



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:02 PM UTC

PDB ID : 8QQM / pdb\_00008qqm  
EMDB ID : EMD-18596  
Title : nicotinic acetylcholine receptor in intact synaptic membrane  
Authors : Unwin, N.  
Deposited on : 2023-10-05  
Resolution : 4.70 Å(reported)  
Based on initial model : 7SMM

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:

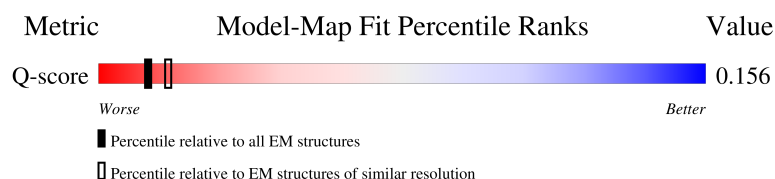
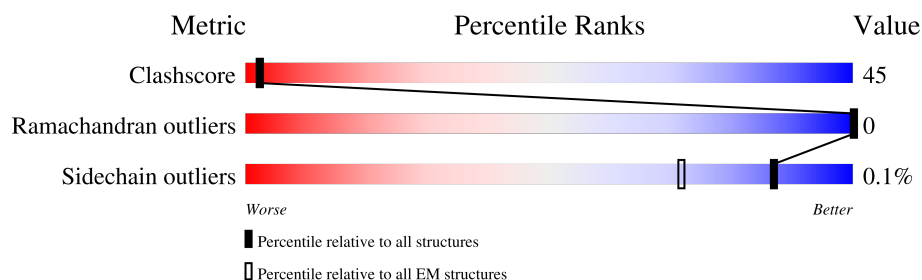
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 4.70 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                       | 1989 ( 4.20 - 5.20 )                                     |

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     | 437    |                  |
| 1   | D     | 437    |                  |
| 2   | B     | 501    |                  |
| 3   | C     | 469    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 4   | E     | 489    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>16%17%•65%</div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7118 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 Acetylcholine receptor subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | A     | 184      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1450  | 964 | 221 | 253 | 12 |         |       |
| 1   | D     | 184      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1450  | 964 | 221 | 253 | 12 |         |       |

- Molecule 2 is a protein called Acetylcholine receptor subunit delta.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1420  | 937 | 226 | 248 | 9 |         |       |

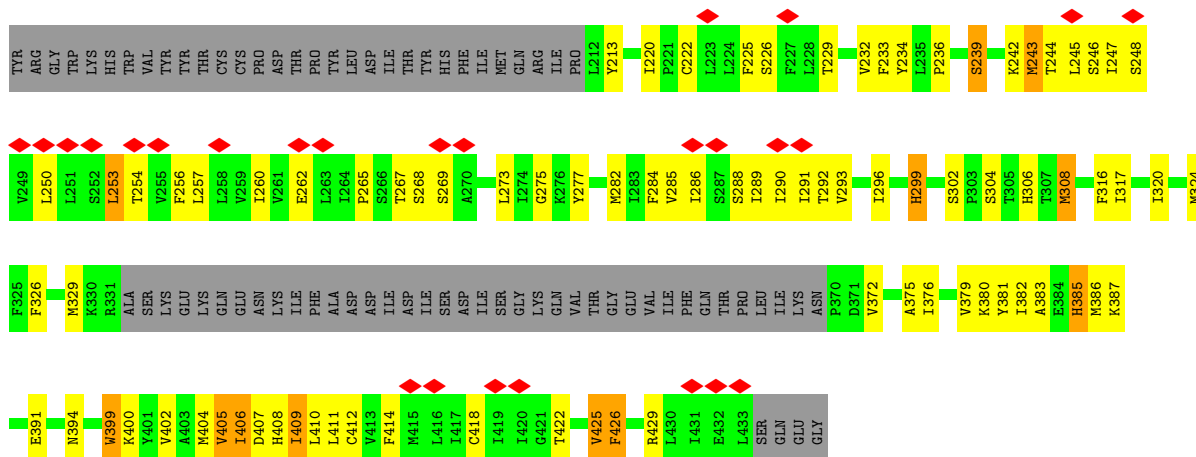
- Molecule 3 is a protein called Acetylcholine receptor subunit beta.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1455  | 980 | 220 | 248 | 7 |         |       |

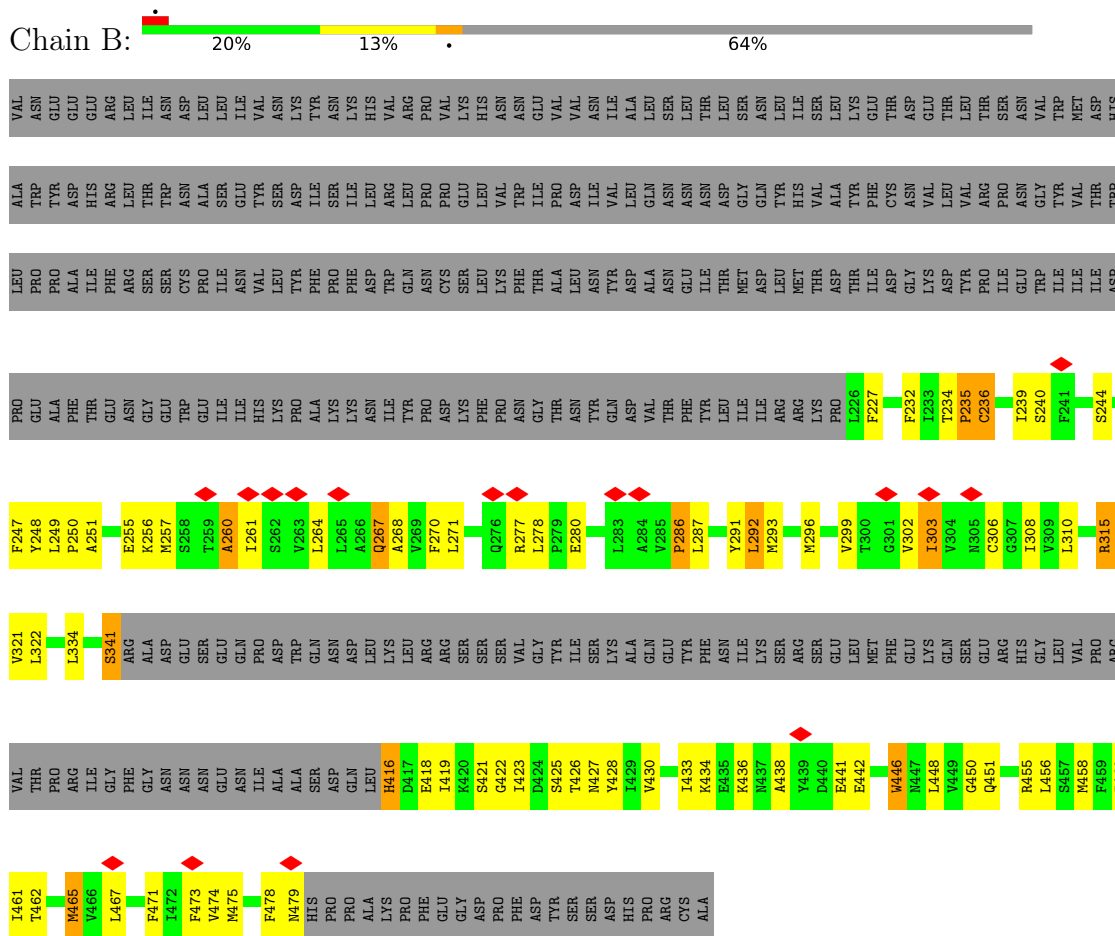
- Molecule 4 is a protein called Acetylcholine receptor subunit gamma.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | E     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1343  | 896 | 208 | 230 | 9 |         |       |

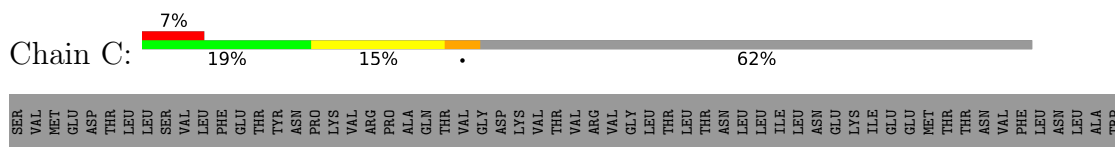




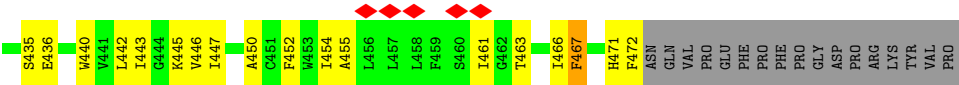
- Molecule 2: Acetylcholine receptor subunit delta



- Molecule 3: Acetylcholine receptor subunit beta







## 4 Experimental information

| Property                             | Value                                                                                         | Source    |
|--------------------------------------|-----------------------------------------------------------------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                                                               | Depositor |
| Imposed symmetry                     | POINT, C1                                                                                     | Depositor |
| Number of particles used             | 107524                                                                                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                                                             | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; Correction performed by standard procedure in RELION | Depositor |
| Microscope                           | FEI TITAN KRIOS                                                                               | Depositor |
| Voltage (kV)                         | 300                                                                                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                                                                            | Depositor |
| Minimum defocus (nm)                 | 1200                                                                                          | Depositor |
| Maximum defocus (nm)                 | 2800                                                                                          | Depositor |
| Magnification                        | 104478                                                                                        | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                                                                      | Depositor |
| Maximum map value                    | 0.001                                                                                         | Depositor |
| Minimum map value                    | -0.001                                                                                        | Depositor |
| Average map value                    | 0.000                                                                                         | Depositor |
| Map value standard deviation         | 0.000                                                                                         | Depositor |
| Recommended contour level            | 0.0005                                                                                        | Depositor |
| Map size (Å)                         | 268.0, 268.0, 268.0                                                                           | wwPDB     |
| Map dimensions                       | 200, 200, 200                                                                                 | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                                                              | wwPDB     |
| Pixel spacing (Å)                    | 1.34, 1.34, 1.34                                                                              | 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     | 2.13         | 9/1482 (0.6%)  | 1.96        | 48/2015 (2.4%)  |
| 1   | D     | 2.09         | 8/1482 (0.5%)  | 1.79        | 27/2015 (1.3%)  |
| 2   | B     | 2.17         | 6/1449 (0.4%)  | 1.94        | 47/1966 (2.4%)  |
| 3   | C     | 2.14         | 6/1493 (0.4%)  | 2.03        | 59/2037 (2.9%)  |
| 4   | E     | 2.20         | 12/1370 (0.9%) | 2.01        | 57/1861 (3.1%)  |
| All | All   | 2.14         | 41/7276 (0.6%) | 1.95        | 238/9894 (2.4%) |

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                   | 1                   |
| 3   | C     | 0                   | 2                   |
| 4   | E     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (41) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 320 | ILE  | CA-CB   | -6.67 | 1.49        | 1.53     |
| 4   | E     | 280 | VAL  | CA-C    | -5.82 | 1.48        | 1.53     |
| 4   | E     | 280 | VAL  | N-CA    | -5.71 | 1.41        | 1.46     |
| 4   | E     | 226 | ILE  | CA-C    | -5.66 | 1.46        | 1.52     |
| 1   | A     | 408 | HIS  | CE1-NE2 | -5.56 | 1.26        | 1.32     |
| 1   | D     | 288 | SER  | C-O     | -5.44 | 1.17        | 1.24     |
| 1   | D     | 220 | ILE  | CA-CB   | 5.42  | 1.57        | 1.54     |
| 2   | B     | 462 | THR  | C-O     | -5.39 | 1.19        | 1.24     |
| 3   | C     | 312 | HIS  | CE1-NE2 | 5.38  | 1.38        | 1.32     |
| 1   | D     | 299 | HIS  | CE1-NE2 | 5.35  | 1.37        | 1.32     |
| 2   | B     | 286 | PRO  | C-O     | -5.32 | 1.17        | 1.23     |
| 1   | D     | 246 | SER  | C-N     | 5.29  | 1.39        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | E     | 249 | GLY  | CA-C    | -5.25 | 1.46        | 1.52     |
| 4   | E     | 236 | LEU  | C-N     | -5.25 | 1.28        | 1.34     |
| 1   | D     | 244 | THR  | C-O     | -5.23 | 1.18        | 1.24     |
| 1   | D     | 391 | GLU  | C-O     | 5.23  | 1.30        | 1.24     |
| 2   | B     | 320 | HIS  | CD2-NE2 | 5.22  | 1.43        | 1.37     |
| 1   | D     | 306 | HIS  | ND1-CE1 | -5.22 | 1.27        | 1.32     |
| 3   | C     | 277 | VAL  | CA-C    | 5.22  | 1.57        | 1.52     |
| 1   | A     | 260 | ILE  | CA-C    | -5.21 | 1.46        | 1.52     |
| 2   | B     | 450 | GLY  | CA-C    | -5.18 | 1.46        | 1.52     |
| 4   | E     | 323 | HIS  | CE1-NE2 | 5.17  | 1.37        | 1.32     |
| 4   | E     | 281 | PRO  | C-O     | -5.16 | 1.17        | 1.23     |
| 1   | A     | 407 | ASP  | C-O     | -5.15 | 1.18        | 1.24     |
| 3   | C     | 227 | PRO  | C-O     | -5.14 | 1.18        | 1.24     |
| 1   | A     | 408 | HIS  | ND1-CE1 | -5.13 | 1.27        | 1.32     |
| 3   | C     | 455 | PHE  | C-O     | -5.11 | 1.18        | 1.24     |
| 3   | C     | 442 | VAL  | CA-C    | -5.09 | 1.46        | 1.52     |
| 2   | B     | 446 | TRP  | NE1-CE2 | 5.09  | 1.43        | 1.37     |
| 4   | E     | 461 | ILE  | N-CA    | -5.09 | 1.40        | 1.46     |
| 2   | B     | 287 | LEU  | C-O     | -5.08 | 1.18        | 1.24     |
| 1   | A     | 306 | HIS  | CE1-NE2 | -5.06 | 1.27        | 1.32     |
| 1   | A     | 293 | VAL  | CA-C    | -5.05 | 1.46        | 1.52     |
| 4   | E     | 316 | SER  | N-CA    | -5.04 | 1.40        | 1.46     |
| 4   | E     | 254 | LEU  | C-O     | -5.04 | 1.18        | 1.24     |
| 4   | E     | 301 | CYS  | C-O     | -5.03 | 1.18        | 1.24     |
| 1   | A     | 289 | ILE  | N-CA    | 5.03  | 1.52        | 1.46     |
| 1   | A     | 419 | ILE  | N-CA    | -5.02 | 1.41        | 1.46     |
| 3   | C     | 433 | MET  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | D     | 409 | ILE  | CA-CB   | 5.01  | 1.60        | 1.54     |
| 4   | E     | 450 | ALA  | C-O     | 5.01  | 1.29        | 1.24     |

All (238) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 426 | PHE  | CA-CB-CG   | 11.07 | 124.87      | 113.80   |
| 1   | A     | 426 | PHE  | CA-CB-CG   | 10.57 | 124.37      | 113.80   |
| 1   | D     | 308 | MET  | O-C-N      | 10.17 | 130.35      | 121.30   |
| 4   | E     | 284 | GLY  | O-C-N      | -9.72 | 112.85      | 122.19   |
| 3   | C     | 314 | MET  | O-C-N      | 9.47  | 129.99      | 121.18   |
| 3   | C     | 333 | GLN  | OE1-CD-NE2 | -9.16 | 113.44      | 122.60   |
| 4   | E     | 248 | GLY  | CA-C-N     | -9.07 | 110.03      | 120.00   |
| 4   | E     | 248 | GLY  | C-N-CA     | -9.07 | 110.03      | 120.00   |
| 1   | D     | 265 | PRO  | O-C-N      | 8.99  | 134.12      | 123.06   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 421 | GLY  | O-C-N      | -8.96 | 113.59      | 122.19   |
| 4   | E     | 248 | GLY  | O-C-N      | 8.91  | 133.20      | 122.60   |
| 1   | A     | 420 | ILE  | CA-C-O     | 8.74  | 130.44      | 121.17   |
| 1   | D     | 422 | THR  | CA-C-O     | -8.58 | 111.81      | 120.82   |
| 4   | E     | 461 | ILE  | O-C-N      | -8.48 | 113.60      | 121.91   |
| 3   | C     | 459 | SER  | CA-C-O     | -8.46 | 109.19      | 119.43   |
| 3   | C     | 282 | ARG  | NE-CZ-NH2  | -8.34 | 111.69      | 119.20   |
| 3   | C     | 267 | ALA  | CA-C-O     | -8.29 | 111.64      | 120.92   |
| 1   | A     | 330 | LYS  | CA-C-O     | 8.14  | 130.18      | 121.55   |
| 4   | E     | 471 | HIS  | CG-CD2-NE2 | -7.98 | 99.22       | 107.20   |
| 1   | D     | 267 | THR  | O-C-N      | -7.94 | 113.31      | 122.68   |
| 3   | C     | 268 | ASP  | O-C-N      | -7.94 | 112.21      | 122.37   |
| 4   | E     | 293 | VAL  | O-C-N      | -7.89 | 113.70      | 121.83   |
| 3   | C     | 254 | SER  | CA-C-O     | 7.83  | 129.03      | 119.79   |
| 1   | D     | 408 | HIS  | CA-C-O     | 7.71  | 129.14      | 120.90   |
| 2   | B     | 240 | SER  | N-CA-C     | -7.70 | 102.01      | 111.40   |
| 2   | B     | 475 | MET  | CA-C-O     | 7.68  | 128.69      | 120.55   |
| 1   | D     | 394 | ASN  | OD1-CG-ND2 | -7.65 | 114.95      | 122.60   |
| 4   | E     | 265 | PHE  | CA-C-N     | -7.65 | 110.03      | 120.28   |
| 4   | E     | 265 | PHE  | C-N-CA     | -7.65 | 110.03      | 120.28   |
| 1   | A     | 320 | ILE  | O-C-N      | -7.64 | 114.65      | 120.07   |
| 4   | E     | 461 | ILE  | CA-C-N     | 7.61  | 128.59      | 119.99   |
| 4   | E     | 461 | ILE  | C-N-CA     | 7.61  | 128.59      | 119.99   |
| 1   | A     | 265 | PRO  | N-CA-CB    | 7.40  | 109.79      | 103.35   |
| 4   | E     | 316 | SER  | CA-C-O     | 7.34  | 129.16      | 120.20   |
| 4   | E     | 271 | GLN  | O-C-N      | -7.33 | 111.73      | 122.43   |
| 3   | C     | 314 | MET  | CA-C-O     | -7.28 | 112.28      | 119.49   |
| 4   | E     | 250 | GLN  | O-C-N      | 7.27  | 130.88      | 122.67   |
| 1   | A     | 391 | GLU  | CA-C-N     | -7.23 | 109.32      | 120.31   |
| 1   | A     | 391 | GLU  | C-N-CA     | -7.23 | 109.32      | 120.31   |
| 3   | C     | 437 | ARG  | NE-CZ-NH2  | -7.23 | 112.69      | 119.20   |
| 1   | A     | 252 | SER  | O-C-N      | -7.20 | 114.66      | 122.07   |
| 1   | D     | 422 | THR  | N-CA-C     | -7.20 | 103.37      | 111.07   |
| 3   | C     | 226 | ILE  | CA-C-N     | -7.14 | 111.07      | 118.85   |
| 3   | C     | 226 | ILE  | C-N-CA     | -7.14 | 111.07      | 118.85   |
| 2   | B     | 467 | LEU  | O-C-N      | -7.08 | 114.44      | 122.09   |
| 1   | D     | 253 | LEU  | O-C-N      | -7.02 | 114.00      | 122.22   |
| 1   | A     | 267 | THR  | O-C-N      | -6.96 | 115.09      | 122.96   |
| 3   | C     | 412 | ALA  | CA-C-O     | 6.90  | 128.07      | 120.82   |
| 1   | D     | 407 | ASP  | O-C-N      | -6.89 | 114.97      | 122.07   |
| 2   | B     | 471 | PHE  | CG-CD1-CE1 | 6.88  | 132.40      | 120.70   |
| 2   | B     | 315 | ARG  | NE-CZ-NH2  | -6.87 | 113.01      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | E     | 321 | ILE  | O-C-N      | 6.86  | 128.53      | 121.87   |
| 2   | B     | 306 | CYS  | O-C-N      | 6.84  | 129.37      | 122.12   |
| 1   | D     | 225 | PHE  | CA-CB-CG   | -6.82 | 106.98      | 113.80   |
| 2   | B     | 240 | SER  | CA-C-O     | -6.81 | 113.27      | 120.55   |
| 3   | C     | 412 | ALA  | O-C-N      | -6.76 | 115.11      | 122.07   |
| 4   | E     | 266 | LEU  | N-CA-CB    | -6.67 | 100.31      | 110.12   |
| 4   | E     | 233 | ILE  | CB-CG1-CD1 | 6.60  | 127.65      | 113.80   |
| 2   | B     | 293 | MET  | CA-C-O     | 6.56  | 127.71      | 120.82   |
| 3   | C     | 328 | PRO  | O-C-N      | -6.55 | 114.71      | 122.24   |
| 3   | C     | 254 | SER  | O-C-N      | -6.53 | 113.58      | 122.33   |
| 1   | A     | 420 | ILE  | O-C-N      | -6.53 | 115.52      | 121.91   |
| 3   | C     | 442 | VAL  | O-C-N      | -6.49 | 115.55      | 121.91   |
| 3   | C     | 229 | ILE  | CA-C-O     | -6.43 | 114.36      | 121.17   |
| 1   | A     | 403 | ALA  | O-C-N      | -6.42 | 115.31      | 122.12   |
| 4   | E     | 232 | LEU  | CA-C-O     | 6.39  | 127.28      | 120.70   |
| 3   | C     | 227 | PRO  | CA-N-CD    | 6.39  | 120.94      | 112.00   |
| 2   | B     | 260 | ALA  | N-CA-C     | -6.37 | 104.42      | 111.36   |
| 1   | D     | 408 | HIS  | O-C-N      | -6.36 | 115.47      | 122.09   |
| 3   | C     | 227 | PRO  | O-C-N      | 6.35  | 130.16      | 122.23   |
| 1   | A     | 301 | ARG  | O-C-N      | -6.31 | 115.27      | 122.97   |
| 4   | E     | 273 | VAL  | N-CA-CB    | -6.31 | 102.37      | 111.21   |
| 2   | B     | 455 | ARG  | CA-C-O     | 6.30  | 127.23      | 120.55   |
| 1   | D     | 243 | MET  | O-C-N      | -6.30 | 114.52      | 122.27   |
| 4   | E     | 273 | VAL  | CA-CB-CG2  | -6.28 | 99.72       | 110.40   |
| 4   | E     | 319 | GLU  | CB-CG-CD   | 6.25  | 123.22      | 112.60   |
| 2   | B     | 467 | LEU  | CA-C-N     | 6.23  | 126.86      | 119.94   |
| 2   | B     | 467 | LEU  | C-N-CA     | 6.23  | 126.86      | 119.94   |
| 1   | D     | 425 | VAL  | CA-CB-CG2  | -6.21 | 99.84       | 110.40   |
| 1   | A     | 413 | VAL  | O-C-N      | -6.20 | 115.44      | 121.83   |
| 4   | E     | 300 | ASN  | OD1-CG-ND2 | -6.18 | 116.42      | 122.60   |
| 3   | C     | 308 | SER  | CA-C-N     | -6.17 | 113.27      | 119.56   |
| 3   | C     | 308 | SER  | C-N-CA     | -6.17 | 113.27      | 119.56   |
| 4   | E     | 271 | GLN  | CA-C-O     | 6.14  | 126.97      | 119.11   |
| 2   | B     | 416 | HIS  | CG-CD2-NE2 | 6.11  | 113.31      | 107.20   |
| 3   | C     | 431 | VAL  | CA-C-O     | 6.11  | 127.30      | 120.95   |
| 1   | A     | 429 | ARG  | NE-CZ-NH2  | 6.10  | 124.69      | 119.20   |
| 3   | C     | 273 | THR  | O-C-N      | -6.07 | 114.98      | 123.11   |
| 2   | B     | 471 | PHE  | CB-CG-CD1  | 6.06  | 131.01      | 120.70   |
| 3   | C     | 415 | LEU  | N-CA-CB    | 6.05  | 118.79      | 110.01   |
| 2   | B     | 293 | MET  | O-C-N      | -6.04 | 115.85      | 122.07   |
| 3   | C     | 243 | PRO  | CA-C-N     | 6.04  | 129.48      | 120.31   |
| 3   | C     | 243 | PRO  | C-N-CA     | 6.04  | 129.48      | 120.31   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 341 | SER  | CA-C-O     | 6.03  | 131.05      | 120.80   |
| 3   | C     | 267 | ALA  | O-C-N      | 6.01  | 129.02      | 122.11   |
| 4   | E     | 276 | THR  | O-C-N      | -6.01 | 115.56      | 122.89   |
| 3   | C     | 402 | LYS  | N-CA-C     | 6.00  | 117.83      | 111.28   |
| 4   | E     | 257 | SER  | O-C-N      | -6.00 | 115.31      | 122.15   |
| 4   | E     | 467 | PHE  | CA-CB-CG   | 6.00  | 119.80      | 113.80   |
| 2   | B     | 474 | VAL  | CA-C-N     | -5.98 | 112.27      | 120.28   |
| 2   | B     | 474 | VAL  | C-N-CA     | -5.98 | 112.27      | 120.28   |
| 4   | E     | 435 | SER  | CA-C-O     | -5.95 | 114.53      | 120.90   |
| 2   | B     | 306 | CYS  | CA-C-N     | -5.94 | 113.46      | 120.00   |
| 2   | B     | 306 | CYS  | C-N-CA     | -5.94 | 113.46      | 120.00   |
| 1   | A     | 255 | VAL  | N-CA-C     | -5.94 | 104.72      | 110.72   |
| 1   | A     | 411 | LEU  | N-CA-C     | 5.93  | 117.42      | 111.07   |
| 1   | A     | 213 | TYR  | CA-C-O     | -5.93 | 114.59      | 120.82   |
| 3   | C     | 419 | SER  | O-C-N      | -5.92 | 115.97      | 122.07   |
| 1   | A     | 253 | LEU  | O-C-N      | -5.92 | 115.85      | 122.12   |
| 2   | B     | 478 | PHE  | N-CA-CB    | -5.91 | 101.58      | 110.91   |
| 3   | C     | 291 | VAL  | O-C-N      | 5.89  | 127.90      | 121.83   |
| 3   | C     | 258 | ALA  | N-CA-C     | -5.88 | 104.79      | 111.14   |
| 2   | B     | 478 | PHE  | CD1-CG-CD2 | -5.86 | 109.81      | 118.60   |
| 4   | E     | 305 | LEU  | O-C-N      | -5.81 | 115.96      | 122.12   |
| 2   | B     | 308 | ILE  | CA-C-O     | -5.81 | 114.69      | 120.85   |
| 4   | E     | 282 | LEU  | O-C-N      | -5.81 | 116.08      | 122.07   |
| 2   | B     | 465 | MET  | CA-C-O     | 5.81  | 126.58      | 120.42   |
| 3   | C     | 229 | ILE  | N-CA-C     | -5.80 | 104.86      | 110.42   |
| 3   | C     | 399 | GLN  | CG-CD-OE1  | -5.79 | 109.21      | 120.80   |
| 2   | B     | 306 | CYS  | N-CA-C     | 5.77  | 117.57      | 111.28   |
| 2   | B     | 416 | HIS  | N-CA-CB    | 5.75  | 120.28      | 110.50   |
| 3   | C     | 438 | LEU  | O-C-N      | -5.74 | 116.04      | 122.12   |
| 1   | D     | 391 | GLU  | O-C-N      | -5.74 | 116.16      | 122.07   |
| 4   | E     | 249 | GLY  | CA-C-O     | -5.73 | 114.58      | 120.66   |
| 4   | E     | 435 | SER  | O-C-N      | 5.73  | 128.05      | 122.09   |
| 1   | A     | 287 | SER  | O-C-N      | 5.72  | 128.18      | 122.12   |
| 1   | A     | 274 | ILE  | O-C-N      | -5.71 | 115.35      | 121.80   |
| 2   | B     | 308 | ILE  | N-CA-C     | -5.71 | 104.96      | 110.72   |
| 3   | C     | 235 | ALA  | N-CA-CB    | -5.71 | 101.44      | 110.28   |
| 3   | C     | 294 | SER  | O-C-N      | -5.71 | 116.07      | 122.12   |
| 3   | C     | 456 | LEU  | CA-C-O     | -5.71 | 114.50      | 120.55   |
| 2   | B     | 321 | VAL  | O-C-N      | 5.70  | 129.41      | 123.26   |
| 3   | C     | 275 | LEU  | CA-C-O     | -5.70 | 114.38      | 120.42   |
| 3   | C     | 268 | ASP  | CA-CB-CG   | 5.69  | 118.29      | 112.60   |
| 4   | E     | 319 | GLU  | CG-CD-OE2  | 5.69  | 131.49      | 118.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 475 | MET  | N-CA-C      | 5.68  | 117.47      | 111.28   |
| 4   | E     | 252 | CYS  | O-C-N       | -5.64 | 116.14      | 122.12   |
| 4   | E     | 315 | HIS  | CG-CD2-NE2  | -5.64 | 101.56      | 107.20   |
| 3   | C     | 334 | ARG  | NE-CZ-NH2   | 5.63  | 124.27      | 119.20   |
| 2   | B     | 268 | ALA  | CA-C-O      | 5.63  | 126.71      | 120.63   |
| 1   | A     | 328 | THR  | CA-C-O      | -5.62 | 112.98      | 119.56   |
| 3   | C     | 235 | ALA  | N-CA-C      | -5.61 | 105.31      | 111.82   |
| 3   | C     | 449 | ILE  | CB-CA-C     | -5.61 | 104.67      | 112.02   |
| 2   | B     | 261 | ILE  | O-C-N       | -5.61 | 115.46      | 121.80   |
| 1   | D     | 385 | HIS  | ND1-CE1-NE2 | -5.60 | 102.80      | 108.40   |
| 2   | B     | 416 | HIS  | ND1-CG-CD2  | -5.59 | 100.51      | 106.10   |
| 4   | E     | 273 | VAL  | O-C-N       | 5.56  | 127.44      | 121.10   |
| 4   | E     | 422 | PHE  | CA-CB-CG    | -5.54 | 108.26      | 113.80   |
| 1   | D     | 275 | GLY  | O-C-N       | 5.54  | 127.50      | 122.18   |
| 1   | D     | 406 | ILE  | CA-C-O      | -5.54 | 115.19      | 120.95   |
| 3   | C     | 414 | GLN  | CA-C-O      | 5.53  | 126.41      | 120.55   |
| 3   | C     | 272 | GLU  | N-CA-C      | 5.52  | 122.56      | 110.80   |
| 3   | C     | 449 | ILE  | CA-CB-CG1   | -5.52 | 101.02      | 110.40   |
| 1   | A     | 226 | SER  | O-C-N       | -5.51 | 116.28      | 122.12   |
| 2   | B     | 280 | GLU  | OE1-CD-OE2  | 5.51  | 136.13      | 122.90   |
| 2   | B     | 292 | LEU  | O-C-N       | -5.50 | 115.88      | 122.15   |
| 3   | C     | 439 | PHE  | O-C-N       | -5.50 | 116.29      | 122.12   |
| 1   | A     | 262 | GLU  | O-C-N       | -5.49 | 114.88      | 122.46   |
| 3   | C     | 258 | ALA  | CB-CA-C     | 5.49  | 119.58      | 110.90   |
| 2   | B     | 236 | CYS  | N-CA-CB     | -5.48 | 102.07      | 110.12   |
| 1   | A     | 217 | ASN  | OD1-CG-ND2  | 5.46  | 128.06      | 122.60   |
| 1   | A     | 258 | LEU  | CA-C-N      | 5.45  | 127.43      | 120.56   |
| 1   | A     | 258 | LEU  | C-N-CA      | 5.45  | 127.43      | 120.56   |
| 2   | B     | 315 | ARG  | CD-NE-CZ    | -5.45 | 116.77      | 124.40   |
| 4   | E     | 258 | VAL  | O-C-N       | -5.45 | 116.37      | 121.87   |
| 3   | C     | 414 | GLN  | O-C-N       | -5.44 | 116.35      | 122.12   |
| 1   | D     | 248 | SER  | CA-CB-OG    | 5.43  | 121.97      | 111.10   |
| 1   | A     | 427 | ALA  | CA-C-N      | -5.43 | 113.95      | 119.98   |
| 1   | A     | 427 | ALA  | C-N-CA      | -5.43 | 113.95      | 119.98   |
| 4   | E     | 284 | GLY  | CA-C-O      | 5.42  | 126.34      | 120.75   |
| 4   | E     | 280 | VAL  | N-CA-C      | 5.42  | 113.29      | 108.63   |
| 1   | D     | 260 | ILE  | O-C-N       | -5.40 | 116.62      | 121.91   |
| 1   | A     | 399 | TRP  | CD2-CE2-CZ2 | -5.38 | 117.03      | 122.40   |
| 2   | B     | 267 | GLN  | O-C-N       | -5.36 | 116.04      | 122.15   |
| 3   | C     | 434 | VAL  | CA-C-O      | -5.35 | 114.69      | 120.47   |
| 1   | A     | 292 | THR  | CA-C-O      | 5.34  | 126.21      | 120.55   |
| 4   | E     | 250 | GLN  | CG-CD-NE2   | -5.34 | 108.39      | 116.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | D     | 399 | TRP  | CD2-CE2-CZ2 | 5.32  | 127.72      | 122.40   |
| 1   | A     | 274 | ILE  | CA-C-N      | 5.31  | 125.83      | 119.94   |
| 1   | A     | 274 | ILE  | C-N-CA      | 5.31  | 125.83      | 119.94   |
| 4   | E     | 225 | ASN  | CA-C-O      | 5.28  | 124.95      | 119.14   |
| 1   | A     | 398 | GLU  | N-CA-C      | 5.27  | 117.02      | 111.28   |
| 3   | C     | 332 | ILE  | O-C-N       | -5.25 | 116.01      | 122.57   |
| 3   | C     | 271 | PRO  | N-CA-C      | 5.25  | 119.44      | 111.15   |
| 4   | E     | 313 | ASN  | OD1-CG-ND2  | -5.24 | 117.36      | 122.60   |
| 1   | A     | 427 | ALA  | N-CA-C      | 5.24  | 117.67      | 111.33   |
| 1   | A     | 269 | SER  | N-CA-CB     | -5.23 | 102.48      | 110.07   |
| 1   | A     | 313 | ARG  | NE-CZ-NH1   | -5.23 | 116.27      | 121.50   |
| 4   | E     | 301 | CYS  | CA-C-O      | 5.23  | 125.96      | 120.42   |
| 3   | C     | 399 | GLN  | CG-CD-NE2   | 5.22  | 124.24      | 116.40   |
| 1   | A     | 313 | ARG  | NE-CZ-NH2   | 5.21  | 123.89      | 119.20   |
| 1   | A     | 260 | ILE  | CB-CG1-CD1  | 5.21  | 124.74      | 113.80   |
| 4   | E     | 300 | ASN  | N-CA-C      | -5.21 | 105.67      | 112.23   |
| 1   | A     | 422 | THR  | CA-C-O      | -5.20 | 115.54      | 121.00   |
| 4   | E     | 472 | PHE  | CD1-CG-CD2  | -5.20 | 110.80      | 118.60   |
| 1   | D     | 308 | MET  | CA-C-O      | -5.19 | 114.87      | 119.75   |
| 2   | B     | 236 | CYS  | O-C-N       | -5.18 | 116.63      | 122.12   |
| 3   | C     | 265 | LEU  | CA-C-O      | -5.18 | 115.39      | 120.82   |
| 3   | C     | 334 | ARG  | NH1-CZ-NH2  | -5.17 | 112.58      | 119.30   |
| 3   | C     | 277 | VAL  | CG1-CB-CG2  | -5.17 | 99.44       | 110.80   |
| 2   | B     | 235 | PRO  | CA-C-N      | -5.17 | 113.36      | 120.28   |
| 2   | B     | 235 | PRO  | C-N-CA      | -5.17 | 113.36      | 120.28   |
| 1   | D     | 239 | SER  | CA-C-O      | -5.16 | 114.77      | 120.60   |
| 4   | E     | 262 | GLN  | CA-C-O      | 5.16  | 126.02      | 120.55   |
| 2   | B     | 474 | VAL  | N-CA-C      | 5.15  | 115.93      | 110.72   |
| 1   | A     | 389 | ASP  | CA-CB-CG    | 5.15  | 117.75      | 112.60   |
| 2   | B     | 471 | PHE  | CA-C-O      | 5.15  | 126.00      | 120.55   |
| 1   | D     | 254 | THR  | CA-C-O      | 5.14  | 125.87      | 120.42   |
| 4   | E     | 315 | HIS  | CA-CB-CG    | 5.13  | 118.93      | 113.80   |
| 2   | B     | 271 | LEU  | CA-C-O      | 5.12  | 125.98      | 120.55   |
| 1   | A     | 326 | PHE  | CA-C-O      | -5.12 | 115.13      | 120.55   |
| 4   | E     | 443 | ILE  | O-C-N       | 5.11  | 126.83      | 121.87   |
| 4   | E     | 443 | ILE  | CA-C-O      | -5.11 | 115.64      | 120.95   |
| 4   | E     | 225 | ASN  | CA-C-N      | -5.11 | 117.75      | 123.16   |
| 4   | E     | 225 | ASN  | C-N-CA      | -5.11 | 117.75      | 123.16   |
| 4   | E     | 307 | VAL  | CA-C-O      | -5.10 | 115.44      | 120.85   |
| 1   | A     | 395 | ALA  | CA-C-O      | 5.09  | 126.17      | 120.82   |
| 2   | B     | 303 | ILE  | N-CA-CB     | -5.09 | 103.61      | 110.54   |
| 1   | D     | 262 | GLU  | O-C-N       | -5.09 | 116.72      | 122.12   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | C     | 227 | PRO  | N-CA-CB    | -5.09 | 97.74       | 103.44   |
| 2   | B     | 455 | ARG  | NE-CZ-NH2  | 5.08  | 123.77      | 119.20   |
| 1   | D     | 405 | VAL  | CB-CA-C    | -5.08 | 104.03      | 112.26   |
| 1   | A     | 421 | GLY  | CA-C-N     | 5.08  | 127.35      | 120.65   |
| 1   | A     | 421 | GLY  | C-N-CA     | 5.08  | 127.35      | 120.65   |
| 4   | E     | 454 | ILE  | O-C-N      | -5.07 | 116.94      | 121.91   |
| 4   | E     | 285 | LYS  | O-C-N      | -5.07 | 116.81      | 122.09   |
| 4   | E     | 275 | GLU  | OE1-CD-OE2 | 5.07  | 135.06      | 122.90   |
| 4   | E     | 463 | THR  | O-C-N      | -5.05 | 116.63      | 122.09   |
| 3   | C     | 291 | VAL  | CA-C-O     | -5.05 | 115.50      | 120.85   |
| 1   | A     | 270 | ALA  | CA-C-O     | 5.04  | 126.85      | 121.45   |
| 4   | E     | 235 | SER  | N-CA-C     | -5.04 | 106.39      | 112.54   |
| 2   | B     | 479 | ASN  | CA-CB-CG   | 5.04  | 117.64      | 112.60   |
| 2   | B     | 478 | PHE  | CG-CD2-CE2 | 5.04  | 129.26      | 120.70   |
| 1   | D     | 269 | SER  | CB-CA-C    | 5.03  | 118.78      | 110.88   |
| 1   | A     | 331 | ARG  | NE-CZ-NH2  | 5.03  | 123.72      | 119.20   |
| 1   | A     | 375 | ALA  | CA-C-O     | -5.03 | 115.54      | 120.82   |
| 3   | C     | 295 | VAL  | N-CA-C     | -5.02 | 105.43      | 110.30   |
| 3   | C     | 459 | SER  | CB-CA-C    | -5.01 | 101.45      | 110.37   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 267 | THR  | Mainchain |
| 3   | C     | 275 | LEU  | Mainchain |
| 3   | C     | 459 | SER  | Mainchain |
| 4   | E     | 315 | HIS  | 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     | 1450  | 0        | 1526     | 199     | 0            |
| 1   | D     | 1450  | 0        | 1526     | 195     | 0            |
| 2   | B     | 1420  | 0        | 1483     | 159     | 0            |
| 3   | C     | 1455  | 0        | 1516     | 195     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | E     | 1343  | 0        | 1424     | 188     | 0            |
| All | All   | 7118  | 0        | 7475     | 652     | 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 45.

All (652) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:231:ILE:HG13 | 3:C:262:PHE:CZ   | 1.72                     | 1.22              |
| 1:A:216:VAL:HG21 | 4:E:280:VAL:CG2  | 1.69                     | 1.21              |
| 4:E:255:SER:HB2  | 4:E:298:VAL:CG2  | 1.69                     | 1.20              |
| 1:A:376:ILE:HD13 | 4:E:412:GLU:C    | 1.65                     | 1.19              |
| 1:D:317:ILE:HD11 | 1:D:402:VAL:CG2  | 1.73                     | 1.19              |
| 1:A:264:ILE:HG21 | 1:A:274:ILE:HD11 | 1.25                     | 1.18              |
| 2:B:422:GLY:CA   | 3:C:405:VAL:HG13 | 1.73                     | 1.18              |
| 4:E:312:PRO:HG3  | 4:E:436:GLU:CD   | 1.68                     | 1.18              |
| 4:E:255:SER:CB   | 4:E:298:VAL:HG22 | 1.74                     | 1.17              |
| 3:C:259:VAL:HG12 | 3:C:288:MET:CE   | 1.74                     | 1.15              |
| 2:B:422:GLY:HA3  | 3:C:405:VAL:HG13 | 1.29                     | 1.14              |
| 4:E:286:TYR:CD1  | 4:E:466:ILE:HG21 | 1.80                     | 1.14              |
| 1:D:253:LEU:HD22 | 1:D:285:VAL:HG21 | 1.25                     | 1.14              |
| 1:A:386:MET:HE1  | 4:E:423:ILE:HG23 | 1.16                     | 1.12              |
| 1:A:375:ALA:CB   | 2:B:423:ILE:HD12 | 1.78                     | 1.12              |
| 1:A:257:LEU:HD13 | 1:A:278:MET:HE1  | 1.19                     | 1.12              |
| 1:A:381:TYR:CD2  | 2:B:430:VAL:HG13 | 1.85                     | 1.11              |
| 3:C:259:VAL:HG12 | 3:C:288:MET:HE2  | 1.26                     | 1.11              |
| 1:A:375:ALA:HB2  | 2:B:423:ILE:CG2  | 1.79                     | 1.11              |
| 1:A:273:LEU:HD22 | 1:A:429:ARG:HG2  | 1.33                     | 1.10              |
| 1:A:291:ILE:CG2  | 1:A:410:LEU:HD13 | 1.82                     | 1.10              |
| 1:A:257:LEU:HD13 | 1:A:278:MET:CE   | 1.81                     | 1.09              |
| 1:A:257:LEU:CD1  | 1:A:278:MET:HE1  | 1.80                     | 1.09              |
| 3:C:411:ILE:HG23 | 1:D:386:MET:CE   | 1.80                     | 1.09              |
| 1:A:307:THR:HG22 | 2:B:341:SER:HB3  | 1.27                     | 1.08              |
| 3:C:408:ILE:HG13 | 1:D:379:VAL:CG1  | 1.83                     | 1.08              |
| 3:C:411:ILE:HG23 | 1:D:386:MET:HE1  | 1.14                     | 1.08              |
| 2:B:421:SER:HB2  | 3:C:409:LYS:NZ   | 1.70                     | 1.07              |
| 4:E:269:ILE:HD13 | 4:E:287:LEU:HG   | 1.36                     | 1.07              |
| 1:A:376:ILE:HD11 | 4:E:413:ILE:HD13 | 1.11                     | 1.07              |
| 2:B:419:ILE:HA   | 3:C:405:VAL:HG21 | 1.09                     | 1.07              |
| 3:C:408:ILE:HG13 | 1:D:379:VAL:HG11 | 1.34                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:262:GLN:HB3  | 4:E:291:MET:HE3  | 1.18                     | 1.07              |
| 1:A:386:MET:CE   | 4:E:423:ILE:HG23 | 1.84                     | 1.06              |
| 2:B:256:LYS:HD3  | 2:B:310:LEU:HD11 | 1.35                     | 1.06              |
| 3:C:266:LEU:HD23 | 3:C:281:ILE:HD13 | 1.35                     | 1.06              |
| 3:C:404:ALA:HB2  | 1:D:376:ILE:HG23 | 1.37                     | 1.05              |
| 1:A:379:VAL:HG12 | 4:E:419:ALA:HB3  | 1.06                     | 1.04              |
| 1:D:302:SER:CB   | 4:E:445:LYS:HE2  | 1.87                     | 1.04              |
| 1:A:216:VAL:HG21 | 4:E:280:VAL:HG22 | 1.40                     | 1.04              |
| 4:E:262:GLN:CB   | 4:E:291:MET:HE3  | 1.87                     | 1.04              |
| 3:C:283:TYR:CE2  | 3:C:455:PHE:HE1  | 1.74                     | 1.03              |
| 1:D:299:HIS:NE2  | 1:D:400:LYS:HG2  | 1.73                     | 1.03              |
| 1:A:378:GLY:CA   | 2:B:430:VAL:HG21 | 1.89                     | 1.03              |
| 2:B:264:LEU:CD2  | 3:C:234:LEU:HD11 | 1.86                     | 1.03              |
| 2:B:239:ILE:HD12 | 2:B:270:PHE:CE2  | 1.93                     | 1.02              |
| 3:C:231:ILE:HG13 | 3:C:262:PHE:CE2  | 1.95                     | 1.02              |
| 3:C:283:TYR:CD1  | 3:C:454:ILE:HG21 | 1.93                     | 1.02              |
| 1:A:375:ALA:CB   | 2:B:423:ILE:HG23 | 1.88                     | 1.01              |
| 1:D:302:SER:HB2  | 4:E:445:LYS:HE2  | 1.02                     | 1.01              |
| 1:A:291:ILE:HG21 | 1:A:410:LEU:HD13 | 1.36                     | 1.01              |
| 1:A:379:VAL:HG12 | 4:E:419:ALA:CB   | 1.92                     | 1.00              |
| 4:E:262:GLN:HB3  | 4:E:291:MET:CE   | 1.93                     | 0.99              |
| 4:E:325:PHE:HD1  | 4:E:446:VAL:CG1  | 1.75                     | 0.99              |
| 1:A:305:THR:HG22 | 2:B:448:LEU:HD22 | 1.46                     | 0.98              |
| 3:C:283:TYR:HD1  | 3:C:454:ILE:HD13 | 1.27                     | 0.98              |
| 1:D:302:SER:HB2  | 4:E:445:LYS:CE   | 1.93                     | 0.98              |
| 1:A:273:LEU:CD2  | 1:A:429:ARG:HG2  | 1.94                     | 0.97              |
| 1:A:305:THR:CG2  | 2:B:448:LEU:HD22 | 1.93                     | 0.97              |
| 2:B:334:LEU:HD13 | 2:B:456:LEU:HD22 | 1.45                     | 0.97              |
| 4:E:237:VAL:HG12 | 4:E:258:VAL:HG11 | 1.43                     | 0.97              |
| 1:A:222:CYS:HG   | 1:A:256:PHE:HE2  | 1.05                     | 0.96              |
| 1:A:216:VAL:HG21 | 4:E:280:VAL:HG21 | 1.44                     | 0.96              |
| 3:C:238:VAL:HA   | 3:C:251:LEU:CD2  | 1.94                     | 0.96              |
| 1:D:232:VAL:HG23 | 1:D:245:LEU:HD23 | 1.48                     | 0.96              |
| 4:E:269:ILE:CD1  | 4:E:287:LEU:HG   | 1.96                     | 0.96              |
| 2:B:264:LEU:HD21 | 3:C:234:LEU:HD11 | 1.47                     | 0.96              |
| 3:C:231:ILE:HG13 | 3:C:262:PHE:HZ   | 1.21                     | 0.95              |
| 1:A:222:CYS:SG   | 1:A:256:PHE:HE2  | 1.89                     | 0.95              |
| 2:B:418:GLU:HG3  | 3:C:402:LYS:HG3  | 1.47                     | 0.95              |
| 2:B:421:SER:HB2  | 3:C:409:LYS:HZ3  | 1.23                     | 0.95              |
| 2:B:247:PHE:CZ   | 2:B:461:ILE:HD13 | 2.01                     | 0.94              |
| 1:D:253:LEU:CD2  | 1:D:285:VAL:HG21 | 1.98                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:286:TYR:HD1  | 4:E:466:ILE:HG21 | 1.30                     | 0.94              |
| 1:D:273:LEU:CD2  | 1:D:429:ARG:HG2  | 1.97                     | 0.93              |
| 2:B:418:GLU:O    | 3:C:405:VAL:HG11 | 1.69                     | 0.93              |
| 4:E:317:LEU:HB2  | 4:E:440:TRP:CZ2  | 2.04                     | 0.93              |
| 3:C:403:GLU:HB3  | 1:D:380:LYS:HD3  | 1.50                     | 0.92              |
| 2:B:419:ILE:CA   | 3:C:405:VAL:HG21 | 1.98                     | 0.92              |
| 3:C:238:VAL:HA   | 3:C:251:LEU:HD23 | 1.49                     | 0.92              |
| 2:B:247:PHE:CE2  | 2:B:461:ILE:HD13 | 2.03                     | 0.91              |
| 3:C:401:LEU:HD22 | 1:D:376:ILE:CD1  | 2.00                     | 0.91              |
| 1:A:382:ILE:HG22 | 4:E:423:ILE:HG12 | 1.52                     | 0.91              |
| 4:E:286:TYR:CE2  | 4:E:467:PHE:CZ   | 2.58                     | 0.91              |
| 2:B:291:TYR:CZ   | 2:B:473:PHE:CZ   | 2.59                     | 0.91              |
| 2:B:334:LEU:CD1  | 2:B:456:LEU:HD22 | 2.00                     | 0.91              |
| 3:C:411:ILE:HD11 | 1:D:382:ILE:HG22 | 1.52                     | 0.91              |
| 3:C:283:TYR:CE2  | 3:C:455:PHE:CE1  | 2.58                     | 0.91              |
| 4:E:325:PHE:HD1  | 4:E:446:VAL:HG12 | 1.34                     | 0.90              |
| 1:D:222:CYS:HG   | 1:D:256:PHE:HE2  | 1.15                     | 0.90              |
| 3:C:283:TYR:OH   | 3:C:451:THR:HG23 | 1.73                     | 0.89              |
| 1:D:277:TYR:CE1  | 1:D:426:PHE:CZ   | 2.60                     | 0.89              |
| 1:D:317:ILE:HD11 | 1:D:402:VAL:HG23 | 1.51                     | 0.89              |
| 1:A:264:ILE:HG21 | 1:A:274:ILE:CD1  | 2.02                     | 0.89              |
| 2:B:291:TYR:CZ   | 2:B:473:PHE:HZ   | 1.91                     | 0.89              |
| 4:E:262:GLN:C    | 4:E:291:MET:HE3  | 1.98                     | 0.88              |
| 1:A:304:SER:OG   | 2:B:448:LEU:HD21 | 1.74                     | 0.88              |
| 2:B:422:GLY:HA3  | 3:C:405:VAL:CG1  | 2.04                     | 0.88              |
| 2:B:232:PHE:HE2  | 2:B:277:ARG:HG3  | 1.39                     | 0.88              |
| 1:A:264:ILE:CG2  | 1:A:274:ILE:HD11 | 2.03                     | 0.87              |
| 4:E:242:PHE:CZ   | 4:E:452:PHE:CE1  | 2.63                     | 0.87              |
| 4:E:237:VAL:CG1  | 4:E:258:VAL:HG11 | 2.04                     | 0.87              |
| 2:B:248:TYR:CE1  | 2:B:458:MET:HE1  | 2.10                     | 0.87              |
| 3:C:410:TYR:HE2  | 1:D:386:MET:CB   | 1.88                     | 0.87              |
| 2:B:418:GLU:CG   | 3:C:402:LYS:HG3  | 2.05                     | 0.87              |
| 2:B:422:GLY:N    | 3:C:405:VAL:HG13 | 1.90                     | 0.86              |
| 1:D:273:LEU:HD22 | 1:D:429:ARG:HG2  | 1.55                     | 0.86              |
| 1:D:222:CYS:SG   | 1:D:256:PHE:HE2  | 1.98                     | 0.86              |
| 1:D:247:ILE:HD13 | 4:E:254:LEU:HD13 | 1.53                     | 0.86              |
| 1:A:273:LEU:HD21 | 1:A:429:ARG:CB   | 2.05                     | 0.86              |
| 1:A:387:LYS:HE3  | 4:E:422:PHE:CE1  | 2.10                     | 0.86              |
| 1:A:307:THR:H    | 2:B:341:SER:CB   | 1.88                     | 0.86              |
| 2:B:232:PHE:CE2  | 2:B:277:ARG:HG3  | 2.11                     | 0.85              |
| 4:E:325:PHE:CD1  | 4:E:446:VAL:HG12 | 2.12                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:252:CYS:SG   | 4:E:302:VAL:HG22 | 2.17                     | 0.85              |
| 1:D:253:LEU:HD22 | 1:D:285:VAL:CG2  | 2.05                     | 0.85              |
| 3:C:408:ILE:CG1  | 1:D:379:VAL:HG11 | 2.07                     | 0.85              |
| 3:C:411:ILE:CD1  | 1:D:382:ILE:HG22 | 2.06                     | 0.85              |
| 2:B:322:LEU:HD13 | 2:B:446:TRP:CH2  | 2.11                     | 0.85              |
| 3:C:407:ALA:HB1  | 1:D:383:ALA:CB   | 2.07                     | 0.85              |
| 1:D:286:ILE:HD12 | 4:E:236:LEU:HD21 | 1.58                     | 0.85              |
| 1:A:375:ALA:HB2  | 2:B:423:ILE:HG23 | 0.92                     | 0.84              |
| 1:D:257:LEU:HD22 | 1:D:282:MET:HE3  | 1.58                     | 0.84              |
| 4:E:241:TYR:OH   | 4:E:297:ILE:HG12 | 1.77                     | 0.84              |
| 3:C:311:THR:HG22 | 1:D:404:MET:SD   | 2.17                     | 0.84              |
| 3:C:283:TYR:CD1  | 3:C:454:ILE:HD13 | 2.12                     | 0.84              |
| 4:E:255:SER:HB2  | 4:E:298:VAL:HG22 | 0.88                     | 0.84              |
| 1:D:247:ILE:HD13 | 4:E:254:LEU:CD1  | 2.06                     | 0.84              |
| 1:A:387:LYS:HE3  | 4:E:422:PHE:CZ   | 2.13                     | 0.84              |
| 1:A:277:TYR:CE2  | 1:A:426:PHE:CZ   | 2.66                     | 0.83              |
| 1:A:293:VAL:HG13 | 2:B:249:LEU:HD13 | 1.59                     | 0.83              |
| 2:B:256:LYS:HD3  | 2:B:310:LEU:CD1  | 2.08                     | 0.83              |
| 2:B:239:ILE:CD1  | 2:B:270:PHE:HE2  | 1.91                     | 0.83              |
| 1:D:233:PHE:CE2  | 1:D:414:PHE:CD2  | 2.66                     | 0.83              |
| 1:D:375:ALA:HB2  | 4:E:417:VAL:HB   | 1.61                     | 0.83              |
| 1:A:374:SER:HB3  | 2:B:427:ASN:HD21 | 1.41                     | 0.83              |
| 3:C:259:VAL:HG12 | 3:C:288:MET:HE3  | 1.60                     | 0.83              |
| 1:A:291:ILE:HD12 | 1:A:414:PHE:CZ   | 2.14                     | 0.83              |
| 4:E:286:TYR:CE2  | 4:E:467:PHE:CE2  | 2.66                     | 0.83              |
| 1:D:320:ILE:CG2  | 1:D:409:ILE:HD11 | 2.08                     | 0.83              |
| 1:A:381:TYR:HE2  | 2:B:433:ILE:HB   | 1.44                     | 0.82              |
| 2:B:317:PRO:HG3  | 2:B:442:GLU:OE2  | 1.80                     | 0.82              |
| 3:C:252:SER:HB2  | 3:C:295:VAL:HG22 | 1.60                     | 0.82              |
| 3:C:410:TYR:OH   | 1:D:387:LYS:HA   | 1.79                     | 0.82              |
| 2:B:239:ILE:CD1  | 2:B:270:PHE:CE2  | 2.62                     | 0.82              |
| 3:C:410:TYR:CE2  | 1:D:386:MET:HB3  | 2.15                     | 0.82              |
| 1:D:372:VAL:HA   | 4:E:417:VAL:HG11 | 1.62                     | 0.82              |
| 4:E:241:TYR:CE2  | 4:E:455:ALA:CB   | 2.62                     | 0.81              |
| 4:E:312:PRO:HG3  | 4:E:436:GLU:OE2  | 1.78                     | 0.81              |
| 3:C:407:ALA:HB1  | 1:D:383:ALA:HB2  | 1.62                     | 0.81              |
| 1:A:277:TYR:CE2  | 1:A:426:PHE:HZ   | 1.99                     | 0.81              |
| 1:A:273:LEU:HD22 | 1:A:429:ARG:CG   | 2.10                     | 0.81              |
| 1:D:320:ILE:CG2  | 1:D:409:ILE:CD1  | 2.59                     | 0.81              |
| 2:B:264:LEU:CD2  | 3:C:234:LEU:CD1  | 2.59                     | 0.81              |
| 1:D:375:ALA:HB2  | 4:E:417:VAL:CB   | 2.11                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:311:THR:HA   | 1:D:404:MET:SD   | 2.21                     | 0.81              |
| 1:D:375:ALA:CB   | 4:E:417:VAL:HA   | 2.09                     | 0.81              |
| 1:A:378:GLY:HA2  | 2:B:430:VAL:HG21 | 1.64                     | 0.80              |
| 1:A:376:ILE:HD11 | 4:E:413:ILE:CD1  | 2.05                     | 0.80              |
| 1:A:380:LYS:HE2  | 4:E:415:SER:OG   | 1.80                     | 0.80              |
| 2:B:418:GLU:HG3  | 3:C:402:LYS:CG   | 2.09                     | 0.80              |
| 3:C:266:LEU:HD23 | 3:C:281:ILE:CD1  | 2.12                     | 0.80              |
| 1:A:277:TYR:CZ   | 1:A:426:PHE:CE2  | 2.69                     | 0.80              |
| 2:B:239:ILE:HD12 | 2:B:270:PHE:CZ   | 2.16                     | 0.80              |
| 3:C:408:ILE:CG1  | 1:D:379:VAL:CG1  | 2.60                     | 0.80              |
| 4:E:230:CYS:HA   | 4:E:265:PHE:CE2  | 2.16                     | 0.80              |
| 4:E:242:PHE:HZ   | 4:E:452:PHE:CE1  | 2.01                     | 0.79              |
| 1:D:277:TYR:CD1  | 1:D:426:PHE:CZ   | 2.71                     | 0.79              |
| 1:D:381:TYR:CZ   | 4:E:428:LYS:HE3  | 2.18                     | 0.79              |
| 1:A:277:TYR:HD1  | 1:A:425:VAL:HG11 | 1.47                     | 0.79              |
| 1:A:375:ALA:HB1  | 2:B:423:ILE:HD12 | 1.64                     | 0.78              |
| 2:B:247:PHE:CE2  | 2:B:461:ILE:HG21 | 2.19                     | 0.78              |
| 2:B:419:ILE:HA   | 3:C:405:VAL:CG2  | 2.04                     | 0.78              |
| 1:D:277:TYR:CE1  | 1:D:426:PHE:CE2  | 2.71                     | 0.78              |
| 1:A:380:LYS:HE2  | 4:E:415:SER:CB   | 2.12                     | 0.78              |
| 1:D:232:VAL:HG23 | 1:D:245:LEU:CD2  | 2.14                     | 0.77              |
| 1:D:317:ILE:HD11 | 1:D:402:VAL:HG22 | 1.66                     | 0.77              |
| 3:C:407:ALA:CA   | 1:D:383:ALA:CB   | 2.62                     | 0.77              |
| 3:C:407:ALA:CA   | 1:D:383:ALA:HB2  | 2.14                     | 0.77              |
| 3:C:283:TYR:CZ   | 3:C:455:PHE:CE1  | 2.72                     | 0.77              |
| 1:D:308:MET:HE1  | 1:D:402:VAL:HG21 | 1.65                     | 0.77              |
| 1:A:379:VAL:O    | 4:E:419:ALA:HB1  | 1.84                     | 0.76              |
| 1:D:375:ALA:HB2  | 4:E:417:VAL:CA   | 2.15                     | 0.76              |
| 4:E:286:TYR:CZ   | 4:E:467:PHE:CE2  | 2.74                     | 0.76              |
| 1:D:234:TYR:HD1  | 1:D:411:LEU:HD22 | 1.49                     | 0.76              |
| 1:D:277:TYR:CZ   | 1:D:426:PHE:CZ   | 2.74                     | 0.76              |
| 1:A:387:LYS:CE   | 4:E:422:PHE:CE1  | 2.69                     | 0.76              |
| 2:B:426:THR:HB   | 3:C:408:ILE:HG21 | 1.68                     | 0.76              |
| 1:A:308:MET:HE1  | 1:A:402:VAL:HG21 | 1.66                     | 0.76              |
| 1:A:386:MET:HE1  | 4:E:423:ILE:CG2  | 2.09                     | 0.76              |
| 1:A:291:ILE:CG2  | 1:A:410:LEU:CD1  | 2.62                     | 0.75              |
| 2:B:317:PRO:HG3  | 2:B:442:GLU:CD   | 2.11                     | 0.75              |
| 1:D:222:CYS:SG   | 1:D:256:PHE:CE2  | 2.77                     | 0.75              |
| 3:C:401:LEU:CD2  | 1:D:376:ILE:HD11 | 2.17                     | 0.75              |
| 3:C:407:ALA:CB   | 1:D:383:ALA:CB   | 2.64                     | 0.75              |
| 4:E:317:LEU:HD13 | 4:E:440:TRP:CH2  | 2.22                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:273:LEU:CD2  | 1:A:429:ARG:CG   | 2.64                     | 0.75              |
| 1:A:379:VAL:HG11 | 4:E:416:CYS:O    | 1.86                     | 0.75              |
| 1:D:299:HIS:CE1  | 1:D:400:LYS:HG2  | 2.22                     | 0.75              |
| 1:D:317:ILE:CD1  | 1:D:402:VAL:CG2  | 2.62                     | 0.74              |
| 2:B:425:SER:CB   | 3:C:409:LYS:HA   | 2.16                     | 0.74              |
| 3:C:407:ALA:HB2  | 1:D:380:LYS:HA   | 1.68                     | 0.74              |
| 3:C:410:TYR:CE2  | 1:D:386:MET:CB   | 2.70                     | 0.74              |
| 3:C:411:ILE:HD11 | 1:D:382:ILE:CG2  | 2.17                     | 0.74              |
| 1:D:233:PHE:CE2  | 1:D:414:PHE:CE2  | 2.76                     | 0.74              |
| 3:C:410:TYR:HE2  | 1:D:386:MET:HB3  | 1.51                     | 0.74              |
| 2:B:291:TYR:CE2  | 2:B:473:PHE:HZ   | 2.06                     | 0.74              |
| 3:C:401:LEU:HD22 | 1:D:376:ILE:HD11 | 1.69                     | 0.74              |
| 1:D:277:TYR:CE2  | 1:D:426:PHE:HZ   | 2.05                     | 0.74              |
| 1:A:381:TYR:CZ   | 2:B:434:LYS:HG3  | 2.22                     | 0.73              |
| 1:A:381:TYR:CE1  | 2:B:434:LYS:HG3  | 2.23                     | 0.73              |
| 1:A:273:LEU:HD21 | 1:A:429:ARG:HB3  | 1.68                     | 0.73              |
| 3:C:407:ALA:HA   | 1:D:383:ALA:CB   | 2.19                     | 0.73              |
| 2:B:291:TYR:CE1  | 2:B:473:PHE:CZ   | 2.77                     | 0.73              |
| 1:D:291:ILE:HD12 | 1:D:414:PHE:HZ   | 1.53                     | 0.73              |
| 1:D:273:LEU:HD21 | 1:D:429:ARG:HG2  | 1.71                     | 0.73              |
| 4:E:312:PRO:HD3  | 4:E:436:GLU:HG2  | 1.71                     | 0.73              |
| 2:B:264:LEU:HD22 | 3:C:234:LEU:HD11 | 1.70                     | 0.73              |
| 3:C:332:ILE:HD11 | 3:C:437:ARG:HG2  | 1.70                     | 0.73              |
| 3:C:407:ALA:C    | 1:D:383:ALA:HB2  | 2.14                     | 0.73              |
| 1:A:299:HIS:NE2  | 1:A:400:LYS:HG2  | 2.04                     | 0.73              |
| 1:A:376:ILE:HA   | 4:E:416:CYS:HB2  | 1.69                     | 0.72              |
| 3:C:225:ILE:HG23 | 3:C:455:PHE:CE2  | 2.24                     | 0.72              |
| 2:B:248:TYR:CD1  | 2:B:458:MET:HE1  | 2.24                     | 0.72              |
| 3:C:236:ILE:HD11 | 3:C:447:CYS:SG   | 2.29                     | 0.72              |
| 2:B:247:PHE:CZ   | 2:B:302:VAL:HG13 | 2.25                     | 0.72              |
| 3:C:401:LEU:CD1  | 1:D:376:ILE:HD11 | 2.20                     | 0.72              |
| 1:D:277:TYR:HD1  | 1:D:425:VAL:HG11 | 1.53                     | 0.72              |
| 3:C:238:VAL:HA   | 3:C:251:LEU:HD21 | 1.69                     | 0.72              |
| 1:D:242:LYS:HE2  | 1:D:292:THR:HG23 | 1.72                     | 0.72              |
| 3:C:294:SER:CB   | 3:C:443:PHE:HE2  | 2.01                     | 0.72              |
| 1:A:291:ILE:HG21 | 1:A:410:LEU:CD1  | 2.17                     | 0.72              |
| 1:A:273:LEU:CD2  | 1:A:429:ARG:CB   | 2.68                     | 0.71              |
| 1:A:374:SER:HB3  | 2:B:427:ASN:ND2  | 2.05                     | 0.71              |
| 2:B:232:PHE:HZ   | 2:B:277:ARG:NE   | 1.87                     | 0.71              |
| 1:A:305:THR:CG2  | 2:B:448:LEU:CD2  | 2.69                     | 0.71              |
| 3:C:311:THR:CB   | 1:D:404:MET:SD   | 2.78                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:243:MET:HE1  | 1:D:293:VAL:HG22 | 1.72                     | 0.71              |
| 1:D:324:MET:HE1  | 1:D:412:CYS:SG   | 2.30                     | 0.71              |
| 3:C:231:ILE:CG1  | 3:C:262:PHE:HZ   | 2.03                     | 0.71              |
| 1:A:381:TYR:CG   | 2:B:430:VAL:HG13 | 2.25                     | 0.71              |
| 1:A:277:TYR:CD1  | 1:A:425:VAL:HG11 | 2.25                     | 0.71              |
| 1:A:277:TYR:CD2  | 1:A:426:PHE:CZ   | 2.79                     | 0.71              |
| 4:E:262:GLN:C    | 4:E:291:MET:CE   | 2.63                     | 0.71              |
| 3:C:411:ILE:CD1  | 1:D:382:ILE:CG2  | 2.68                     | 0.71              |
| 1:A:324:MET:HE1  | 1:A:412:CYS:SG   | 2.31                     | 0.70              |
| 1:A:374:SER:CB   | 2:B:427:ASN:HD21 | 2.04                     | 0.70              |
| 3:C:410:TYR:CE1  | 1:D:387:LYS:HD3  | 2.26                     | 0.70              |
| 1:D:320:ILE:HG21 | 1:D:409:ILE:HG13 | 1.73                     | 0.70              |
| 3:C:401:LEU:HD13 | 1:D:376:ILE:HD11 | 1.72                     | 0.70              |
| 4:E:241:TYR:CZ   | 4:E:455:ALA:HB2  | 2.27                     | 0.70              |
| 4:E:251:LYS:HB3  | 4:E:301:CYS:HB3  | 1.72                     | 0.70              |
| 4:E:325:PHE:HD1  | 4:E:446:VAL:HG11 | 1.56                     | 0.70              |
| 3:C:407:ALA:CB   | 1:D:380:LYS:HA   | 2.22                     | 0.70              |
| 3:C:407:ALA:CB   | 1:D:383:ALA:HB2  | 2.20                     | 0.69              |
| 1:D:234:TYR:CD1  | 1:D:411:LEU:HD22 | 2.27                     | 0.69              |
| 1:A:324:MET:CE   | 1:A:412:CYS:SG   | 2.80                     | 0.69              |
| 1:D:299:HIS:CD2  | 1:D:400:LYS:HA   | 2.27                     | 0.69              |
| 1:A:213:TYR:CB   | 4:E:277:SER:HB2  | 2.23                     | 0.69              |
| 1:A:382:ILE:HG22 | 4:E:423:ILE:CG1  | 2.23                     | 0.69              |
| 1:D:316:PHE:O    | 1:D:405:VAL:HG11 | 1.93                     | 0.69              |
| 1:A:306:HIS:HA   | 2:B:341:SER:HB2  | 1.74                     | 0.69              |
| 1:D:375:ALA:HA   | 4:E:421:ASN:OD1  | 1.92                     | 0.69              |
| 1:A:379:VAL:CG1  | 4:E:419:ALA:HB3  | 2.02                     | 0.68              |
| 1:D:277:TYR:CZ   | 1:D:426:PHE:HZ   | 2.08                     | 0.68              |
| 3:C:403:GLU:CB   | 1:D:380:LYS:HD3  | 2.21                     | 0.68              |
| 1:A:382:ILE:CG2  | 4:E:423:ILE:CD1  | 2.71                     | 0.68              |
| 1:D:406:ILE:HG22 | 1:D:410:LEU:HD12 | 1.76                     | 0.68              |
| 3:C:294:SER:HA   | 3:C:443:PHE:CE2  | 2.29                     | 0.68              |
| 1:D:243:MET:HB2  | 4:E:250:GLN:OE1  | 1.93                     | 0.68              |
| 1:A:233:PHE:CZ   | 1:A:288:SER:HB2  | 2.29                     | 0.68              |
| 1:A:380:LYS:HE2  | 4:E:415:SER:HB2  | 1.74                     | 0.67              |
| 4:E:230:CYS:HA   | 4:E:265:PHE:CZ   | 2.29                     | 0.67              |
| 1:A:387:LYS:CE   | 4:E:422:PHE:CZ   | 2.77                     | 0.67              |
| 2:B:247:PHE:CZ   | 2:B:461:ILE:CD1  | 2.76                     | 0.67              |
| 2:B:264:LEU:HD21 | 3:C:234:LEU:CD1  | 2.19                     | 0.67              |
| 1:A:307:THR:H    | 2:B:341:SER:HB3  | 1.59                     | 0.67              |
| 3:C:294:SER:CB   | 3:C:443:PHE:CE2  | 2.78                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:320:ILE:HG22 | 1:D:409:ILE:HD11 | 1.75                     | 0.67              |
| 1:A:376:ILE:HD13 | 4:E:413:ILE:N    | 2.10                     | 0.66              |
| 1:D:382:ILE:CD1  | 4:E:423:ILE:HG22 | 2.25                     | 0.66              |
| 3:C:404:ALA:HB2  | 1:D:376:ILE:CG2  | 2.22                     | 0.66              |
| 3:C:239:PHE:CE2  | 3:C:294:SER:HB2  | 2.30                     | 0.66              |
| 3:C:311:THR:CG2  | 1:D:404:MET:SD   | 2.83                     | 0.66              |
| 2:B:425:SER:OG   | 3:C:409:LYS:HA   | 1.95                     | 0.66              |
| 1:D:375:ALA:HB1  | 4:E:417:VAL:HA   | 1.78                     | 0.66              |
| 1:A:305:THR:HG21 | 2:B:451:GLN:OE1  | 1.95                     | 0.66              |
| 3:C:238:VAL:HG23 | 3:C:251:LEU:HD23 | 1.78                     | 0.66              |
| 1:A:291:ILE:HG22 | 1:A:410:LEU:HD13 | 1.75                     | 0.65              |
| 3:C:294:SER:CA   | 3:C:443:PHE:CE2  | 2.79                     | 0.65              |
| 1:A:307:THR:N    | 2:B:341:SER:CB   | 2.58                     | 0.65              |
| 3:C:408:ILE:HG13 | 1:D:379:VAL:HG13 | 1.75                     | 0.65              |
| 3:C:294:SER:CA   | 3:C:443:PHE:HE2  | 2.09                     | 0.65              |
| 2:B:421:SER:HB2  | 3:C:409:LYS:HZ1  | 1.57                     | 0.65              |
| 4:E:286:TYR:CD2  | 4:E:467:PHE:CZ   | 2.84                     | 0.65              |
| 2:B:248:TYR:HE1  | 2:B:458:MET:HE1  | 1.61                     | 0.65              |
| 2:B:278:LEU:HD13 | 2:B:286:PRO:HG3  | 1.79                     | 0.65              |
| 1:D:382:ILE:HD13 | 4:E:423:ILE:HG22 | 1.77                     | 0.65              |
| 1:A:295:VAL:HG11 | 1:A:407:ASP:OD1  | 1.98                     | 0.64              |
| 4:E:262:GLN:HE22 | 4:E:294:SER:CB   | 2.09                     | 0.64              |
| 1:A:253:LEU:HD21 | 1:A:281:THR:HG22 | 1.80                     | 0.64              |
| 3:C:266:LEU:CD2  | 3:C:281:ILE:HD13 | 2.20                     | 0.64              |
| 1:A:382:ILE:HB   | 4:E:423:ILE:HD11 | 1.79                     | 0.64              |
| 4:E:241:TYR:CZ   | 4:E:455:ALA:CB   | 2.80                     | 0.64              |
| 4:E:245:ALA:HB1  | 4:E:304:VAL:CG1  | 2.27                     | 0.64              |
| 3:C:407:ALA:HB1  | 1:D:383:ALA:HB3  | 1.80                     | 0.64              |
| 3:C:248:LYS:HB2  | 3:C:302:LEU:HD11 | 1.78                     | 0.64              |
| 3:C:280:ILE:O    | 3:C:284:LEU:HD23 | 1.98                     | 0.64              |
| 2:B:425:SER:HB3  | 3:C:409:LYS:HA   | 1.78                     | 0.64              |
| 1:A:257:LEU:HD13 | 1:A:278:MET:HE2  | 1.78                     | 0.64              |
| 3:C:407:ALA:CB   | 1:D:383:ALA:HB3  | 2.28                     | 0.64              |
| 4:E:230:CYS:CA   | 4:E:265:PHE:CE2  | 2.81                     | 0.64              |
| 1:A:375:ALA:HB3  | 2:B:423:ILE:HD12 | 1.77                     | 0.63              |
| 4:E:286:TYR:CD1  | 4:E:466:ILE:CG2  | 2.70                     | 0.63              |
| 3:C:311:THR:O    | 1:D:329:MET:HA   | 1.98                     | 0.63              |
| 1:D:247:ILE:CD1  | 4:E:254:LEU:CD1  | 2.77                     | 0.63              |
| 1:A:304:SER:HG   | 2:B:448:LEU:HD21 | 1.61                     | 0.63              |
| 4:E:312:PRO:HG3  | 4:E:436:GLU:CG   | 2.29                     | 0.63              |
| 3:C:238:VAL:CA   | 3:C:251:LEU:CD2  | 2.76                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:411:ILE:HA   | 1:D:386:MET:SD   | 2.39                     | 0.63              |
| 1:A:284:PHE:CZ   | 1:A:418:CYS:HB2  | 2.34                     | 0.63              |
| 1:D:257:LEU:HD22 | 1:D:282:MET:CE   | 2.28                     | 0.63              |
| 2:B:247:PHE:HE2  | 2:B:461:ILE:HG21 | 1.61                     | 0.63              |
| 1:D:375:ALA:HB2  | 4:E:417:VAL:HA   | 1.76                     | 0.63              |
| 1:A:375:ALA:HB1  | 2:B:423:ILE:CD1  | 2.29                     | 0.63              |
| 1:A:378:GLY:HA3  | 2:B:430:VAL:HG21 | 1.80                     | 0.62              |
| 1:A:375:ALA:CB   | 2:B:423:ILE:CD1  | 2.66                     | 0.62              |
| 1:A:378:GLY:C    | 2:B:430:VAL:HG21 | 2.24                     | 0.62              |
| 3:C:314:MET:HA   | 3:C:428:TRP:CZ2  | 2.35                     | 0.62              |
| 1:A:381:TYR:CD1  | 2:B:434:LYS:HE3  | 2.35                     | 0.62              |
| 2:B:260:ALA:HB1  | 2:B:303:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:307:THR:HG22 | 2:B:341:SER:CB   | 2.16                     | 0.62              |
| 4:E:245:ALA:HB1  | 4:E:304:VAL:HG12 | 1.82                     | 0.62              |
| 2:B:267:GLN:HB3  | 2:B:296:MET:HE3  | 1.79                     | 0.62              |
| 3:C:294:SER:HB3  | 3:C:443:PHE:HE2  | 1.62                     | 0.62              |
| 1:D:243:MET:HE1  | 1:D:293:VAL:CG2  | 2.29                     | 0.62              |
| 1:A:253:LEU:HD22 | 1:A:285:VAL:HG21 | 1.82                     | 0.62              |
| 3:C:401:LEU:HD22 | 1:D:376:ILE:HD13 | 1.79                     | 0.61              |
| 1:A:293:VAL:HG13 | 2:B:249:LEU:CD1  | 2.28                     | 0.61              |
| 1:D:243:MET:CE   | 1:D:293:VAL:HG22 | 2.30                     | 0.61              |
| 1:D:308:MET:CE   | 1:D:402:VAL:HG21 | 2.29                     | 0.61              |
| 1:D:320:ILE:HG23 | 1:D:409:ILE:CD1  | 2.30                     | 0.61              |
| 4:E:313:ASN:OD1  | 4:E:314:THR:N    | 2.33                     | 0.61              |
| 1:A:216:VAL:HG11 | 4:E:280:VAL:HG21 | 1.81                     | 0.61              |
| 4:E:283:ILE:O    | 4:E:287:LEU:HD23 | 1.99                     | 0.61              |
| 3:C:231:ILE:CG1  | 3:C:262:PHE:CZ   | 2.67                     | 0.61              |
| 4:E:262:GLN:CA   | 4:E:291:MET:HE3  | 2.30                     | 0.61              |
| 1:A:243:MET:HB2  | 2:B:255:GLU:CD   | 2.26                     | 0.61              |
| 3:C:407:ALA:HB3  | 1:D:379:VAL:HG12 | 1.82                     | 0.61              |
| 1:D:268:SER:HB3  | 4:E:221:PHE:HB2  | 1.82                     | 0.61              |
| 1:A:375:ALA:HB2  | 2:B:423:ILE:HD12 | 1.75                     | 0.61              |
| 1:D:317:ILE:CD1  | 1:D:402:VAL:HG22 | 2.27                     | 0.61              |
| 1:A:376:ILE:CD1  | 4:E:412:GLU:HB3  | 2.30                     | 0.60              |
| 3:C:403:GLU:HB3  | 1:D:380:LYS:CD   | 2.28                     | 0.60              |
| 1:A:386:MET:HE3  | 4:E:423:ILE:HG12 | 1.82                     | 0.60              |
| 3:C:259:VAL:HG11 | 3:C:288:MET:HA   | 1.83                     | 0.60              |
| 3:C:283:TYR:CG   | 3:C:454:ILE:HG21 | 2.34                     | 0.60              |
| 1:D:375:ALA:CB   | 4:E:417:VAL:CB   | 2.79                     | 0.60              |
| 1:D:326:PHE:CE1  | 1:D:412:CYS:SG   | 2.94                     | 0.60              |
| 1:A:306:HIS:CA   | 2:B:341:SER:HB2  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:376:ILE:HG12 | 4:E:416:CYS:HB2  | 1.83                     | 0.60              |
| 1:A:382:ILE:HG21 | 4:E:423:ILE:HD13 | 1.83                     | 0.60              |
| 1:D:233:PHE:HE2  | 1:D:414:PHE:CD2  | 2.20                     | 0.60              |
| 2:B:248:TYR:CD1  | 2:B:458:MET:CE   | 2.85                     | 0.60              |
| 4:E:262:GLN:CB   | 4:E:291:MET:CE   | 2.63                     | 0.60              |
| 1:A:376:ILE:CD1  | 4:E:413:ILE:HD13 | 2.07                     | 0.59              |
| 2:B:256:LYS:HD2  | 2:B:310:LEU:HD21 | 1.84                     | 0.59              |
| 1:D:293:VAL:HG13 | 4:E:243:LEU:HD23 | 1.85                     | 0.59              |
| 3:C:408:ILE:CD1  | 1:D:379:VAL:HG11 | 2.31                     | 0.59              |
| 1:D:385:HIS:NE2  | 4:E:431:ASN:CG   | 2.61                     | 0.59              |
| 1:D:375:ALA:CB   | 4:E:417:VAL:CA   | 2.77                     | 0.59              |
| 3:C:311:THR:CA   | 1:D:404:MET:SD   | 2.90                     | 0.59              |
| 3:C:239:PHE:HE2  | 3:C:294:SER:HB2  | 1.68                     | 0.59              |
| 2:B:247:PHE:CE2  | 2:B:461:ILE:CD1  | 2.83                     | 0.58              |
| 3:C:401:LEU:CD2  | 1:D:376:ILE:CD1  | 2.75                     | 0.58              |
| 1:A:222:CYS:SG   | 1:A:256:PHE:CE2  | 2.75                     | 0.58              |
| 1:A:216:VAL:CG2  | 4:E:280:VAL:HG21 | 2.27                     | 0.58              |
| 1:A:284:PHE:HZ   | 1:A:418:CYS:HB2  | 1.67                     | 0.58              |
| 1:A:381:TYR:OH   | 2:B:433:ILE:HG22 | 2.02                     | 0.58              |
| 3:C:408:ILE:CG1  | 1:D:379:VAL:HG13 | 2.31                     | 0.58              |
| 1:D:250:LEU:HD21 | 4:E:236:LEU:HD13 | 1.84                     | 0.58              |
| 1:A:376:ILE:HG12 | 4:E:416:CYS:CB   | 2.33                     | 0.58              |
| 3:C:407:ALA:O    | 1:D:383:ALA:HB2  | 2.04                     | 0.58              |
| 1:A:277:TYR:CD2  | 1:A:426:PHE:HZ   | 2.21                     | 0.58              |
| 3:C:311:THR:HB   | 1:D:404:MET:SD   | 2.44                     | 0.58              |
| 4:E:269:ILE:HD13 | 4:E:287:LEU:CG   | 2.24                     | 0.58              |
| 4:E:325:PHE:CD1  | 4:E:446:VAL:CG1  | 2.67                     | 0.58              |
| 1:A:380:LYS:CE   | 4:E:415:SER:HB2  | 2.33                     | 0.57              |
| 3:C:231:ILE:CG1  | 3:C:262:PHE:CE2  | 2.79                     | 0.57              |
| 1:D:293:VAL:HG13 | 4:E:243:LEU:CD2  | 2.35                     | 0.57              |
| 1:A:291:ILE:HD12 | 1:A:414:PHE:HZ   | 1.65                     | 0.57              |
| 2:B:291:TYR:CZ   | 2:B:473:PHE:CE2  | 2.93                     | 0.57              |
| 2:B:422:GLY:N    | 3:C:405:VAL:CG1  | 2.64                     | 0.57              |
| 1:A:305:THR:HG23 | 2:B:448:LEU:CD2  | 2.35                     | 0.57              |
| 1:A:273:LEU:HD21 | 1:A:429:ARG:HB2  | 1.86                     | 0.57              |
| 1:A:277:TYR:CZ   | 1:A:426:PHE:HE2  | 2.20                     | 0.57              |
| 1:A:297:ASN:OD1  | 2:B:250:PRO:HD3  | 2.05                     | 0.56              |
| 3:C:411:ILE:HG12 | 1:D:386:MET:HE3  | 1.87                     | 0.56              |
| 1:A:284:PHE:CE1  | 1:A:417:ILE:HG22 | 2.40                     | 0.56              |
| 3:C:231:ILE:HG21 | 3:C:262:PHE:HE2  | 1.71                     | 0.56              |
| 3:C:411:ILE:CG2  | 1:D:386:MET:CE   | 2.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:288:SER:HA   | 1:A:414:PHE:CE2  | 2.41                     | 0.56              |
| 2:B:422:GLY:HA3  | 3:C:405:VAL:CB   | 2.35                     | 0.56              |
| 1:A:324:MET:HE2  | 1:A:412:CYS:SG   | 2.45                     | 0.56              |
| 2:B:256:LYS:HD3  | 2:B:310:LEU:CG   | 2.35                     | 0.56              |
| 1:D:372:VAL:HA   | 4:E:417:VAL:CG1  | 2.34                     | 0.56              |
| 4:E:286:TYR:CE2  | 4:E:467:PHE:HZ   | 2.20                     | 0.56              |
| 1:A:376:ILE:HG21 | 4:E:412:GLU:CA   | 2.35                     | 0.56              |
| 1:A:381:TYR:CE2  | 2:B:433:ILE:HB   | 2.34                     | 0.56              |
| 1:D:253:LEU:CD2  | 1:D:285:VAL:CG2  | 2.73                     | 0.56              |
| 1:D:382:ILE:HD11 | 4:E:424:ALA:N    | 2.21                     | 0.55              |
| 1:A:380:LYS:CE   | 4:E:415:SER:CB   | 2.83                     | 0.55              |
| 1:D:277:TYR:CD2  | 1:D:426:PHE:HZ   | 2.24                     | 0.55              |
| 1:A:383:ALA:O    | 4:E:422:PHE:CE2  | 2.60                     | 0.55              |
| 1:D:277:TYR:CZ   | 1:D:426:PHE:CE2  | 2.94                     | 0.55              |
| 1:D:277:TYR:CG   | 1:D:426:PHE:CZ   | 2.94                     | 0.55              |
| 1:A:291:ILE:HD12 | 1:A:414:PHE:CE1  | 2.42                     | 0.55              |
| 3:C:231:ILE:CB   | 3:C:262:PHE:HE2  | 2.19                     | 0.55              |
| 1:D:233:PHE:CZ   | 1:D:414:PHE:CE2  | 2.95                     | 0.55              |
| 1:D:379:VAL:CG2  | 4:E:420:CYS:SG   | 2.94                     | 0.55              |
| 2:B:239:ILE:HD13 | 2:B:270:PHE:HE2  | 1.67                     | 0.55              |
| 1:D:253:LEU:HD22 | 1:D:285:VAL:HG11 | 1.88                     | 0.55              |
| 2:B:418:GLU:HG2  | 3:C:402:LYS:HG3  | 1.87                     | 0.54              |
| 2:B:248:TYR:CD1  | 2:B:458:MET:SD   | 3.00                     | 0.54              |
| 1:D:326:PHE:CZ   | 1:D:412:CYS:SG   | 3.00                     | 0.54              |
| 4:E:237:VAL:HG12 | 4:E:258:VAL:CG1  | 2.27                     | 0.54              |
| 1:A:307:THR:N    | 2:B:341:SER:HB3  | 2.23                     | 0.54              |
| 3:C:408:ILE:HD11 | 1:D:379:VAL:HG21 | 1.88                     | 0.54              |
| 1:A:305:THR:O    | 2:B:341:SER:HB2  | 2.07                     | 0.54              |
| 1:D:320:ILE:HG23 | 1:D:409:ILE:HD11 | 1.85                     | 0.54              |
| 3:C:314:MET:CA   | 3:C:428:TRP:CZ2  | 2.90                     | 0.54              |
| 3:C:410:TYR:HE2  | 1:D:386:MET:HB2  | 1.71                     | 0.54              |
| 1:D:375:ALA:CB   | 4:E:417:VAL:HB   | 2.37                     | 0.54              |
| 2:B:267:GLN:HE22 | 2:B:299:VAL:HG11 | 1.72                     | 0.54              |
| 1:D:242:LYS:HB2  | 1:D:296:ILE:HD11 | 1.90                     | 0.54              |
| 1:A:257:LEU:CG   | 1:A:278:MET:HE1  | 2.35                     | 0.54              |
| 4:E:245:ALA:CB   | 4:E:304:VAL:CG1  | 2.86                     | 0.54              |
| 4:E:241:TYR:CE2  | 4:E:455:ALA:HB1  | 2.43                     | 0.54              |
| 1:A:376:ILE:CG2  | 4:E:412:GLU:O    | 2.56                     | 0.53              |
| 1:A:277:TYR:CZ   | 1:A:426:PHE:CZ   | 2.95                     | 0.53              |
| 2:B:291:TYR:CE1  | 2:B:473:PHE:CE2  | 2.97                     | 0.53              |
| 2:B:317:PRO:CG   | 2:B:442:GLU:CD   | 2.81                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:386:MET:HB2  | 4:E:422:PHE:HE2  | 1.73                     | 0.53              |
| 1:D:247:ILE:CD1  | 4:E:254:LEU:HD12 | 2.39                     | 0.53              |
| 3:C:263:LEU:HD11 | 3:C:285:MET:HE2  | 1.90                     | 0.53              |
| 3:C:283:TYR:CD1  | 3:C:454:ILE:CD1  | 2.89                     | 0.53              |
| 1:A:233:PHE:CE2  | 1:A:288:SER:HB2  | 2.44                     | 0.52              |
| 3:C:314:MET:HB2  | 3:C:428:TRP:CZ2  | 2.44                     | 0.52              |
| 1:A:376:ILE:HD13 | 4:E:412:GLU:CB   | 2.38                     | 0.52              |
| 4:E:241:TYR:CE2  | 4:E:455:ALA:HB3  | 2.42                     | 0.52              |
| 1:A:376:ILE:CA   | 4:E:416:CYS:HB2  | 2.39                     | 0.52              |
| 3:C:238:VAL:CA   | 3:C:251:LEU:HD21 | 2.39                     | 0.52              |
| 1:D:273:LEU:HD21 | 1:D:429:ARG:CG   | 2.38                     | 0.52              |
| 2:B:422:GLY:H    | 3:C:405:VAL:CG1  | 2.23                     | 0.52              |
| 1:A:305:THR:CG2  | 2:B:451:GLN:OE1  | 2.57                     | 0.52              |
| 1:D:317:ILE:CG1  | 1:D:402:VAL:HG22 | 2.39                     | 0.52              |
| 2:B:418:GLU:OE2  | 3:C:402:LYS:HE3  | 2.09                     | 0.52              |
| 1:A:307:THR:CG2  | 2:B:341:SER:HB3  | 2.19                     | 0.52              |
| 1:A:385:HIS:CE1  | 2:B:436:LYS:HZ1  | 2.28                     | 0.52              |
| 2:B:426:THR:CB   | 3:C:408:ILE:HG21 | 2.40                     | 0.52              |
| 1:A:277:TYR:CE1  | 1:A:426:PHE:CE2  | 2.98                     | 0.52              |
| 4:E:286:TYR:HD1  | 4:E:466:ILE:HD13 | 1.74                     | 0.52              |
| 1:A:299:HIS:CE1  | 1:A:400:LYS:HG2  | 2.44                     | 0.51              |
| 1:D:290:ILE:HG12 | 4:E:239:LEU:HD21 | 1.91                     | 0.51              |
| 4:E:325:PHE:CZ   | 4:E:447:ILE:HG12 | 2.45                     | 0.51              |
| 1:A:253:LEU:CD2  | 1:A:285:VAL:HG21 | 2.41                     | 0.51              |
| 3:C:266:LEU:HD22 | 3:C:284:LEU:HG   | 1.92                     | 0.51              |
| 1:A:383:ALA:HB1  | 4:E:422:PHE:CD2  | 2.45                     | 0.51              |
| 1:A:382:ILE:HG13 | 2:B:430:VAL:HG22 | 1.92                     | 0.51              |
| 1:D:375:ALA:HB3  | 4:E:417:VAL:HG12 | 1.92                     | 0.51              |
| 1:D:381:TYR:CZ   | 4:E:428:LYS:CE   | 2.90                     | 0.51              |
| 3:C:314:MET:HE3  | 3:C:431:VAL:HG21 | 1.92                     | 0.51              |
| 3:C:411:ILE:CG2  | 1:D:386:MET:HE1  | 2.10                     | 0.51              |
| 4:E:269:ILE:CD1  | 4:E:287:LEU:CG   | 2.79                     | 0.51              |
| 1:A:257:LEU:CB   | 1:A:278:MET:HE1  | 2.41                     | 0.51              |
| 1:A:295:VAL:HG21 | 1:A:407:ASP:OD1  | 2.10                     | 0.51              |
| 1:A:382:ILE:HG22 | 4:E:423:ILE:CD1  | 2.38                     | 0.51              |
| 2:B:456:LEU:HG   | 2:B:460:ILE:HD12 | 1.92                     | 0.51              |
| 1:D:234:TYR:CD1  | 1:D:411:LEU:CD2  | 2.93                     | 0.51              |
| 1:A:256:PHE:O    | 1:A:260:ILE:HD12 | 2.10                     | 0.51              |
| 1:A:376:ILE:CD1  | 4:E:412:GLU:CB   | 2.89                     | 0.51              |
| 1:A:380:LYS:HA   | 4:E:419:ALA:HB2  | 1.93                     | 0.50              |
| 1:D:250:LEU:HD13 | 1:D:289:ILE:CD1  | 2.40                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:242:PHE:HZ   | 4:E:452:PHE:HE1  | 1.58                     | 0.50              |
| 2:B:234:THR:CG2  | 2:B:235:PRO:HD3  | 2.41                     | 0.50              |
| 2:B:438:ALA:O    | 2:B:441:GLU:HG3  | 2.11                     | 0.50              |
| 3:C:410:TYR:CE2  | 1:D:386:MET:HB2  | 2.47                     | 0.50              |
| 1:D:324:MET:SD   | 1:D:409:ILE:HD13 | 2.51                     | 0.50              |
| 1:A:308:MET:HE3  | 1:A:399:TRP:CZ3  | 2.47                     | 0.50              |
| 3:C:410:TYR:CE2  | 1:D:387:LYS:N    | 2.80                     | 0.50              |
| 1:A:213:TYR:CG   | 4:E:277:SER:CB   | 2.94                     | 0.50              |
| 2:B:251:ALA:HB1  | 2:B:310:LEU:CD2  | 2.42                     | 0.50              |
| 1:A:299:HIS:CD2  | 1:A:400:LYS:HG2  | 2.47                     | 0.50              |
| 1:A:376:ILE:HD12 | 4:E:412:GLU:HB3  | 1.93                     | 0.50              |
| 2:B:426:THR:N    | 3:C:408:ILE:CG2  | 2.75                     | 0.50              |
| 3:C:283:TYR:OH   | 3:C:455:PHE:CE1  | 2.65                     | 0.50              |
| 4:E:233:ILE:HD12 | 4:E:265:PHE:CZ   | 2.47                     | 0.50              |
| 1:A:213:TYR:HB2  | 4:E:277:SER:HB2  | 1.94                     | 0.49              |
| 2:B:248:TYR:HD1  | 2:B:458:MET:CE   | 2.25                     | 0.49              |
| 1:D:381:TYR:OH   | 4:E:428:LYS:CE   | 2.60                     | 0.49              |
| 1:A:246:SER:HB2  | 1:A:289:ILE:HG12 | 1.92                     | 0.49              |
| 1:A:297:ASN:HA   | 2:B:250:PRO:HG3  | 1.94                     | 0.49              |
| 1:D:320:ILE:CG2  | 1:D:409:ILE:HG13 | 2.42                     | 0.49              |
| 4:E:237:VAL:CG1  | 4:E:258:VAL:CG1  | 2.85                     | 0.49              |
| 1:D:253:LEU:HD22 | 1:D:285:VAL:CB   | 2.42                     | 0.49              |
| 4:E:237:VAL:HG11 | 4:E:294:SER:OG   | 2.11                     | 0.49              |
| 1:D:239:SER:O    | 1:D:239:SER:OG   | 2.25                     | 0.49              |
| 1:A:302:SER:CB   | 2:B:451:GLN:HE22 | 2.26                     | 0.49              |
| 1:A:382:ILE:CB   | 4:E:423:ILE:HD11 | 2.42                     | 0.49              |
| 3:C:411:ILE:HD13 | 1:D:382:ILE:CG2  | 2.43                     | 0.49              |
| 1:A:376:ILE:HD13 | 4:E:412:GLU:O    | 2.07                     | 0.49              |
| 1:A:386:MET:SD   | 4:E:426:SER:HB2  | 2.53                     | 0.49              |
| 3:C:226:ILE:HB   | 3:C:227:PRO:HD3  | 1.94                     | 0.49              |
| 3:C:235:ALA:O    | 3:C:238:VAL:HG12 | 2.13                     | 0.49              |
| 3:C:225:ILE:HG23 | 3:C:455:PHE:CZ   | 2.48                     | 0.48              |
| 1:D:232:VAL:HA   | 1:D:245:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:317:ILE:HD11 | 1:A:402:VAL:CG2  | 2.43                     | 0.48              |
| 3:C:225:ILE:CG2  | 3:C:455:PHE:CE2  | 2.95                     | 0.48              |
| 1:A:381:TYR:OH   | 2:B:434:LYS:HG3  | 2.13                     | 0.48              |
| 4:E:243:LEU:HD11 | 4:E:254:LEU:HD23 | 1.95                     | 0.48              |
| 1:D:302:SER:CB   | 4:E:445:LYS:CE   | 2.70                     | 0.48              |
| 1:A:213:TYR:CG   | 4:E:277:SER:HB3  | 2.49                     | 0.48              |
| 3:C:238:VAL:CA   | 3:C:251:LEU:HD23 | 2.33                     | 0.48              |
| 1:A:262:GLU:OE2  | 4:E:267:PHE:CE1  | 2.67                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:256:LYS:CD   | 2:B:310:LEU:HD21 | 2.43                     | 0.48              |
| 4:E:312:PRO:CD   | 4:E:436:GLU:HG2  | 2.43                     | 0.47              |
| 1:A:243:MET:HB2  | 2:B:255:GLU:OE1  | 2.13                     | 0.47              |
| 1:A:383:ALA:O    | 4:E:422:PHE:HE2  | 1.97                     | 0.47              |
| 3:C:231:ILE:HD12 | 3:C:258:ALA:HB1  | 1.95                     | 0.47              |
| 4:E:242:PHE:CZ   | 4:E:452:PHE:HE1  | 2.29                     | 0.47              |
| 4:E:312:PRO:CG   | 4:E:436:GLU:OE2  | 2.57                     | 0.47              |
| 2:B:267:GLN:NE2  | 2:B:299:VAL:HG11 | 2.29                     | 0.47              |
| 1:D:299:HIS:NE2  | 1:D:400:LYS:CG   | 2.63                     | 0.47              |
| 1:D:381:TYR:OH   | 4:E:428:LYS:HE3  | 2.14                     | 0.47              |
| 4:E:230:CYS:CB   | 4:E:265:PHE:CE2  | 2.97                     | 0.47              |
| 1:A:378:GLY:O    | 2:B:430:VAL:CG2  | 2.63                     | 0.47              |
| 3:C:248:LYS:HD2  | 3:C:302:LEU:HG   | 1.96                     | 0.47              |
| 3:C:314:MET:CB   | 3:C:428:TRP:CZ2  | 2.97                     | 0.47              |
| 1:A:376:ILE:HG21 | 4:E:412:GLU:HB3  | 1.96                     | 0.47              |
| 2:B:315:ARG:HD3  | 2:B:320:HIS:CD2  | 2.50                     | 0.47              |
| 1:A:268:SER:OG   | 2:B:227:PHE:CD1  | 2.56                     | 0.47              |
| 2:B:244:SER:OG   | 2:B:465:MET:HE1  | 2.15                     | 0.47              |
| 2:B:260:ALA:HB1  | 2:B:303:ILE:HG23 | 1.97                     | 0.47              |
| 3:C:238:VAL:HG23 | 3:C:251:LEU:HB3  | 1.96                     | 0.47              |
| 3:C:407:ALA:HA   | 1:D:383:ALA:HB1  | 1.95                     | 0.47              |
| 1:D:382:ILE:HD13 | 4:E:423:ILE:CG2  | 2.43                     | 0.47              |
| 1:D:291:ILE:HD12 | 1:D:414:PHE:CZ   | 2.41                     | 0.47              |
| 4:E:325:PHE:CD1  | 4:E:446:VAL:HG11 | 2.45                     | 0.47              |
| 2:B:426:THR:HB   | 3:C:408:ILE:CG2  | 2.43                     | 0.46              |
| 2:B:418:GLU:HG3  | 3:C:402:LYS:HG2  | 1.96                     | 0.46              |
| 3:C:239:PHE:CE2  | 3:C:443:PHE:CD2  | 3.04                     | 0.46              |
| 3:C:231:ILE:CG2  | 3:C:262:PHE:HE2  | 2.28                     | 0.46              |
| 2:B:244:SER:OG   | 2:B:465:MET:CE   | 2.64                     | 0.46              |
| 4:E:317:LEU:HD13 | 4:E:440:TRP:CZ3  | 2.51                     | 0.46              |
| 3:C:294:SER:HB3  | 3:C:443:PHE:CE2  | 2.45                     | 0.46              |
| 3:C:314:MET:HB2  | 3:C:428:TRP:CE2  | 2.51                     | 0.46              |
| 3:C:410:TYR:OH   | 1:D:387:LYS:CA   | 2.58                     | 0.46              |
| 1:A:376:ILE:HG21 | 4:E:412:GLU:HA   | 1.97                     | 0.46              |
| 1:A:213:TYR:HB3  | 4:E:277:SER:HB2  | 1.97                     | 0.45              |
| 1:D:320:ILE:CG2  | 1:D:409:ILE:CG1  | 2.94                     | 0.45              |
| 1:A:386:MET:HE3  | 4:E:423:ILE:HG23 | 1.89                     | 0.45              |
| 2:B:428:TYR:OH   | 3:C:416:GLU:HG3  | 2.16                     | 0.45              |
| 3:C:274:SER:HB3  | 1:D:213:TYR:HB2  | 1.98                     | 0.45              |
| 1:D:382:ILE:HD11 | 4:E:423:ILE:HG22 | 1.97                     | 0.45              |
| 1:A:381:TYR:OH   | 2:B:434:LYS:HA   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:259:VAL:CG1  | 3:C:288:MET:HE3  | 2.38                     | 0.45              |
| 1:A:381:TYR:OH   | 2:B:434:LYS:CA   | 2.64                     | 0.45              |
| 3:C:410:TYR:CE2  | 1:D:387:LYS:HG2  | 2.52                     | 0.45              |
| 1:D:284:PHE:HZ   | 1:D:418:CYS:HB2  | 1.81                     | 0.45              |
| 1:A:233:PHE:HZ   | 1:A:288:SER:HB2  | 1.79                     | 0.44              |
| 1:A:268:SER:OG   | 2:B:227:PHE:CE1  | 2.66                     | 0.44              |
| 1:A:386:MET:HB2  | 4:E:422:PHE:CE2  | 2.52                     | 0.44              |
| 4:E:243:LEU:HD11 | 4:E:254:LEU:CD2  | 2.48                     | 0.44              |
| 3:C:236:ILE:HD11 | 3:C:447:CYS:CB   | 2.48                     | 0.44              |
| 1:D:304:SER:OG   | 4:E:442:LEU:CD2  | 2.65                     | 0.44              |
| 2:B:423:ILE:HA   | 2:B:426:THR:HG22 | 2.00                     | 0.44              |
| 3:C:332:ILE:O    | 3:C:333:GLN:C    | 2.60                     | 0.44              |
| 4:E:228:ALA:HB3  | 4:E:229:PRO:HD3  | 1.99                     | 0.44              |
| 4:E:241:TYR:OH   | 4:E:455:ALA:HB2  | 2.17                     | 0.44              |
| 1:A:299:HIS:HB2  | 1:A:403:ALA:CB   | 2.47                     | 0.44              |
| 1:A:381:TYR:CE1  | 2:B:434:LYS:HE3  | 2.53                     | 0.44              |
| 3:C:238:VAL:HG23 | 3:C:251:LEU:CD2  | 2.45                     | 0.43              |
| 3:C:238:VAL:HB   | 3:C:251:LEU:HG   | 2.01                     | 0.43              |
| 1:A:384:GLU:O    | 1:A:387:LYS:HB2  | 2.17                     | 0.43              |
| 3:C:407:ALA:HB1  | 1:D:379:VAL:O    | 2.19                     | 0.43              |
| 3:C:314:MET:HE2  | 3:C:319:ARG:HB2  | 2.01                     | 0.43              |
| 1:D:226:SER:O    | 1:D:229:THR:HG22 | 2.18                     | 0.43              |
| 3:C:226:ILE:N    | 3:C:227:PRO:CD   | 2.81                     | 0.43              |
| 3:C:238:VAL:HG23 | 3:C:251:LEU:CG   | 2.48                     | 0.43              |
| 2:B:416:HIS:O    | 2:B:416:HIS:ND1  | 2.52                     | 0.43              |
| 1:D:308:MET:HE2  | 1:D:399:TRP:CZ3  | 2.53                     | 0.43              |
| 2:B:236:CYS:SG   | 2:B:292:LEU:HD21 | 2.59                     | 0.43              |
| 2:B:426:THR:N    | 3:C:408:ILE:HG21 | 2.33                     | 0.43              |
| 4:E:237:VAL:HG13 | 4:E:258:VAL:HG11 | 1.97                     | 0.43              |
| 3:C:306:HIS:CD2  | 1:D:239:SER:HB3  | 2.54                     | 0.42              |
| 1:D:284:PHE:CZ   | 1:D:418:CYS:HB2  | 2.54                     | 0.42              |
| 1:D:317:ILE:HG13 | 1:D:402:VAL:HG22 | 1.99                     | 0.42              |
| 3:C:283:TYR:CD1  | 3:C:454:ILE:CG2  | 2.84                     | 0.42              |
| 3:C:303:ASN:ND2  | 1:D:236:PRO:HD3  | 2.34                     | 0.42              |
| 1:A:376:ILE:HD13 | 4:E:412:GLU:CA   | 2.42                     | 0.42              |
| 1:D:277:TYR:CD2  | 1:D:426:PHE:CZ   | 3.06                     | 0.42              |
| 1:D:317:ILE:HD11 | 1:D:402:VAL:HG21 | 1.86                     | 0.42              |
| 1:A:264:ILE:CG2  | 1:A:274:ILE:CD1  | 2.80                     | 0.42              |
| 3:C:239:PHE:HZ   | 3:C:294:SER:HA   | 1.84                     | 0.42              |
| 3:C:327:PRO:N    | 3:C:328:PRO:HD2  | 2.34                     | 0.42              |
| 4:E:269:ILE:HG22 | 4:E:269:ILE:O    | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:421:SER:CB   | 3:C:409:LYS:NZ   | 2.61                     | 0.42              |
| 3:C:305:HIS:O    | 3:C:429:GLN:HG2  | 2.20                     | 0.42              |
| 4:E:286:TYR:CD1  | 4:E:466:ILE:HD13 | 2.52                     | 0.42              |
| 1:A:306:HIS:HA   | 2:B:341:SER:CB   | 2.45                     | 0.42              |
| 3:C:410:TYR:CZ   | 1:D:387:LYS:HA   | 2.55                     | 0.42              |
| 3:C:411:ILE:HD13 | 1:D:382:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:380:LYS:HA   | 4:E:419:ALA:CB   | 2.49                     | 0.42              |
| 1:A:381:TYR:OH   | 2:B:434:LYS:N    | 2.53                     | 0.42              |
| 3:C:277:VAL:O    | 3:C:282:ARG:NH1  | 2.53                     | 0.42              |
| 2:B:267:GLN:O    | 2:B:296:MET:CE   | 2.68                     | 0.41              |
| 3:C:231:ILE:HG21 | 3:C:262:PHE:CE2  | 2.52                     | 0.41              |
| 1:A:273:LEU:CD2  | 1:A:429:ARG:HB2  | 2.47                     | 0.41              |
| 1:D:406:ILE:HG22 | 1:D:410:LEU:CD1  | 2.48                     | 0.41              |
| 1:A:383:ALA:CB   | 4:E:422:PHE:HD2  | 2.33                     | 0.41              |
| 2:B:267:GLN:O    | 2:B:296:MET:HE3  | 2.21                     | 0.41              |
| 3:C:410:TYR:CZ   | 1:D:387:LYS:HG2  | 2.54                     | 0.41              |
| 1:A:213:TYR:CB   | 4:E:277:SER:CB   | 2.94                     | 0.41              |
| 1:A:260:ILE:HD12 | 1:A:260:ILE:H    | 1.86                     | 0.41              |
| 1:A:376:ILE:HG21 | 4:E:412:GLU:CB   | 2.50                     | 0.41              |
| 1:A:376:ILE:HG21 | 4:E:412:GLU:O    | 2.20                     | 0.41              |
| 1:A:381:TYR:CZ   | 2:B:433:ILE:HG22 | 2.55                     | 0.41              |
| 1:A:385:HIS:CE1  | 2:B:436:LYS:NZ   | 2.88                     | 0.41              |
| 3:C:398:PRO:N    | 3:C:402:LYS:HZ3  | 2.18                     | 0.41              |
| 1:A:376:ILE:HG23 | 4:E:412:GLU:O    | 2.21                     | 0.41              |
| 3:C:400:ASP:O    | 1:D:376:ILE:HG21 | 2.21                     | 0.41              |
| 1:A:376:ILE:HD13 | 4:E:412:GLU:HB3  | 2.00                     | 0.41              |
| 2:B:257:MET:HE2  | 3:C:241:LEU:HD11 | 2.02                     | 0.41              |
| 1:D:253:LEU:CD2  | 1:D:285:VAL:CB   | 2.99                     | 0.41              |
| 4:E:286:TYR:CD2  | 4:E:467:PHE:HZ   | 2.35                     | 0.41              |
| 3:C:238:VAL:CG2  | 3:C:251:LEU:HD23 | 2.50                     | 0.41              |
| 3:C:283:TYR:HH   | 3:C:451:THR:HG23 | 1.80                     | 0.41              |
| 2:B:418:GLU:OE2  | 3:C:402:LYS:CE   | 2.69                     | 0.41              |
| 1:D:253:LEU:HD22 | 1:D:285:VAL:CG1  | 2.51                     | 0.41              |
| 1:D:375:ALA:CB   | 4:E:417:VAL:HG12 | 2.51                     | 0.41              |
| 2:B:232:PHE:CZ   | 2:B:277:ARG:NE   | 2.79                     | 0.41              |
| 2:B:256:LYS:HB2  | 2:B:310:LEU:HD11 | 2.02                     | 0.41              |
| 2:B:278:LEU:CD1  | 2:B:286:PRO:HG3  | 2.49                     | 0.41              |
| 1:D:326:PHE:HE1  | 1:D:412:CYS:SG   | 2.43                     | 0.40              |
| 3:C:449:ILE:HD12 | 3:C:449:ILE:HG23 | 1.93                     | 0.40              |
| 4:E:251:LYS:HD3  | 4:E:301:CYS:HB3  | 2.03                     | 0.40              |
| 4:E:255:SER:OG   | 4:E:298:VAL:HG13 | 2.20                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:B:418:GLU:CG   | 3:C:402:LYS:CG  | 2.83                     | 0.40              |
| 3:C:231:ILE:HB   | 3:C:262:PHE:HE2 | 1.87                     | 0.40              |
| 3:C:303:ASN:ND2  | 1:D:234:TYR:O   | 2.55                     | 0.40              |
| 3:C:449:ILE:HD13 | 3:C:449:ILE:HA  | 1.83                     | 0.40              |
| 1:A:235:LEU:HD12 | 1:A:236:PRO:HD2 | 2.03                     | 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     | 180/437 (41%)  | 173 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | D     | 180/437 (41%)  | 174 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 2   | B     | 176/501 (35%)  | 173 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 3   | C     | 176/469 (38%)  | 170 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 4   | E     | 169/489 (35%)  | 167 (99%) | 2 (1%)  | 0        | 100         | 100 |
| All | All   | 881/2333 (38%) | 857 (97%) | 24 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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     | 171/405 (42%)  | 171 (100%) | 0        | 100         | 100 |
| 1   | D     | 171/405 (42%)  | 171 (100%) | 0        | 100         | 100 |
| 2   | B     | 162/458 (35%)  | 162 (100%) | 0        | 100         | 100 |
| 3   | C     | 165/431 (38%)  | 164 (99%)  | 1 (1%)   | 78          | 81  |
| 4   | E     | 154/446 (34%)  | 154 (100%) | 0        | 100         | 100 |
| All | All   | 823/2145 (38%) | 822 (100%) | 1 (0%)   | 87          | 88  |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 405 | VAL  |

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     | 300 | HIS  |
| 1   | A     | 394 | ASN  |
| 2   | B     | 267 | GLN  |
| 3   | C     | 306 | HIS  |
| 3   | C     | 414 | GLN  |
| 3   | C     | 429 | GLN  |
| 1   | D     | 408 | HIS  |
| 4   | E     | 225 | ASN  |
| 4   | E     | 262 | GLN  |
| 4   | E     | 300 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18596. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

#### 6.1.1 Primary map



X



Y



Z

#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

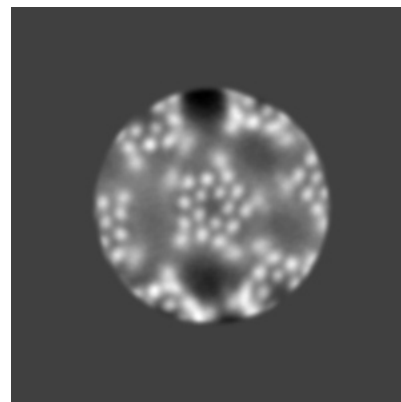
### 6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

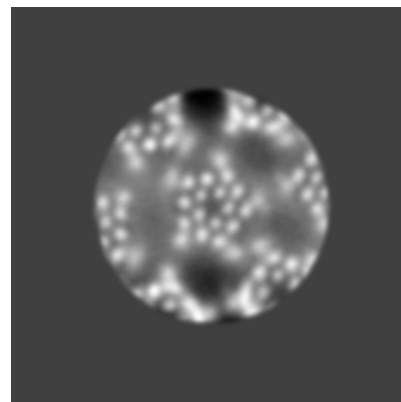
### 6.2.2 Raw map



X Index: 100



Y Index: 100



Z Index: 100

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: 111



Y Index: 112



Z Index: 76

### 6.3.2 Raw map



X Index: 111



Y Index: 112

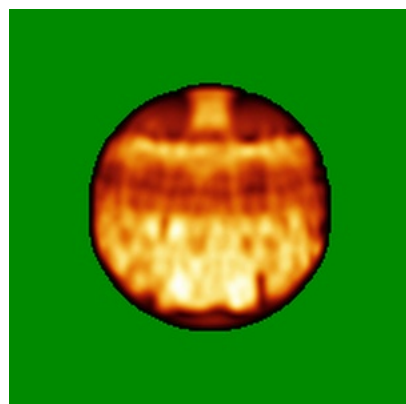


Z Index: 76

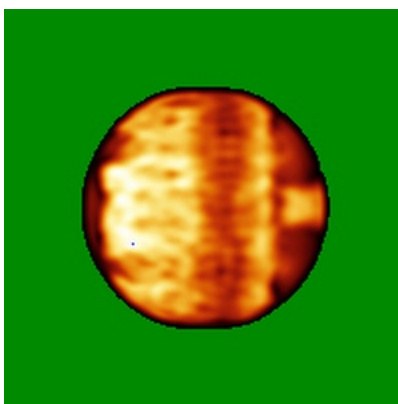
The images above show the largest variance slices of the map in three orthogonal directions.

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

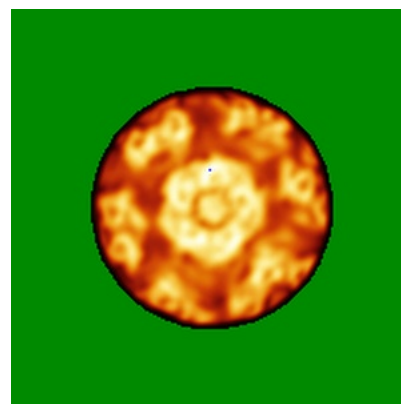
### 6.4.1 Primary map



X

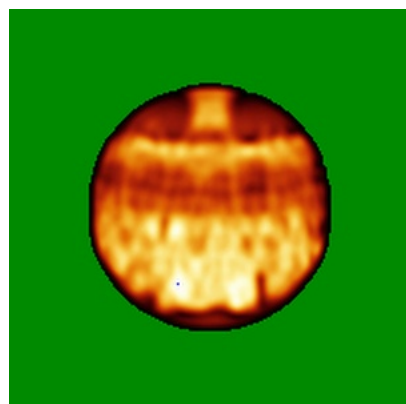


Y

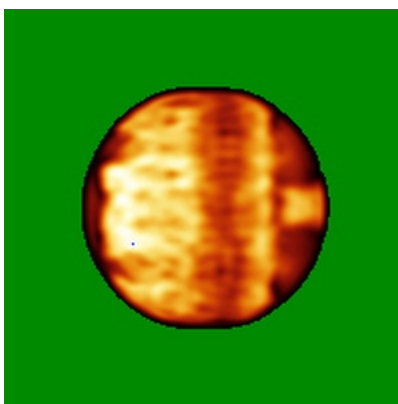


Z

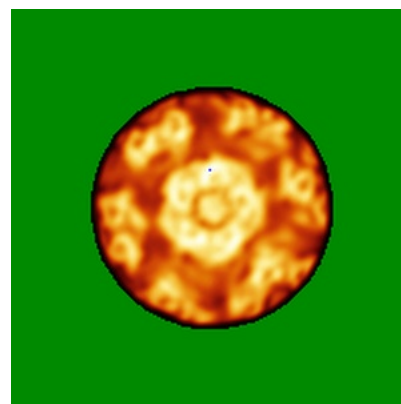
### 6.4.2 Raw map



X



Y

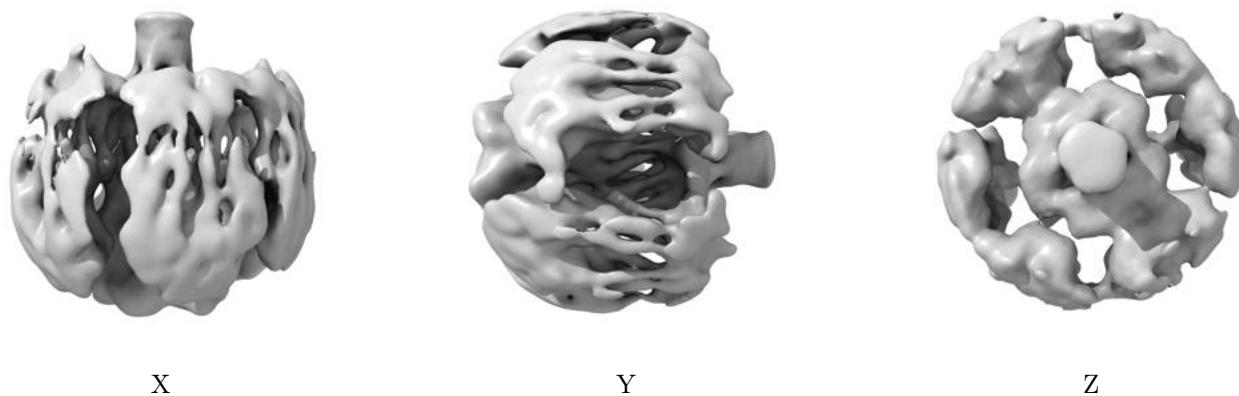


Z

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

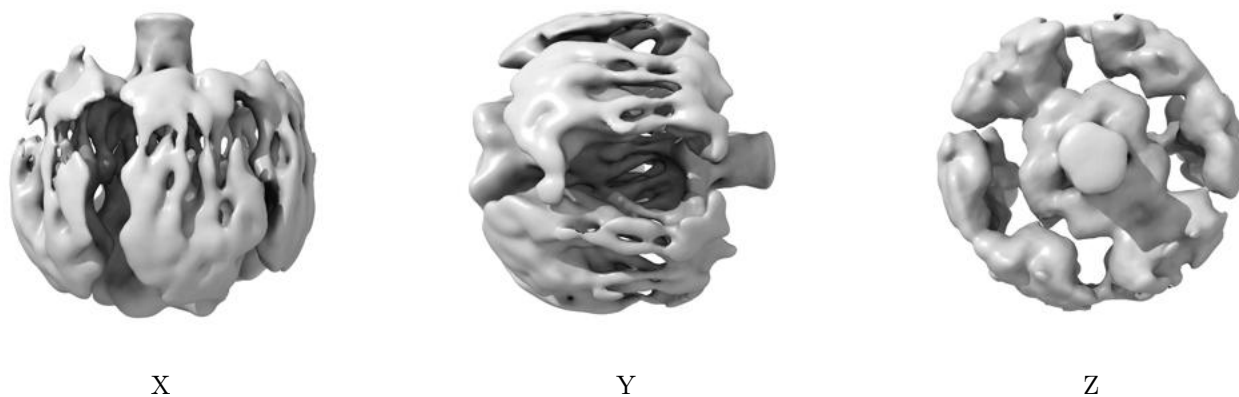
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

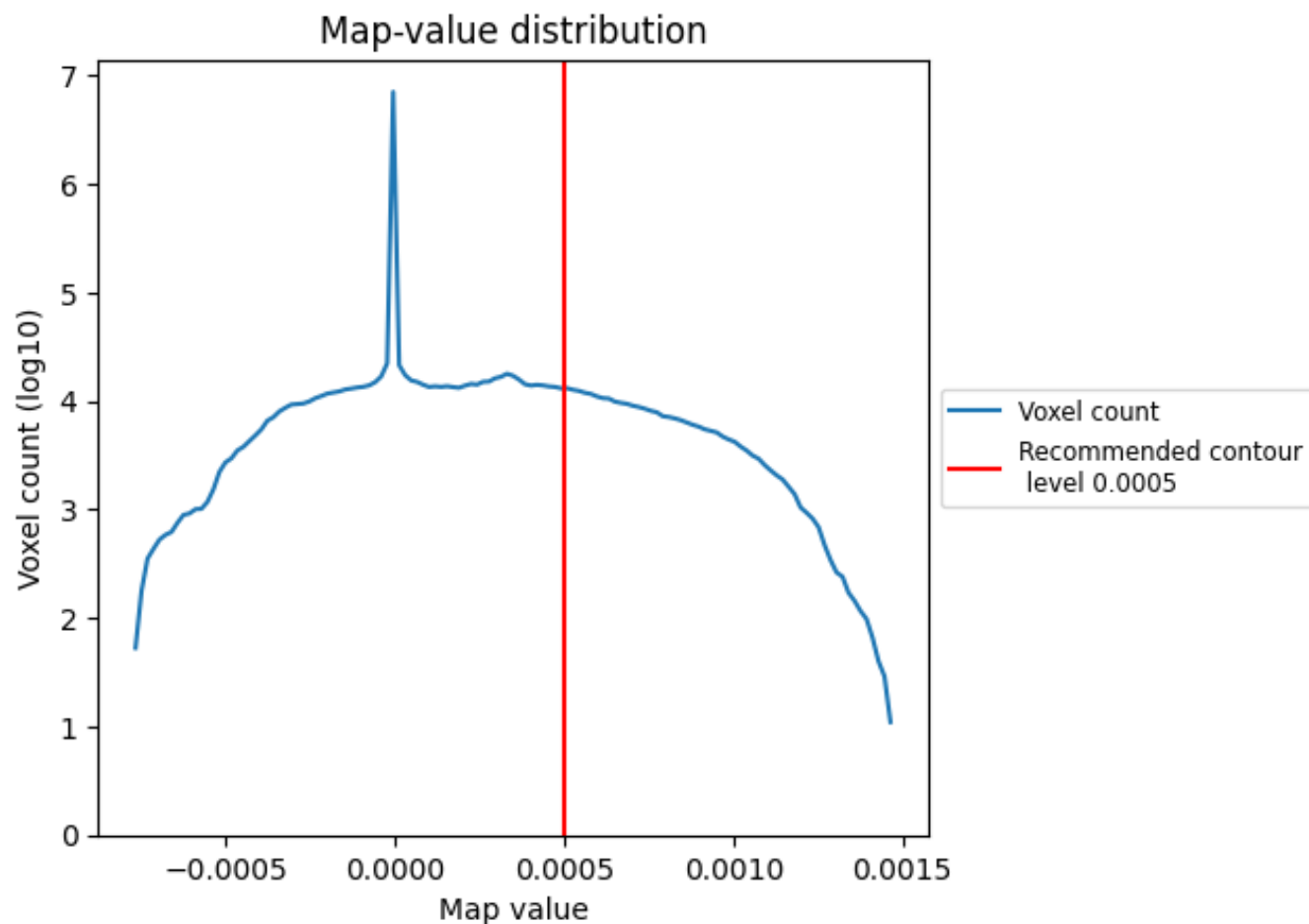
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

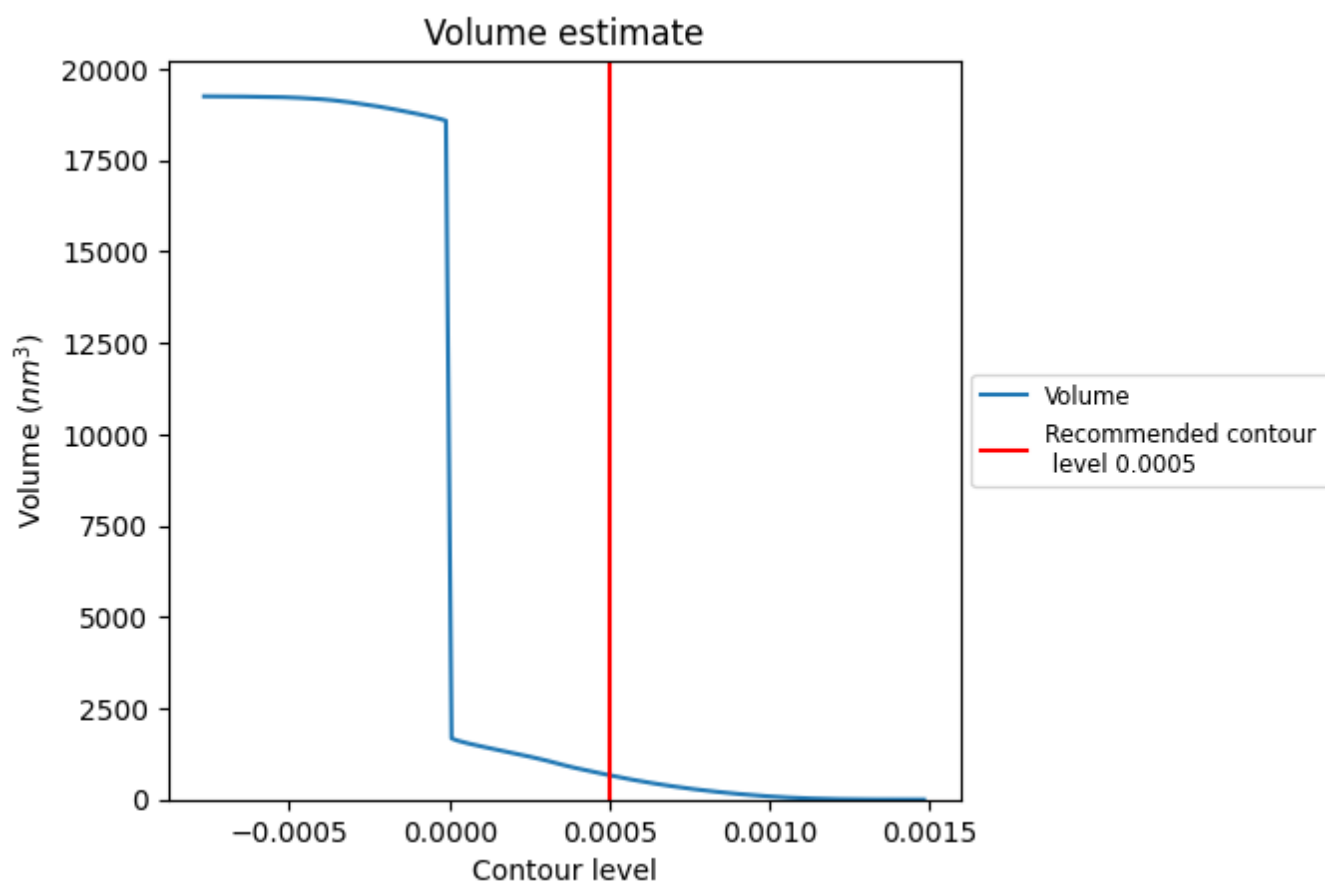
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

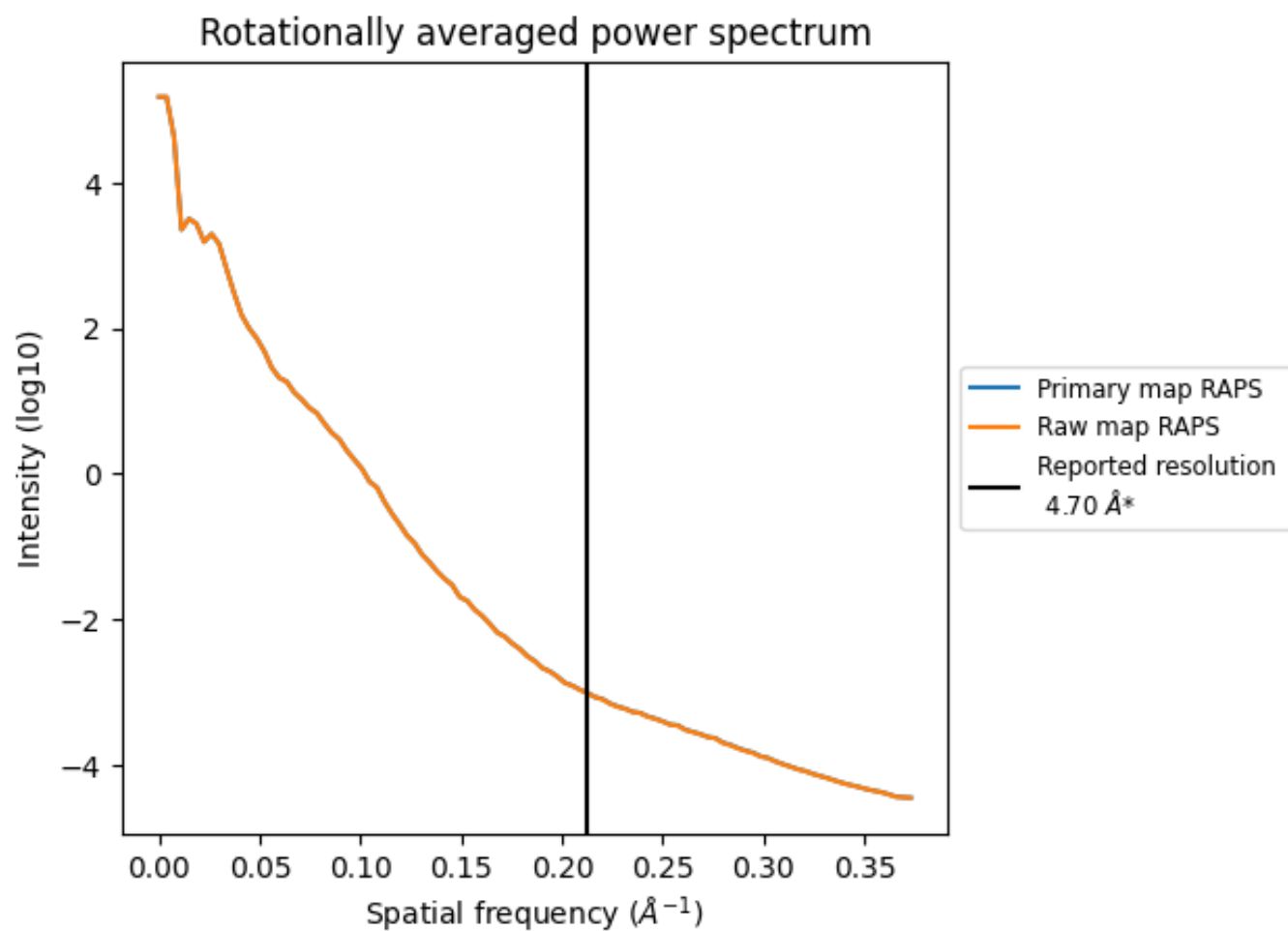
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 666 nm<sup>3</sup>; this corresponds to an approximate mass of 602 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 ⓘ

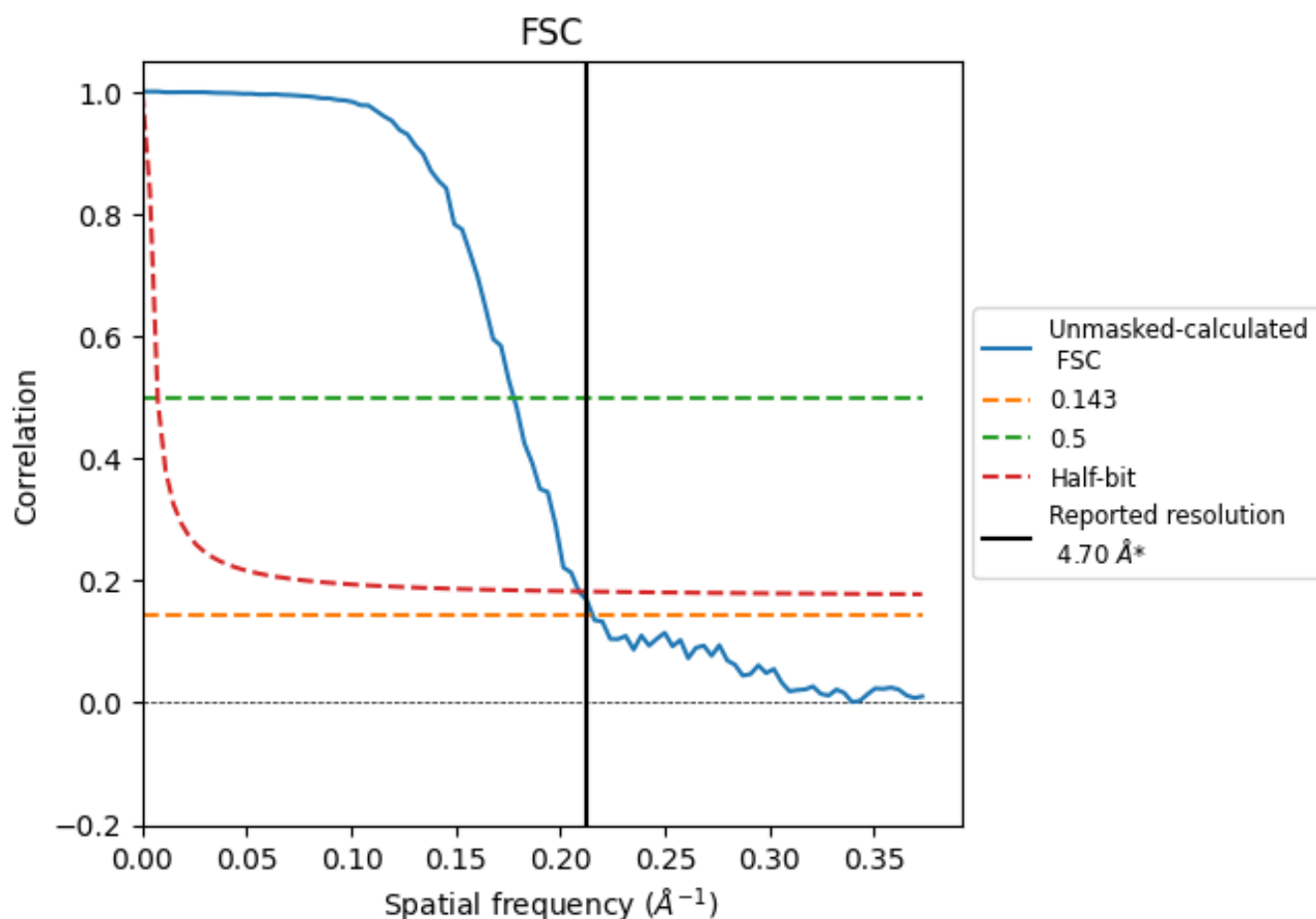


\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.213  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.70                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.64                               | 5.63 | 4.79     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

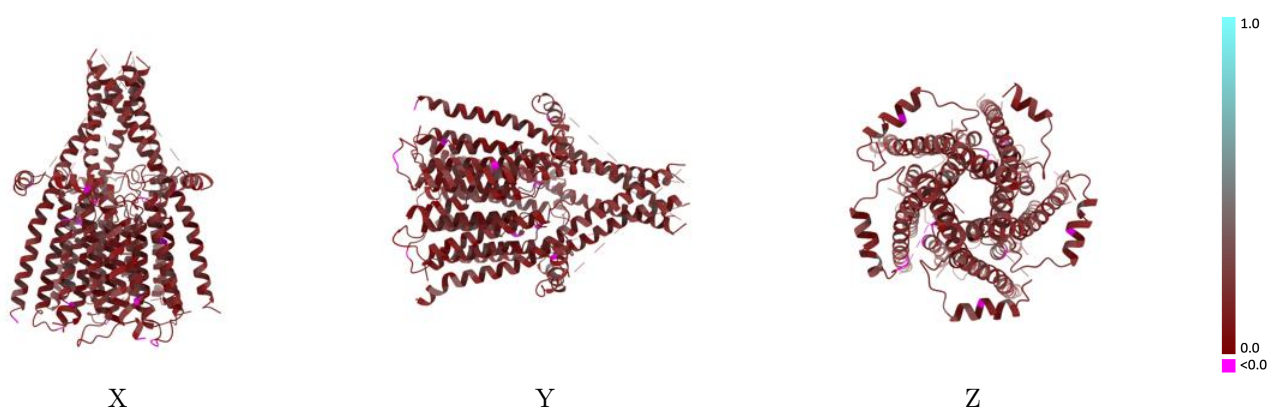
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18596 and PDB model 8QQM. Per-residue inclusion information can be found in section 3 on page 5.

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

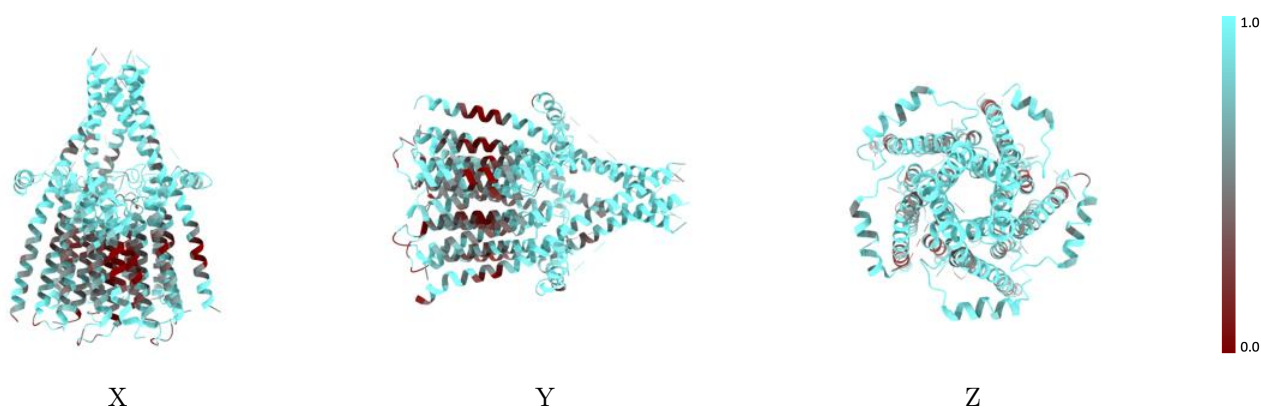
This section was not generated.

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



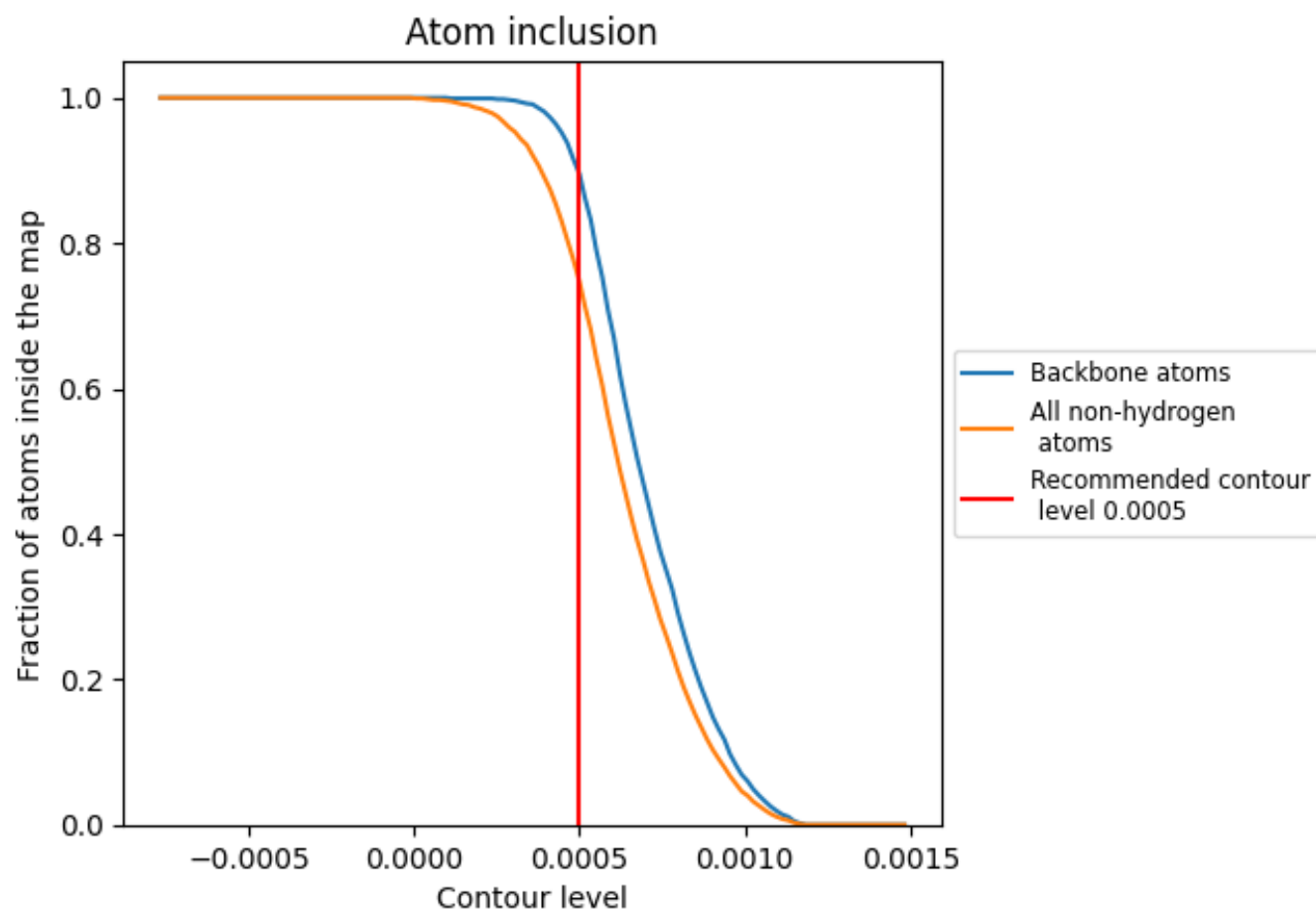
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 75% 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 (0.0005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7470 | <div></div> 0.1560 |
| A     | <div></div> 0.7290 | <div></div> 0.1580 |
| B     | <div></div> 0.7740 | <div></div> 0.1590 |
| C     | <div></div> 0.7210 | <div></div> 0.1530 |
| D     | <div></div> 0.7530 | <div></div> 0.1550 |
| E     | <div></div> 0.7600 | <div></div> 0.1540 |

