |
| 1:C:2424:SER:OG   | 1:C:2425:ASP:N    | 2.40                     | 0.51              |
| 1:A:1131:UNK:O    | 1:A:1132:UNK:C    | 2.57                     | 0.51              |
| 1:B:1776:UNK:O    | 1:B:1780:UNK:N    | 2.44                     | 0.51              |
| 1:C:2522:GLU:O    | 1:C:2523:GLU:C    | 2.53                     | 0.51              |
| 1:A:2037:LEU:O    | 1:A:2038:TYR:C    | 2.52                     | 0.51              |
| 1:A:2519:LEU:O    | 1:A:2520:GLU:C    | 2.53                     | 0.51              |
| 1:B:233:UNK:HA    | 1:B:255:UNK:CB    | 2.40                     | 0.51              |
| 1:C:2060:TRP:O    | 1:C:2061:MET:C    | 2.54                     | 0.51              |
| 1:C:2409:GLN:OE1  | 1:C:2411:GLY:HA3  | 2.11                     | 0.51              |
| 1:A:2410:VAL:CG2  | 1:A:2426:PHE:CG   | 2.93                     | 0.51              |
| 1:B:1136:UNK:C    | 1:B:1138:UNK:N    | 2.72                     | 0.51              |
| 1:B:2409:GLN:HG2  | 1:B:2410:VAL:C    | 2.36                     | 0.51              |
| 1:B:2429:TRP:HZ2  | 1:C:2299:PRO:CG   | 2.23                     | 0.51              |
| 1:B:2522:GLU:O    | 1:B:2523:GLU:C    | 2.53                     | 0.51              |
| 1:C:2519:LEU:O    | 1:C:2520:GLU:C    | 2.53                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1776:UNK:O    | 1:A:1780:UNK:N    | 2.43                     | 0.51              |
| 1:A:2299:PRO:HB3  | 1:C:2406:ARG:HH12 | 1.75                     | 0.51              |
| 1:B:1747:UNK:O    | 1:B:1748:UNK:C    | 2.58                     | 0.51              |
| 1:B:1791:UNK:C    | 1:B:1793:UNK:N    | 2.73                     | 0.51              |
| 1:C:1747:UNK:O    | 1:C:1748:UNK:C    | 2.58                     | 0.51              |
| 1:A:1747:UNK:O    | 1:A:1748:UNK:C    | 2.58                     | 0.51              |
| 1:B:2050:GLN:N    | 1:B:2051:VAL:CB   | 2.73                     | 0.51              |
| 1:A:1510:UNK:C    | 1:A:1512:UNK:N    | 2.73                     | 0.51              |
| 1:B:265:UNK:HA    | 1:B:2528:LYS:CB   | 2.40                     | 0.51              |
| 1:B:1751:UNK:O    | 1:B:1755:UNK:N    | 2.44                     | 0.51              |
| 1:B:2046:LYS:HA   | 1:B:2050:GLN:N    | 2.26                     | 0.51              |
| 1:C:265:UNK:HA    | 1:C:2528:LYS:CB   | 2.40                     | 0.51              |
| 1:C:2425:ASP:C    | 1:C:2426:PHE:CD1  | 2.89                     | 0.51              |
| 1:A:1140:UNK:C    | 1:A:1142:UNK:N    | 2.73                     | 0.51              |
| 1:B:242:UNK:C     | 1:B:244:UNK:N     | 2.73                     | 0.51              |
| 1:C:244:UNK:N     | 1:C:247:UNK:CB    | 2.73                     | 0.51              |
| 1:A:1136:UNK:C    | 1:A:1138:UNK:N    | 2.72                     | 0.50              |
| 1:A:1751:UNK:O    | 1:A:1755:UNK:N    | 2.44                     | 0.50              |
| 1:A:2409:GLN:CA   | 1:A:2410:VAL:HG23 | 2.26                     | 0.50              |
| 1:A:2043:VAL:O    | 1:A:2044:LEU:C    | 2.54                     | 0.50              |
| 1:A:2299:PRO:HG3  | 1:C:2429:TRP:CZ2  | 2.46                     | 0.50              |
| 1:B:2041:LYS:O    | 1:B:2043:VAL:C    | 2.45                     | 0.50              |
| 1:B:2409:GLN:C    | 1:B:2410:VAL:HG13 | 2.36                     | 0.50              |
| 1:A:245:UNK:C     | 1:A:247:UNK:N     | 2.73                     | 0.50              |
| 1:A:1130:UNK:C    | 1:A:1132:UNK:N    | 2.74                     | 0.50              |
| 1:B:222:UNK:CA    | 1:B:266:UNK:CB    | 2.88                     | 0.50              |
| 1:B:2519:LEU:O    | 1:B:2520:GLU:C    | 2.53                     | 0.50              |
| 1:C:2052:VAL:HA   | 1:C:2056:ALA:HB2  | 1.93                     | 0.50              |
| 1:C:2220:VAL:HG13 | 1:C:2280:ASP:OD1  | 2.11                     | 0.50              |
| 1:A:2429:TRP:HH2  | 1:B:2299:PRO:CD   | 2.24                     | 0.50              |
| 1:B:2220:VAL:HG13 | 1:B:2280:ASP:OD1  | 2.11                     | 0.50              |
| 1:C:1142:UNK:C    | 1:C:1144:UNK:N    | 2.73                     | 0.50              |
| 1:A:2050:GLN:CB   | 1:A:2051:VAL:CA   | 2.86                     | 0.50              |
| 1:A:2220:VAL:HG13 | 1:A:2280:ASP:OD1  | 2.12                     | 0.50              |
| 1:A:2513:VAL:H    | 1:B:2491:SER:CB   | 2.24                     | 0.50              |
| 1:C:1776:UNK:O    | 1:C:1780:UNK:N    | 2.44                     | 0.50              |
| 1:A:2042:THR:O    | 1:A:2043:VAL:C    | 2.52                     | 0.50              |
| 1:B:235:UNK:C     | 1:B:237:UNK:N     | 2.73                     | 0.50              |
| 1:B:1140:UNK:C    | 1:B:1142:UNK:N    | 2.73                     | 0.50              |
| 1:B:2011:LEU:O    | 1:B:2015:GLN:CB   | 2.60                     | 0.50              |
| 1:B:2038:TYR:O    | 1:B:2039:LEU:C    | 2.52                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:2143:THR:O    | 1:C:2147:LEU:N   | 2.41                     | 0.50              |
| 1:B:2424:SER:N    | 1:B:2426:PHE:CE1 | 2.80                     | 0.50              |
| 1:C:1751:UNK:O    | 1:C:1755:UNK:N   | 2.44                     | 0.50              |
| 1:B:2219:VAL:CG1  | 1:B:2220:VAL:H   | 2.13                     | 0.49              |
| 1:C:2408:GLU:C    | 1:C:2426:PHE:CD2 | 2.90                     | 0.49              |
| 1:A:295:UNK:N     | 1:A:447:UNK:N    | 2.56                     | 0.49              |
| 1:B:222:UNK:CB    | 1:B:266:UNK:CA   | 2.90                     | 0.49              |
| 1:C:234:UNK:O     | 1:C:237:UNK:N    | 2.45                     | 0.49              |
| 1:A:2076:ASN:C    | 1:A:2083:TYR:CB  | 2.86                     | 0.49              |
| 1:B:2003:ALA:CB   | 1:B:2102:PRO:CA  | 2.90                     | 0.49              |
| 1:C:1134:UNK:O    | 1:C:1135:UNK:C   | 2.60                     | 0.49              |
| 1:C:2076:ASN:C    | 1:C:2083:TYR:CB  | 2.86                     | 0.49              |
| 1:A:1130:UNK:O    | 1:A:1132:UNK:N   | 2.46                     | 0.49              |
| 1:B:2076:ASN:C    | 1:B:2083:TYR:CB  | 2.85                     | 0.49              |
| 1:B:2429:TRP:HZ2  | 1:C:2299:PRO:HG2 | 1.78                     | 0.49              |
| 1:C:2011:LEU:O    | 1:C:2015:GLN:CB  | 2.60                     | 0.49              |
| 1:C:2409:GLN:HB2  | 1:C:2410:VAL:CG2 | 2.23                     | 0.49              |
| 1:A:2298:PRO:CG   | 1:C:2408:GLU:HB2 | 2.42                     | 0.49              |
| 1:C:241:UNK:CA    | 1:C:248:UNK:CB   | 2.85                     | 0.49              |
| 1:B:234:UNK:O     | 1:B:237:UNK:N    | 2.45                     | 0.49              |
| 1:C:2012:SER:O    | 1:C:2016:VAL:N   | 2.39                     | 0.49              |
| 1:C:2409:GLN:CA   | 1:C:2426:PHE:CD2 | 2.96                     | 0.49              |
| 1:A:1130:UNK:O    | 1:A:1131:UNK:C   | 2.60                     | 0.49              |
| 1:A:1990:ILE:N    | 1:A:1991:ILE:CA  | 2.75                     | 0.49              |
| 1:B:2049:PHE:C    | 1:B:2051:VAL:CB  | 2.86                     | 0.49              |
| 1:B:2297:SER:O    | 1:B:2301:ARG:N   | 2.44                     | 0.49              |
| 1:A:2408:GLU:HG3  | 1:A:2429:TRP:HZ3 | 1.74                     | 0.49              |
| 1:C:2048:ALA:C    | 1:C:2051:VAL:CB  | 2.86                     | 0.49              |
| 1:B:233:UNK:C     | 1:B:255:UNK:CB   | 2.91                     | 0.48              |
| 1:B:2048:ALA:C    | 1:B:2051:VAL:CB  | 2.86                     | 0.48              |
| 1:C:2041:LYS:O    | 1:C:2043:VAL:N   | 2.47                     | 0.48              |
| 1:A:1792:UNK:O    | 1:A:1796:UNK:CB  | 2.61                     | 0.48              |
| 1:A:2297:SER:OG   | 1:A:2300:SER:CB  | 2.45                     | 0.48              |
| 1:B:2409:GLN:HG3  | 1:B:2411:GLY:H   | 1.78                     | 0.48              |
| 1:A:2146:THR:O    | 1:A:2150:SER:N   | 2.47                     | 0.48              |
| 1:A:2299:PRO:HD2  | 1:C:2408:GLU:CG  | 2.42                     | 0.48              |
| 1:B:2296:ILE:HD11 | 1:B:2300:SER:C   | 2.38                     | 0.48              |
| 1:B:2407:ARG:HG3  | 1:B:2407:ARG:O   | 2.12                     | 0.48              |
| 1:C:1776:UNK:CB   | 1:C:1781:UNK:CA  | 2.85                     | 0.48              |
| 1:A:2522:GLU:C    | 1:A:2524:GLU:N   | 2.72                     | 0.48              |
| 1:B:2211:SER:C    | 1:B:2213:ILE:H   | 2.21                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:2429:TRP:CZ2 | 1:C:2297:SER:OG  | 2.66                     | 0.48              |
| 1:A:2012:SER:O   | 1:A:2016:VAL:N   | 2.39                     | 0.48              |
| 1:B:884:UNK:O    | 1:B:887:UNK:N    | 2.47                     | 0.48              |
| 1:B:2051:VAL:O   | 1:B:2053:LEU:N   | 2.37                     | 0.48              |
| 1:C:2052:VAL:C   | 1:C:2056:ALA:HB2 | 2.39                     | 0.48              |
| 1:C:2500:VAL:O   | 1:C:2504:LEU:N   | 2.36                     | 0.48              |
| 1:A:2298:PRO:CD  | 1:C:2408:GLU:CB  | 2.91                     | 0.48              |
| 1:C:2041:LYS:O   | 1:C:2044:LEU:CB  | 2.61                     | 0.48              |
| 1:C:2409:GLN:C   | 1:C:2410:VAL:CG1 | 2.78                     | 0.48              |
| 1:A:2101:TYR:O   | 1:A:2104:ARG:CB  | 2.61                     | 0.48              |
| 1:B:2003:ALA:HB1 | 1:B:2102:PRO:HA  | 1.96                     | 0.48              |
| 1:B:2101:TYR:O   | 1:B:2104:ARG:CB  | 2.61                     | 0.48              |
| 1:C:1983:ALA:O   | 1:C:1987:ASP:N   | 2.47                     | 0.48              |
| 1:B:233:UNK:CA   | 1:B:255:UNK:CB   | 2.92                     | 0.48              |
| 1:B:2146:THR:O   | 1:B:2150:SER:N   | 2.47                     | 0.48              |
| 1:B:2298:PRO:O   | 1:B:2301:ARG:CB  | 2.59                     | 0.48              |
| 1:C:2101:TYR:O   | 1:C:2104:ARG:CB  | 2.61                     | 0.48              |
| 1:B:241:UNK:CA   | 1:B:248:UNK:CB   | 2.87                     | 0.47              |
| 1:B:1368:UNK:O   | 1:B:1372:UNK:N   | 2.47                     | 0.47              |
| 1:B:2046:LYS:HA  | 1:B:2050:GLN:CA  | 2.44                     | 0.47              |
| 1:B:2050:GLN:CB  | 1:B:2051:VAL:HA  | 2.43                     | 0.47              |
| 1:A:211:UNK:CB   | 1:A:277:UNK:CB   | 2.92                     | 0.47              |
| 1:A:1368:UNK:O   | 1:A:1372:UNK:N   | 2.47                     | 0.47              |
| 1:A:2046:LYS:C   | 1:A:2048:ALA:H   | 2.22                     | 0.47              |
| 1:A:2106:LEU:O   | 1:A:2110:LEU:CB  | 2.62                     | 0.47              |
| 1:B:234:UNK:C    | 1:B:236:UNK:N    | 2.74                     | 0.47              |
| 1:B:2052:VAL:O   | 1:B:2056:ALA:HA  | 2.14                     | 0.47              |
| 1:B:2106:LEU:O   | 1:B:2110:LEU:CB  | 2.62                     | 0.47              |
| 1:C:2046:LYS:HA  | 1:C:2049:PHE:CB  | 2.44                     | 0.47              |
| 1:C:2222:GLN:OE1 | 1:C:2282:VAL:CG1 | 2.62                     | 0.47              |
| 1:C:2409:GLN:CD  | 1:C:2426:PHE:CZ  | 2.85                     | 0.47              |
| 1:A:2153:MET:CA  | 1:A:2156:GLU:CB  | 2.85                     | 0.47              |
| 1:A:2222:GLN:OE1 | 1:A:2282:VAL:CG1 | 2.62                     | 0.47              |
| 1:B:2041:LYS:O   | 1:B:2043:VAL:CA  | 2.62                     | 0.47              |
| 1:B:2041:LYS:HA  | 1:B:2044:LEU:CB  | 2.44                     | 0.47              |
| 1:C:1974:THR:C   | 1:C:1976:VAL:N   | 2.71                     | 0.47              |
| 1:C:2146:THR:O   | 1:C:2150:SER:N   | 2.47                     | 0.47              |
| 1:A:237:UNK:CA   | 1:A:252:UNK:CA   | 2.28                     | 0.47              |
| 1:A:1974:THR:C   | 1:A:1976:VAL:N   | 2.71                     | 0.47              |
| 1:A:2406:ARG:NH2 | 1:A:2429:TRP:CZ2 | 2.82                     | 0.47              |
| 1:A:201:UNK:N    | 1:A:288:UNK:CB   | 2.75                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:241:UNK:CA    | 1:A:248:UNK:CB    | 2.85                     | 0.47              |
| 1:C:2003:ALA:CB   | 1:C:2102:PRO:CA   | 2.89                     | 0.47              |
| 1:C:2106:LEU:O    | 1:C:2110:LEU:CB   | 2.62                     | 0.47              |
| 1:A:2406:ARG:NH2  | 1:A:2429:TRP:HZ2  | 2.13                     | 0.47              |
| 1:B:1776:UNK:CB   | 1:B:1781:UNK:CA   | 2.85                     | 0.47              |
| 1:B:2222:GLN:OE1  | 1:B:2282:VAL:CG1  | 2.62                     | 0.47              |
| 1:B:2299:PRO:C    | 1:B:2301:ARG:H    | 2.19                     | 0.47              |
| 1:C:2044:LEU:O    | 1:C:2047:LEU:CB   | 2.63                     | 0.47              |
| 1:C:2176:PRO:O    | 1:C:2180:GLY:N    | 2.45                     | 0.47              |
| 1:A:1793:UNK:C    | 1:A:1797:UNK:CB   | 2.93                     | 0.47              |
| 1:A:2049:PHE:N    | 1:A:2051:VAL:CB   | 2.78                     | 0.47              |
| 1:A:2077:ALA:N    | 1:A:2083:TYR:CB   | 2.78                     | 0.47              |
| 1:A:2297:SER:CB   | 1:C:2429:TRP:CH2  | 2.98                     | 0.47              |
| 1:B:2051:VAL:C    | 1:B:2053:LEU:N    | 2.73                     | 0.47              |
| 1:B:2077:ALA:N    | 1:B:2083:TYR:CB   | 2.78                     | 0.47              |
| 1:B:2219:VAL:C    | 1:B:2452:LYS:HE3  | 2.33                     | 0.47              |
| 1:B:2297:SER:O    | 1:B:2298:PRO:C    | 2.58                     | 0.47              |
| 1:C:1368:UNK:O    | 1:C:1372:UNK:N    | 2.47                     | 0.47              |
| 1:C:1994:GLY:C    | 1:C:1996:TRP:H    | 2.16                     | 0.47              |
| 1:C:2223:PRO:O    | 1:C:2248:ILE:HD13 | 2.15                     | 0.47              |
| 1:A:204:UNK:CB    | 1:A:284:UNK:CA    | 2.90                     | 0.47              |
| 1:A:2297:SER:HB3  | 1:C:2429:TRP:CE2  | 2.50                     | 0.47              |
| 1:B:2209:PHE:C    | 1:B:2211:SER:N    | 2.73                     | 0.47              |
| 1:B:2522:GLU:C    | 1:B:2524:GLU:N    | 2.72                     | 0.47              |
| 1:A:2406:ARG:NH2  | 1:A:2406:ARG:CG   | 2.73                     | 0.47              |
| 1:C:2058:HIS:C    | 1:C:2060:TRP:N    | 2.71                     | 0.47              |
| 1:B:251:UNK:C     | 1:B:253:UNK:N     | 2.77                     | 0.46              |
| 1:C:2077:ALA:N    | 1:C:2083:TYR:CB   | 2.78                     | 0.46              |
| 1:A:1990:ILE:CB   | 1:A:1991:ILE:HA   | 2.45                     | 0.46              |
| 1:B:2211:SER:C    | 1:B:2213:ILE:N    | 2.73                     | 0.46              |
| 1:B:2429:TRP:CZ2  | 1:C:2299:PRO:CD   | 2.97                     | 0.46              |
| 1:A:1776:UNK:CB   | 1:A:1781:UNK:CA   | 2.85                     | 0.46              |
| 1:B:2245:GLN:NE2  | 1:C:2339:LYS:HE3  | 2.30                     | 0.46              |
| 1:C:2003:ALA:HB1  | 1:C:2102:PRO:HA   | 1.96                     | 0.46              |
| 1:C:2003:ALA:HB2  | 1:C:2102:PRO:HA   | 1.96                     | 0.46              |
| 1:A:2003:ALA:CB   | 1:A:2102:PRO:CA   | 2.90                     | 0.46              |
| 1:A:2046:LYS:C    | 1:A:2048:ALA:N    | 2.73                     | 0.46              |
| 1:A:2050:GLN:C    | 1:A:2055:VAL:H    | 2.23                     | 0.46              |
| 1:A:2410:VAL:HG23 | 1:A:2426:PHE:CG   | 2.51                     | 0.46              |
| 1:B:2299:PRO:CG   | 1:B:2300:SER:N    | 2.78                     | 0.46              |
| 1:C:2522:GLU:C    | 1:C:2524:GLU:N    | 2.72                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1137:UNK:O    | 1:A:1141:UNK:N    | 2.48                     | 0.46              |
| 1:A:2500:VAL:O    | 1:A:2504:LEU:N    | 2.36                     | 0.46              |
| 1:B:251:UNK:O     | 1:B:255:UNK:CB    | 2.64                     | 0.46              |
| 1:B:2408:GLU:C    | 1:B:2426:PHE:CB   | 2.89                     | 0.46              |
| 1:B:2409:GLN:HG3  | 1:B:2410:VAL:CA   | 2.46                     | 0.46              |
| 1:C:2058:HIS:O    | 1:C:2060:TRP:N    | 2.49                     | 0.46              |
| 1:C:2496:GLU:O    | 1:C:2499:CYS:O    | 2.34                     | 0.46              |
| 1:B:2223:PRO:O    | 1:B:2248:ILE:HD13 | 2.15                     | 0.46              |
| 1:A:2054:VAL:C    | 1:A:2056:ALA:H    | 2.24                     | 0.46              |
| 1:A:2407:ARG:CG   | 1:A:2426:PHE:HB2  | 2.19                     | 0.46              |
| 1:B:2221:ASN:O    | 1:B:2450:SER:HB2  | 2.16                     | 0.46              |
| 1:A:2003:ALA:HB1  | 1:A:2102:PRO:HA   | 1.96                     | 0.46              |
| 1:A:2293:LEU:H    | 1:B:2295:ARG:HB2  | 1.81                     | 0.46              |
| 1:A:2299:PRO:CD   | 1:C:2408:GLU:CG   | 2.87                     | 0.46              |
| 1:A:236:UNK:C     | 1:A:238:UNK:N     | 2.73                     | 0.46              |
| 1:A:2425:ASP:O    | 1:A:2426:PHE:HD1  | 1.99                     | 0.46              |
| 1:B:240:UNK:C     | 1:B:248:UNK:HA    | 2.45                     | 0.46              |
| 1:B:283:UNK:O     | 1:B:284:UNK:C     | 2.64                     | 0.46              |
| 1:A:2245:GLN:HE22 | 1:B:2339:LYS:NZ   | 2.14                     | 0.45              |
| 1:A:2382:PRO:CD   | 1:C:2328:ALA:HB2  | 2.31                     | 0.45              |
| 1:B:2057:ILE:HA   | 1:B:2060:TRP:CB   | 2.45                     | 0.45              |
| 1:C:248:UNK:O     | 1:C:252:UNK:CA    | 2.64                     | 0.45              |
| 1:C:2213:ILE:C    | 1:C:2215:SER:N    | 2.73                     | 0.45              |
| 1:A:2057:ILE:O    | 1:A:2061:MET:N    | 2.46                     | 0.45              |
| 1:A:2221:ASN:O    | 1:A:2450:SER:HB2  | 2.16                     | 0.45              |
| 1:A:2223:PRO:O    | 1:A:2248:ILE:HD13 | 2.15                     | 0.45              |
| 1:B:2299:PRO:CG   | 1:B:2300:SER:H    | 2.29                     | 0.45              |
| 1:B:2496:GLU:O    | 1:B:2499:CYS:O    | 2.34                     | 0.45              |
| 1:C:2012:SER:O    | 1:C:2016:VAL:CB   | 2.64                     | 0.45              |
| 1:B:2012:SER:O    | 1:B:2016:VAL:CB   | 2.64                     | 0.45              |
| 1:B:2221:ASN:C    | 1:B:2222:GLN:HE21 | 2.24                     | 0.45              |
| 1:B:2297:SER:HB2  | 1:B:2299:PRO:HD2  | 1.99                     | 0.45              |
| 1:B:2500:VAL:O    | 1:B:2504:LEU:N    | 2.36                     | 0.45              |
| 1:A:2012:SER:O    | 1:A:2016:VAL:CB   | 2.64                     | 0.45              |
| 1:A:2220:VAL:HG11 | 1:A:2279:GLU:O    | 2.17                     | 0.45              |
| 1:A:2298:PRO:HD2  | 1:C:2408:GLU:HG3  | 1.94                     | 0.45              |
| 1:B:1790:UNK:O    | 1:B:1793:UNK:N    | 2.50                     | 0.45              |
| 1:B:2406:ARG:HH12 | 1:C:2299:PRO:CD   | 2.21                     | 0.45              |
| 1:C:2221:ASN:O    | 1:C:2450:SER:HB2  | 2.16                     | 0.45              |
| 1:A:204:UNK:CA    | 1:A:284:UNK:CB    | 2.94                     | 0.45              |
| 1:A:1787:UNK:O    | 1:A:1788:UNK:C    | 2.64                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2408:GLU:O    | 1:B:2426:PHE:HB2  | 2.17                     | 0.45              |
| 1:B:2425:ASP:N    | 1:B:2425:ASP:OD1  | 2.49                     | 0.45              |
| 1:A:1748:UNK:HA   | 1:A:1751:UNK:CB   | 2.47                     | 0.45              |
| 1:A:2299:PRO:CG   | 1:C:2406:ARG:HH12 | 2.28                     | 0.45              |
| 1:B:2409:GLN:HG3  | 1:B:2410:VAL:C    | 2.41                     | 0.45              |
| 1:A:2003:ALA:HB2  | 1:A:2102:PRO:HA   | 1.96                     | 0.45              |
| 1:A:2408:GLU:CG   | 1:A:2429:TRP:CH2  | 2.99                     | 0.45              |
| 1:A:2496:GLU:O    | 1:A:2499:CYS:O    | 2.34                     | 0.45              |
| 1:B:237:UNK:HA    | 1:B:252:UNK:CA    | 2.45                     | 0.45              |
| 1:C:2055:VAL:C    | 1:C:2057:ILE:N    | 2.74                     | 0.45              |
| 1:C:2220:VAL:HG11 | 1:C:2279:GLU:O    | 2.17                     | 0.45              |
| 1:B:2221:ASN:O    | 1:B:2450:SER:CB   | 2.65                     | 0.45              |
| 1:B:2409:GLN:C    | 1:B:2410:VAL:CG1  | 2.90                     | 0.45              |
| 1:A:2221:ASN:C    | 1:A:2222:GLN:HE21 | 2.24                     | 0.44              |
| 1:B:1141:UNK:O    | 1:B:1145:UNK:N    | 2.50                     | 0.44              |
| 1:C:2153:MET:CA   | 1:C:2156:GLU:CB   | 2.85                     | 0.44              |
| 1:A:1121:UNK:O    | 1:A:1125:UNK:CB   | 2.66                     | 0.44              |
| 1:A:2044:LEU:HA   | 1:A:2047:LEU:CB   | 2.47                     | 0.44              |
| 1:A:2176:PRO:O    | 1:A:2180:GLY:N    | 2.45                     | 0.44              |
| 1:A:2408:GLU:OE1  | 1:A:2429:TRP:CH2  | 2.70                     | 0.44              |
| 1:B:2527:ALA:O    | 1:B:2531:PHE:N    | 2.50                     | 0.44              |
| 1:B:1748:UNK:HA   | 1:B:1751:UNK:CB   | 2.47                     | 0.44              |
| 1:B:1974:THR:C    | 1:B:1976:VAL:N    | 2.72                     | 0.44              |
| 1:B:2212:LEU:C    | 1:B:2214:ARG:N    | 2.73                     | 0.44              |
| 1:B:2220:VAL:HG11 | 1:B:2279:GLU:O    | 2.17                     | 0.44              |
| 1:C:2408:GLU:O    | 1:C:2426:PHE:CD2  | 2.70                     | 0.44              |
| 1:A:265:UNK:CA    | 1:A:2528:LYS:CB   | 2.96                     | 0.44              |
| 1:A:1488:UNK:O    | 1:A:1492:UNK:CB   | 2.66                     | 0.44              |
| 1:A:2221:ASN:O    | 1:A:2450:SER:CB   | 2.65                     | 0.44              |
| 1:B:1121:UNK:O    | 1:B:1125:UNK:CB   | 2.66                     | 0.44              |
| 1:B:2153:MET:C    | 1:B:2156:GLU:H    | 2.25                     | 0.44              |
| 1:B:2408:GLU:N    | 1:B:2408:GLU:CD   | 2.73                     | 0.44              |
| 1:C:2153:MET:C    | 1:C:2156:GLU:H    | 2.25                     | 0.44              |
| 1:C:2206:PRO:O    | 1:C:2210:MET:N    | 2.47                     | 0.44              |
| 1:C:2221:ASN:C    | 1:C:2222:GLN:HE21 | 2.24                     | 0.44              |
| 1:A:1137:UNK:O    | 1:A:1141:UNK:CB   | 2.66                     | 0.44              |
| 1:B:1488:UNK:O    | 1:B:1492:UNK:CB   | 2.66                     | 0.44              |
| 1:A:1136:UNK:O    | 1:A:1138:UNK:N    | 2.50                     | 0.44              |
| 1:A:1747:UNK:O    | 1:A:1750:UNK:CA   | 2.65                     | 0.44              |
| 1:A:2211:SER:C    | 1:A:2213:ILE:N    | 2.73                     | 0.44              |
| 1:B:251:UNK:O     | 1:B:255:UNK:N     | 2.50                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:265:UNK:CA    | 1:B:2528:LYS:CB  | 2.96                     | 0.44              |
| 1:C:1748:UNK:HA   | 1:C:1751:UNK:CB  | 2.47                     | 0.44              |
| 1:A:2424:SER:O    | 1:A:2426:PHE:CE1 | 2.71                     | 0.44              |
| 1:A:2429:TRP:CZ2  | 1:B:2299:PRO:HD2 | 2.53                     | 0.44              |
| 1:B:1795:UNK:O    | 1:B:1798:UNK:N   | 2.51                     | 0.44              |
| 1:B:2297:SER:OG   | 1:B:2300:SER:HB2 | 2.17                     | 0.44              |
| 1:B:2408:GLU:OE1  | 1:B:2429:TRP:CH2 | 2.70                     | 0.44              |
| 1:C:2221:ASN:O    | 1:C:2450:SER:CB  | 2.65                     | 0.44              |
| 1:A:1773:UNK:HA   | 1:A:1776:UNK:CB  | 2.48                     | 0.44              |
| 1:B:1773:UNK:HA   | 1:B:1776:UNK:CB  | 2.48                     | 0.44              |
| 1:C:1747:UNK:O    | 1:C:1750:UNK:CA  | 2.65                     | 0.44              |
| 1:A:2409:GLN:OE1  | 1:A:2426:PHE:CZ  | 2.70                     | 0.44              |
| 1:A:2528:LYS:HA   | 1:A:2531:PHE:CB  | 2.48                     | 0.44              |
| 1:C:1121:UNK:O    | 1:C:1125:UNK:CB  | 2.66                     | 0.44              |
| 1:A:1132:UNK:C    | 1:A:1134:UNK:N   | 2.79                     | 0.43              |
| 1:A:2153:MET:C    | 1:A:2156:GLU:H   | 2.25                     | 0.43              |
| 1:A:2217:VAL:CB   | 1:A:2455:PRO:CD  | 2.96                     | 0.43              |
| 1:A:2527:ALA:O    | 1:A:2531:PHE:N   | 2.50                     | 0.43              |
| 1:C:1773:UNK:HA   | 1:C:1776:UNK:CB  | 2.48                     | 0.43              |
| 1:B:2224:ILE:HG12 | 1:B:2224:ILE:H   | 1.56                     | 0.43              |
| 1:B:2406:ARG:HH22 | 1:C:2299:PRO:HG3 | 1.81                     | 0.43              |
| 1:C:1488:UNK:O    | 1:C:1492:UNK:CB  | 2.66                     | 0.43              |
| 1:C:2424:SER:O    | 1:C:2426:PHE:HD1 | 2.01                     | 0.43              |
| 1:C:2425:ASP:O    | 1:C:2426:PHE:CD1 | 2.70                     | 0.43              |
| 1:A:2410:VAL:N    | 1:B:2425:ASP:OD2 | 2.51                     | 0.43              |
| 1:B:1747:UNK:O    | 1:B:1750:UNK:CA  | 2.65                     | 0.43              |
| 1:B:2050:GLN:N    | 1:B:2051:VAL:HA  | 2.33                     | 0.43              |
| 1:B:2406:ARG:HH12 | 1:C:2299:PRO:CB  | 2.28                     | 0.43              |
| 1:B:2409:GLN:CD   | 1:B:2426:PHE:CE1 | 2.96                     | 0.43              |
| 1:A:884:UNK:O     | 1:A:885:UNK:C    | 2.64                     | 0.43              |
| 1:A:2299:PRO:HD3  | 1:C:2408:GLU:CG  | 2.43                     | 0.43              |
| 1:B:2153:MET:CA   | 1:B:2156:GLU:CB  | 2.85                     | 0.43              |
| 1:C:2146:THR:O    | 1:C:2150:SER:HA  | 2.19                     | 0.43              |
| 1:C:2306:GLN:NE2  | 1:C:2310:ASN:OD1 | 2.51                     | 0.43              |
| 1:C:2424:SER:O    | 1:C:2426:PHE:CD1 | 2.70                     | 0.43              |
| 1:A:1794:UNK:O    | 1:A:1798:UNK:N   | 2.51                     | 0.43              |
| 1:A:2407:ARG:HE   | 1:A:2426:PHE:N   | 2.14                     | 0.43              |
| 1:A:2531:PHE:O    | 1:A:2535:SER:N   | 2.50                     | 0.43              |
| 1:B:2215:SER:O    | 1:B:2216:VAL:CB  | 2.67                     | 0.43              |
| 1:B:2409:GLN:CA   | 1:B:2426:PHE:HB3 | 2.47                     | 0.43              |
| 1:A:2406:ARG:NH1  | 1:A:2429:TRP:HZ2 | 2.15                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:2146:THR:O    | 1:B:2150:SER:HA  | 2.19                     | 0.43              |
| 1:B:2429:TRP:CZ2  | 1:C:2299:PRO:CG  | 3.01                     | 0.43              |
| 1:A:2406:ARG:CZ   | 1:A:2429:TRP:HZ2 | 2.28                     | 0.43              |
| 1:B:884:UNK:O     | 1:B:885:UNK:C    | 2.65                     | 0.43              |
| 1:B:2219:VAL:CG2  | 1:B:2220:VAL:H   | 2.28                     | 0.43              |
| 1:B:1136:UNK:O    | 1:B:1138:UNK:N   | 2.52                     | 0.43              |
| 1:B:2519:LEU:O    | 1:B:2521:LEU:N   | 2.52                     | 0.43              |
| 1:C:1749:UNK:HA   | 1:C:1752:UNK:CB  | 2.49                     | 0.43              |
| 1:A:2146:THR:O    | 1:A:2150:SER:HA  | 2.19                     | 0.43              |
| 1:B:1749:UNK:HA   | 1:B:1752:UNK:CB  | 2.49                     | 0.43              |
| 1:B:2003:ALA:HB2  | 1:B:2102:PRO:HA  | 1.96                     | 0.43              |
| 1:B:2528:LYS:HA   | 1:B:2531:PHE:CB  | 2.48                     | 0.43              |
| 1:A:2406:ARG:NH1  | 1:B:2299:PRO:CD  | 2.70                     | 0.43              |
| 1:B:2176:PRO:O    | 1:B:2180:GLY:N   | 2.45                     | 0.43              |
| 1:C:265:UNK:CA    | 1:C:2528:LYS:CB  | 2.96                     | 0.43              |
| 1:C:2527:ALA:O    | 1:C:2531:PHE:N   | 2.50                     | 0.43              |
| 1:C:2528:LYS:HA   | 1:C:2531:PHE:CB  | 2.48                     | 0.42              |
| 1:A:1791:UNK:O    | 1:A:1795:UNK:N   | 2.52                     | 0.42              |
| 1:B:1140:UNK:O    | 1:B:1142:UNK:N   | 2.52                     | 0.42              |
| 1:B:2407:ARG:HD3  | 1:B:2426:PHE:CD2 | 2.55                     | 0.42              |
| 1:C:2045:GLY:C    | 1:C:2047:LEU:N   | 2.73                     | 0.42              |
| 1:A:1749:UNK:HA   | 1:A:1752:UNK:CB  | 2.49                     | 0.42              |
| 1:C:2318:ARG:HD2  | 1:C:2339:LYS:HD2 | 2.01                     | 0.42              |
| 1:A:2308:LEU:HB3  | 1:A:2355:ALA:HB2 | 2.01                     | 0.42              |
| 1:B:1133:UNK:O    | 1:B:1137:UNK:CB  | 2.68                     | 0.42              |
| 1:B:2306:GLN:NE2  | 1:B:2310:ASN:OD1 | 2.51                     | 0.42              |
| 1:A:2318:ARG:HD2  | 1:A:2339:LYS:HD2 | 2.01                     | 0.42              |
| 1:C:2055:VAL:O    | 1:C:2057:ILE:N   | 2.52                     | 0.42              |
| 1:A:2426:PHE:O    | 1:A:2427:LEU:O   | 2.38                     | 0.42              |
| 1:B:1136:UNK:O    | 1:B:1137:UNK:C   | 2.68                     | 0.42              |
| 1:C:226:UNK:CB    | 1:C:263:UNK:CB   | 2.97                     | 0.42              |
| 1:C:2519:LEU:O    | 1:C:2521:LEU:N   | 2.52                     | 0.42              |
| 1:A:1133:UNK:O    | 1:A:1137:UNK:CB  | 2.68                     | 0.42              |
| 1:B:2429:TRP:CH2  | 1:C:2297:SER:CA  | 3.01                     | 0.42              |
| 1:C:1137:UNK:O    | 1:C:1141:UNK:CB  | 2.67                     | 0.42              |
| 1:A:2003:ALA:HB1  | 1:A:2102:PRO:CA  | 2.50                     | 0.42              |
| 1:B:2224:ILE:HD11 | 1:B:2324:GLN:HG2 | 2.02                     | 0.42              |
| 1:C:2003:ALA:HB1  | 1:C:2102:PRO:CA  | 2.50                     | 0.42              |
| 1:C:2538:THR:O    | 1:C:2542:TRP:N   | 2.47                     | 0.42              |
| 1:A:2426:PHE:CD1  | 1:A:2426:PHE:N   | 2.87                     | 0.41              |
| 1:B:1788:UNK:C    | 1:B:1790:UNK:N   | 2.83                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2318:ARG:HD2  | 1:B:2339:LYS:HD2  | 2.01                     | 0.41              |
| 1:A:2054:VAL:O    | 1:A:2056:ALA:N    | 2.45                     | 0.41              |
| 1:A:2224:ILE:HD11 | 1:A:2324:GLN:HG2  | 2.02                     | 0.41              |
| 1:A:2299:PRO:HG3  | 1:C:2406:ARG:CZ   | 2.49                     | 0.41              |
| 1:A:2306:GLN:NE2  | 1:A:2310:ASN:OD1  | 2.51                     | 0.41              |
| 1:A:2519:LEU:O    | 1:A:2521:LEU:N    | 2.52                     | 0.41              |
| 1:B:2003:ALA:HB1  | 1:B:2102:PRO:CA   | 2.50                     | 0.41              |
| 1:C:2308:LEU:HB3  | 1:C:2355:ALA:HB2  | 2.02                     | 0.41              |
| 1:B:2293:LEU:HD11 | 1:B:2427:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:2224:ILE:HD11 | 1:C:2324:GLN:HG2  | 2.02                     | 0.41              |
| 1:A:2045:GLY:C    | 1:A:2047:LEU:N    | 2.78                     | 0.41              |
| 1:A:2426:PHE:HD1  | 1:A:2426:PHE:N    | 2.18                     | 0.41              |
| 1:B:564:UNK:C     | 1:B:566:UNK:N     | 2.83                     | 0.41              |
| 1:C:2410:VAL:CG2  | 1:C:2426:PHE:CD1  | 3.01                     | 0.41              |
| 1:C:2211:SER:C    | 1:C:2213:ILE:N    | 2.78                     | 0.41              |
| 1:C:2213:ILE:O    | 1:C:2215:SER:N    | 2.53                     | 0.41              |
| 1:B:2268:LEU:HD23 | 1:B:2268:LEU:HA   | 1.88                     | 0.41              |
| 1:C:240:UNK:CB    | 1:C:248:UNK:HA    | 2.50                     | 0.41              |
| 1:C:2425:ASP:OD1  | 1:C:2426:PHE:N    | 2.54                     | 0.41              |
| 1:A:1136:UNK:O    | 1:A:1137:UNK:C    | 2.69                     | 0.41              |
| 1:C:564:UNK:C     | 1:C:566:UNK:N     | 2.83                     | 0.41              |
| 1:C:2003:ALA:CB   | 1:C:2102:PRO:CB   | 2.99                     | 0.41              |
| 1:B:2308:LEU:HB3  | 1:B:2355:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:250:UNK:O     | 1:A:252:UNK:N     | 2.53                     | 0.41              |
| 1:A:2045:GLY:C    | 1:A:2047:LEU:H    | 2.28                     | 0.41              |
| 1:A:2206:PRO:O    | 1:A:2210:MET:N    | 2.47                     | 0.41              |
| 1:B:240:UNK:C     | 1:B:247:UNK:C     | 2.99                     | 0.41              |
| 1:C:1991:ILE:O    | 1:C:1992:ILE:C    | 2.62                     | 0.41              |
| 1:C:2213:ILE:C    | 1:C:2215:SER:H    | 2.29                     | 0.41              |
| 1:C:2293:LEU:HD11 | 1:C:2427:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:2152:TRP:O    | 1:A:2155:VAL:N    | 2.54                     | 0.40              |
| 1:B:241:UNK:O     | 1:B:242:UNK:C     | 2.69                     | 0.40              |
| 1:B:2212:LEU:O    | 1:B:2214:ARG:N    | 2.54                     | 0.40              |
| 1:B:2219:VAL:CG2  | 1:B:2220:VAL:HG23 | 2.44                     | 0.40              |
| 1:B:2429:TRP:HZ3  | 1:C:2298:PRO:HD2  | 1.34                     | 0.40              |
| 1:A:2409:GLN:NE2  | 1:A:2410:VAL:C    | 2.73                     | 0.40              |
| 1:B:2531:PHE:O    | 1:B:2535:SER:N    | 2.50                     | 0.40              |
| 1:C:2152:TRP:O    | 1:C:2155:VAL:N    | 2.55                     | 0.40              |
| 1:A:2003:ALA:CB   | 1:A:2102:PRO:CB   | 2.99                     | 0.40              |
| 1:A:2003:ALA:HB1  | 1:A:2102:PRO:CB   | 2.52                     | 0.40              |
| 1:A:2382:PRO:HG3  | 1:C:2328:ALA:CA   | 2.51                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:2003:ALA:CB | 1:B:2102:PRO:CB  | 2.99                     | 0.40              |
| 1:C:2217:VAL:CB | 1:C:2455:PRO:CD  | 2.99                     | 0.40              |
| 1:A:1986:VAL:O  | 1:A:1989:ILE:N   | 2.55                     | 0.40              |
| 1:A:2297:SER:O  | 1:A:2301:ARG:N   | 2.42                     | 0.40              |
| 1:B:2056:ALA:C  | 1:B:2058:HIS:N   | 2.79                     | 0.40              |
| 1:A:2044:LEU:O  | 1:A:2045:GLY:C   | 2.64                     | 0.40              |
| 1:A:2425:ASP:C  | 1:A:2426:PHE:CD1 | 2.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | A     | 568/2553 (22%)  | 512 (90%)  | 31 (6%) | 25 (4%)  | 2           | 17 |
| 1   | B     | 568/2553 (22%)  | 513 (90%)  | 27 (5%) | 28 (5%)  | 1           | 16 |
| 1   | C     | 568/2553 (22%)  | 513 (90%)  | 27 (5%) | 28 (5%)  | 1           | 16 |
| All | All   | 1704/7659 (22%) | 1538 (90%) | 85 (5%) | 81 (5%)  | 3           | 16 |

All (81) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1992 | ILE  |
| 1   | A     | 1993 | PHE  |
| 1   | A     | 2025 | LEU  |
| 1   | A     | 2043 | VAL  |
| 1   | A     | 2051 | VAL  |
| 1   | A     | 2054 | VAL  |
| 1   | A     | 2059 | ILE  |
| 1   | A     | 2061 | MET  |
| 1   | A     | 2065 | LEU  |
| 1   | A     | 2066 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2174 | LYS  |
| 1   | A     | 2216 | VAL  |
| 1   | A     | 2217 | VAL  |
| 1   | A     | 2410 | VAL  |
| 1   | A     | 2456 | PRO  |
| 1   | A     | 2523 | GLU  |
| 1   | B     | 1990 | ILE  |
| 1   | B     | 2025 | LEU  |
| 1   | B     | 2041 | LYS  |
| 1   | B     | 2042 | THR  |
| 1   | B     | 2052 | VAL  |
| 1   | B     | 2058 | HIS  |
| 1   | B     | 2065 | LEU  |
| 1   | B     | 2066 | PRO  |
| 1   | B     | 2174 | LYS  |
| 1   | B     | 2216 | VAL  |
| 1   | B     | 2217 | VAL  |
| 1   | B     | 2410 | VAL  |
| 1   | B     | 2427 | LEU  |
| 1   | B     | 2456 | PRO  |
| 1   | B     | 2523 | GLU  |
| 1   | C     | 1991 | ILE  |
| 1   | C     | 1992 | ILE  |
| 1   | C     | 1995 | PHE  |
| 1   | C     | 2025 | LEU  |
| 1   | C     | 2041 | LYS  |
| 1   | C     | 2055 | VAL  |
| 1   | C     | 2058 | HIS  |
| 1   | C     | 2060 | TRP  |
| 1   | C     | 2065 | LEU  |
| 1   | C     | 2066 | PRO  |
| 1   | C     | 2174 | LYS  |
| 1   | C     | 2410 | VAL  |
| 1   | C     | 2456 | PRO  |
| 1   | C     | 2523 | GLU  |
| 1   | A     | 2055 | VAL  |
| 1   | A     | 2215 | SER  |
| 1   | A     | 2458 | LEU  |
| 1   | B     | 2059 | ILE  |
| 1   | B     | 2219 | VAL  |
| 1   | B     | 2409 | GLN  |
| 1   | B     | 2458 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2042 | THR  |
| 1   | C     | 2051 | VAL  |
| 1   | C     | 2216 | VAL  |
| 1   | C     | 2458 | LEU  |
| 1   | A     | 1994 | GLY  |
| 1   | A     | 2111 | THR  |
| 1   | A     | 2520 | GLU  |
| 1   | A     | 2526 | TYR  |
| 1   | B     | 2111 | THR  |
| 1   | B     | 2210 | MET  |
| 1   | B     | 2520 | GLU  |
| 1   | B     | 2526 | TYR  |
| 1   | C     | 2056 | ALA  |
| 1   | C     | 2111 | THR  |
| 1   | C     | 2520 | GLU  |
| 1   | C     | 2526 | TYR  |
| 1   | A     | 2078 | VAL  |
| 1   | B     | 2055 | VAL  |
| 1   | B     | 2078 | VAL  |
| 1   | C     | 2045 | GLY  |
| 1   | C     | 2078 | VAL  |
| 1   | A     | 2081 | LEU  |
| 1   | B     | 2081 | LEU  |
| 1   | B     | 2206 | PRO  |
| 1   | C     | 2081 | LEU  |
| 1   | C     | 2214 | ARG  |
| 1   | C     | 1994 | GLY  |
| 1   | C     | 2059 | ILE  |
| 1   | B     | 1994 | GLY  |

### 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     | 200/522 (38%) | 193 (96%) | 7 (4%)   | 32          | 53 |
| 1   | B     | 200/522 (38%) | 188 (94%) | 12 (6%)  | 17          | 39 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | C     | 200/522 (38%)  | 194 (97%) | 6 (3%)   | 36          | 57 |
| All | All   | 600/1566 (38%) | 575 (96%) | 25 (4%)  | 28          | 48 |

All (25) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2220 | VAL  |
| 1   | A     | 2224 | ILE  |
| 1   | A     | 2295 | ARG  |
| 1   | A     | 2391 | GLN  |
| 1   | A     | 2408 | GLU  |
| 1   | A     | 2410 | VAL  |
| 1   | A     | 2427 | LEU  |
| 1   | B     | 2220 | VAL  |
| 1   | B     | 2224 | ILE  |
| 1   | B     | 2295 | ARG  |
| 1   | B     | 2297 | SER  |
| 1   | B     | 2300 | SER  |
| 1   | B     | 2391 | GLN  |
| 1   | B     | 2407 | ARG  |
| 1   | B     | 2408 | GLU  |
| 1   | B     | 2409 | GLN  |
| 1   | B     | 2410 | VAL  |
| 1   | B     | 2425 | ASP  |
| 1   | B     | 2426 | PHE  |
| 1   | C     | 2220 | VAL  |
| 1   | C     | 2224 | ILE  |
| 1   | C     | 2295 | ARG  |
| 1   | C     | 2391 | GLN  |
| 1   | C     | 2409 | GLN  |
| 1   | C     | 2454 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2245 | GLN  |
| 1   | A     | 2356 | GLN  |
| 1   | A     | 2380 | ASN  |
| 1   | A     | 2409 | GLN  |
| 1   | B     | 2245 | GLN  |
| 1   | B     | 2356 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2380 | ASN  |
| 1   | B     | 2409 | GLN  |
| 1   | C     | 2245 | GLN  |
| 1   | C     | 2356 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

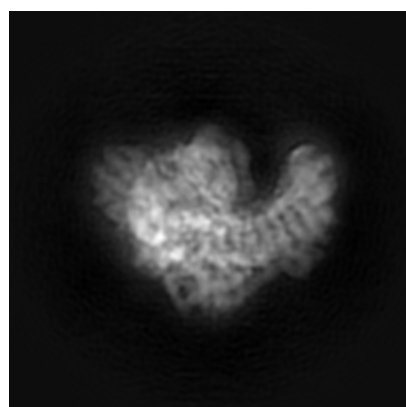
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6343. These allow visual inspection of the internal detail of the map and identification of artifacts.

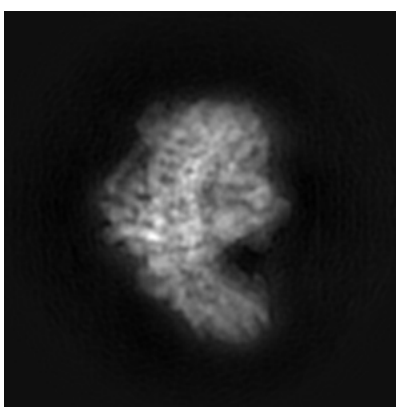
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

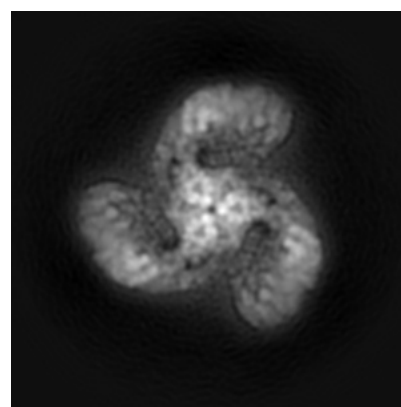
#### 6.1.1 Primary map



X



Y

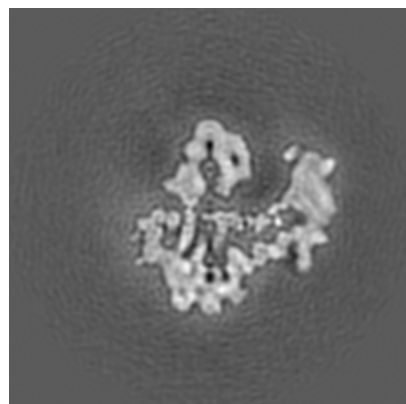


Z

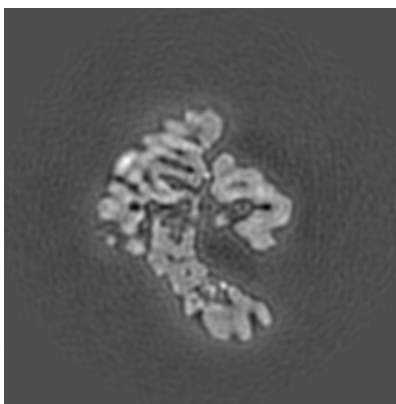
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

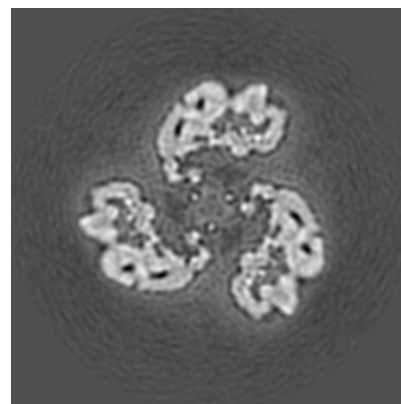
#### 6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

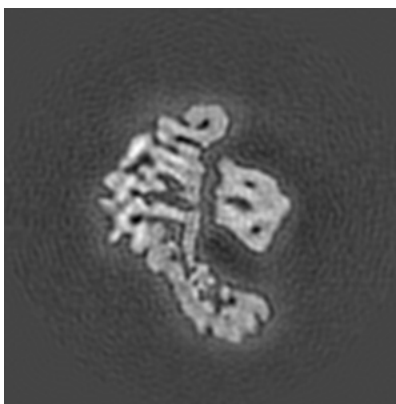
The images above show central slices of the map in three orthogonal directions.

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

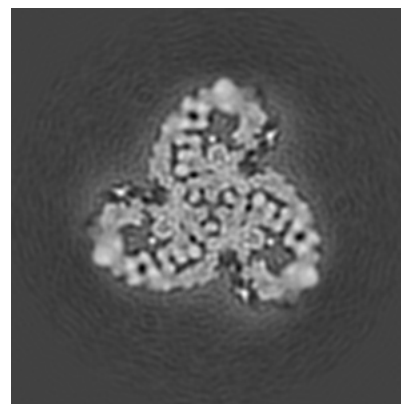
### 6.3.1 Primary map



X Index: 107



Y Index: 115

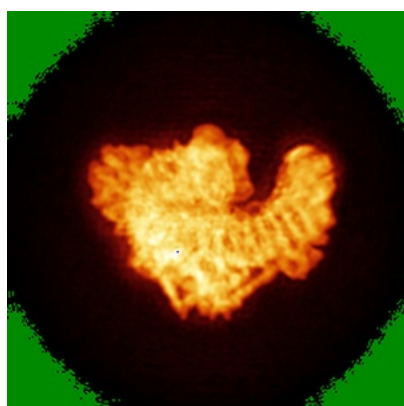


Z Index: 112

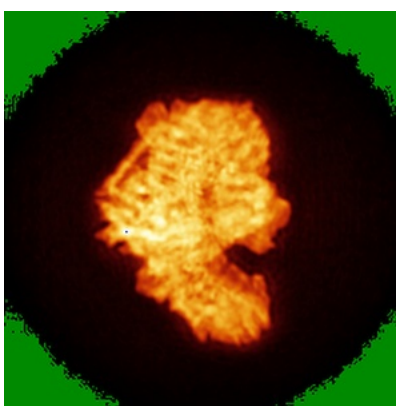
The images above show the largest variance slices of the map in three orthogonal directions.

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

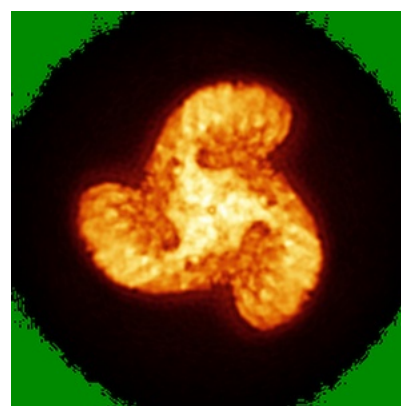
### 6.4.1 Primary map



X



Y

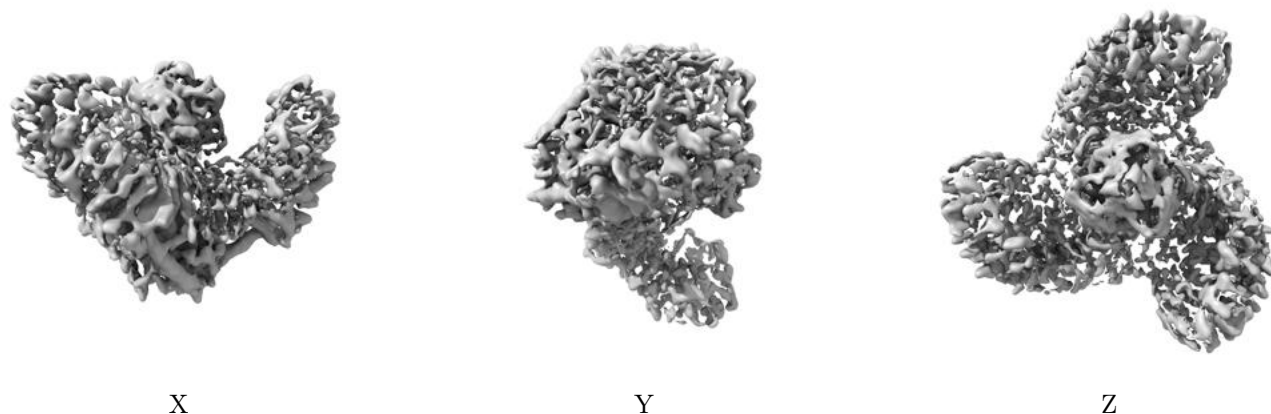


Z

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 0.0273. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

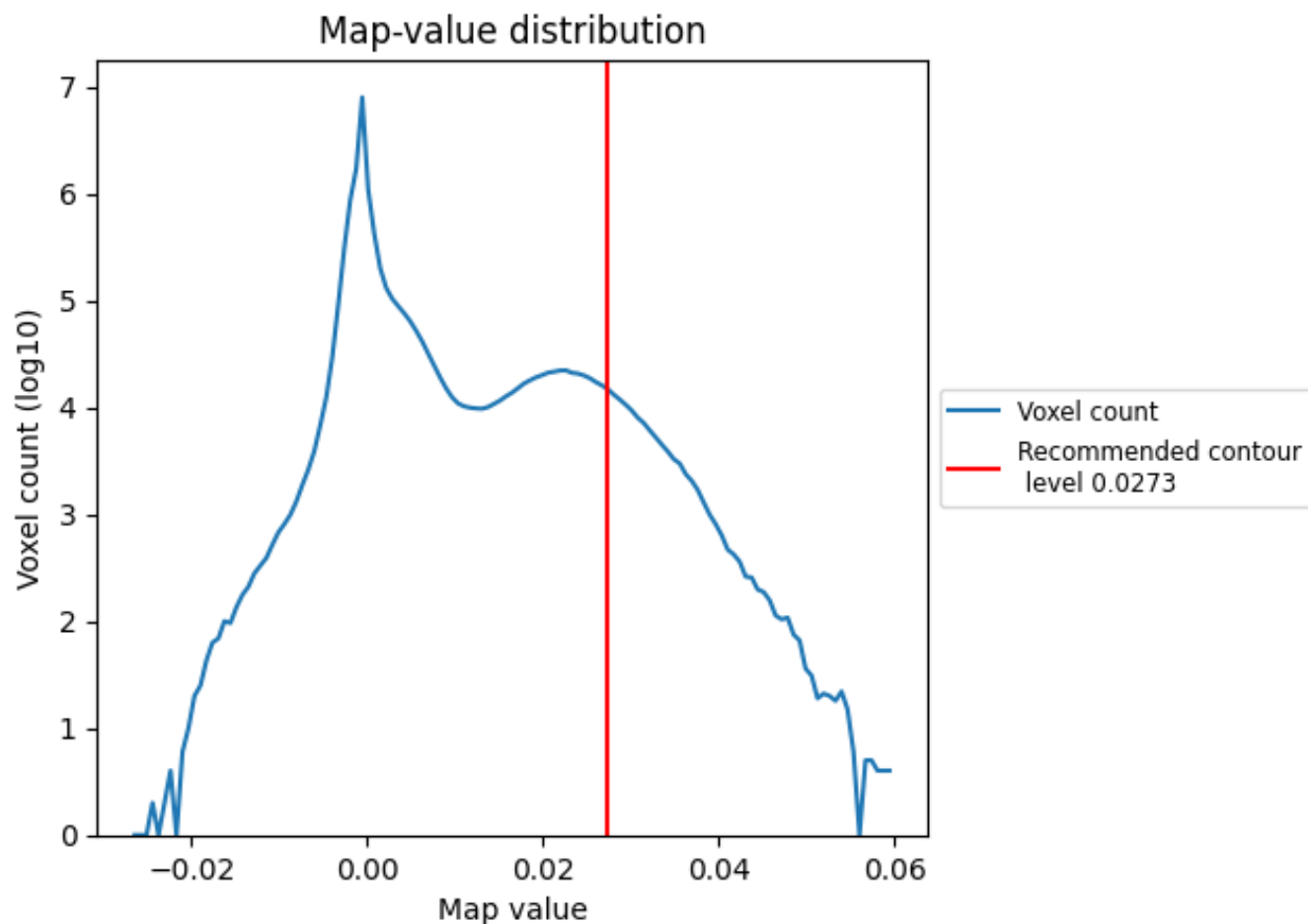
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

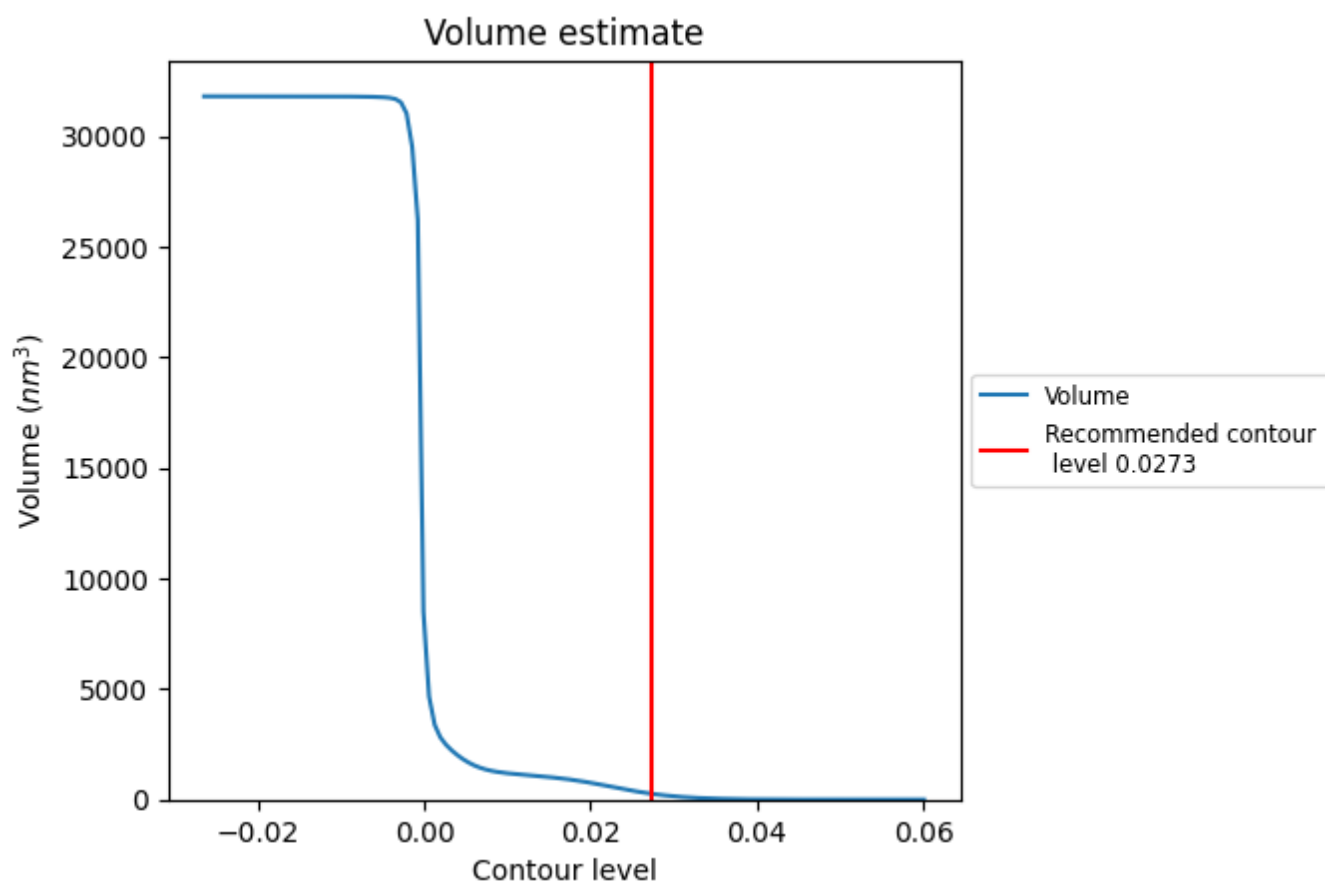
This section contains the results of statistical analysis of the map.

### 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.

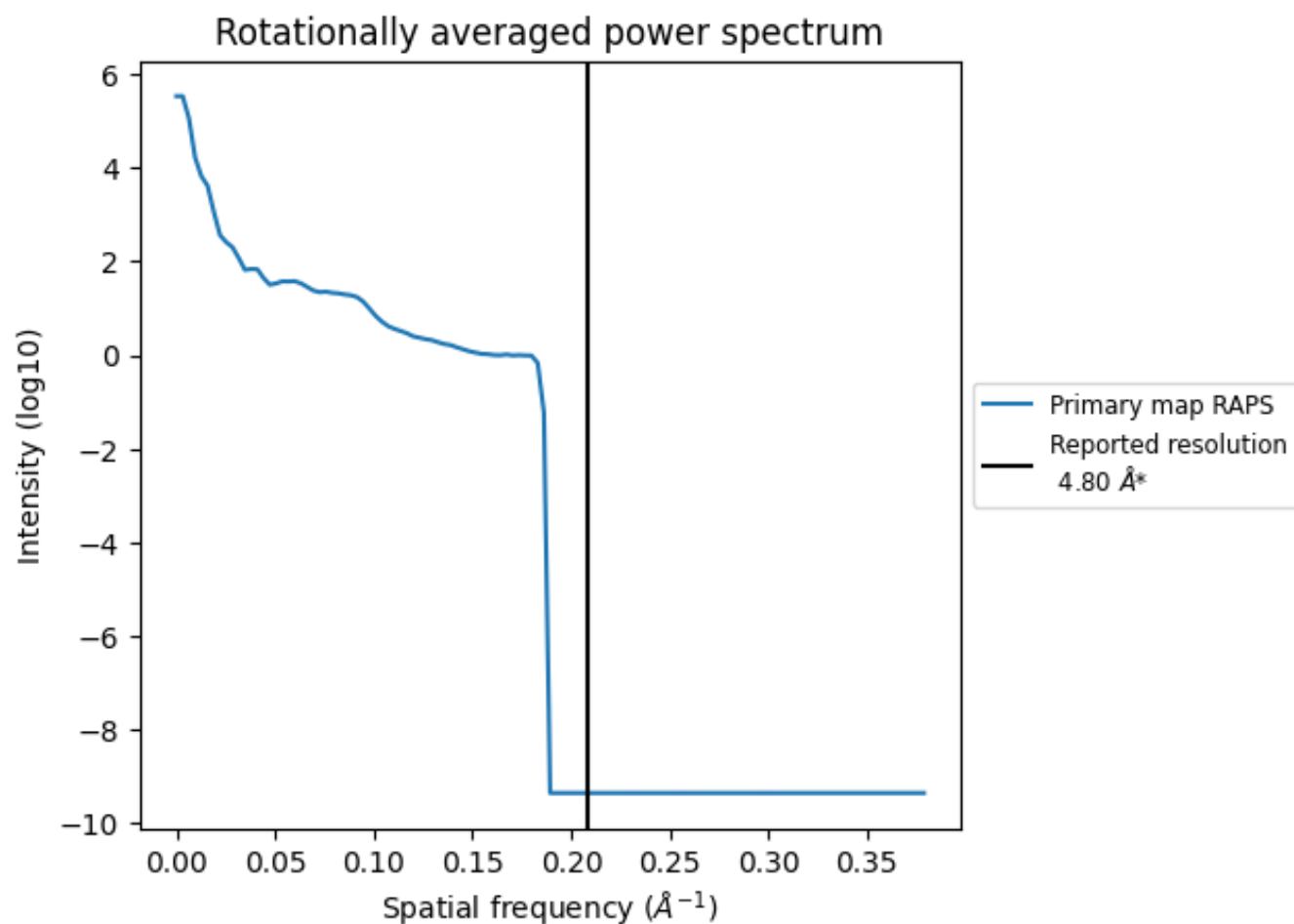
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm<sup>3</sup>; this corresponds to an approximate mass of 240 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 0.208 Å<sup>-1</sup>

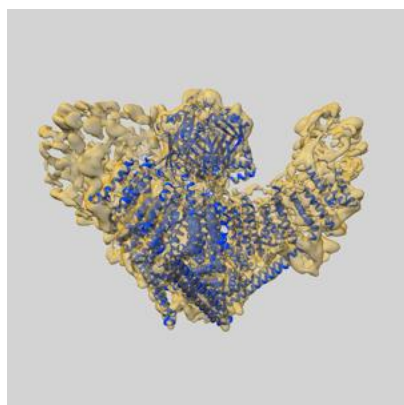
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

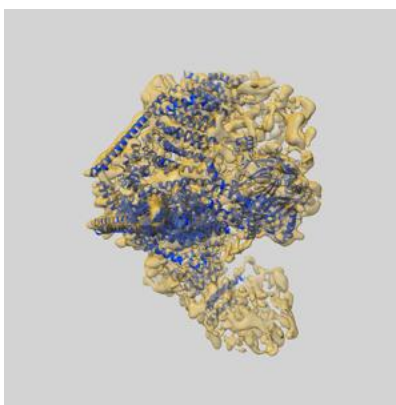
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6343 and PDB model 3JAC. Per-residue inclusion information can be found in section [3](#) on page [4](#).

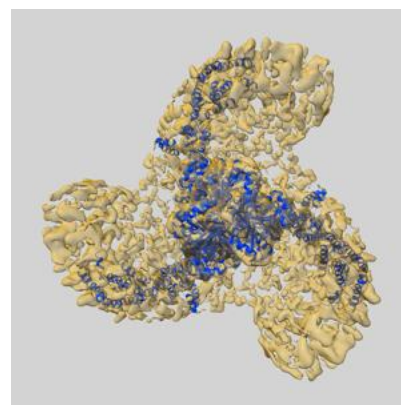
### 9.1 Map-model overlay [i](#)



X



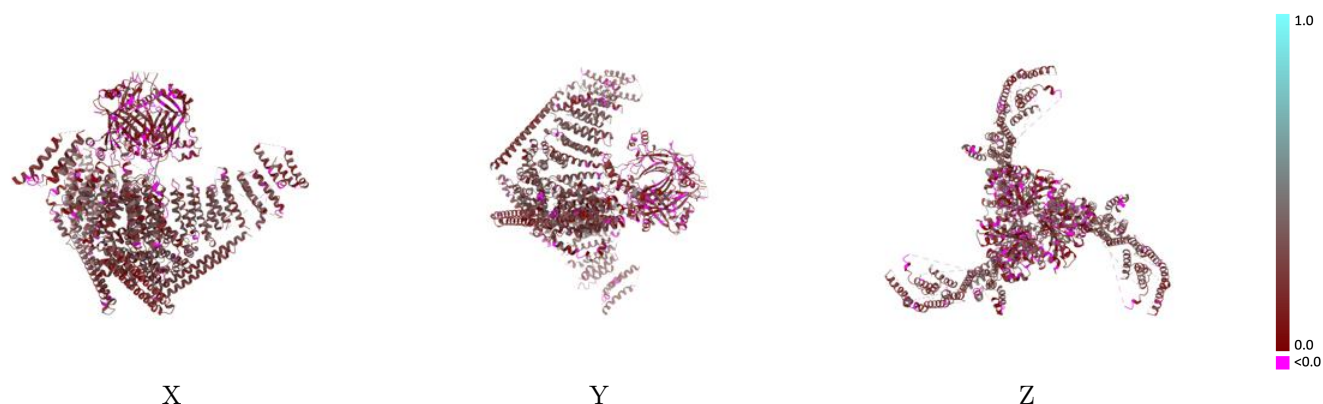
Y



Z

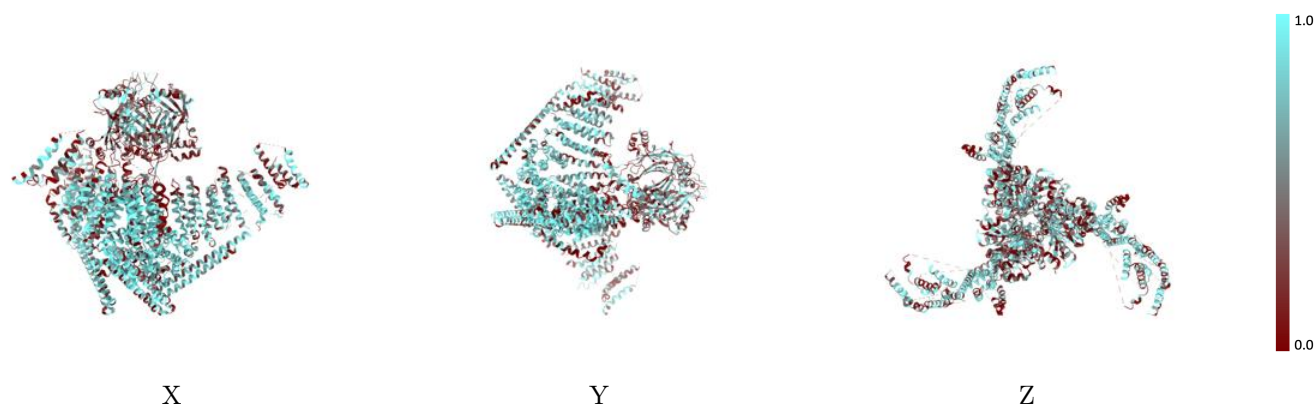
The images above show the 3D surface view of the map at the recommended contour level 0.0273 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



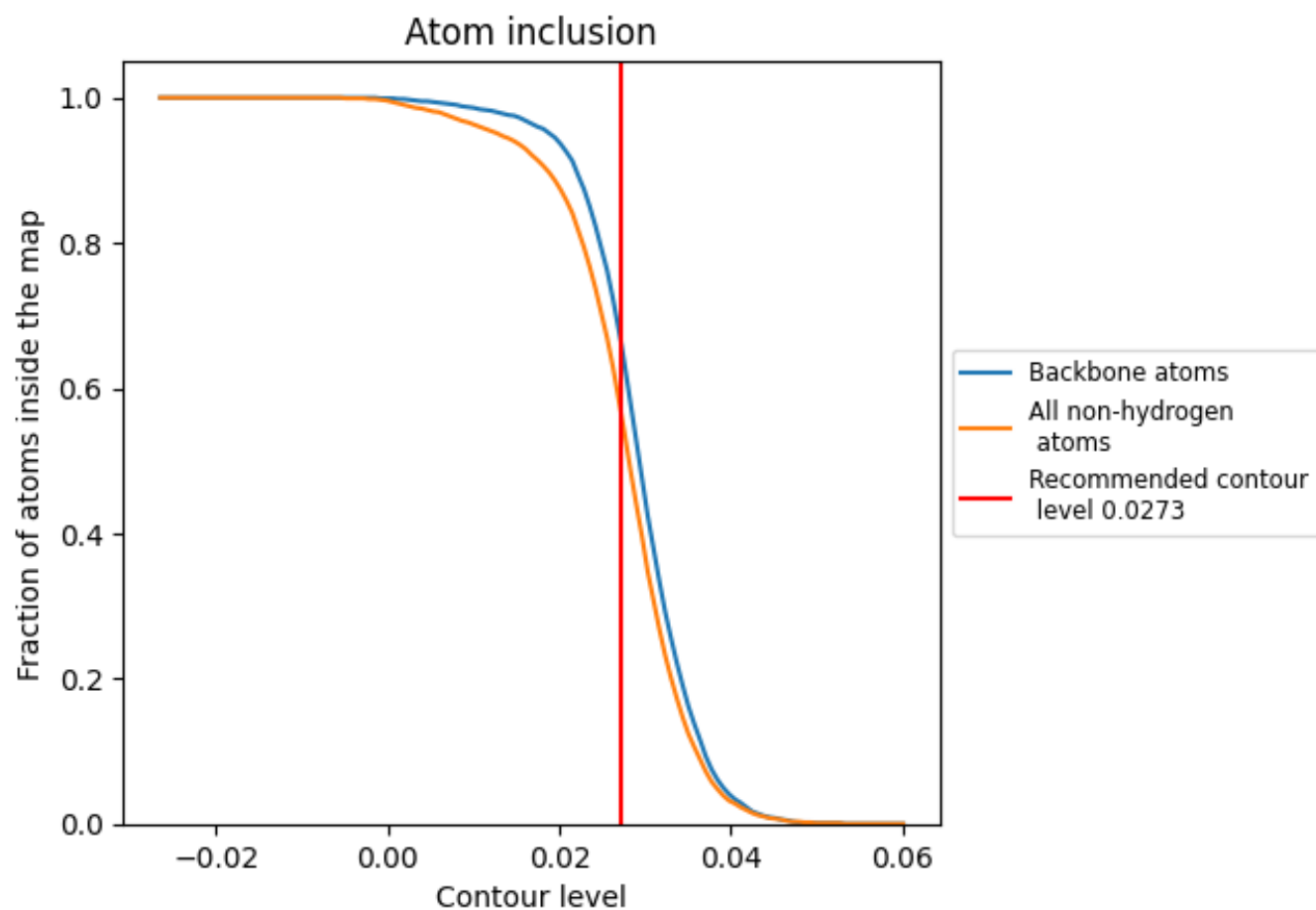
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0273).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 56% 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 (0.0273) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.5610 | <div></div> 0.1900 |
| A     | <div></div> 0.5610 | <div></div> 0.1890 |
| B     | <div></div> 0.5620 | <div></div> 0.1880 |
| C     | <div></div> 0.5600 | <div></div> 0.1920 |

