



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:58 PM UTC

PDB ID : 8Y45 / pdb\_00008y45  
EMDB ID : EMD-38909  
Title : Cryo-EM structure of opioid receptor with biased agonist  
Authors : Lin, C.; Chang, Z.  
Deposited on : 2024-01-30  
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

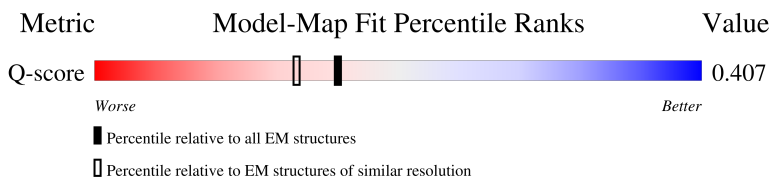
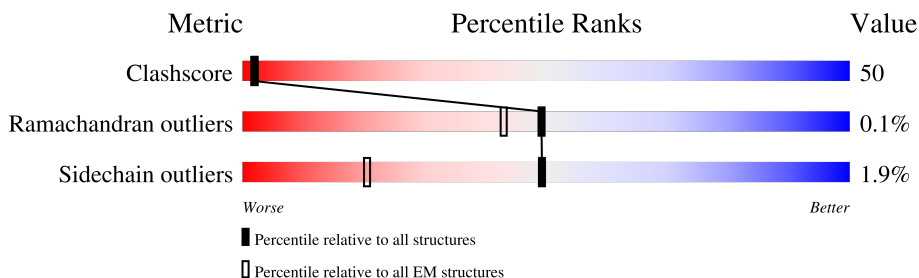
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.45 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                       | 13836 ( 2.95 - 3.95 )                                    |

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     | 325    |                  |
| 2   | B     | 358    |                  |
| 3   | D     | 355    |                  |
| 4   | S     | 266    |                  |

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| Mol | Chain | Length | Quality of chain    |
|-----|-------|--------|---------------------|
| 5   | C     | 71     | <br>28% 30% 23% 20% |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8867 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 Delta-type opioid receptor.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 1   | A     | 286      | 2244  | 1486 | 367 | 370 | 21 | 0       | 0     |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 28      | ASP      | -      | expression tag | UNP P41143 |
| A     | 29      | TYR      | -      | expression tag | UNP P41143 |
| A     | 30      | LYS      | -      | expression tag | UNP P41143 |
| A     | 31      | ASP      | -      | expression tag | UNP P41143 |
| A     | 32      | ASP      | -      | expression tag | UNP P41143 |
| A     | 33      | ASP      | -      | expression tag | UNP P41143 |
| A     | 34      | ASP      | -      | expression tag | UNP P41143 |
| A     | 35      | ALA      | -      | expression tag | UNP P41143 |

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 2   | B     | 340      | 2603  | 1606 | 469 | 508 | 20 | 0       | 0     |

There are 19 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | -17     | MET      | -      | initiating methionine | UNP P62873 |
| B     | -16     | PRO      | -      | expression tag        | UNP P62873 |
| B     | -15     | PRO      | -      | expression tag        | UNP P62873 |
| B     | -14     | HIS      | -      | expression tag        | UNP P62873 |
| B     | -13     | HIS      | -      | expression tag        | UNP P62873 |
| B     | -12     | HIS      | -      | expression tag        | UNP P62873 |
| B     | -11     | HIS      | -      | expression tag        | UNP P62873 |
| B     | -10     | LEU      | -      | expression tag        | UNP P62873 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -9      | GLU      | -      | expression tag | UNP P62873 |
| B     | -8      | VAL      | -      | expression tag | UNP P62873 |
| B     | -7      | LEU      | -      | expression tag | UNP P62873 |
| B     | -6      | PHE      | -      | expression tag | UNP P62873 |
| B     | -5      | GLN      | -      | expression tag | UNP P62873 |
| B     | -4      | GLY      | -      | expression tag | UNP P62873 |
| B     | -3      | PRO      | -      | expression tag | UNP P62873 |
| B     | -2      | GLY      | -      | expression tag | UNP P62873 |
| B     | -1      | SER      | -      | expression tag | UNP P62873 |
| B     | 0       | SER      | -      | expression tag | UNP P62873 |
| B     | 1       | GLY      | -      | expression tag | UNP P62873 |

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | D     | 223      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1786  | 1138 | 297 | 339 | 12 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 5       | LEU      | VAL    | variant  | UNP P04899 |
| D     | 47      | ASN      | SER    | conflict | UNP P04899 |
| D     | 204     | ALA      | GLY    | conflict | UNP P04899 |
| D     | 246     | ALA      | GLU    | conflict | UNP P04899 |
| D     | 327     | SER      | ALA    | conflict | UNP P04899 |

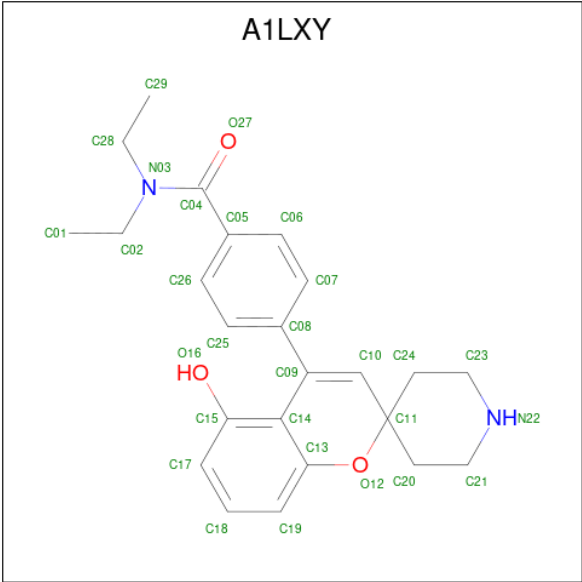
- Molecule 4 is a protein called scFv16.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | S     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 1121 | 291 | 346 | 9 |         |       |

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | C     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 274 | 77 | 84 | 3 |         |       |

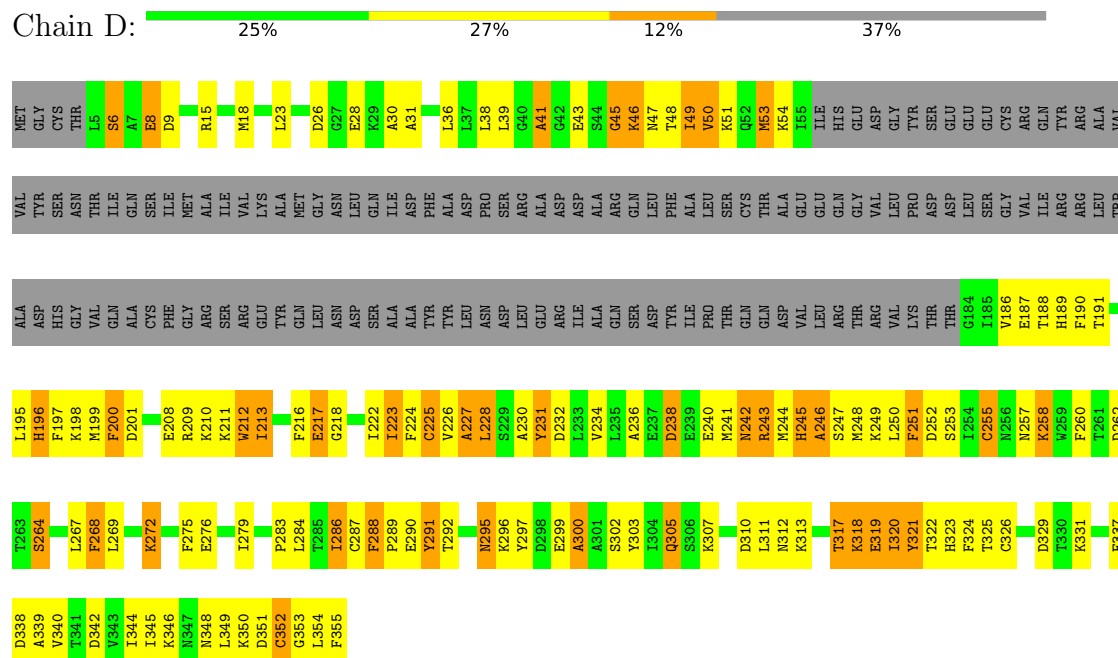
- Molecule 6 is {N}, {N}-diethyl-4-(5-oxidanylspiro[chromene-2,4'-piperidine]-4-yl)benzamid e (CCD ID: A1LXY) (formula: C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>3</sub>).



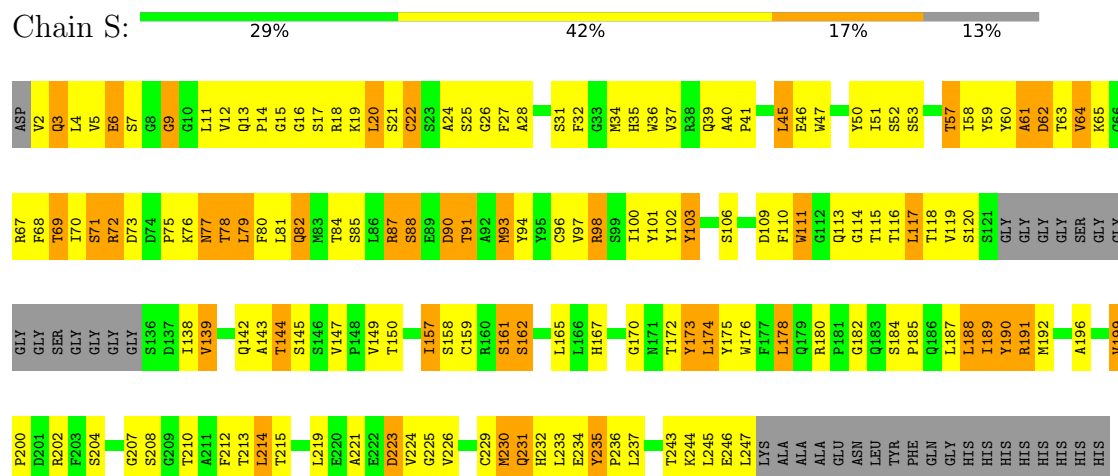
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
|     |       |          | Total | C  | N | O |         |
| 6   | A     | 1        | 29    | 24 | 2 | 3 | 0       |



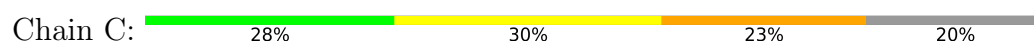
- Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-2



- Molecule 4: scFv16



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



|     |     |     |     |     |     |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | SER | ASN | ASN | THR | A7 | S8 | I9 | A10 | Q11 | A12 | R13 | K14 | L15 | V16 | E17 | Q18 | L19 | K20 | M21 | E22 | I25 | D26 | R27 | I28 | K29 | V30 | S31 | K32 | A33 | A34 | M38 | A39 | Y40 | C41 | D48 | P49 | L50 | L51 | T52 | F53 | V54 | S57 | E58 | F61 | R62 | E63 | LYS | PHE | PHE | CYS | ALA | ILE |
|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

LEU

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 676428                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TECNAI SPIRIT                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 65                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.707                                   | Depositor |
| Minimum map value                    | -3.056                                  | Depositor |
| Average map value                    | -0.002                                  | Depositor |
| Map value standard deviation         | 0.080                                   | Depositor |
| Recommended contour level            | 0.013                                   | Depositor |
| Map size (Å)                         | 217.6, 217.6, 217.6                     | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.85, 0.85, 0.85                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LXY

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     | 1.82         | 85/2297 (3.7%)  | 2.13        | 145/3132 (4.6%)  |
| 2   | B     | 1.83         | 87/2650 (3.3%)  | 1.73        | 92/3592 (2.6%)   |
| 3   | D     | 1.71         | 69/1817 (3.8%)  | 1.40        | 32/2438 (1.3%)   |
| 4   | S     | 1.92         | 71/1811 (3.9%)  | 1.60        | 46/2458 (1.9%)   |
| 5   | C     | 2.32         | 24/444 (5.4%)   | 2.67        | 54/599 (9.0%)    |
| All | All   | 1.85         | 336/9019 (3.7%) | 1.82        | 369/12219 (3.0%) |

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                   |
| 2   | B     | 0                   | 1                   |
| 4   | S     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (336) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 93  | ILE  | C-N   | 20.99 | 1.58        | 1.33     |
| 1   | A     | 54  | ALA  | C-N   | 20.89 | 1.58        | 1.33     |
| 2   | B     | 21  | ALA  | C-N   | 20.11 | 1.59        | 1.33     |
| 4   | S     | 7   | SER  | C-N   | 18.43 | 1.60        | 1.33     |
| 1   | A     | 159 | PHE  | C-N   | 18.34 | 1.56        | 1.33     |
| 2   | B     | 18  | ILE  | C-N   | 17.41 | 1.57        | 1.33     |
| 5   | C     | 9   | ILE  | C-N   | 16.11 | 1.55        | 1.33     |
| 2   | B     | 188 | MET  | C-N   | 15.65 | 1.52        | 1.33     |
| 4   | S     | 91  | THR  | C-N   | 14.82 | 1.51        | 1.33     |
| 5   | C     | 14  | LYS  | C-N   | 14.53 | 1.52        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | D     | 225 | CYS  | C-N   | 14.45  | 1.51        | 1.33     |
| 4   | S     | 90  | ASP  | C-N   | 14.22  | 1.53        | 1.33     |
| 2   | B     | 205 | ASP  | C-N   | 14.12  | 1.51        | 1.33     |
| 2   | B     | 14  | LEU  | C-N   | 13.87  | 1.52        | 1.33     |
| 3   | D     | 307 | LYS  | C-N   | 13.87  | 1.53        | 1.33     |
| 2   | B     | 253 | PHE  | C-N   | 13.71  | 1.53        | 1.33     |
| 3   | D     | 350 | LYS  | C-N   | 13.57  | 1.51        | 1.33     |
| 4   | S     | 188 | LEU  | C-N   | 13.18  | 1.51        | 1.33     |
| 4   | S     | 3   | GLN  | C-N   | 13.16  | 1.50        | 1.33     |
| 4   | S     | 18  | ARG  | C-N   | 12.97  | 1.52        | 1.33     |
| 3   | D     | 292 | THR  | C-N   | 12.78  | 1.47        | 1.33     |
| 4   | S     | 61  | ALA  | C-N   | 12.76  | 1.50        | 1.33     |
| 1   | A     | 180 | GLY  | C-N   | 12.52  | 1.50        | 1.34     |
| 5   | C     | 13  | ARG  | C-N   | 12.48  | 1.50        | 1.33     |
| 2   | B     | 243 | THR  | C-N   | 12.46  | 1.50        | 1.33     |
| 4   | S     | 185 | PRO  | C-N   | 12.39  | 1.48        | 1.33     |
| 4   | S     | 100 | ILE  | C-N   | 12.15  | 1.49        | 1.33     |
| 1   | A     | 292 | ARG  | C-N   | 11.89  | 1.49        | 1.33     |
| 4   | S     | 230 | MET  | C-N   | 11.83  | 1.50        | 1.33     |
| 5   | C     | 11  | GLN  | C-N   | 11.75  | 1.48        | 1.33     |
| 2   | B     | 59  | TYR  | C-N   | 11.67  | 1.48        | 1.33     |
| 1   | A     | 314 | ASN  | C-N   | -11.66 | 1.23        | 1.33     |
| 5   | C     | 17  | GLU  | C-N   | 11.65  | 1.49        | 1.33     |
| 4   | S     | 71  | SER  | C-N   | 11.64  | 1.49        | 1.33     |
| 4   | S     | 5   | VAL  | C-N   | 11.51  | 1.49        | 1.33     |
| 4   | S     | 147 | VAL  | C-N   | 11.47  | 1.47        | 1.33     |
| 2   | B     | 204 | CYS  | C-N   | 11.33  | 1.48        | 1.33     |
| 4   | S     | 28  | ALA  | C-N   | 11.31  | 1.49        | 1.33     |
| 1   | A     | 52  | ILE  | C-N   | 11.20  | 1.48        | 1.33     |
| 5   | C     | 27  | ARG  | C-N   | 11.11  | 1.43        | 1.33     |
| 4   | S     | 191 | ARG  | C-N   | 10.94  | 1.47        | 1.33     |
| 2   | B     | 117 | LEU  | C-N   | 10.93  | 1.50        | 1.33     |
| 1   | A     | 316 | VAL  | C-N   | 10.90  | 1.48        | 1.33     |
| 1   | A     | 219 | LEU  | C-N   | 10.83  | 1.49        | 1.34     |
| 4   | S     | 64  | VAL  | C-N   | 10.73  | 1.47        | 1.33     |
| 5   | C     | 49  | PRO  | C-N   | 10.61  | 1.49        | 1.33     |
| 2   | B     | 169 | TRP  | C-N   | -10.59 | 1.20        | 1.33     |
| 3   | D     | 310 | ASP  | C-N   | 10.48  | 1.49        | 1.33     |
| 1   | A     | 315 | PRO  | C-N   | -10.48 | 1.20        | 1.33     |
| 4   | S     | 213 | THR  | C-N   | 10.37  | 1.47        | 1.33     |
| 4   | S     | 20  | LEU  | C-N   | 10.30  | 1.47        | 1.33     |
| 2   | B     | 41  | GLY  | C-N   | 10.24  | 1.47        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | D     | 289 | PRO  | C-N   | 10.24  | 1.50        | 1.33     |
| 3   | D     | 288 | PHE  | C-N   | -10.16 | 1.21        | 1.33     |
| 3   | D     | 300 | ALA  | C-N   | -10.13 | 1.20        | 1.33     |
| 2   | B     | 153 | ASP  | C-N   | -10.10 | 1.21        | 1.33     |
| 5   | C     | 12  | ALA  | C-N   | 10.06  | 1.47        | 1.33     |
| 5   | C     | 8   | SER  | C-N   | 10.04  | 1.46        | 1.33     |
| 1   | A     | 164 | LYS  | C-N   | 10.02  | 1.46        | 1.33     |
| 3   | D     | 216 | PHE  | C-N   | 10.00  | 1.46        | 1.33     |
| 2   | B     | 208 | ALA  | C-N   | 9.98   | 1.47        | 1.33     |
| 1   | A     | 323 | GLU  | C-N   | 9.97   | 1.47        | 1.33     |
| 2   | B     | 92  | ALA  | C-N   | 9.94   | 1.42        | 1.33     |
| 2   | B     | 277 | SER  | C-N   | -9.86  | 1.21        | 1.33     |
| 3   | D     | 319 | GLU  | C-N   | 9.85   | 1.47        | 1.33     |
| 3   | D     | 339 | ALA  | C-N   | -9.80  | 1.22        | 1.33     |
| 2   | B     | 50  | THR  | C-N   | 9.75   | 1.49        | 1.33     |
| 1   | A     | 317 | LEU  | C-N   | 9.72   | 1.50        | 1.33     |
| 2   | B     | 285 | LEU  | C-N   | 9.71   | 1.47        | 1.33     |
| 1   | A     | 214 | LYS  | C-N   | 9.70   | 1.46        | 1.33     |
| 4   | S     | 199 | VAL  | C-N   | 9.64   | 1.45        | 1.33     |
| 1   | A     | 262 | MET  | C-N   | -9.61  | 1.23        | 1.34     |
| 4   | S     | 224 | VAL  | C-N   | 9.56   | 1.42        | 1.33     |
| 2   | B     | 47  | THR  | C-N   | -9.55  | 1.21        | 1.33     |
| 4   | S     | 143 | ALA  | C-N   | -9.54  | 1.20        | 1.33     |
| 2   | B     | 271 | CYS  | C-N   | 9.51   | 1.50        | 1.33     |
| 3   | D     | 217 | GLU  | C-N   | 9.51   | 1.48        | 1.33     |
| 2   | B     | 323 | ASP  | C-N   | 9.49   | 1.45        | 1.33     |
| 4   | S     | 111 | TRP  | C-N   | 9.48   | 1.47        | 1.33     |
| 1   | A     | 70  | VAL  | C-N   | -9.46  | 1.21        | 1.33     |
| 3   | D     | 228 | LEU  | C-N   | 9.46   | 1.45        | 1.33     |
| 1   | A     | 59  | VAL  | C-N   | 9.45   | 1.45        | 1.33     |
| 3   | D     | 321 | TYR  | C-N   | 9.39   | 1.47        | 1.33     |
| 4   | S     | 225 | GLY  | C-N   | 9.34   | 1.45        | 1.33     |
| 4   | S     | 45  | LEU  | C-N   | 9.30   | 1.45        | 1.33     |
| 3   | D     | 253 | SER  | C-N   | -9.28  | 1.21        | 1.33     |
| 2   | B     | 178 | THR  | C-N   | 9.27   | 1.46        | 1.33     |
| 5   | C     | 10  | ALA  | C-N   | 9.25   | 1.46        | 1.33     |
| 1   | A     | 185 | VAL  | C-N   | -9.25  | 1.21        | 1.33     |
| 2   | B     | 226 | GLU  | C-N   | 9.24   | 1.41        | 1.33     |
| 1   | A     | 148 | ILE  | C-N   | 9.23   | 1.46        | 1.33     |
| 1   | A     | 222 | PHE  | C-N   | 9.19   | 1.44        | 1.33     |
| 2   | B     | 326 | ALA  | C-N   | -9.03  | 1.22        | 1.33     |
| 2   | B     | 240 | ALA  | C-N   | -9.02  | 1.22        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 162 | PRO  | C-N   | -8.91 | 1.22        | 1.33     |
| 3   | D     | 226 | VAL  | C-N   | -8.89 | 1.20        | 1.33     |
| 2   | B     | 274 | THR  | C-N   | 8.88  | 1.44        | 1.33     |
| 1   | A     | 89  | PHE  | C-N   | -8.86 | 1.22        | 1.33     |
| 1   | A     | 141 | MET  | C-N   | -8.85 | 1.22        | 1.33     |
| 1   | A     | 154 | VAL  | C-N   | 8.84  | 1.47        | 1.33     |
| 1   | A     | 296 | VAL  | C-N   | -8.83 | 1.22        | 1.33     |
| 5   | C     | 28  | ILE  | C-N   | 8.80  | 1.45        | 1.33     |
| 1   | A     | 223 | VAL  | C-N   | 8.75  | 1.45        | 1.34     |
| 4   | S     | 67  | ARG  | C-N   | -8.67 | 1.21        | 1.33     |
| 5   | C     | 25  | ILE  | C-N   | 8.67  | 1.45        | 1.33     |
| 4   | S     | 98  | ARG  | C-N   | -8.66 | 1.22        | 1.33     |
| 2   | B     | 71  | VAL  | C-N   | -8.65 | 1.21        | 1.33     |
| 5   | C     | 40  | TYR  | C-N   | -8.65 | 1.22        | 1.34     |
| 2   | B     | 282 | GLY  | C-N   | -8.57 | 1.22        | 1.33     |
| 4   | S     | 158 | SER  | C-N   | 8.54  | 1.45        | 1.33     |
| 2   | B     | 318 | LEU  | C-N   | 8.51  | 1.46        | 1.33     |
| 5   | C     | 57  | SER  | C-N   | 8.51  | 1.45        | 1.34     |
| 3   | D     | 223 | ILE  | C-N   | -8.48 | 1.22        | 1.33     |
| 1   | A     | 241 | ARG  | C-N   | 8.40  | 1.46        | 1.33     |
| 5   | C     | 29  | LYS  | C-N   | 8.36  | 1.44        | 1.33     |
| 2   | B     | 309 | ALA  | C-N   | -8.35 | 1.21        | 1.33     |
| 2   | B     | 192 | LEU  | C-N   | 8.34  | 1.48        | 1.33     |
| 2   | B     | 209 | LYS  | C-N   | -8.30 | 1.21        | 1.33     |
| 4   | S     | 34  | MET  | C-N   | -8.30 | 1.21        | 1.33     |
| 4   | S     | 78  | THR  | C-N   | -8.29 | 1.23        | 1.33     |
| 1   | A     | 168 | ILE  | C-N   | -8.25 | 1.23        | 1.33     |
| 2   | B     | 322 | ASP  | C-N   | -8.21 | 1.22        | 1.33     |
| 3   | D     | 195 | LEU  | C-N   | -8.20 | 1.22        | 1.33     |
| 2   | B     | 159 | THR  | C-N   | 8.18  | 1.44        | 1.33     |
| 1   | A     | 285 | THR  | C-N   | 8.11  | 1.44        | 1.33     |
| 3   | D     | 305 | GLN  | C-N   | 8.10  | 1.45        | 1.33     |
| 2   | B     | 194 | PRO  | C-N   | -8.08 | 1.23        | 1.33     |
| 1   | A     | 62  | VAL  | C-N   | 8.08  | 1.45        | 1.33     |
| 3   | D     | 302 | SER  | C-N   | -8.06 | 1.23        | 1.33     |
| 1   | A     | 166 | LYS  | C-N   | -8.05 | 1.23        | 1.33     |
| 1   | A     | 218 | PHE  | C-N   | 8.00  | 1.43        | 1.33     |
| 3   | D     | 272 | LYS  | C-N   | -7.88 | 1.23        | 1.33     |
| 3   | D     | 46  | LYS  | C-N   | -7.79 | 1.23        | 1.33     |
| 1   | A     | 280 | PHE  | C-N   | -7.75 | 1.24        | 1.33     |
| 2   | B     | 222 | PHE  | C-N   | 7.75  | 1.44        | 1.33     |
| 3   | D     | 317 | THR  | C-N   | 7.75  | 1.43        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 287 | ALA  | C-N   | 7.74  | 1.38        | 1.33     |
| 1   | A     | 144 | VAL  | C-N   | -7.72 | 1.23        | 1.33     |
| 3   | D     | 36  | LEU  | C-N   | -7.67 | 1.22        | 1.33     |
| 2   | B     | 127 | LYS  | C-N   | -7.65 | 1.23        | 1.33     |
| 1   | A     | 176 | ALA  | C-N   | -7.63 | 1.23        | 1.33     |
| 2   | B     | 293 | ASN  | C-N   | -7.62 | 1.23        | 1.33     |
| 1   | A     | 103 | PRO  | C-N   | -7.60 | 1.24        | 1.33     |
| 2   | B     | 197 | ARG  | C-N   | 7.56  | 1.45        | 1.33     |
| 2   | B     | 290 | ASP  | C-N   | 7.55  | 1.44        | 1.33     |
| 3   | D     | 238 | ASP  | C-N   | 7.55  | 1.45        | 1.33     |
| 3   | D     | 287 | CYS  | C-N   | 7.54  | 1.49        | 1.33     |
| 5   | C     | 16  | VAL  | C-N   | 7.53  | 1.43        | 1.33     |
| 4   | S     | 69  | THR  | C-N   | -7.53 | 1.25        | 1.33     |
| 4   | S     | 187 | LEU  | C-N   | 7.48  | 1.44        | 1.33     |
| 2   | B     | 265 | SER  | C-N   | -7.44 | 1.23        | 1.33     |
| 4   | S     | 24  | ALA  | C-N   | 7.42  | 1.43        | 1.33     |
| 3   | D     | 320 | ILE  | C-N   | -7.37 | 1.22        | 1.33     |
| 3   | D     | 41  | ALA  | C-N   | 7.37  | 1.44        | 1.33     |
| 4   | S     | 47  | TRP  | C-N   | 7.37  | 1.44        | 1.33     |
| 1   | A     | 252 | LYS  | C-N   | 7.36  | 1.44        | 1.34     |
| 1   | A     | 303 | CYS  | C-N   | 7.34  | 1.43        | 1.34     |
| 4   | S     | 53  | SER  | C-N   | -7.34 | 1.22        | 1.33     |
| 4   | S     | 178 | LEU  | C-N   | -7.33 | 1.23        | 1.33     |
| 4   | S     | 62  | ASP  | C-N   | 7.28  | 1.44        | 1.33     |
| 4   | S     | 145 | SER  | C-N   | 7.28  | 1.42        | 1.33     |
| 1   | A     | 253 | ASP  | C-N   | 7.26  | 1.43        | 1.34     |
| 4   | S     | 231 | GLN  | C-N   | 7.24  | 1.43        | 1.33     |
| 3   | D     | 200 | PHE  | C-N   | -7.24 | 1.23        | 1.33     |
| 4   | S     | 200 | PRO  | C-N   | 7.23  | 1.44        | 1.33     |
| 1   | A     | 290 | ASP  | C-N   | 7.21  | 1.42        | 1.33     |
| 3   | D     | 353 | GLY  | C-N   | 7.20  | 1.42        | 1.33     |
| 1   | A     | 82  | THR  | C-N   | -7.18 | 1.24        | 1.34     |
| 2   | B     | 170 | ASP  | C-N   | 7.17  | 1.43        | 1.33     |
| 3   | D     | 227 | ALA  | C-N   | 7.16  | 1.43        | 1.33     |
| 3   | D     | 240 | GLU  | C-N   | -7.14 | 1.24        | 1.33     |
| 1   | A     | 187 | ALA  | C-N   | 7.14  | 1.43        | 1.33     |
| 3   | D     | 191 | THR  | C-N   | -7.14 | 1.23        | 1.33     |
| 2   | B     | 229 | ILE  | C-N   | -7.13 | 1.24        | 1.33     |
| 2   | B     | 58  | ILE  | C-N   | 7.11  | 1.43        | 1.33     |
| 4   | S     | 235 | TYR  | C-N   | -7.10 | 1.25        | 1.33     |
| 3   | D     | 213 | ILE  | C-N   | 7.09  | 1.43        | 1.33     |
| 3   | D     | 323 | HIS  | C-N   | -7.08 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 306 | LEU  | C-N   | 7.06  | 1.41        | 1.33     |
| 3   | D     | 311 | LEU  | C-N   | -7.05 | 1.23        | 1.33     |
| 4   | S     | 196 | ALA  | C-N   | 7.05  | 1.43        | 1.33     |
| 4   | S     | 17  | SER  | C-N   | 7.05  | 1.42        | 1.33     |
| 4   | S     | 52  | SER  | CA-CB | -7.03 | 1.42        | 1.53     |
| 3   | D     | 6   | SER  | C-N   | -6.97 | 1.24        | 1.33     |
| 5   | C     | 32  | LYS  | C-N   | 6.97  | 1.43        | 1.34     |
| 2   | B     | 131 | GLY  | C-N   | 6.95  | 1.43        | 1.33     |
| 2   | B     | 311 | HIS  | C-N   | -6.95 | 1.24        | 1.33     |
| 3   | D     | 234 | VAL  | C-N   | -6.93 | 1.24        | 1.33     |
| 1   | A     | 281 | VAL  | C-N   | -6.92 | 1.25        | 1.33     |
| 4   | S     | 192 | MET  | C-N   | 6.90  | 1.43        | 1.33     |
| 2   | B     | 327 | VAL  | C-N   | 6.87  | 1.43        | 1.33     |
| 3   | D     | 258 | LYS  | C-N   | -6.87 | 1.23        | 1.33     |
| 3   | D     | 290 | GLU  | C-N   | -6.84 | 1.23        | 1.33     |
| 1   | A     | 74  | ILE  | C-N   | -6.83 | 1.25        | 1.33     |
| 3   | D     | 53  | MET  | C-N   | -6.82 | 1.24        | 1.33     |
| 3   | D     | 232 | ASP  | C-N   | 6.81  | 1.41        | 1.33     |
| 1   | A     | 244 | ARG  | C-N   | -6.79 | 1.24        | 1.33     |
| 1   | A     | 86  | ILE  | C-N   | -6.78 | 1.24        | 1.33     |
| 3   | D     | 318 | LYS  | C-N   | -6.77 | 1.23        | 1.33     |
| 2   | B     | 195 | ASP  | C-N   | 6.77  | 1.43        | 1.33     |
| 2   | B     | 100 | VAL  | C-N   | -6.75 | 1.22        | 1.33     |
| 1   | A     | 99  | THR  | C-N   | -6.74 | 1.24        | 1.33     |
| 1   | A     | 320 | PHE  | C-N   | 6.74  | 1.44        | 1.33     |
| 1   | A     | 227 | LEU  | C-N   | 6.72  | 1.42        | 1.33     |
| 2   | B     | 219 | ARG  | C-N   | -6.70 | 1.25        | 1.33     |
| 1   | A     | 80  | MET  | C-N   | -6.70 | 1.24        | 1.33     |
| 4   | S     | 167 | HIS  | C-N   | -6.69 | 1.25        | 1.33     |
| 1   | A     | 178 | GLY  | C-N   | -6.68 | 1.25        | 1.33     |
| 3   | D     | 313 | LYS  | C-N   | -6.66 | 1.24        | 1.33     |
| 3   | D     | 245 | HIS  | C-N   | -6.63 | 1.25        | 1.33     |
| 2   | B     | 331 | SER  | C-N   | -6.58 | 1.24        | 1.33     |
| 2   | B     | 36  | ASN  | C-N   | 6.57  | 1.43        | 1.33     |
| 3   | D     | 337 | PHE  | C-N   | 6.56  | 1.42        | 1.33     |
| 3   | D     | 231 | TYR  | C-N   | 6.51  | 1.42        | 1.33     |
| 4   | S     | 60  | TYR  | C-N   | -6.51 | 1.24        | 1.33     |
| 5   | C     | 15  | LEU  | C-N   | 6.44  | 1.42        | 1.33     |
| 2   | B     | 119 | ASN  | C-N   | -6.42 | 1.25        | 1.33     |
| 1   | A     | 104 | PHE  | C-N   | -6.39 | 1.24        | 1.33     |
| 2   | B     | 55  | LEU  | C-N   | -6.39 | 1.23        | 1.33     |
| 3   | D     | 243 | ARG  | C-N   | -6.37 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | D     | 196 | HIS  | C-N   | 6.37  | 1.42        | 1.33     |
| 4   | S     | 32  | PHE  | C-N   | -6.37 | 1.21        | 1.33     |
| 1   | A     | 264 | LEU  | C-N   | 6.35  | 1.41        | 1.33     |
| 5   | C     | 58  | GLU  | C-N   | -6.34 | 1.22        | 1.33     |
| 3   | D     | 286 | ILE  | C-N   | -6.33 | 1.24        | 1.33     |
| 4   | S     | 150 | THR  | C-N   | -6.25 | 1.25        | 1.33     |
| 1   | A     | 84  | THR  | C-N   | 6.25  | 1.42        | 1.33     |
| 4   | S     | 144 | THR  | C-N   | 6.24  | 1.42        | 1.33     |
| 2   | B     | 310 | GLY  | C-N   | -6.23 | 1.24        | 1.33     |
| 1   | A     | 53  | THR  | C-N   | 6.21  | 1.41        | 1.33     |
| 2   | B     | 177 | THR  | C-N   | -6.21 | 1.25        | 1.33     |
| 4   | S     | 170 | GLY  | C-N   | -6.18 | 1.26        | 1.33     |
| 1   | A     | 98  | ALA  | C-N   | 6.17  | 1.42        | 1.33     |
| 3   | D     | 295 | ASN  | C-N   | -6.17 | 1.25        | 1.33     |
| 2   | B     | 152 | LEU  | C-N   | 6.12  | 1.42        | 1.33     |
| 1   | A     | 115 | PRO  | C-N   | -6.12 | 1.24        | 1.33     |
| 4   | S     | 173 | TYR  | C-N   | 6.10  | 1.41        | 1.33     |
| 2   | B     | 87  | THR  | C-N   | 6.10  | 1.41        | 1.33     |
| 2   | B     | 125 | ASN  | C-N   | -6.10 | 1.25        | 1.33     |
| 2   | B     | 221 | THR  | C-N   | 6.09  | 1.42        | 1.33     |
| 2   | B     | 176 | GLN  | C-N   | -6.08 | 1.25        | 1.33     |
| 3   | D     | 296 | LYS  | C-N   | 6.03  | 1.41        | 1.33     |
| 5   | C     | 18  | GLN  | C-N   | 6.02  | 1.42        | 1.33     |
| 1   | A     | 68  | VAL  | C-N   | -6.01 | 1.26        | 1.33     |
| 3   | D     | 268 | PHE  | C-N   | -5.99 | 1.25        | 1.33     |
| 1   | A     | 196 | VAL  | C-N   | -5.97 | 1.25        | 1.33     |
| 4   | S     | 75  | PRO  | C-N   | 5.96  | 1.42        | 1.33     |
| 2   | B     | 228 | ASP  | C-N   | -5.93 | 1.25        | 1.33     |
| 2   | B     | 84  | SER  | CA-CB | -5.90 | 1.44        | 1.53     |
| 4   | S     | 207 | GLY  | C-N   | 5.89  | 1.40        | 1.33     |
| 1   | A     | 102 | LEU  | C-N   | 5.88  | 1.42        | 1.34     |
| 1   | A     | 245 | LEU  | C-N   | -5.84 | 1.24        | 1.33     |
| 2   | B     | 90  | VAL  | C-N   | -5.82 | 1.26        | 1.33     |
| 3   | D     | 338 | ASP  | C-N   | -5.82 | 1.26        | 1.33     |
| 2   | B     | 218 | CYS  | C-N   | -5.80 | 1.25        | 1.33     |
| 4   | S     | 190 | TYR  | C-N   | -5.80 | 1.25        | 1.33     |
| 2   | B     | 75  | GLN  | C-N   | 5.80  | 1.42        | 1.33     |
| 3   | D     | 260 | PHE  | C-N   | 5.74  | 1.41        | 1.34     |
| 3   | D     | 352 | CYS  | C-N   | -5.74 | 1.25        | 1.33     |
| 4   | S     | 215 | THR  | C-N   | 5.73  | 1.40        | 1.33     |
| 3   | D     | 30  | ALA  | C-N   | 5.68  | 1.42        | 1.33     |
| 1   | A     | 140 | THR  | C-N   | 5.68  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | C     | 52  | THR  | C-N   | -5.65 | 1.26        | 1.33     |
| 3   | D     | 264 | SER  | C-N   | 5.63  | 1.40        | 1.33     |
| 1   | A     | 171 | CYS  | C-N   | 5.63  | 1.41        | 1.33     |
| 2   | B     | 56  | ALA  | C-N   | -5.63 | 1.26        | 1.33     |
| 3   | D     | 251 | PHE  | C-N   | 5.62  | 1.41        | 1.33     |
| 2   | B     | 276 | VAL  | C-N   | 5.61  | 1.41        | 1.33     |
| 2   | B     | 333 | ASP  | C-N   | 5.60  | 1.41        | 1.33     |
| 3   | D     | 31  | ALA  | C-N   | -5.59 | 1.23        | 1.33     |
| 1   | A     | 76  | ARG  | C-N   | 5.59  | 1.42        | 1.33     |
| 1   | A     | 138 | THR  | C-N   | -5.59 | 1.26        | 1.34     |
| 4   | S     | 21  | SER  | C-N   | -5.57 | 1.26        | 1.33     |
| 4   | S     | 6   | GLU  | C-N   | 5.57  | 1.40        | 1.33     |
| 3   | D     | 255 | CYS  | C-N   | 5.57  | 1.41        | 1.33     |
| 1   | A     | 137 | PHE  | C-N   | -5.56 | 1.26        | 1.33     |
| 4   | S     | 189 | ILE  | C-N   | -5.54 | 1.25        | 1.33     |
| 2   | B     | 19  | ARG  | C-N   | -5.52 | 1.26        | 1.33     |
| 1   | A     | 270 | PHE  | C-N   | 5.52  | 1.40        | 1.33     |
| 1   | A     | 79  | LYS  | C-N   | -5.51 | 1.25        | 1.33     |
| 4   | S     | 162 | SER  | C-N   | 5.49  | 1.40        | 1.33     |
| 2   | B     | 335 | PHE  | C-N   | -5.49 | 1.25        | 1.33     |
| 3   | D     | 26  | ASP  | C-N   | -5.49 | 1.27        | 1.34     |
| 1   | A     | 77  | TYR  | C-N   | -5.48 | 1.26        | 1.33     |
| 4   | S     | 22  | CYS  | C-N   | 5.47  | 1.41        | 1.33     |
| 3   | D     | 211 | LYS  | C-N   | -5.45 | 1.25        | 1.33     |
| 4   | S     | 223 | ASP  | C-N   | -5.45 | 1.27        | 1.33     |
| 2   | B     | 232 | ILE  | C-N   | 5.44  | 1.40        | 1.33     |
| 4   | S     | 208 | SER  | C-N   | -5.44 | 1.25        | 1.33     |
| 1   | A     | 120 | LEU  | C-N   | -5.42 | 1.26        | 1.34     |
| 1   | A     | 269 | ALA  | C-N   | -5.42 | 1.26        | 1.34     |
| 1   | A     | 310 | ASN  | C-O   | -5.41 | 1.17        | 1.24     |
| 1   | A     | 121 | CYS  | C-N   | -5.40 | 1.25        | 1.33     |
| 3   | D     | 28  | GLU  | C-N   | 5.39  | 1.41        | 1.34     |
| 1   | A     | 88  | ILE  | C-N   | -5.39 | 1.26        | 1.33     |
| 2   | B     | 45  | MET  | C-N   | -5.37 | 1.26        | 1.33     |
| 2   | B     | 316 | SER  | CA-CB | -5.35 | 1.44        | 1.53     |
| 4   | S     | 117 | LEU  | C-N   | -5.35 | 1.26        | 1.33     |
| 3   | D     | 218 | GLY  | C-N   | -5.33 | 1.21        | 1.33     |
| 2   | B     | 136 | SER  | CA-CB | -5.33 | 1.46        | 1.53     |
| 1   | A     | 139 | LEU  | C-O   | -5.32 | 1.17        | 1.24     |
| 5   | C     | 7   | ALA  | C-N   | 5.32  | 1.41        | 1.33     |
| 4   | S     | 174 | LEU  | C-N   | -5.31 | 1.25        | 1.33     |
| 2   | B     | 42  | ARG  | C-N   | -5.30 | 1.26        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 78  | THR  | C-N   | -5.29 | 1.26        | 1.33     |
| 3   | D     | 236 | ALA  | C-N   | -5.29 | 1.26        | 1.33     |
| 2   | B     | 116 | GLY  | C-N   | -5.28 | 1.26        | 1.33     |
| 2   | B     | 80  | ILE  | C-N   | 5.28  | 1.40        | 1.33     |
| 1   | A     | 308 | TYR  | C-N   | -5.27 | 1.25        | 1.33     |
| 2   | B     | 81  | ILE  | C-N   | -5.26 | 1.27        | 1.33     |
| 2   | B     | 299 | ALA  | C-N   | -5.25 | 1.26        | 1.33     |
| 4   | S     | 161 | SER  | C-N   | -5.25 | 1.26        | 1.33     |
| 4   | S     | 15  | GLY  | C-N   | -5.24 | 1.24        | 1.33     |
| 2   | B     | 308 | LEU  | C-N   | 5.23  | 1.40        | 1.33     |
| 1   | A     | 81  | LYS  | C-N   | -5.23 | 1.25        | 1.33     |
| 5   | C     | 54  | VAL  | C-N   | 5.22  | 1.40        | 1.33     |
| 4   | S     | 214 | LEU  | C-N   | 5.22  | 1.41        | 1.33     |
| 2   | B     | 235 | PHE  | C-N   | -5.20 | 1.27        | 1.33     |
| 1   | A     | 111 | MET  | C-N   | 5.20  | 1.41        | 1.33     |
| 2   | B     | 129 | ARG  | C-N   | -5.19 | 1.27        | 1.34     |
| 1   | A     | 304 | ILE  | C-O   | 5.19  | 1.30        | 1.24     |
| 4   | S     | 103 | TYR  | C-N   | -5.18 | 1.26        | 1.33     |
| 5   | C     | 50  | LEU  | C-N   | 5.17  | 1.41        | 1.33     |
| 2   | B     | 88  | ASN  | C-N   | 5.17  | 1.40        | 1.33     |
| 4   | S     | 35  | HIS  | C-N   | 5.14  | 1.40        | 1.33     |
| 3   | D     | 230 | ALA  | C-N   | -5.12 | 1.26        | 1.33     |
| 4   | S     | 31  | SER  | C-N   | 5.12  | 1.40        | 1.33     |
| 1   | A     | 238 | LEU  | C-N   | 5.12  | 1.41        | 1.34     |
| 4   | S     | 159 | CYS  | C-N   | 5.11  | 1.41        | 1.33     |
| 3   | D     | 39  | LEU  | C-N   | 5.11  | 1.39        | 1.33     |
| 1   | A     | 95  | ASP  | C-N   | -5.09 | 1.27        | 1.33     |
| 1   | A     | 220 | PHE  | C-N   | -5.05 | 1.26        | 1.33     |
| 2   | B     | 143 | THR  | C-N   | 5.05  | 1.38        | 1.32     |
| 3   | D     | 15  | ARG  | C-N   | -5.05 | 1.27        | 1.33     |
| 1   | A     | 67  | ASN  | C-N   | -5.04 | 1.26        | 1.33     |
| 1   | A     | 71  | MET  | C-N   | -5.03 | 1.27        | 1.33     |

All (369) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 52  | ILE  | O-C-N   | 20.90  | 142.37      | 121.89   |
| 1   | A     | 52  | ILE  | CA-C-N  | -17.45 | 97.76       | 120.44   |
| 1   | A     | 52  | ILE  | C-N-CA  | -17.45 | 97.76       | 120.44   |
| 1   | A     | 53  | THR  | O-C-N   | 15.88  | 138.42      | 122.07   |
| 1   | A     | 130 | TYR  | CB-CA-C | -15.09 | 86.39       | 110.08   |
| 4   | S     | 77  | ASN  | O-C-N   | 14.10  | 140.04      | 122.55   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 177 | SER  | CA-C-N  | -14.02 | 104.33      | 120.03   |
| 1   | A     | 177 | SER  | C-N-CA  | -14.02 | 104.33      | 120.03   |
| 5   | C     | 12  | ALA  | O-C-N   | 13.94  | 136.59      | 122.09   |
| 5   | C     | 11  | GLN  | O-C-N   | 13.58  | 136.51      | 122.12   |
| 2   | B     | 14  | LEU  | O-C-N   | 13.38  | 136.30      | 122.12   |
| 5   | C     | 8   | SER  | O-C-N   | 13.20  | 136.11      | 122.12   |
| 2   | B     | 244 | GLY  | O-C-N   | -12.65 | 111.80      | 123.57   |
| 4   | S     | 77  | ASN  | CA-C-N  | -12.57 | 103.08      | 122.81   |
| 4   | S     | 77  | ASN  | C-N-CA  | -12.57 | 103.08      | 122.81   |
| 1   | A     | 223 | VAL  | CA-C-N  | -12.34 | 112.47      | 120.24   |
| 1   | A     | 223 | VAL  | C-N-CA  | -12.34 | 112.47      | 120.24   |
| 1   | A     | 53  | THR  | CA-C-N  | -12.05 | 104.27      | 120.54   |
| 1   | A     | 53  | THR  | C-N-CA  | -12.05 | 104.27      | 120.54   |
| 2   | B     | 192 | LEU  | O-C-N   | -11.75 | 111.82      | 123.46   |
| 5   | C     | 9   | ILE  | O-C-N   | 11.66  | 133.18      | 121.87   |
| 5   | C     | 15  | LEU  | O-C-N   | 11.65  | 134.07      | 122.07   |
| 5   | C     | 16  | VAL  | O-C-N   | 11.48  | 133.00      | 121.87   |
| 1   | A     | 269 | ALA  | O-C-N   | 11.42  | 133.83      | 122.07   |
| 5   | C     | 10  | ALA  | O-C-N   | 11.17  | 133.96      | 122.12   |
| 1   | A     | 56  | TYR  | N-CA-C  | -10.86 | 99.44       | 111.28   |
| 5   | C     | 13  | ARG  | O-C-N   | 10.69  | 133.45      | 122.12   |
| 1   | A     | 283 | VAL  | O-C-N   | 10.48  | 132.80      | 121.90   |
| 3   | D     | 226 | VAL  | O-C-N   | -10.48 | 112.28      | 123.18   |
| 4   | S     | 67  | ARG  | O-C-N   | 10.41  | 137.14      | 122.36   |
| 4   | S     | 67  | ARG  | CA-C-N  | -10.34 | 104.72      | 122.92   |
| 4   | S     | 67  | ARG  | C-N-CA  | -10.34 | 104.72      | 122.92   |
| 1   | A     | 216 | CYS  | CB-CA-C | -10.33 | 94.67       | 110.88   |
| 2   | B     | 20  | ASP  | O-C-N   | 10.32  | 133.06      | 122.12   |
| 2   | B     | 14  | LEU  | CA-C-N  | -10.29 | 106.49      | 120.28   |
| 2   | B     | 14  | LEU  | C-N-CA  | -10.29 | 106.49      | 120.28   |
| 1   | A     | 58  | ALA  | O-C-N   | 10.28  | 132.65      | 122.07   |
| 4   | S     | 187 | LEU  | O-C-N   | 10.21  | 134.81      | 123.27   |
| 2   | B     | 18  | ILE  | O-C-N   | 10.01  | 131.58      | 121.87   |
| 5   | C     | 14  | LYS  | O-C-N   | 9.98   | 132.87      | 122.09   |
| 1   | A     | 269 | ALA  | CA-C-N  | -9.91  | 105.24      | 120.31   |
| 1   | A     | 269 | ALA  | C-N-CA  | -9.91  | 105.24      | 120.31   |
| 5   | C     | 10  | ALA  | CA-C-N  | -9.86  | 107.06      | 120.28   |
| 5   | C     | 10  | ALA  | C-N-CA  | -9.86  | 107.06      | 120.28   |
| 3   | D     | 228 | LEU  | O-C-N   | 9.86   | 132.57      | 122.12   |
| 1   | A     | 54  | ALA  | O-C-N   | 9.79   | 132.27      | 122.09   |
| 5   | C     | 7   | ALA  | CA-C-N  | -9.57  | 107.46      | 120.28   |
| 5   | C     | 7   | ALA  | C-N-CA  | -9.57  | 107.46      | 120.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 52  | THR  | CA-C-N  | -9.45 | 110.31      | 119.85   |
| 5   | C     | 52  | THR  | C-N-CA  | -9.45 | 110.31      | 119.85   |
| 1   | A     | 55  | LEU  | O-C-N   | 9.36  | 132.09      | 122.08   |
| 4   | S     | 79  | LEU  | O-C-N   | 9.27  | 134.12      | 123.27   |
| 3   | D     | 320 | ILE  | O-C-N   | -9.19 | 113.26      | 123.18   |
| 2   | B     | 204 | CYS  | O-C-N   | -9.11 | 111.77      | 122.15   |
| 2   | B     | 286 | LEU  | O-C-N   | -9.02 | 113.07      | 123.27   |
| 1   | A     | 117 | GLY  | O-C-N   | 8.97  | 134.36      | 122.70   |
| 1   | A     | 224 | VAL  | O-C-N   | 8.94  | 126.42      | 120.07   |
| 1   | A     | 57  | SER  | O-C-N   | 8.93  | 131.64      | 122.08   |
| 2   | B     | 243 | THR  | CA-C-N  | -8.90 | 112.18      | 121.35   |
| 2   | B     | 243 | THR  | C-N-CA  | -8.90 | 112.18      | 121.35   |
| 2   | B     | 320 | VAL  | O-C-N   | -8.89 | 113.50      | 122.93   |
| 5   | C     | 7   | ALA  | O-C-N   | 8.88  | 137.20      | 123.00   |
| 5   | C     | 13  | ARG  | CA-C-N  | -8.86 | 108.39      | 120.44   |
| 5   | C     | 13  | ARG  | C-N-CA  | -8.86 | 108.39      | 120.44   |
| 1   | A     | 279 | ILE  | O-C-N   | -8.53 | 113.60      | 121.87   |
| 4   | S     | 101 | TYR  | O-C-N   | -8.50 | 113.41      | 123.27   |
| 1   | A     | 309 | ALA  | CB-CA-C | -8.42 | 94.11       | 110.11   |
| 3   | D     | 50  | VAL  | O-C-N   | 8.42  | 130.04      | 121.87   |
| 2   | B     | 298 | ASP  | O-C-N   | -8.41 | 112.97      | 123.06   |
| 3   | D     | 49  | ILE  | N-CA-C  | -8.40 | 101.54      | 110.36   |
| 5   | C     | 8   | SER  | CA-C-N  | -8.36 | 109.01      | 120.46   |
| 5   | C     | 8   | SER  | C-N-CA  | -8.36 | 109.01      | 120.46   |
| 2   | B     | 190 | LEU  | O-C-N   | 8.20  | 132.91      | 123.31   |
| 2   | B     | 210 | LEU  | O-C-N   | 8.20  | 132.79      | 123.19   |
| 5   | C     | 17  | GLU  | O-C-N   | 8.17  | 130.78      | 122.12   |
| 3   | D     | 291 | TYR  | O-C-N   | -8.15 | 113.51      | 123.04   |
| 1   | A     | 54  | ALA  | CA-C-N  | -8.14 | 109.47      | 120.79   |
| 1   | A     | 54  | ALA  | C-N-CA  | -8.14 | 109.47      | 120.79   |
| 1   | A     | 310 | ASN  | N-CA-C  | -8.14 | 100.74      | 111.24   |
| 1   | A     | 308 | TYR  | N-CA-C  | -8.06 | 102.54      | 112.38   |
| 5   | C     | 12  | ALA  | CA-C-N  | -8.02 | 109.53      | 120.28   |
| 5   | C     | 12  | ALA  | C-N-CA  | -8.02 | 109.53      | 120.28   |
| 2   | B     | 266 | HIS  | O-C-N   | -8.00 | 114.00      | 123.27   |
| 1   | A     | 299 | ALA  | O-C-N   | 7.99  | 130.66      | 122.03   |
| 1   | A     | 315 | PRO  | CA-C-N  | -7.85 | 109.27      | 120.42   |
| 1   | A     | 315 | PRO  | C-N-CA  | -7.85 | 109.27      | 120.42   |
| 2   | B     | 163 | ASP  | O-C-N   | 7.83  | 131.33      | 122.32   |
| 3   | D     | 228 | LEU  | CA-C-N  | -7.78 | 110.70      | 122.21   |
| 3   | D     | 228 | LEU  | C-N-CA  | -7.78 | 110.70      | 122.21   |
| 2   | B     | 257 | ALA  | N-CA-C  | -7.76 | 100.08      | 110.55   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | S     | 115 | THR  | O-C-N  | 7.75  | 131.74      | 123.06   |
| 1   | A     | 229 | ILE  | O-C-N  | -7.74 | 113.05      | 121.80   |
| 4   | S     | 79  | LEU  | CA-C-N | -7.65 | 112.25      | 123.11   |
| 4   | S     | 79  | LEU  | C-N-CA | -7.65 | 112.25      | 123.11   |
| 1   | A     | 173 | TRP  | O-C-N  | 7.64  | 130.91      | 122.20   |
| 5   | C     | 18  | GLN  | O-C-N  | 7.64  | 130.21      | 122.12   |
| 5   | C     | 11  | GLN  | CA-C-N | -7.60 | 110.28      | 120.54   |
| 5   | C     | 11  | GLN  | C-N-CA | -7.60 | 110.28      | 120.54   |
| 4   | S     | 113 | GLN  | CA-C-N | -7.60 | 113.58      | 122.77   |
| 4   | S     | 113 | GLN  | C-N-CA | -7.60 | 113.58      | 122.77   |
| 1   | A     | 283 | VAL  | CA-C-N | -7.58 | 110.12      | 120.28   |
| 1   | A     | 283 | VAL  | C-N-CA | -7.58 | 110.12      | 120.28   |
| 2   | B     | 27  | ASP  | N-CA-C | -7.54 | 104.22      | 113.19   |
| 2   | B     | 20  | ASP  | CA-C-N | -7.53 | 109.60      | 120.29   |
| 2   | B     | 20  | ASP  | C-N-CA | -7.53 | 109.60      | 120.29   |
| 1   | A     | 58  | ALA  | CA-C-N | -7.51 | 109.75      | 120.42   |
| 1   | A     | 58  | ALA  | C-N-CA | -7.51 | 109.75      | 120.42   |
| 1   | A     | 325 | PHE  | O-C-N  | -7.50 | 113.05      | 122.27   |
| 1   | A     | 254 | ARG  | O-C-N  | 7.50  | 130.99      | 122.22   |
| 1   | A     | 293 | ASP  | O-C-N  | -7.49 | 114.98      | 121.35   |
| 2   | B     | 60  | ALA  | O-C-N  | -7.45 | 115.13      | 123.48   |
| 5   | C     | 9   | ILE  | CA-C-N | -7.45 | 110.30      | 120.28   |
| 5   | C     | 9   | ILE  | C-N-CA | -7.45 | 110.30      | 120.28   |
| 3   | D     | 213 | ILE  | O-C-N  | 7.43  | 132.14      | 122.26   |
| 5   | C     | 15  | LEU  | CA-C-N | -7.33 | 110.42      | 120.46   |
| 5   | C     | 15  | LEU  | C-N-CA | -7.33 | 110.42      | 120.46   |
| 2   | B     | 13  | GLN  | O-C-N  | 7.30  | 129.86      | 122.12   |
| 2   | B     | 243 | THR  | O-C-N  | 7.30  | 132.64      | 123.15   |
| 1   | A     | 222 | PHE  | CA-C-N | -7.27 | 112.01      | 120.88   |
| 1   | A     | 222 | PHE  | C-N-CA | -7.27 | 112.01      | 120.88   |
| 1   | A     | 123 | ALA  | O-C-N  | 7.25  | 129.81      | 122.12   |
| 1   | A     | 300 | LEU  | O-C-N  | 7.25  | 130.45      | 122.11   |
| 2   | B     | 229 | ILE  | O-C-N  | 7.20  | 130.69      | 122.99   |
| 2   | B     | 252 | LEU  | O-C-N  | -7.17 | 114.84      | 123.29   |
| 5   | C     | 16  | VAL  | CA-C-N | -7.16 | 110.68      | 120.28   |
| 5   | C     | 16  | VAL  | C-N-CA | -7.16 | 110.68      | 120.28   |
| 3   | D     | 213 | ILE  | CA-C-N | -7.14 | 110.80      | 122.65   |
| 3   | D     | 213 | ILE  | C-N-CA | -7.14 | 110.80      | 122.65   |
| 1   | A     | 284 | TRP  | O-C-N  | 7.06  | 129.60      | 122.12   |
| 3   | D     | 226 | VAL  | CA-C-N | 7.04  | 131.94      | 121.72   |
| 3   | D     | 226 | VAL  | C-N-CA | 7.04  | 131.94      | 121.72   |
| 1   | A     | 226 | ILE  | O-C-N  | 7.02  | 128.68      | 121.87   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 272 | VAL  | CB-CA-C | -7.02 | 102.82      | 111.87   |
| 1   | A     | 144 | VAL  | O-C-N   | -6.98 | 115.10      | 121.87   |
| 5   | C     | 54  | VAL  | O-C-N   | 6.93  | 129.00      | 121.10   |
| 1   | A     | 256 | LEU  | N-CA-C  | -6.92 | 103.74      | 111.28   |
| 4   | S     | 61  | ALA  | O-C-N   | 6.91  | 130.80      | 121.74   |
| 1   | A     | 300 | LEU  | CA-C-N  | -6.91 | 109.81      | 120.31   |
| 1   | A     | 300 | LEU  | C-N-CA  | -6.91 | 109.81      | 120.31   |
| 2   | B     | 244 | GLY  | CA-C-N  | 6.91  | 133.65      | 122.53   |
| 2   | B     | 244 | GLY  | C-N-CA  | 6.91  | 133.65      | 122.53   |
| 1   | A     | 224 | VAL  | CA-C-N  | -6.85 | 111.45      | 119.05   |
| 1   | A     | 224 | VAL  | C-N-CA  | -6.85 | 111.45      | 119.05   |
| 1   | A     | 264 | LEU  | CA-C-N  | -6.80 | 111.86      | 120.56   |
| 1   | A     | 264 | LEU  | C-N-CA  | -6.80 | 111.86      | 120.56   |
| 3   | D     | 286 | ILE  | O-C-N   | -6.79 | 115.24      | 121.89   |
| 2   | B     | 207 | SER  | O-C-N   | -6.77 | 115.54      | 123.25   |
| 1   | A     | 315 | PRO  | O-C-N   | 6.72  | 133.28      | 122.52   |
| 1   | A     | 222 | PHE  | O-C-N   | 6.69  | 130.15      | 122.25   |
| 1   | A     | 253 | ASP  | O-C-N   | 6.69  | 130.50      | 122.27   |
| 2   | B     | 203 | ALA  | CA-C-N  | 6.66  | 129.75      | 120.29   |
| 2   | B     | 203 | ALA  | C-N-CA  | 6.66  | 129.75      | 120.29   |
| 1   | A     | 325 | PHE  | CA-C-N  | 6.66  | 129.09      | 120.44   |
| 1   | A     | 325 | PHE  | C-N-CA  | 6.66  | 129.09      | 120.44   |
| 2   | B     | 300 | LEU  | N-CA-C  | -6.65 | 105.17      | 113.55   |
| 1   | A     | 126 | SER  | CB-CA-C | -6.62 | 99.79       | 110.79   |
| 4   | S     | 187 | LEU  | CA-C-N  | -6.61 | 110.56      | 122.46   |
| 4   | S     | 187 | LEU  | C-N-CA  | -6.61 | 110.56      | 122.46   |
| 2   | B     | 286 | LEU  | CA-C-N  | 6.60  | 132.31      | 123.00   |
| 2   | B     | 286 | LEU  | C-N-CA  | 6.60  | 132.31      | 123.00   |
| 2   | B     | 307 | VAL  | CA-C-N  | -6.60 | 112.18      | 122.08   |
| 2   | B     | 307 | VAL  | C-N-CA  | -6.60 | 112.18      | 122.08   |
| 1   | A     | 117 | GLY  | CA-C-N  | -6.58 | 110.32      | 122.09   |
| 1   | A     | 117 | GLY  | C-N-CA  | -6.58 | 110.32      | 122.09   |
| 1   | A     | 185 | VAL  | O-C-N   | 6.57  | 130.51      | 121.84   |
| 5   | C     | 41  | CYS  | O-C-N   | -6.53 | 114.24      | 122.27   |
| 1   | A     | 229 | ILE  | CA-C-N  | 6.51  | 129.29      | 120.44   |
| 1   | A     | 229 | ILE  | C-N-CA  | 6.51  | 129.29      | 120.44   |
| 1   | A     | 223 | VAL  | O-C-N   | 6.50  | 129.87      | 121.94   |
| 5   | C     | 54  | VAL  | CA-C-N  | -6.46 | 113.12      | 119.78   |
| 5   | C     | 54  | VAL  | C-N-CA  | -6.46 | 113.12      | 119.78   |
| 5   | C     | 20  | LYS  | O-C-N   | -6.45 | 115.29      | 122.12   |
| 2   | B     | 231 | ALA  | O-C-N   | -6.44 | 115.50      | 123.36   |
| 1   | A     | 324 | ASN  | O-C-N   | -6.42 | 115.32      | 122.12   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 91  | HIS  | CA-C-N   | 6.41  | 131.60      | 121.72   |
| 2   | B     | 91  | HIS  | C-N-CA   | 6.41  | 131.60      | 121.72   |
| 3   | D     | 291 | TYR  | CA-C-N   | 6.40  | 132.17      | 122.95   |
| 3   | D     | 291 | TYR  | C-N-CA   | 6.40  | 132.17      | 122.95   |
| 4   | S     | 101 | TYR  | CA-C-N   | 6.39  | 133.82      | 122.45   |
| 4   | S     | 101 | TYR  | C-N-CA   | 6.39  | 133.82      | 122.45   |
| 2   | B     | 91  | HIS  | CA-CB-CG | 6.37  | 120.17      | 113.80   |
| 1   | A     | 126 | SER  | N-CA-C   | 6.37  | 118.22      | 111.28   |
| 2   | B     | 266 | HIS  | CA-C-N   | 6.35  | 129.96      | 120.31   |
| 2   | B     | 266 | HIS  | C-N-CA   | 6.35  | 129.96      | 120.31   |
| 1   | A     | 315 | PRO  | N-CA-C   | -6.34 | 105.80      | 114.80   |
| 3   | D     | 252 | ASP  | O-C-N    | -6.32 | 114.94      | 122.15   |
| 2   | B     | 45  | MET  | O-C-N    | 6.30  | 130.05      | 122.68   |
| 1   | A     | 299 | ALA  | CA-C-N   | -6.29 | 111.39      | 120.82   |
| 1   | A     | 299 | ALA  | C-N-CA   | -6.29 | 111.39      | 120.82   |
| 2   | B     | 18  | ILE  | CA-C-N   | -6.28 | 111.38      | 120.29   |
| 2   | B     | 18  | ILE  | C-N-CA   | -6.28 | 111.38      | 120.29   |
| 2   | B     | 75  | GLN  | O-C-N    | -6.25 | 113.74      | 122.37   |
| 1   | A     | 240 | LEU  | N-CA-C   | -6.25 | 105.14      | 112.89   |
| 4   | S     | 221 | ALA  | O-C-N    | 6.25  | 128.74      | 122.12   |
| 2   | B     | 198 | LEU  | O-C-N    | -6.24 | 115.56      | 123.24   |
| 2   | B     | 158 | VAL  | O-C-N    | -6.21 | 114.33      | 122.47   |
| 5   | C     | 14  | LYS  | CA-C-N   | -6.15 | 112.44      | 120.44   |
| 5   | C     | 14  | LYS  | C-N-CA   | -6.15 | 112.44      | 120.44   |
| 1   | A     | 175 | LEU  | O-C-N    | -6.15 | 115.19      | 122.20   |
| 2   | B     | 203 | ALA  | O-C-N    | -6.14 | 113.97      | 121.83   |
| 2   | B     | 30  | LEU  | N-CA-C   | -6.13 | 106.20      | 113.38   |
| 2   | B     | 60  | ALA  | CA-C-N   | 6.12  | 130.71      | 121.40   |
| 2   | B     | 60  | ALA  | C-N-CA   | 6.12  | 130.71      | 121.40   |
| 2   | B     | 178 | THR  | O-C-N    | -6.12 | 115.63      | 122.91   |
| 1   | A     | 272 | VAL  | N-CA-C   | 6.12  | 116.17      | 110.42   |
| 2   | B     | 13  | GLN  | CA-C-N   | -6.12 | 112.08      | 120.28   |
| 2   | B     | 13  | GLN  | C-N-CA   | -6.12 | 112.08      | 120.28   |
| 4   | S     | 7   | SER  | O-C-N    | -6.11 | 116.64      | 123.48   |
| 2   | B     | 210 | LEU  | CA-C-N   | -6.10 | 112.56      | 122.81   |
| 2   | B     | 210 | LEU  | C-N-CA   | -6.10 | 112.56      | 122.81   |
| 1   | A     | 62  | VAL  | O-C-N    | -6.09 | 115.96      | 121.87   |
| 3   | D     | 242 | ASN  | CA-C-N   | -6.08 | 111.69      | 120.82   |
| 3   | D     | 242 | ASN  | C-N-CA   | -6.08 | 111.69      | 120.82   |
| 3   | D     | 320 | ILE  | CA-C-N   | 6.08  | 132.35      | 122.81   |
| 3   | D     | 320 | ILE  | C-N-CA   | 6.08  | 132.35      | 122.81   |
| 3   | D     | 227 | ALA  | O-C-N    | 6.07  | 130.49      | 123.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 52  | THR  | O-C-N   | 6.04  | 131.50      | 121.59   |
| 4   | S     | 93  | MET  | N-CA-C  | -6.00 | 102.44      | 110.55   |
| 2   | B     | 54  | HIS  | O-C-N   | -6.00 | 115.66      | 122.68   |
| 5   | C     | 20  | LYS  | CA-C-N  | 6.00  | 129.43      | 120.31   |
| 5   | C     | 20  | LYS  | C-N-CA  | 6.00  | 129.43      | 120.31   |
| 1   | A     | 250 | LYS  | N-CA-C  | -5.96 | 105.10      | 112.38   |
| 1   | A     | 251 | GLU  | CA-C-N  | -5.96 | 113.19      | 122.67   |
| 1   | A     | 251 | GLU  | C-N-CA  | -5.96 | 113.19      | 122.67   |
| 2   | B     | 180 | PHE  | O-C-N   | 5.92  | 129.59      | 122.85   |
| 1   | A     | 253 | ASP  | CA-C-N  | -5.91 | 111.76      | 120.28   |
| 1   | A     | 253 | ASP  | C-N-CA  | -5.91 | 111.76      | 120.28   |
| 1   | A     | 293 | ASP  | CA-C-N  | 5.90  | 127.00      | 120.45   |
| 1   | A     | 293 | ASP  | C-N-CA  | 5.90  | 127.00      | 120.45   |
| 2   | B     | 39  | PRO  | CB-CA-C | -5.89 | 103.85      | 111.39   |
| 1   | A     | 259 | ILE  | N-CA-C  | -5.89 | 104.61      | 110.62   |
| 4   | S     | 57  | THR  | N-CA-C  | 5.88  | 118.79      | 108.56   |
| 1   | A     | 183 | ILE  | CB-CA-C | -5.87 | 104.36      | 111.88   |
| 2   | B     | 151 | PHE  | O-C-N   | -5.87 | 115.60      | 123.23   |
| 1   | A     | 109 | TYR  | N-CA-C  | -5.86 | 104.24      | 111.33   |
| 1   | A     | 216 | CYS  | N-CA-C  | 5.85  | 117.33      | 111.07   |
| 1   | A     | 254 | ARG  | CA-C-N  | -5.84 | 111.43      | 120.31   |
| 1   | A     | 254 | ARG  | C-N-CA  | -5.84 | 111.43      | 120.31   |
| 1   | A     | 226 | ILE  | CA-C-N  | -5.84 | 112.50      | 120.44   |
| 1   | A     | 226 | ILE  | C-N-CA  | -5.84 | 112.50      | 120.44   |
| 1   | A     | 55  | LEU  | N-CA-C  | 5.82  | 118.12      | 111.02   |
| 4   | S     | 52  | SER  | CA-C-O  | -5.82 | 115.45      | 122.03   |
| 1   | A     | 304 | ILE  | O-C-N   | 5.82  | 127.78      | 121.90   |
| 3   | D     | 212 | TRP  | O-C-N   | 5.82  | 129.53      | 122.20   |
| 2   | B     | 192 | LEU  | CA-C-N  | 5.82  | 133.35      | 121.48   |
| 2   | B     | 192 | LEU  | C-N-CA  | 5.82  | 133.35      | 121.48   |
| 4   | S     | 71  | SER  | O-C-N   | 5.81  | 129.71      | 122.92   |
| 3   | D     | 246 | ALA  | N-CA-C  | -5.75 | 105.03      | 112.68   |
| 2   | B     | 97  | SER  | O-C-N   | -5.75 | 116.17      | 122.84   |
| 5   | C     | 18  | GLN  | CA-C-N  | -5.74 | 112.14      | 120.29   |
| 5   | C     | 18  | GLN  | C-N-CA  | -5.74 | 112.14      | 120.29   |
| 2   | B     | 163 | ASP  | CA-C-N  | -5.72 | 111.79      | 121.18   |
| 2   | B     | 163 | ASP  | C-N-CA  | -5.72 | 111.79      | 121.18   |
| 1   | A     | 262 | MET  | O-C-N   | 5.72  | 127.97      | 122.07   |
| 4   | S     | 139 | VAL  | O-C-N   | 5.72  | 128.87      | 122.75   |
| 3   | D     | 53  | MET  | N-CA-C  | -5.72 | 106.26      | 113.18   |
| 2   | B     | 232 | ILE  | O-C-N   | 5.70  | 129.02      | 123.03   |
| 4   | S     | 157 | ILE  | O-C-N   | -5.70 | 117.05      | 122.98   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 143 | SER  | O-C-N   | -5.68 | 115.67      | 122.15   |
| 2   | B     | 228 | ASP  | CA-C-N  | -5.67 | 115.53      | 123.13   |
| 2   | B     | 228 | ASP  | C-N-CA  | -5.67 | 115.53      | 123.13   |
| 1   | A     | 236 | MET  | CA-C-N  | -5.66 | 111.70      | 120.31   |
| 1   | A     | 236 | MET  | C-N-CA  | -5.66 | 111.70      | 120.31   |
| 1   | A     | 297 | VAL  | O-C-N   | 5.66  | 127.36      | 121.87   |
| 1   | A     | 123 | ALA  | CA-C-N  | -5.66 | 113.32      | 120.56   |
| 1   | A     | 123 | ALA  | C-N-CA  | -5.66 | 113.32      | 120.56   |
| 4   | S     | 87  | ARG  | N-CA-C  | -5.65 | 104.98      | 112.94   |
| 1   | A     | 279 | ILE  | CA-C-N  | 5.62  | 128.26      | 120.29   |
| 1   | A     | 279 | ILE  | C-N-CA  | 5.62  | 128.26      | 120.29   |
| 3   | D     | 45  | GLY  | O-C-N   | -5.62 | 115.49      | 122.34   |
| 2   | B     | 31  | SER  | N-CA-C  | -5.61 | 105.22      | 112.68   |
| 5   | C     | 22  | GLU  | O-C-N   | -5.60 | 115.38      | 122.27   |
| 1   | A     | 266 | VAL  | CA-C-N  | -5.60 | 113.38      | 120.60   |
| 1   | A     | 266 | VAL  | C-N-CA  | -5.60 | 113.38      | 120.60   |
| 4   | S     | 115 | THR  | CA-C-N  | -5.59 | 114.52      | 122.41   |
| 4   | S     | 115 | THR  | C-N-CA  | -5.59 | 114.52      | 122.41   |
| 4   | S     | 182 | GLY  | O-C-N   | 5.58  | 129.02      | 122.38   |
| 4   | S     | 15  | GLY  | CA-C-N  | -5.56 | 115.41      | 122.19   |
| 4   | S     | 15  | GLY  | C-N-CA  | -5.56 | 115.41      | 122.19   |
| 5   | C     | 21  | MET  | O-C-N   | -5.55 | 115.44      | 122.27   |
| 1   | A     | 266 | VAL  | O-C-N   | 5.54  | 127.32      | 121.89   |
| 2   | B     | 317 | CYS  | O-C-N   | -5.54 | 116.84      | 123.27   |
| 2   | B     | 12  | GLU  | N-CA-C  | -5.53 | 105.33      | 111.36   |
| 4   | S     | 72  | ARG  | O-C-N   | -5.53 | 116.86      | 123.27   |
| 4   | S     | 224 | VAL  | O-C-N   | -5.51 | 116.66      | 122.67   |
| 1   | A     | 186 | MET  | CA-C-N  | -5.51 | 114.43      | 122.19   |
| 1   | A     | 186 | MET  | C-N-CA  | -5.51 | 114.43      | 122.19   |
| 5   | C     | 32  | LYS  | O-C-N   | -5.48 | 115.90      | 122.15   |
| 4   | S     | 188 | LEU  | O-C-N   | 5.48  | 128.83      | 122.09   |
| 2   | B     | 239 | ASN  | O-C-N   | 5.46  | 128.75      | 122.25   |
| 1   | A     | 55  | LEU  | CB-CA-C | -5.46 | 102.24      | 110.92   |
| 1   | A     | 185 | VAL  | CA-C-N  | -5.45 | 113.77      | 122.66   |
| 1   | A     | 185 | VAL  | C-N-CA  | -5.45 | 113.77      | 122.66   |
| 1   | A     | 158 | ASP  | O-C-N   | 5.44  | 130.44      | 122.39   |
| 1   | A     | 144 | VAL  | CA-C-N  | 5.43  | 127.56      | 120.28   |
| 1   | A     | 144 | VAL  | C-N-CA  | 5.43  | 127.56      | 120.28   |
| 2   | B     | 160 | SER  | O-C-N   | 5.43  | 129.81      | 122.96   |
| 1   | A     | 214 | LYS  | CA-C-N  | 5.42  | 128.12      | 120.42   |
| 1   | A     | 214 | LYS  | C-N-CA  | 5.42  | 128.12      | 120.42   |
| 1   | A     | 262 | MET  | CA-C-N  | -5.42 | 111.80      | 120.86   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 262 | MET  | C-N-CA | -5.42 | 111.80      | 120.86   |
| 2   | B     | 93  | ILE  | O-C-N  | 5.42  | 125.69      | 121.46   |
| 1   | A     | 265 | VAL  | N-CA-C | 5.41  | 115.62      | 110.53   |
| 4   | S     | 184 | SER  | CA-C-N | 5.41  | 125.40      | 120.21   |
| 4   | S     | 184 | SER  | C-N-CA | 5.41  | 125.40      | 120.21   |
| 1   | A     | 173 | TRP  | CA-C-N | -5.40 | 113.02      | 120.74   |
| 1   | A     | 173 | TRP  | C-N-CA | -5.40 | 113.02      | 120.74   |
| 2   | B     | 45  | MET  | CA-C-N | -5.39 | 113.40      | 122.29   |
| 2   | B     | 45  | MET  | C-N-CA | -5.39 | 113.40      | 122.29   |
| 1   | A     | 217 | VAL  | CA-C-N | -5.38 | 113.45      | 120.44   |
| 1   | A     | 217 | VAL  | C-N-CA | -5.38 | 113.45      | 120.44   |
| 2   | B     | 8   | ARG  | N-CA-C | -5.38 | 105.50      | 111.36   |
| 2   | B     | 204 | CYS  | CA-C-N | 5.38  | 130.75      | 120.97   |
| 2   | B     | 204 | CYS  | C-N-CA | 5.38  | 130.75      | 120.97   |
| 2   | B     | 281 | SER  | O-C-N  | -5.37 | 115.24      | 122.43   |
| 4   | S     | 60  | TYR  | O-C-N  | 5.32  | 129.14      | 122.92   |
| 1   | A     | 57  | SER  | CA-C-N | -5.31 | 113.53      | 120.44   |
| 1   | A     | 57  | SER  | C-N-CA | -5.31 | 113.53      | 120.44   |
| 4   | S     | 214 | LEU  | O-C-N  | -5.29 | 117.00      | 123.30   |
| 4   | S     | 75  | PRO  | O-C-N  | 5.29  | 129.05      | 122.22   |
| 5   | C     | 19  | LEU  | O-C-N  | 5.29  | 128.18      | 122.15   |
| 1   | A     | 302 | LEU  | O-C-N  | 5.28  | 127.72      | 122.12   |
| 3   | D     | 227 | ALA  | CA-C-N | -5.28 | 113.21      | 120.28   |
| 3   | D     | 227 | ALA  | C-N-CA | -5.28 | 113.21      | 120.28   |
| 1   | A     | 158 | ASP  | CA-C-N | -5.27 | 113.96      | 122.24   |
| 1   | A     | 158 | ASP  | C-N-CA | -5.27 | 113.96      | 122.24   |
| 1   | A     | 207 | TRP  | O-C-N  | 5.27  | 128.12      | 121.64   |
| 3   | D     | 30  | ALA  | O-C-N  | -5.27 | 115.75      | 122.34   |
| 2   | B     | 228 | ASP  | O-C-N  | 5.25  | 129.22      | 122.23   |
| 1   | A     | 121 | CYS  | N-CA-C | -5.24 | 105.69      | 111.71   |
| 5   | C     | 17  | GLU  | CA-C-N | -5.19 | 113.33      | 120.28   |
| 5   | C     | 17  | GLU  | C-N-CA | -5.19 | 113.33      | 120.28   |
| 3   | D     | 8   | GLU  | O-C-N  | 5.17  | 128.46      | 122.25   |
| 3   | D     | 252 | ASP  | CA-C-N | 5.17  | 127.62      | 120.29   |
| 3   | D     | 252 | ASP  | C-N-CA | 5.17  | 127.62      | 120.29   |
| 1   | A     | 239 | ARG  | CA-C-N | -5.16 | 112.11      | 121.14   |
| 1   | A     | 239 | ARG  | C-N-CA | -5.16 | 112.11      | 121.14   |
| 1   | A     | 258 | ARG  | CA-C-N | -5.16 | 113.39      | 120.46   |
| 1   | A     | 258 | ARG  | C-N-CA | -5.16 | 113.39      | 120.46   |
| 1   | A     | 313 | LEU  | N-CA-C | -5.16 | 105.84      | 111.82   |
| 1   | A     | 131 | ASN  | N-CA-C | -5.15 | 104.93      | 111.11   |
| 5   | C     | 22  | GLU  | CA-C-N | 5.15  | 127.61      | 120.29   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | C     | 22  | GLU  | C-N-CA | 5.15  | 127.61      | 120.29   |
| 1   | A     | 323 | GLU  | CA-C-N | -5.15 | 113.38      | 120.28   |
| 1   | A     | 323 | GLU  | C-N-CA | -5.15 | 113.38      | 120.28   |
| 4   | S     | 15  | GLY  | O-C-N  | 5.14  | 128.34      | 122.23   |
| 4   | S     | 61  | ALA  | CA-C-N | -5.13 | 112.96      | 122.60   |
| 4   | S     | 61  | ALA  | C-N-CA | -5.13 | 112.96      | 122.60   |
| 1   | A     | 118 | GLU  | CA-C-N | -5.11 | 113.80      | 120.44   |
| 1   | A     | 118 | GLU  | C-N-CA | -5.11 | 113.80      | 120.44   |
| 2   | B     | 208 | ALA  | CA-C-N | -5.10 | 115.28      | 122.94   |
| 2   | B     | 208 | ALA  | C-N-CA | -5.10 | 115.28      | 122.94   |
| 1   | A     | 122 | LYS  | CA-C-N | -5.10 | 113.44      | 120.28   |
| 1   | A     | 122 | LYS  | C-N-CA | -5.10 | 113.44      | 120.28   |
| 1   | A     | 214 | LYS  | O-C-N  | -5.10 | 115.11      | 122.36   |
| 4   | S     | 9   | GLY  | O-C-N  | -5.09 | 118.43      | 122.81   |
| 5   | C     | 21  | MET  | CA-C-N | 5.09  | 128.04      | 120.31   |
| 5   | C     | 21  | MET  | C-N-CA | 5.09  | 128.04      | 120.31   |
| 2   | B     | 178 | THR  | CA-C-N | 5.06  | 129.56      | 121.66   |
| 2   | B     | 178 | THR  | C-N-CA | 5.06  | 129.56      | 121.66   |
| 2   | B     | 320 | VAL  | CA-C-N | 5.06  | 130.18      | 120.97   |
| 2   | B     | 320 | VAL  | C-N-CA | 5.06  | 130.18      | 120.97   |
| 4   | S     | 57  | THR  | CA-C-O | -5.04 | 116.57      | 122.37   |
| 2   | B     | 118 | ASP  | CA-C-N | 5.03  | 131.14      | 121.54   |
| 2   | B     | 118 | ASP  | C-N-CA | 5.03  | 131.14      | 121.54   |
| 2   | B     | 275 | SER  | CA-C-N | -5.02 | 115.48      | 122.71   |
| 2   | B     | 275 | SER  | C-N-CA | -5.02 | 115.48      | 122.71   |
| 1   | A     | 108 | LYS  | CA-C-N | -5.01 | 113.52      | 120.38   |
| 1   | A     | 108 | LYS  | C-N-CA | -5.01 | 113.52      | 120.38   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 171 | CYS  | Mainchain |
| 2   | B     | 148 | CYS  | Mainchain |
| 4   | S     | 82  | GLN  | 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     | 2244  | 0        | 2363     | 352     | 0            |
| 2   | B     | 2603  | 0        | 2506     | 261     | 0            |
| 3   | D     | 1786  | 0        | 1772     | 143     | 0            |
| 4   | S     | 1767  | 0        | 1686     | 116     | 0            |
| 5   | C     | 438   | 0        | 443      | 69      | 0            |
| 6   | A     | 29    | 0        | 0        | 3       | 0            |
| All | All   | 8867  | 0        | 8770     | 875     | 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 50.

All (875) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:126:SER:HB3 | 1:A:184:MET:SD   | 1.43                     | 1.56              |
| 2:B:283:ARG:NE  | 2:B:300:LEU:HD12 | 1.29                     | 1.44              |
| 1:A:126:SER:CB  | 1:A:184:MET:SD   | 2.04                     | 1.44              |
| 2:B:22:ARG:CG   | 5:C:30:VAL:HG11  | 1.51                     | 1.36              |
| 3:D:275:PHE:O   | 3:D:279:ILE:HG23 | 1.25                     | 1.35              |
| 2:B:34:THR:HG22 | 5:C:38:MET:SD    | 1.67                     | 1.32              |
| 5:C:8:SER:O     | 5:C:12:ALA:N     | 1.57                     | 1.32              |
| 2:B:22:ARG:HG3  | 5:C:30:VAL:CG1   | 1.61                     | 1.28              |
| 2:B:281:SER:HB3 | 5:C:48:ASP:CB    | 1.59                     | 1.26              |
| 1:A:312:SER:O   | 1:A:316:VAL:HG23 | 1.33                     | 1.25              |
| 2:B:250:CYS:SG  | 2:B:273:ILE:HD13 | 1.81                     | 1.20              |
| 5:C:12:ALA:O    | 5:C:16:VAL:N     | 1.74                     | 1.19              |
| 3:D:275:PHE:O   | 3:D:279:ILE:CG2  | 1.94                     | 1.15              |
| 2:B:26:ALA:HB1  | 2:B:33:ILE:HD11  | 1.23                     | 1.15              |
| 4:S:91:THR:HG23 | 4:S:118:THR:HA   | 1.29                     | 1.14              |
| 2:B:281:SER:CB  | 5:C:48:ASP:HB2   | 1.77                     | 1.14              |
| 3:D:48:THR:HA   | 3:D:51:LYS:CB    | 1.79                     | 1.13              |
| 5:C:14:LYS:O    | 5:C:18:GLN:N     | 1.82                     | 1.12              |
| 2:B:26:ALA:CB   | 2:B:33:ILE:HD11  | 1.78                     | 1.12              |
| 1:A:313:LEU:HA  | 1:A:316:VAL:HB   | 1.30                     | 1.11              |
| 1:A:52:ILE:CG2  | 1:A:56:TYR:CE1   | 2.35                     | 1.09              |
| 4:S:70:ILE:HD12 | 4:S:81:LEU:HD12  | 1.26                     | 1.09              |
| 1:A:116:PHE:CD2 | 1:A:120:LEU:HB2  | 1.88                     | 1.08              |
| 2:B:15:LYS:HZ1  | 2:B:258:ASP:HB2  | 1.07                     | 1.07              |
| 4:S:11:LEU:HD11 | 4:S:120:SER:HB2  | 1.30                     | 1.07              |
| 5:C:15:LEU:O    | 5:C:19:LEU:N     | 1.87                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:250:CYS:SG   | 2:B:273:ILE:CD1  | 2.44                     | 1.05              |
| 5:C:9:ILE:HA     | 5:C:12:ALA:HB3   | 1.32                     | 1.05              |
| 1:A:245:LEU:CD1  | 3:D:342:ASP:OD1  | 2.03                     | 1.05              |
| 1:A:246:LEU:HD13 | 3:D:355:PHE:HE1  | 1.18                     | 1.05              |
| 3:D:48:THR:HA    | 3:D:51:LYS:HB2   | 1.11                     | 1.05              |
| 4:S:70:ILE:HA    | 4:S:81:LEU:HA    | 1.39                     | 1.05              |
| 1:A:77:TYR:CE2   | 1:A:328:CYS:SG   | 2.50                     | 1.05              |
| 4:S:71:SER:O     | 4:S:79:LEU:HD12  | 1.58                     | 1.04              |
| 2:B:26:ALA:HB1   | 2:B:33:ILE:CD1   | 1.87                     | 1.03              |
| 1:A:257:ARG:O    | 1:A:260:THR:HG22 | 1.60                     | 1.02              |
| 3:D:49:ILE:HG22  | 3:D:53:MET:HE3   | 1.40                     | 1.02              |
| 4:S:71:SER:N     | 4:S:80:PHE:O     | 1.94                     | 1.01              |
| 2:B:283:ARG:CD   | 2:B:300:LEU:HD12 | 1.89                     | 1.00              |
| 3:D:186:VAL:HB   | 3:D:201:ASP:HB3  | 1.43                     | 1.00              |
| 3:D:224:PHE:CE2  | 3:D:251:PHE:HD2  | 1.79                     | 1.00              |
| 3:D:349:LEU:HG   | 3:D:355:PHE:HB2  | 1.01                     | 1.00              |
| 4:S:142:GLN:NE2  | 4:S:229:CYS:SG   | 2.35                     | 1.00              |
| 1:A:67:ASN:ND2   | 1:A:95:ASP:HB3   | 1.77                     | 1.00              |
| 1:A:299:ALA:HA   | 1:A:302:LEU:HB2  | 1.37                     | 1.00              |
| 2:B:15:LYS:NZ    | 2:B:258:ASP:HB2  | 1.76                     | 0.99              |
| 1:A:52:ILE:CG2   | 1:A:56:TYR:CZ    | 2.47                     | 0.98              |
| 4:S:70:ILE:HD12  | 4:S:81:LEU:CD1   | 1.91                     | 0.98              |
| 2:B:283:ARG:NE   | 2:B:300:LEU:CD1  | 2.26                     | 0.98              |
| 1:A:245:LEU:HD11 | 3:D:342:ASP:OD1  | 1.61                     | 0.98              |
| 2:B:197:ARG:HE   | 2:B:214:ARG:NH2  | 1.61                     | 0.98              |
| 1:A:313:LEU:HA   | 1:A:316:VAL:CB   | 1.93                     | 0.97              |
| 1:A:150:VAL:HG21 | 1:A:236:MET:HG3  | 1.45                     | 0.97              |
| 4:S:138:ILE:HB   | 4:S:231:GLN:OE1  | 1.64                     | 0.97              |
| 3:D:349:LEU:CG   | 3:D:355:PHE:HB2  | 1.93                     | 0.97              |
| 1:A:313:LEU:CA   | 1:A:316:VAL:HB   | 1.95                     | 0.96              |
| 3:D:272:LYS:HB2  | 3:D:326:CYS:SG   | 2.06                     | 0.96              |
| 3:D:228:LEU:HD21 | 3:D:269:LEU:HD13 | 1.45                     | 0.95              |
| 1:A:116:PHE:HE2  | 1:A:120:LEU:N    | 1.65                     | 0.95              |
| 5:C:16:VAL:O     | 5:C:20:LYS:N     | 1.99                     | 0.95              |
| 1:A:125:LEU:HD11 | 1:A:198:CYS:SG   | 2.05                     | 0.95              |
| 2:B:22:ARG:HA    | 5:C:30:VAL:HG12  | 1.46                     | 0.94              |
| 5:C:13:ARG:O     | 5:C:17:GLU:HB2   | 1.69                     | 0.93              |
| 1:A:126:SER:HB2  | 1:A:184:MET:SD   | 2.07                     | 0.93              |
| 2:B:340:ASN:HD22 | 5:C:61:PHE:HB2   | 1.34                     | 0.92              |
| 3:D:349:LEU:HG   | 3:D:355:PHE:CB   | 1.96                     | 0.92              |
| 1:A:52:ILE:O     | 1:A:56:TYR:N     | 2.03                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:9:ILE:HA     | 5:C:12:ALA:CB    | 2.00                     | 0.92              |
| 3:D:269:LEU:O    | 3:D:325:THR:OG1  | 1.88                     | 0.92              |
| 1:A:246:LEU:HD13 | 3:D:355:PHE:CE1  | 2.05                     | 0.92              |
| 3:D:53:MET:SD    | 3:D:199:MET:SD   | 2.67                     | 0.91              |
| 4:S:70:ILE:HG13  | 4:S:81:LEU:HB2   | 1.52                     | 0.90              |
| 1:A:312:SER:O    | 1:A:316:VAL:CG2  | 2.18                     | 0.90              |
| 4:S:64:VAL:CG1   | 4:S:68:PHE:CD2   | 2.55                     | 0.90              |
| 2:B:283:ARG:HE   | 2:B:300:LEU:HD12 | 1.08                     | 0.89              |
| 5:C:7:ALA:O      | 5:C:11:GLN:N     | 2.05                     | 0.89              |
| 4:S:64:VAL:HG11  | 4:S:68:PHE:CD2   | 2.08                     | 0.88              |
| 1:A:56:TYR:CE1   | 1:A:305:ALA:HB2  | 2.08                     | 0.88              |
| 1:A:54:ALA:O     | 1:A:58:ALA:N     | 2.05                     | 0.87              |
| 1:A:74:ILE:HD13  | 1:A:88:ILE:HG23  | 1.56                     | 0.87              |
| 1:A:102:LEU:HD23 | 1:A:103:PRO:HD3  | 1.57                     | 0.87              |
| 2:B:250:CYS:HG   | 2:B:273:ILE:HD13 | 1.37                     | 0.87              |
| 1:A:176:ALA:O    | 1:A:179:VAL:N    | 2.07                     | 0.87              |
| 1:A:119:LEU:HA   | 1:A:122:LYS:HZ3  | 1.40                     | 0.86              |
| 1:A:202:PHE:CD2  | 1:A:210:ASP:HB2  | 2.10                     | 0.86              |
| 1:A:52:ILE:HG23  | 1:A:56:TYR:CE1   | 2.10                     | 0.86              |
| 2:B:256:ARG:H    | 2:B:256:ARG:HD2  | 1.39                     | 0.86              |
| 1:A:108:LYS:O    | 1:A:112:GLU:N    | 2.08                     | 0.86              |
| 2:B:283:ARG:HE   | 2:B:300:LEU:CD1  | 1.89                     | 0.85              |
| 1:A:299:ALA:O    | 1:A:302:LEU:N    | 2.09                     | 0.85              |
| 1:A:146:ARG:HD2  | 3:D:354:LEU:HD12 | 1.58                     | 0.85              |
| 2:B:340:ASN:ND2  | 5:C:61:PHE:HB2   | 1.91                     | 0.85              |
| 1:A:53:THR:O     | 1:A:57:SER:N     | 2.08                     | 0.85              |
| 4:S:71:SER:O     | 4:S:80:PHE:N     | 2.09                     | 0.85              |
| 1:A:52:ILE:HG22  | 1:A:56:TYR:CE1   | 2.11                     | 0.84              |
| 3:D:48:THR:CA    | 3:D:51:LYS:HB2   | 2.03                     | 0.84              |
| 1:A:91:LEU:HD22  | 1:A:138:THR:HG21 | 1.60                     | 0.84              |
| 2:B:15:LYS:HG2   | 5:C:27:ARG:HH22  | 1.42                     | 0.83              |
| 4:S:64:VAL:HG12  | 4:S:68:PHE:CG    | 2.12                     | 0.83              |
| 1:A:306:LEU:O    | 1:A:309:ALA:HB3  | 1.79                     | 0.83              |
| 2:B:310:GLY:O    | 2:B:337:LYS:NZ   | 2.12                     | 0.83              |
| 2:B:119:ASN:ND2  | 2:B:144:GLY:O    | 2.11                     | 0.83              |
| 2:B:47:THR:HG22  | 2:B:339:TRP:CD1  | 2.14                     | 0.83              |
| 1:A:52:ILE:HG21  | 1:A:56:TYR:CZ    | 2.13                     | 0.82              |
| 2:B:227:SER:OG   | 2:B:246:ASP:HB3  | 1.79                     | 0.82              |
| 2:B:281:SER:CB   | 5:C:48:ASP:CB    | 2.43                     | 0.82              |
| 2:B:3:GLU:HG2    | 5:C:16:VAL:HG11  | 1.60                     | 0.82              |
| 2:B:26:ALA:CA    | 2:B:33:ILE:HD11  | 2.10                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:161:SER:HB3  | 2:B:187:VAL:HG21 | 1.60                     | 0.81              |
| 2:B:278:PHE:HE2  | 2:B:282:GLY:HA2  | 1.43                     | 0.81              |
| 2:B:15:LYS:HG2   | 5:C:27:ARG:NH2   | 1.94                     | 0.81              |
| 1:A:64:LEU:HA    | 1:A:99:THR:HG21  | 1.62                     | 0.81              |
| 3:D:224:PHE:CE2  | 3:D:251:PHE:CD2  | 2.68                     | 0.81              |
| 3:D:49:ILE:CG2   | 3:D:53:MET:HE3   | 2.10                     | 0.81              |
| 1:A:260:THR:O    | 1:A:263:VAL:HG22 | 1.80                     | 0.81              |
| 1:A:153:PRO:HG3  | 3:D:345:ILE:HD11 | 1.63                     | 0.80              |
| 3:D:264:SER:OG   | 3:D:319:GLU:OE2  | 2.00                     | 0.80              |
| 1:A:54:ALA:O     | 1:A:57:SER:HB3   | 1.82                     | 0.80              |
| 2:B:26:ALA:CB    | 2:B:33:ILE:CD1   | 2.53                     | 0.80              |
| 1:A:56:TYR:HA    | 1:A:59:VAL:CG1   | 2.12                     | 0.79              |
| 1:A:146:ARG:HD2  | 3:D:354:LEU:CD1  | 2.11                     | 0.79              |
| 1:A:133:PHE:CE2  | 1:A:179:VAL:HG11 | 2.17                     | 0.79              |
| 2:B:281:SER:HB3  | 5:C:48:ASP:HB2   | 0.84                     | 0.79              |
| 1:A:313:LEU:HA   | 1:A:316:VAL:CG2  | 2.12                     | 0.79              |
| 1:A:299:ALA:CA   | 1:A:302:LEU:HB2  | 2.12                     | 0.79              |
| 1:A:72:PHE:O     | 1:A:75:VAL:N     | 2.15                     | 0.79              |
| 1:A:245:LEU:CG   | 3:D:342:ASP:OD1  | 2.31                     | 0.79              |
| 1:A:272:VAL:O    | 1:A:276:PRO:HD3  | 1.82                     | 0.78              |
| 1:A:311:SER:O    | 1:A:315:PRO:HD2  | 1.84                     | 0.78              |
| 1:A:52:ILE:HA    | 1:A:55:LEU:HB3   | 1.66                     | 0.78              |
| 4:S:138:ILE:HG13 | 4:S:231:GLN:HE22 | 1.47                     | 0.78              |
| 4:S:64:VAL:HG11  | 4:S:68:PHE:CE2   | 2.18                     | 0.78              |
| 1:A:202:PHE:HD2  | 1:A:210:ASP:HB2  | 1.47                     | 0.78              |
| 5:C:9:ILE:CA     | 5:C:12:ALA:HB3   | 2.13                     | 0.78              |
| 1:A:313:LEU:O    | 1:A:316:VAL:N    | 2.17                     | 0.77              |
| 1:A:51:ALA:O     | 1:A:55:LEU:N     | 2.16                     | 0.77              |
| 2:B:278:PHE:CE2  | 2:B:282:GLY:HA2  | 2.19                     | 0.77              |
| 2:B:228:ASP:O    | 2:B:245:SER:HA   | 1.85                     | 0.77              |
| 4:S:98:ARG:HD3   | 4:S:110:PHE:HB3  | 1.66                     | 0.77              |
| 4:S:6:GLU:OE2    | 4:S:96:CYS:SG    | 2.43                     | 0.77              |
| 2:B:18:ILE:O     | 2:B:22:ARG:N     | 2.17                     | 0.76              |
| 1:A:56:TYR:HA    | 1:A:59:VAL:HG12  | 1.66                     | 0.76              |
| 3:D:272:LYS:HD3  | 3:D:324:PHE:HB3  | 1.66                     | 0.76              |
| 1:A:67:ASN:HD21  | 1:A:95:ASP:HB3   | 1.49                     | 0.76              |
| 1:A:130:TYR:HE1  | 1:A:177:SER:N    | 1.82                     | 0.76              |
| 2:B:283:ARG:CD   | 2:B:300:LEU:CD1  | 2.64                     | 0.76              |
| 4:S:64:VAL:CG1   | 4:S:68:PHE:CG    | 2.67                     | 0.76              |
| 3:D:227:ALA:O    | 3:D:244:MET:HE2  | 1.86                     | 0.76              |
| 3:D:54:LYS:HD2   | 3:D:190:PHE:HB3  | 1.68                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:PHE:HB2  | 1:A:210:ASP:OD2  | 1.86                     | 0.75              |
| 3:D:245:HIS:HA   | 3:D:248:MET:SD   | 2.27                     | 0.75              |
| 4:S:244:LYS:C    | 4:S:245:LEU:HD12 | 2.11                     | 0.75              |
| 1:A:302:LEU:O    | 1:A:305:ALA:HB3  | 1.86                     | 0.75              |
| 2:B:48:ARG:HG2   | 2:B:340:ASN:HB3  | 1.68                     | 0.75              |
| 3:D:6:SER:OG     | 3:D:9:ASP:OD1    | 2.03                     | 0.75              |
| 3:D:47:ASN:O     | 3:D:51:LYS:N     | 2.20                     | 0.75              |
| 1:A:78:THR:HG21  | 1:A:85:ASN:ND2   | 2.02                     | 0.75              |
| 3:D:188:THR:O    | 3:D:198:LYS:HA   | 1.87                     | 0.75              |
| 1:A:51:ALA:O     | 1:A:54:ALA:HB3   | 1.86                     | 0.75              |
| 4:S:70:ILE:CD1   | 4:S:81:LEU:HD12  | 2.10                     | 0.75              |
| 1:A:245:LEU:HD13 | 3:D:346:LYS:HB2  | 1.68                     | 0.75              |
| 4:S:2:VAL:HG12   | 4:S:26:GLY:O     | 1.86                     | 0.74              |
| 1:A:141:MET:HE2  | 1:A:168:ILE:HD13 | 1.69                     | 0.74              |
| 1:A:52:ILE:HG22  | 1:A:56:TYR:CZ    | 2.22                     | 0.74              |
| 1:A:72:PHE:O     | 1:A:75:VAL:HB    | 1.88                     | 0.74              |
| 1:A:257:ARG:C    | 1:A:260:THR:HG22 | 2.12                     | 0.74              |
| 3:D:272:LYS:CD   | 3:D:324:PHE:HB3  | 2.18                     | 0.74              |
| 3:D:272:LYS:HG3  | 3:D:325:THR:O    | 1.88                     | 0.74              |
| 1:A:56:TYR:HE1   | 1:A:305:ALA:HB2  | 1.52                     | 0.74              |
| 1:A:224:VAL:HA   | 1:A:227:LEU:HG   | 1.68                     | 0.74              |
| 1:A:56:TYR:CA    | 1:A:59:VAL:HG12  | 2.16                     | 0.73              |
| 2:B:283:ARG:O    | 2:B:299:ALA:N    | 2.18                     | 0.73              |
| 4:S:244:LYS:O    | 4:S:245:LEU:HD12 | 1.86                     | 0.73              |
| 1:A:176:ALA:O    | 1:A:177:SER:C    | 2.28                     | 0.73              |
| 4:S:90:ASP:OD1   | 4:S:119:VAL:HG21 | 1.87                     | 0.73              |
| 1:A:170:ILE:O    | 1:A:174:VAL:HG22 | 1.89                     | 0.73              |
| 1:A:67:ASN:ND2   | 1:A:96:ALA:N     | 2.36                     | 0.73              |
| 2:B:47:THR:HG22  | 2:B:339:TRP:NE1  | 2.03                     | 0.73              |
| 2:B:318:LEU:HG   | 2:B:329:THR:HG22 | 1.71                     | 0.73              |
| 1:A:243:VAL:HG12 | 1:A:245:LEU:H    | 1.53                     | 0.73              |
| 1:A:245:LEU:HG   | 3:D:342:ASP:OD1  | 1.88                     | 0.73              |
| 1:A:246:LEU:CD2  | 1:A:259:ILE:HD12 | 2.19                     | 0.73              |
| 2:B:22:ARG:CG    | 5:C:30:VAL:CG1   | 2.41                     | 0.73              |
| 1:A:313:LEU:O    | 1:A:316:VAL:HB   | 1.88                     | 0.73              |
| 5:C:14:LYS:O     | 5:C:17:GLU:HB3   | 1.88                     | 0.73              |
| 1:A:91:LEU:HD22  | 1:A:138:THR:CG2  | 2.20                     | 0.72              |
| 1:A:299:ALA:O    | 1:A:303:CYS:N    | 2.23                     | 0.72              |
| 2:B:15:LYS:NZ    | 2:B:258:ASP:O    | 2.23                     | 0.72              |
| 1:A:116:PHE:HD2  | 1:A:120:LEU:HB2  | 1.49                     | 0.72              |
| 2:B:161:SER:HB3  | 2:B:187:VAL:CG2  | 2.19                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:10:ALA:O     | 5:C:14:LYS:N      | 2.23                     | 0.72              |
| 2:B:34:THR:CG2   | 5:C:38:MET:SD     | 2.64                     | 0.71              |
| 4:S:71:SER:C     | 4:S:79:LEU:HD12   | 2.13                     | 0.71              |
| 1:A:311:SER:O    | 1:A:314:ASN:HB2   | 1.89                     | 0.71              |
| 2:B:197:ARG:HE   | 2:B:214:ARG:CZ    | 2.02                     | 0.71              |
| 1:A:90:ASN:OD1   | 1:A:169:ASN:ND2   | 2.24                     | 0.71              |
| 3:D:187:GLU:OE1  | 3:D:200:PHE:HD1   | 1.74                     | 0.71              |
| 2:B:61:MET:SD    | 2:B:70:LEU:HD11   | 2.31                     | 0.71              |
| 2:B:283:ARG:HD2  | 2:B:300:LEU:CD1   | 2.20                     | 0.71              |
| 3:D:255:CYS:SG   | 3:D:318:LYS:NZ    | 2.63                     | 0.71              |
| 5:C:16:VAL:O     | 5:C:20:LYS:HG3    | 1.91                     | 0.71              |
| 2:B:22:ARG:CB    | 5:C:30:VAL:HG11   | 2.21                     | 0.70              |
| 1:A:246:LEU:HD21 | 1:A:259:ILE:HD12  | 1.73                     | 0.70              |
| 1:A:243:VAL:HG12 | 1:A:244:ARG:N     | 2.06                     | 0.70              |
| 1:A:56:TYR:CE1   | 1:A:305:ALA:CB    | 2.74                     | 0.70              |
| 1:A:130:TYR:OH   | 1:A:177:SER:HB3   | 1.92                     | 0.70              |
| 1:A:132:MET:HE2  | 6:A:401:A1LXY:C19 | 2.22                     | 0.70              |
| 1:A:52:ILE:O     | 1:A:55:LEU:HB3    | 1.93                     | 0.69              |
| 2:B:26:ALA:HB2   | 5:C:31:SER:HB2    | 1.73                     | 0.69              |
| 2:B:314:ARG:C    | 2:B:331:SER:HG    | 1.99                     | 0.69              |
| 4:S:226:VAL:HG22 | 4:S:244:LYS:HD3   | 1.75                     | 0.69              |
| 1:A:51:ALA:O     | 1:A:54:ALA:N      | 2.26                     | 0.69              |
| 4:S:70:ILE:CG1   | 4:S:81:LEU:HB2    | 2.23                     | 0.69              |
| 2:B:15:LYS:NZ    | 2:B:258:ASP:C     | 2.51                     | 0.69              |
| 2:B:22:ARG:CA    | 5:C:30:VAL:HG12   | 2.23                     | 0.68              |
| 3:D:224:PHE:HE1  | 3:D:250:LEU:HD22  | 1.58                     | 0.68              |
| 2:B:60:ALA:HB3   | 2:B:73:ALA:HB3    | 1.75                     | 0.68              |
| 1:A:197:VAL:HB   | 1:A:199:MET:HE3   | 1.75                     | 0.68              |
| 1:A:251:GLU:HG2  | 1:A:252:LYS:HE3   | 1.76                     | 0.68              |
| 2:B:82:TRP:HB3   | 2:B:89:LYS:HA     | 1.75                     | 0.68              |
| 2:B:248:ALA:HB2  | 2:B:271:CYS:O     | 1.92                     | 0.68              |
| 3:D:188:THR:HB   | 3:D:199:MET:HB2   | 1.76                     | 0.68              |
| 1:A:313:LEU:C    | 1:A:316:VAL:HB    | 2.17                     | 0.68              |
| 2:B:15:LYS:NZ    | 2:B:258:ASP:CB    | 2.56                     | 0.68              |
| 4:S:202:ARG:NH2  | 4:S:223:ASP:OD1   | 2.27                     | 0.68              |
| 1:A:299:ALA:O    | 1:A:300:LEU:C     | 2.38                     | 0.67              |
| 3:D:209:ARG:HA   | 3:D:212:TRP:NE1   | 2.09                     | 0.67              |
| 5:C:13:ARG:O     | 5:C:17:GLU:CB     | 2.40                     | 0.67              |
| 1:A:55:LEU:O     | 1:A:59:VAL:HG12   | 1.94                     | 0.67              |
| 1:A:257:ARG:O    | 1:A:260:THR:CG2   | 2.39                     | 0.67              |
| 4:S:72:ARG:HA    | 4:S:79:LEU:HA     | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:82:TRP:CB    | 2:B:89:LYS:HA    | 2.24                     | 0.67              |
| 4:S:19:LYS:HB3   | 4:S:82:GLN:NE2   | 2.10                     | 0.67              |
| 1:A:52:ILE:HA    | 1:A:55:LEU:CB    | 2.25                     | 0.67              |
| 1:A:273:CYS:HB3  | 1:A:310:ASN:HB3  | 1.75                     | 0.67              |
| 4:S:64:VAL:CG1   | 4:S:68:PHE:CE2   | 2.77                     | 0.67              |
| 3:D:224:PHE:CD2  | 3:D:251:PHE:CD2  | 2.83                     | 0.67              |
| 1:A:56:TYR:O     | 1:A:60:CYS:N     | 2.13                     | 0.67              |
| 1:A:282:ILE:HA   | 1:A:285:THR:OG1  | 1.94                     | 0.67              |
| 2:B:257:ALA:HB1  | 2:B:259:GLN:NE2  | 2.10                     | 0.67              |
| 1:A:146:ARG:HH11 | 3:D:354:LEU:HD11 | 1.60                     | 0.67              |
| 1:A:78:THR:CG2   | 1:A:85:ASN:ND2   | 2.57                     | 0.66              |
| 3:D:54:LYS:CD    | 3:D:190:PHE:HB3  | 2.25                     | 0.66              |
| 3:D:305:GLN:HG2  | 3:D:322:THR:HG21 | 1.78                     | 0.66              |
| 1:A:244:ARG:NH2  | 3:D:321:TYR:CE1  | 2.64                     | 0.66              |
| 2:B:168:LEU:HB3  | 2:B:177:THR:O    | 1.96                     | 0.66              |
| 4:S:139:VAL:CG1  | 4:S:162:SER:OG   | 2.43                     | 0.66              |
| 2:B:3:GLU:CG     | 5:C:16:VAL:HG11  | 2.26                     | 0.66              |
| 2:B:253:PHE:HD1  | 2:B:260:GLU:HA   | 1.59                     | 0.66              |
| 1:A:314:ASN:HB2  | 1:A:315:PRO:HD3  | 1.78                     | 0.66              |
| 1:A:125:LEU:CD1  | 1:A:198:CYS:SG   | 2.82                     | 0.66              |
| 1:A:74:ILE:HG12  | 1:A:325:PHE:HZ   | 1.61                     | 0.66              |
| 1:A:257:ARG:HA   | 1:A:260:THR:HG22 | 1.78                     | 0.66              |
| 4:S:12:VAL:HG12  | 4:S:13:GLN:H     | 1.59                     | 0.66              |
| 4:S:138:ILE:CG1  | 4:S:231:GLN:HE22 | 2.09                     | 0.66              |
| 1:A:70:VAL:O     | 1:A:71:MET:C     | 2.39                     | 0.65              |
| 1:A:159:PHE:HA   | 1:A:164:LYS:HE3  | 1.77                     | 0.65              |
| 2:B:30:LEU:HD13  | 5:C:34:ALA:HB2   | 1.78                     | 0.65              |
| 2:B:26:ALA:C     | 2:B:28:ALA:H     | 2.05                     | 0.65              |
| 2:B:163:ASP:O    | 2:B:186:ASP:HA   | 1.96                     | 0.65              |
| 2:B:215:GLU:HG3  | 2:B:217:MET:HE2  | 1.78                     | 0.65              |
| 2:B:43:ILE:HD13  | 2:B:284:LEU:HD11 | 1.77                     | 0.65              |
| 1:A:225:PRO:O    | 1:A:229:ILE:HG22 | 1.96                     | 0.65              |
| 2:B:314:ARG:O    | 2:B:331:SER:OG   | 2.10                     | 0.65              |
| 3:D:246:ALA:O    | 3:D:249:LYS:N    | 2.30                     | 0.65              |
| 3:D:187:GLU:OE1  | 3:D:200:PHE:CD1  | 2.50                     | 0.65              |
| 1:A:78:THR:HG21  | 1:A:85:ASN:HD21  | 1.62                     | 0.64              |
| 2:B:3:GLU:OE1    | 2:B:7:LEU:HD12   | 1.97                     | 0.64              |
| 3:D:244:MET:HA   | 3:D:247:SER:HB2  | 1.79                     | 0.64              |
| 1:A:95:ASP:OD2   | 1:A:315:PRO:CG   | 2.45                     | 0.64              |
| 2:B:215:GLU:HG3  | 2:B:217:MET:SD   | 2.37                     | 0.64              |
| 1:A:258:ARG:NH2  | 3:D:355:PHE:OXT  | 2.31                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:18:ILE:HD11  | 5:C:27:ARG:HB2    | 1.79                     | 0.64              |
| 1:A:116:PHE:CE2  | 1:A:120:LEU:HB2   | 2.32                     | 0.64              |
| 2:B:189:SER:OG   | 2:B:232:ILE:HG12  | 1.98                     | 0.64              |
| 2:B:48:ARG:NH1   | 5:C:63:GLU:OE2    | 2.28                     | 0.63              |
| 1:A:116:PHE:CD2  | 1:A:120:LEU:CB    | 2.74                     | 0.63              |
| 2:B:113:ALA:HB2  | 2:B:151:PHE:HE1   | 1.64                     | 0.63              |
| 2:B:199:PHE:HE1  | 2:B:213:VAL:HG22  | 1.62                     | 0.63              |
| 1:A:222:PHE:O    | 1:A:226:ILE:HD12  | 1.98                     | 0.63              |
| 3:D:46:LYS:O     | 3:D:50:VAL:HG23   | 1.98                     | 0.63              |
| 3:D:224:PHE:CD2  | 3:D:251:PHE:HD2   | 2.16                     | 0.63              |
| 1:A:223:VAL:HG12 | 1:A:227:LEU:HD23  | 1.78                     | 0.63              |
| 2:B:48:ARG:CG    | 2:B:340:ASN:HB3   | 2.28                     | 0.63              |
| 3:D:187:GLU:OE2  | 3:D:200:PHE:CE1   | 2.51                     | 0.63              |
| 4:S:70:ILE:HG13  | 4:S:81:LEU:CB     | 2.26                     | 0.63              |
| 2:B:232:ILE:HG22 | 2:B:243:THR:OG1   | 1.98                     | 0.63              |
| 4:S:94:TYR:O     | 4:S:114:GLY:HA3   | 1.98                     | 0.63              |
| 2:B:30:LEU:HD23  | 2:B:33:ILE:HD12   | 1.81                     | 0.63              |
| 2:B:200:VAL:HA   | 2:B:210:LEU:HA    | 1.81                     | 0.63              |
| 4:S:139:VAL:HG13 | 4:S:162:SER:CB    | 2.28                     | 0.63              |
| 2:B:22:ARG:CB    | 5:C:30:VAL:CG1    | 2.77                     | 0.63              |
| 2:B:11:ALA:O     | 2:B:15:LYS:N      | 2.29                     | 0.62              |
| 3:D:49:ILE:HD12  | 3:D:225:CYS:SG    | 2.39                     | 0.62              |
| 1:A:56:TYR:HE1   | 1:A:305:ALA:CB    | 2.12                     | 0.62              |
| 1:A:77:TYR:CZ    | 1:A:328:CYS:SG    | 2.92                     | 0.62              |
| 2:B:82:TRP:HB2   | 2:B:88:ASN:O      | 2.00                     | 0.62              |
| 1:A:116:PHE:CE2  | 1:A:120:LEU:HG    | 2.33                     | 0.62              |
| 1:A:250:LYS:HA   | 1:A:253:ASP:HB2   | 1.82                     | 0.62              |
| 1:A:133:PHE:CD2  | 1:A:179:VAL:HG11  | 2.33                     | 0.62              |
| 1:A:300:LEU:HD21 | 6:A:401:A1LXY:O27 | 2.00                     | 0.62              |
| 1:A:219:LEU:HD12 | 1:A:223:VAL:HG21  | 1.81                     | 0.62              |
| 1:A:218:PHE:CE1  | 1:A:278:HIS:HB3   | 2.34                     | 0.62              |
| 2:B:27:ASP:C     | 2:B:29:THR:H      | 2.07                     | 0.62              |
| 3:D:48:THR:HA    | 3:D:51:LYS:HB3    | 1.78                     | 0.62              |
| 4:S:176:TRP:CD1  | 4:S:189:ILE:HB    | 2.33                     | 0.62              |
| 2:B:29:THR:C     | 2:B:31:SER:H      | 2.08                     | 0.61              |
| 1:A:71:MET:O     | 1:A:75:VAL:HG23   | 2.00                     | 0.61              |
| 1:A:108:LYS:O    | 1:A:109:TYR:C     | 2.38                     | 0.61              |
| 1:A:170:ILE:O    | 1:A:174:VAL:HG13  | 2.00                     | 0.61              |
| 1:A:270:PHE:HD1  | 1:A:274:TRP:CE3   | 2.19                     | 0.61              |
| 2:B:3:GLU:O      | 2:B:6:GLN:HG3     | 2.00                     | 0.61              |
| 2:B:54:HIS:ND1   | 2:B:74:SER:HB2    | 2.15                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:116:PHE:HE2  | 1:A:120:LEU:H    | 0.81                     | 0.61              |
| 1:A:271:VAL:O    | 1:A:275:ALA:HB2  | 2.01                     | 0.61              |
| 3:D:45:GLY:O     | 3:D:48:THR:HG22  | 2.01                     | 0.61              |
| 1:A:214:LYS:HE2  | 1:A:281:VAL:HB   | 1.83                     | 0.60              |
| 1:A:225:PRO:HA   | 1:A:228:ILE:HG22 | 1.82                     | 0.60              |
| 1:A:243:VAL:CG1  | 1:A:244:ARG:N    | 2.64                     | 0.60              |
| 4:S:139:VAL:HG13 | 4:S:162:SER:HB3  | 1.84                     | 0.60              |
| 1:A:219:LEU:HD12 | 1:A:223:VAL:CG2  | 2.31                     | 0.60              |
| 2:B:200:VAL:HG22 | 2:B:210:LEU:HD12 | 1.83                     | 0.60              |
| 3:D:38:LEU:HD21  | 3:D:50:VAL:CG2   | 2.30                     | 0.60              |
| 4:S:37:VAL:HA    | 4:S:46:GLU:O     | 2.02                     | 0.60              |
| 4:S:173:TYR:HD2  | 4:S:233:LEU:HA   | 1.66                     | 0.60              |
| 4:S:51:ILE:HD13  | 4:S:79:LEU:HD11  | 1.82                     | 0.60              |
| 4:S:174:LEU:HD12 | 4:S:230:MET:O    | 2.02                     | 0.60              |
| 3:D:275:PHE:O    | 3:D:279:ILE:HG21 | 1.97                     | 0.60              |
| 1:A:126:SER:OG   | 1:A:184:MET:SD   | 2.59                     | 0.60              |
| 2:B:187:VAL:HA   | 2:B:203:ALA:HA   | 1.82                     | 0.60              |
| 2:B:277:SER:OG   | 2:B:278:PHE:N    | 2.32                     | 0.60              |
| 1:A:310:ASN:OD1  | 1:A:311:SER:N    | 2.35                     | 0.60              |
| 2:B:102:THR:HG21 | 2:B:148:CYS:HA   | 1.84                     | 0.60              |
| 2:B:130:GLU:OE2  | 4:S:27:PHE:HA    | 2.01                     | 0.60              |
| 3:D:187:GLU:OE2  | 3:D:200:PHE:HE1  | 1.83                     | 0.60              |
| 1:A:49:ALA:O     | 1:A:53:THR:HG23  | 2.02                     | 0.59              |
| 1:A:52:ILE:CA    | 1:A:55:LEU:HB3   | 2.31                     | 0.59              |
| 1:A:120:LEU:HA   | 1:A:123:ALA:HB3  | 1.83                     | 0.59              |
| 1:A:257:ARG:CA   | 1:A:260:THR:HG22 | 2.32                     | 0.59              |
| 1:A:311:SER:O    | 1:A:315:PRO:CD   | 2.49                     | 0.59              |
| 2:B:121:CYS:HB2  | 2:B:146:LEU:CD2  | 2.32                     | 0.59              |
| 5:C:12:ALA:O     | 5:C:16:VAL:CB    | 2.50                     | 0.59              |
| 1:A:52:ILE:HG22  | 1:A:56:TYR:CD1   | 2.38                     | 0.59              |
| 1:A:77:TYR:CD2   | 1:A:328:CYS:SG   | 2.88                     | 0.59              |
| 1:A:244:ARG:NH2  | 3:D:321:TYR:HE1  | 2.00                     | 0.59              |
| 1:A:314:ASN:HB2  | 1:A:315:PRO:CD   | 2.32                     | 0.59              |
| 2:B:28:ALA:O     | 2:B:30:LEU:HG    | 2.02                     | 0.59              |
| 2:B:228:ASP:O    | 2:B:245:SER:CB   | 2.51                     | 0.59              |
| 3:D:242:ASN:O    | 3:D:243:ARG:C    | 2.42                     | 0.59              |
| 1:A:74:ILE:HD13  | 1:A:88:ILE:CG2   | 2.30                     | 0.59              |
| 1:A:298:ALA:O    | 1:A:302:LEU:N    | 2.34                     | 0.59              |
| 2:B:340:ASN:HD22 | 5:C:61:PHE:CB    | 2.11                     | 0.59              |
| 2:B:30:LEU:HD11  | 5:C:30:VAL:HG22  | 1.83                     | 0.59              |
| 1:A:116:PHE:CE2  | 1:A:120:LEU:CB   | 2.86                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:12:GLU:O     | 2:B:16:ASN:N     | 2.33                     | 0.59              |
| 2:B:274:THR:HG23 | 2:B:315:VAL:O    | 2.03                     | 0.59              |
| 1:A:245:LEU:CD1  | 3:D:346:LYS:HB2  | 2.33                     | 0.59              |
| 1:A:272:VAL:O    | 1:A:276:PRO:CD   | 2.50                     | 0.59              |
| 1:A:267:VAL:O    | 1:A:271:VAL:HG23 | 2.02                     | 0.58              |
| 2:B:33:ILE:HG22  | 2:B:33:ILE:O     | 2.02                     | 0.58              |
| 1:A:79:LYS:NZ    | 1:A:80:MET:HE1   | 2.18                     | 0.58              |
| 2:B:49:ARG:HH12  | 5:C:61:PHE:HD1   | 1.49                     | 0.58              |
| 1:A:67:ASN:ND2   | 1:A:95:ASP:CB    | 2.60                     | 0.58              |
| 2:B:14:LEU:O     | 2:B:18:ILE:HG12  | 2.02                     | 0.58              |
| 2:B:231:ALA:CB   | 2:B:275:SER:HA   | 2.32                     | 0.58              |
| 2:B:258:ASP:N    | 2:B:258:ASP:OD2  | 2.35                     | 0.58              |
| 2:B:200:VAL:HG22 | 2:B:210:LEU:HG   | 1.84                     | 0.58              |
| 2:B:228:ASP:O    | 2:B:245:SER:CA   | 2.51                     | 0.58              |
| 2:B:234:PHE:HA   | 2:B:241:PHE:HA   | 1.86                     | 0.58              |
| 1:A:257:ARG:HD3  | 1:A:260:THR:HG21 | 1.85                     | 0.58              |
| 1:A:298:ALA:O    | 1:A:302:LEU:HG   | 2.03                     | 0.58              |
| 1:A:65:LEU:O     | 1:A:68:VAL:HB    | 2.04                     | 0.58              |
| 1:A:181:VAL:HG23 | 1:A:182:PRO:HD3  | 1.86                     | 0.58              |
| 2:B:200:VAL:HG23 | 2:B:234:PHE:CZ   | 2.39                     | 0.58              |
| 1:A:171:CYS:HA   | 1:A:174:VAL:HG22 | 1.85                     | 0.58              |
| 1:A:176:ALA:C    | 1:A:178:GLY:N    | 2.61                     | 0.58              |
| 1:A:299:ALA:O    | 1:A:302:LEU:HB2  | 2.04                     | 0.58              |
| 4:S:139:VAL:HG12 | 4:S:162:SER:OG   | 2.03                     | 0.58              |
| 2:B:200:VAL:HG22 | 2:B:210:LEU:CG   | 2.34                     | 0.58              |
| 1:A:119:LEU:HA   | 1:A:122:LYS:NZ   | 2.16                     | 0.57              |
| 1:A:257:ARG:HD3  | 1:A:260:THR:CG2  | 2.33                     | 0.57              |
| 2:B:199:PHE:CZ   | 2:B:211:TRP:HB2  | 2.39                     | 0.57              |
| 3:D:248:MET:CE   | 3:D:288:PHE:HZ   | 2.17                     | 0.57              |
| 4:S:139:VAL:HG13 | 4:S:162:SER:OG   | 2.03                     | 0.57              |
| 1:A:72:PHE:O     | 1:A:73:GLY:C     | 2.45                     | 0.57              |
| 2:B:90:VAL:HG13  | 4:S:102:TYR:HB2  | 1.86                     | 0.57              |
| 3:D:188:THR:O    | 3:D:199:MET:N    | 2.35                     | 0.57              |
| 2:B:317:CYS:SG   | 2:B:330:GLY:HA3  | 2.44                     | 0.57              |
| 1:A:91:LEU:CD2   | 1:A:138:THR:CG2  | 2.82                     | 0.57              |
| 2:B:200:VAL:HG22 | 2:B:210:LEU:CD1  | 2.34                     | 0.57              |
| 1:A:67:ASN:ND2   | 1:A:95:ASP:C     | 2.62                     | 0.57              |
| 3:D:47:ASN:O     | 3:D:51:LYS:HB2   | 2.04                     | 0.57              |
| 1:A:168:ILE:O    | 1:A:172:ILE:HG13 | 2.04                     | 0.57              |
| 2:B:274:THR:CG2  | 2:B:315:VAL:O    | 2.53                     | 0.57              |
| 1:A:111:MET:C    | 1:A:113:THR:H    | 2.13                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:144:THR:HG22 | 4:S:243:THR:HG23 | 1.87                     | 0.57              |
| 1:A:139:LEU:CD2  | 1:A:229:ILE:HD12 | 2.34                     | 0.57              |
| 4:S:4:LEU:HD21   | 4:S:27:PHE:CZ    | 2.40                     | 0.57              |
| 1:A:58:ALA:O     | 1:A:62:VAL:HG23  | 2.05                     | 0.57              |
| 1:A:60:CYS:HB2   | 1:A:102:LEU:HD11 | 1.86                     | 0.57              |
| 3:D:272:LYS:HE2  | 3:D:326:CYS:SG   | 2.44                     | 0.57              |
| 2:B:39:PRO:HG3   | 2:B:301:LYS:NZ   | 2.20                     | 0.56              |
| 4:S:39:GLN:HB2   | 4:S:45:LEU:HD23  | 1.87                     | 0.56              |
| 3:D:189:HIS:CG   | 3:D:198:LYS:HG2  | 2.39                     | 0.56              |
| 4:S:9:GLY:HA2    | 4:S:117:LEU:CD1  | 2.34                     | 0.56              |
| 1:A:91:LEU:CD2   | 1:A:138:THR:HG22 | 2.35                     | 0.56              |
| 1:A:300:LEU:O    | 1:A:304:ILE:HG13 | 2.05                     | 0.56              |
| 2:B:228:ASP:O    | 2:B:245:SER:OG   | 2.16                     | 0.56              |
| 3:D:224:PHE:HE1  | 3:D:250:LEU:CD2  | 2.18                     | 0.56              |
| 3:D:262:ASP:OD1  | 3:D:317:THR:OG1  | 2.18                     | 0.56              |
| 4:S:98:ARG:HD3   | 4:S:110:PHE:CB   | 2.34                     | 0.56              |
| 2:B:47:THR:HG22  | 2:B:339:TRP:HE1  | 1.69                     | 0.56              |
| 2:B:30:LEU:CD2   | 2:B:33:ILE:HD12  | 2.36                     | 0.56              |
| 4:S:40:ALA:HB1   | 4:S:41:PRO:HD2   | 1.86                     | 0.56              |
| 1:A:259:ILE:O    | 1:A:263:VAL:HG13 | 2.06                     | 0.56              |
| 2:B:161:SER:CB   | 2:B:187:VAL:HG21 | 2.35                     | 0.56              |
| 2:B:233:CYS:O    | 2:B:241:PHE:HB2  | 2.06                     | 0.56              |
| 4:S:12:VAL:HG12  | 4:S:13:GLN:N     | 2.20                     | 0.56              |
| 1:A:51:ALA:C     | 1:A:53:THR:N     | 2.61                     | 0.56              |
| 3:D:340:VAL:O    | 3:D:344:ILE:HG13 | 2.06                     | 0.56              |
| 1:A:224:VAL:HA   | 1:A:227:LEU:CG   | 2.35                     | 0.56              |
| 1:A:130:TYR:HH   | 1:A:177:SER:HB3  | 1.71                     | 0.56              |
| 2:B:26:ALA:C     | 2:B:28:ALA:N     | 2.63                     | 0.56              |
| 2:B:308:LEU:O    | 2:B:339:TRP:CH2  | 2.58                     | 0.56              |
| 1:A:212:VAL:HG12 | 1:A:212:VAL:O    | 2.06                     | 0.56              |
| 1:A:275:ALA:HB3  | 1:A:276:PRO:HD3  | 1.88                     | 0.55              |
| 2:B:29:THR:C     | 2:B:31:SER:N     | 2.62                     | 0.55              |
| 2:B:191:SER:O    | 2:B:199:PHE:HB2  | 2.06                     | 0.55              |
| 1:A:270:PHE:CD1  | 1:A:274:TRP:CE3  | 2.95                     | 0.55              |
| 4:S:71:SER:O     | 4:S:79:LEU:CD1   | 2.45                     | 0.55              |
| 1:A:74:ILE:HG12  | 1:A:325:PHE:CZ   | 2.40                     | 0.55              |
| 1:A:240:LEU:HD21 | 1:A:246:LEU:CD2  | 2.36                     | 0.55              |
| 4:S:11:LEU:HD11  | 4:S:120:SER:CB   | 2.21                     | 0.55              |
| 1:A:54:ALA:C     | 1:A:57:SER:HB3   | 2.31                     | 0.55              |
| 1:A:95:ASP:OD2   | 1:A:315:PRO:HG2  | 2.07                     | 0.55              |
| 2:B:104:ALA:HB2  | 2:B:149:CYS:O    | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:153:ASP:OD2  | 2:B:196:THR:HG23 | 2.07                     | 0.55              |
| 1:A:119:LEU:HD12 | 1:A:122:LYS:NZ   | 2.22                     | 0.55              |
| 2:B:139:LEU:HD23 | 2:B:169:TRP:CD2  | 2.42                     | 0.55              |
| 1:A:313:LEU:C    | 1:A:316:VAL:H    | 2.15                     | 0.55              |
| 1:A:146:ARG:NH1  | 3:D:354:LEU:HG   | 2.21                     | 0.55              |
| 1:A:74:ILE:CD1   | 1:A:88:ILE:HG12  | 2.37                     | 0.54              |
| 1:A:75:VAL:O     | 1:A:79:LYS:HD3   | 2.07                     | 0.54              |
| 2:B:3:GLU:CG     | 5:C:16:VAL:CG1   | 2.85                     | 0.54              |
| 4:S:9:GLY:HA2    | 4:S:117:LEU:HD13 | 1.89                     | 0.54              |
| 4:S:62:ASP:OD1   | 4:S:63:THR:N     | 2.40                     | 0.54              |
| 3:D:47:ASN:O     | 3:D:51:LYS:HE2   | 2.08                     | 0.54              |
| 1:A:249:SER:C    | 1:A:251:GLU:N    | 2.65                     | 0.54              |
| 1:A:310:ASN:O    | 1:A:311:SER:C    | 2.50                     | 0.54              |
| 1:A:119:LEU:HD12 | 1:A:122:LYS:HE2  | 1.90                     | 0.54              |
| 1:A:146:ARG:HD3  | 3:D:352:CYS:SG   | 2.47                     | 0.54              |
| 1:A:146:ARG:O    | 1:A:150:VAL:HG22 | 2.07                     | 0.54              |
| 1:A:77:TYR:O     | 1:A:79:LYS:N     | 2.40                     | 0.54              |
| 3:D:190:PHE:HE2  | 3:D:199:MET:HE2  | 1.71                     | 0.54              |
| 4:S:61:ALA:O     | 4:S:65:LYS:HB2   | 2.08                     | 0.54              |
| 1:A:107:ALA:HA   | 1:A:110:LEU:HB3  | 1.88                     | 0.54              |
| 1:A:297:VAL:HG13 | 1:A:301:HIS:CD2  | 2.42                     | 0.54              |
| 1:A:313:LEU:O    | 1:A:316:VAL:CB   | 2.56                     | 0.54              |
| 1:A:53:THR:O     | 1:A:57:SER:CB    | 2.56                     | 0.54              |
| 1:A:53:THR:O     | 1:A:54:ALA:C     | 2.48                     | 0.54              |
| 4:S:71:SER:OG    | 4:S:80:PHE:HB2   | 2.07                     | 0.54              |
| 1:A:56:TYR:C     | 1:A:59:VAL:HG12  | 2.31                     | 0.54              |
| 1:A:171:CYS:O    | 1:A:175:LEU:HD13 | 2.07                     | 0.54              |
| 2:B:273:ILE:HG22 | 2:B:289:TYR:CD2  | 2.43                     | 0.54              |
| 1:A:181:VAL:CG2  | 1:A:182:PRO:HD3  | 2.37                     | 0.54              |
| 1:A:313:LEU:CA   | 1:A:316:VAL:CG2  | 2.85                     | 0.54              |
| 2:B:43:ILE:HD12  | 2:B:284:LEU:HD21 | 1.89                     | 0.54              |
| 2:B:183:HIS:NE2  | 2:B:211:TRP:HZ2  | 2.06                     | 0.54              |
| 2:B:197:ARG:HE   | 2:B:214:ARG:HH22 | 1.48                     | 0.54              |
| 1:A:303:CYS:SG   | 1:A:304:ILE:N    | 2.81                     | 0.53              |
| 3:D:188:THR:HG21 | 3:D:199:MET:HE3  | 1.89                     | 0.53              |
| 4:S:20:LEU:HD12  | 4:S:36:TRP:HZ3   | 1.72                     | 0.53              |
| 1:A:69:LEU:O     | 1:A:70:VAL:C     | 2.50                     | 0.53              |
| 2:B:80:ILE:HD11  | 3:D:23:LEU:HD11  | 1.89                     | 0.53              |
| 3:D:244:MET:O    | 3:D:247:SER:HB2  | 2.07                     | 0.53              |
| 1:A:177:SER:O    | 1:A:178:GLY:C    | 2.43                     | 0.53              |
| 5:C:12:ALA:O     | 5:C:16:VAL:CA    | 2.55                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:12:ALA:HA    | 5:C:15:LEU:HB3   | 1.89                     | 0.53              |
| 1:A:305:ALA:C    | 1:A:307:GLY:N    | 2.67                     | 0.53              |
| 1:A:313:LEU:O    | 1:A:316:VAL:CA   | 2.56                     | 0.53              |
| 2:B:168:LEU:HD23 | 2:B:169:TRP:N    | 2.23                     | 0.53              |
| 2:B:215:GLU:HG3  | 2:B:217:MET:CE   | 2.37                     | 0.53              |
| 3:D:228:LEU:O    | 3:D:244:MET:CE   | 2.57                     | 0.53              |
| 3:D:349:LEU:HD21 | 3:D:355:PHE:HD1  | 1.73                     | 0.53              |
| 1:A:79:LYS:HZ3   | 1:A:80:MET:HE1   | 1.72                     | 0.53              |
| 3:D:49:ILE:CG2   | 3:D:53:MET:CE    | 2.84                     | 0.53              |
| 1:A:250:LYS:H    | 1:A:250:LYS:HD2  | 1.73                     | 0.53              |
| 3:D:238:ASP:HB3  | 3:D:241:MET:HG2  | 1.89                     | 0.53              |
| 5:C:11:GLN:HA    | 5:C:14:LYS:HB3   | 1.89                     | 0.53              |
| 1:A:299:ALA:HA   | 1:A:302:LEU:CB   | 2.26                     | 0.53              |
| 1:A:91:LEU:HD21  | 1:A:138:THR:HG22 | 1.91                     | 0.53              |
| 3:D:228:LEU:HG   | 3:D:269:LEU:HB3  | 1.91                     | 0.53              |
| 4:S:172:THR:O    | 4:S:191:ARG:HG2  | 2.08                     | 0.53              |
| 1:A:243:VAL:CG1  | 1:A:244:ARG:H    | 2.22                     | 0.52              |
| 3:D:209:ARG:O    | 3:D:213:ILE:HB   | 2.10                     | 0.52              |
| 4:S:190:TYR:O    | 4:S:191:ARG:C    | 2.50                     | 0.52              |
| 1:A:171:CYS:CA   | 1:A:174:VAL:HG22 | 2.39                     | 0.52              |
| 2:B:61:MET:HA    | 2:B:71:VAL:O     | 2.09                     | 0.52              |
| 2:B:68:ARG:HG2   | 4:S:103:TYR:CZ   | 2.45                     | 0.52              |
| 2:B:168:LEU:C    | 2:B:169:TRP:CD1  | 2.87                     | 0.52              |
| 2:B:278:PHE:O    | 2:B:320:VAL:HG11 | 2.09                     | 0.52              |
| 4:S:97:VAL:HG22  | 4:S:111:TRP:CD2  | 2.44                     | 0.52              |
| 1:A:246:LEU:HD22 | 1:A:259:ILE:HD12 | 1.92                     | 0.52              |
| 3:D:54:LYS:HD2   | 3:D:190:PHE:CB   | 2.38                     | 0.52              |
| 3:D:267:LEU:HB3  | 3:D:321:TYR:O    | 2.09                     | 0.52              |
| 1:A:54:ALA:HA    | 1:A:57:SER:HB3   | 1.92                     | 0.52              |
| 1:A:219:LEU:HD12 | 1:A:223:VAL:HB   | 1.92                     | 0.52              |
| 2:B:27:ASP:O     | 2:B:29:THR:N     | 2.41                     | 0.52              |
| 2:B:163:ASP:OD1  | 2:B:164:THR:N    | 2.42                     | 0.52              |
| 2:B:273:ILE:HG22 | 2:B:289:TYR:CE2  | 2.43                     | 0.52              |
| 3:D:224:PHE:CE1  | 3:D:250:LEU:HD22 | 2.43                     | 0.52              |
| 1:A:294:PRO:HG2  | 1:A:295:LEU:HD12 | 1.90                     | 0.52              |
| 2:B:186:ASP:O    | 2:B:188:MET:HG3  | 2.09                     | 0.52              |
| 1:A:116:PHE:CE2  | 1:A:120:LEU:N    | 2.53                     | 0.52              |
| 1:A:171:CYS:HA   | 1:A:174:VAL:CG2  | 2.40                     | 0.52              |
| 1:A:257:ARG:HA   | 1:A:260:THR:CG2  | 2.38                     | 0.52              |
| 2:B:15:LYS:HZ1   | 2:B:258:ASP:CB   | 1.99                     | 0.52              |
| 2:B:199:PHE:CE2  | 2:B:211:TRP:CD1  | 2.98                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:225:HIS:NE2  | 2:B:251:ARG:HG3  | 2.24                     | 0.52              |
| 3:D:43:GLU:C     | 3:D:243:ARG:HH22 | 2.18                     | 0.52              |
| 3:D:48:THR:CA    | 3:D:51:LYS:CB    | 2.70                     | 0.52              |
| 3:D:49:ILE:HG22  | 3:D:53:MET:CE    | 2.27                     | 0.52              |
| 1:A:171:CYS:O    | 1:A:175:LEU:HB2  | 2.09                     | 0.52              |
| 2:B:43:ILE:CD1   | 2:B:284:LEU:HD11 | 2.40                     | 0.52              |
| 1:A:146:ARG:NH1  | 3:D:354:LEU:CG   | 2.73                     | 0.52              |
| 2:B:19:ARG:HA    | 2:B:22:ARG:HB3   | 1.92                     | 0.52              |
| 2:B:295:ASN:OD1  | 2:B:307:VAL:HG13 | 2.09                     | 0.52              |
| 3:D:305:GLN:CG   | 3:D:322:THR:HG21 | 2.39                     | 0.52              |
| 1:A:282:ILE:HA   | 1:A:285:THR:HG1  | 1.73                     | 0.51              |
| 4:S:51:ILE:HG23  | 4:S:58:ILE:HG13  | 1.92                     | 0.51              |
| 1:A:219:LEU:HD12 | 1:A:223:VAL:CB   | 2.41                     | 0.51              |
| 4:S:93:MET:HE3   | 4:S:116:THR:HG23 | 1.92                     | 0.51              |
| 1:A:101:THR:HG21 | 1:A:128:ASP:CG   | 2.36                     | 0.51              |
| 1:A:51:ALA:O     | 1:A:54:ALA:CB    | 2.57                     | 0.51              |
| 2:B:13:GLN:O     | 2:B:17:GLN:N     | 2.38                     | 0.51              |
| 2:B:22:ARG:HG3   | 5:C:30:VAL:HG11  | 0.65                     | 0.51              |
| 2:B:104:ALA:HB3  | 2:B:113:ALA:HB3  | 1.92                     | 0.51              |
| 2:B:233:CYS:O    | 2:B:242:ALA:N    | 2.42                     | 0.51              |
| 2:B:26:ALA:HA    | 2:B:33:ILE:HD11  | 1.90                     | 0.51              |
| 2:B:251:ARG:NH1  | 2:B:260:GLU:OE1  | 2.43                     | 0.51              |
| 2:B:121:CYS:HB2  | 2:B:146:LEU:HD22 | 1.91                     | 0.51              |
| 4:S:4:LEU:HD21   | 4:S:27:PHE:HZ    | 1.76                     | 0.51              |
| 2:B:315:VAL:HA   | 2:B:331:SER:HA   | 1.93                     | 0.51              |
| 1:A:139:LEU:HD21 | 1:A:229:ILE:CD1  | 2.41                     | 0.51              |
| 1:A:214:LYS:CE   | 1:A:281:VAL:HB   | 2.40                     | 0.51              |
| 1:A:307:GLY:C    | 1:A:309:ALA:N    | 2.60                     | 0.51              |
| 1:A:72:PHE:C     | 1:A:75:VAL:H     | 2.18                     | 0.51              |
| 3:D:48:THR:C     | 3:D:51:LYS:H     | 2.20                     | 0.51              |
| 1:A:201:GLN:N    | 1:A:201:GLN:OE1  | 2.43                     | 0.50              |
| 2:B:40:VAL:HG21  | 5:C:51:LEU:HD11  | 1.93                     | 0.50              |
| 1:A:314:ASN:CB   | 1:A:315:PRO:HD3  | 2.40                     | 0.50              |
| 3:D:283:PRO:HG2  | 3:D:286:ILE:HG13 | 1.93                     | 0.50              |
| 1:A:199:MET:C    | 1:A:200:LEU:HD12 | 2.36                     | 0.50              |
| 2:B:18:ILE:HG13  | 5:C:27:ARG:HD3   | 1.92                     | 0.50              |
| 2:B:29:THR:HG21  | 2:B:32:GLN:HE21  | 1.76                     | 0.50              |
| 2:B:84:SER:O     | 2:B:85:TYR:C     | 2.54                     | 0.50              |
| 3:D:228:LEU:O    | 3:D:244:MET:HE1  | 2.11                     | 0.50              |
| 2:B:215:GLU:HG3  | 2:B:217:MET:HG2  | 1.94                     | 0.50              |
| 2:B:152:LEU:HD23 | 2:B:157:ILE:HG21 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:183:HIS:HE2  | 2:B:211:TRP:HZ2  | 1.60                     | 0.50              |
| 3:D:47:ASN:O     | 3:D:51:LYS:CA    | 2.59                     | 0.50              |
| 1:A:215:ILE:O    | 1:A:218:PHE:HB3  | 2.12                     | 0.50              |
| 4:S:139:VAL:CG1  | 4:S:162:SER:CB   | 2.90                     | 0.50              |
| 4:S:144:THR:CG2  | 4:S:243:THR:HG23 | 2.41                     | 0.50              |
| 4:S:20:LEU:HD12  | 4:S:36:TRP:CZ3   | 2.47                     | 0.49              |
| 4:S:58:ILE:HD12  | 4:S:58:ILE:H     | 1.77                     | 0.49              |
| 5:C:12:ALA:O     | 5:C:16:VAL:HB    | 2.12                     | 0.49              |
| 1:A:283:VAL:O    | 1:A:287:VAL:N    | 2.40                     | 0.49              |
| 1:A:314:ASN:CB   | 1:A:315:PRO:CD   | 2.90                     | 0.49              |
| 2:B:4:LEU:HA     | 5:C:19:LEU:CD2   | 2.41                     | 0.49              |
| 2:B:283:ARG:HD2  | 2:B:300:LEU:HD11 | 1.93                     | 0.49              |
| 3:D:48:THR:O     | 3:D:51:LYS:HB3   | 2.12                     | 0.49              |
| 4:S:72:ARG:HB3   | 4:S:79:LEU:HD13  | 1.93                     | 0.49              |
| 4:S:73:ASP:O     | 4:S:77:ASN:N     | 2.45                     | 0.49              |
| 1:A:52:ILE:C     | 1:A:55:LEU:HB3   | 2.37                     | 0.49              |
| 1:A:170:ILE:O    | 1:A:174:VAL:CG2  | 2.60                     | 0.49              |
| 1:A:297:VAL:CG1  | 1:A:301:HIS:HD2  | 2.26                     | 0.49              |
| 2:B:241:PHE:O    | 2:B:252:LEU:HD12 | 2.12                     | 0.49              |
| 3:D:38:LEU:HD21  | 3:D:50:VAL:HG22  | 1.95                     | 0.49              |
| 1:A:130:TYR:O    | 1:A:131:ASN:C    | 2.54                     | 0.49              |
| 2:B:68:ARG:NE    | 2:B:83:ASP:OD1   | 2.42                     | 0.49              |
| 2:B:232:ILE:HG22 | 2:B:243:THR:CB   | 2.42                     | 0.49              |
| 3:D:246:ALA:O    | 3:D:247:SER:C    | 2.56                     | 0.49              |
| 1:A:52:ILE:C     | 1:A:55:LEU:N     | 2.70                     | 0.49              |
| 1:A:204:SER:HB2  | 1:A:210:ASP:CG   | 2.38                     | 0.49              |
| 2:B:256:ARG:HD2  | 2:B:256:ARG:N    | 2.17                     | 0.49              |
| 3:D:272:LYS:HD2  | 3:D:324:PHE:HB3  | 1.94                     | 0.49              |
| 4:S:84:THR:OG1   | 4:S:85:SER:N     | 2.43                     | 0.49              |
| 1:A:262:MET:O    | 1:A:263:VAL:C    | 2.52                     | 0.48              |
| 2:B:17:GLN:O     | 2:B:21:ALA:N     | 2.40                     | 0.48              |
| 4:S:157:ILE:HG23 | 4:S:243:THR:HG21 | 1.94                     | 0.48              |
| 1:A:198:CYS:C    | 1:A:199:MET:HE2  | 2.38                     | 0.48              |
| 1:A:274:TRP:CH2  | 1:A:314:ASN:OD1  | 2.66                     | 0.48              |
| 2:B:57:LYS:NZ    | 3:D:217:GLU:OE2  | 2.47                     | 0.48              |
| 2:B:166:CYS:HB2  | 2:B:180:PHE:HD2  | 1.77                     | 0.48              |
| 1:A:119:LEU:HD12 | 1:A:122:LYS:CE   | 2.43                     | 0.48              |
| 1:A:313:LEU:HA   | 1:A:316:VAL:HG21 | 1.92                     | 0.48              |
| 1:A:67:ASN:HD22  | 1:A:96:ALA:N     | 2.11                     | 0.48              |
| 1:A:299:ALA:C    | 1:A:302:LEU:HB2  | 2.38                     | 0.48              |
| 1:A:324:ASN:OD1  | 1:A:325:PHE:N    | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:51:LEU:HB2   | 2:B:336:LEU:HB2  | 1.94                     | 0.48              |
| 1:A:72:PHE:O     | 1:A:75:VAL:CB    | 2.61                     | 0.48              |
| 1:A:297:VAL:CG1  | 1:A:301:HIS:CD2  | 2.96                     | 0.48              |
| 2:B:80:ILE:HG22  | 2:B:82:TRP:HE3   | 1.77                     | 0.48              |
| 4:S:88:SER:HA    | 4:S:119:VAL:CG1  | 2.44                     | 0.48              |
| 1:A:67:ASN:HD21  | 1:A:96:ALA:N     | 2.09                     | 0.48              |
| 1:A:67:ASN:O     | 1:A:68:VAL:C     | 2.55                     | 0.48              |
| 1:A:111:MET:C    | 1:A:113:THR:N    | 2.72                     | 0.48              |
| 1:A:116:PHE:CE2  | 1:A:120:LEU:CG   | 2.96                     | 0.48              |
| 2:B:4:LEU:HA     | 5:C:19:LEU:HD23  | 1.96                     | 0.48              |
| 2:B:32:GLN:C     | 2:B:34:THR:H     | 2.21                     | 0.48              |
| 2:B:199:PHE:CE2  | 2:B:211:TRP:HB2  | 2.49                     | 0.48              |
| 3:D:189:HIS:HA   | 3:D:197:PHE:O    | 2.14                     | 0.48              |
| 1:A:240:LEU:CD2  | 1:A:246:LEU:HD23 | 2.44                     | 0.48              |
| 3:D:222:ILE:O    | 3:D:223:ILE:C    | 2.56                     | 0.48              |
| 4:S:6:GLU:HG3    | 4:S:22:CYS:SG    | 2.54                     | 0.48              |
| 2:B:45:MET:SD    | 2:B:308:LEU:HD21 | 2.54                     | 0.48              |
| 3:D:190:PHE:CE2  | 3:D:199:MET:HE2  | 2.48                     | 0.48              |
| 1:A:130:TYR:CE1  | 1:A:177:SER:CA   | 2.97                     | 0.48              |
| 1:A:252:LYS:O    | 1:A:255:SER:HB2  | 2.13                     | 0.48              |
| 1:A:299:ALA:O    | 1:A:302:LEU:CA   | 2.62                     | 0.48              |
| 1:A:303:CYS:C    | 1:A:305:ALA:N    | 2.70                     | 0.48              |
| 3:D:53:MET:SD    | 3:D:199:MET:CE   | 3.02                     | 0.47              |
| 2:B:22:ARG:HH21  | 2:B:259:GLN:CD   | 2.22                     | 0.47              |
| 4:S:98:ARG:CD    | 4:S:110:PHE:HB3  | 2.41                     | 0.47              |
| 2:B:215:GLU:HG3  | 2:B:217:MET:CG   | 2.44                     | 0.47              |
| 4:S:246:GLU:C    | 4:S:247:LEU:HD12 | 2.39                     | 0.47              |
| 1:A:305:ALA:C    | 1:A:307:GLY:H    | 2.22                     | 0.47              |
| 2:B:153:ASP:OD2  | 2:B:196:THR:CG2  | 2.63                     | 0.47              |
| 1:A:70:VAL:HG13  | 1:A:71:MET:N     | 2.30                     | 0.47              |
| 1:A:258:ARG:O    | 1:A:259:ILE:C    | 2.53                     | 0.47              |
| 1:A:307:GLY:C    | 1:A:309:ALA:H    | 2.21                     | 0.47              |
| 2:B:27:ASP:C     | 2:B:29:THR:N     | 2.70                     | 0.47              |
| 5:C:8:SER:O      | 5:C:11:GLN:HB2   | 2.14                     | 0.47              |
| 1:A:283:VAL:C    | 1:A:286:LEU:H    | 2.23                     | 0.47              |
| 2:B:16:ASN:O     | 2:B:20:ASP:N     | 2.33                     | 0.47              |
| 2:B:22:ARG:CA    | 5:C:30:VAL:CG1   | 2.93                     | 0.47              |
| 2:B:51:LEU:HD23  | 2:B:82:TRP:CZ2   | 2.50                     | 0.47              |
| 2:B:250:CYS:SG   | 2:B:273:ILE:HD12 | 2.50                     | 0.47              |
| 3:D:349:LEU:HD21 | 3:D:355:PHE:CD1  | 2.49                     | 0.47              |
| 4:S:88:SER:HA    | 4:S:119:VAL:HG11 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:12:ALA:O     | 5:C:16:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:218:PHE:HE1  | 1:A:278:HIS:HB3  | 1.75                     | 0.47              |
| 1:A:297:VAL:HG12 | 1:A:301:HIS:HD2  | 1.80                     | 0.47              |
| 1:A:311:SER:HA   | 1:A:314:ASN:OD1  | 2.15                     | 0.47              |
| 2:B:123:ILE:HG13 | 2:B:171:ILE:HD12 | 1.97                     | 0.47              |
| 2:B:208:ALA:N    | 2:B:222:PHE:O    | 2.48                     | 0.47              |
| 2:B:331:SER:HG   | 2:B:332:TRP:H    | 1.63                     | 0.47              |
| 3:D:6:SER:C      | 3:D:8:GLU:H      | 2.21                     | 0.47              |
| 3:D:188:THR:HG21 | 3:D:199:MET:CE   | 2.45                     | 0.47              |
| 1:A:102:LEU:CD2  | 1:A:103:PRO:HD3  | 2.36                     | 0.47              |
| 1:A:130:TYR:CE1  | 1:A:177:SER:N    | 2.73                     | 0.47              |
| 1:A:243:VAL:HG12 | 1:A:245:LEU:N    | 2.26                     | 0.47              |
| 2:B:18:ILE:CD1   | 5:C:27:ARG:HB2   | 2.44                     | 0.47              |
| 3:D:49:ILE:HD13  | 3:D:268:PHE:CD2  | 2.50                     | 0.47              |
| 1:A:48:LEU:O     | 1:A:51:ALA:HB3   | 2.15                     | 0.47              |
| 3:D:349:LEU:CD2  | 3:D:355:PHE:CD1  | 2.98                     | 0.47              |
| 4:S:232:HIS:CD2  | 4:S:237:LEU:HD21 | 2.50                     | 0.47              |
| 1:A:67:ASN:HD22  | 1:A:95:ASP:C     | 2.23                     | 0.46              |
| 1:A:74:ILE:HD11  | 1:A:88:ILE:HG12  | 1.96                     | 0.46              |
| 2:B:119:ASN:ND2  | 2:B:144:GLY:C    | 2.74                     | 0.46              |
| 4:S:50:TYR:C     | 4:S:51:ILE:HG13  | 2.40                     | 0.46              |
| 1:A:64:LEU:HA    | 1:A:99:THR:CG2   | 2.37                     | 0.46              |
| 1:A:108:LYS:O    | 1:A:111:MET:N    | 2.46                     | 0.46              |
| 4:S:64:VAL:HG13  | 4:S:68:PHE:CE1   | 2.50                     | 0.46              |
| 5:C:9:ILE:O      | 5:C:12:ALA:HB3   | 2.14                     | 0.46              |
| 1:A:172:ILE:C    | 1:A:174:VAL:N    | 2.71                     | 0.46              |
| 1:A:299:ALA:C    | 1:A:302:LEU:H    | 2.22                     | 0.46              |
| 1:A:313:LEU:O    | 1:A:317:LEU:N    | 2.47                     | 0.46              |
| 4:S:73:ASP:O     | 4:S:78:THR:N     | 2.36                     | 0.46              |
| 1:A:130:TYR:CE1  | 1:A:177:SER:HA   | 2.51                     | 0.46              |
| 1:A:243:VAL:HG12 | 1:A:244:ARG:H    | 1.79                     | 0.46              |
| 2:B:191:SER:OG   | 2:B:192:LEU:N    | 2.49                     | 0.46              |
| 1:A:279:ILE:O    | 1:A:282:ILE:HG22 | 2.16                     | 0.46              |
| 2:B:239:ASN:HB2  | 2:B:256:ARG:CZ   | 2.45                     | 0.46              |
| 4:S:70:ILE:HB    | 4:S:81:LEU:HD12  | 1.97                     | 0.46              |
| 1:A:251:GLU:O    | 1:A:252:LYS:HE2  | 2.16                     | 0.46              |
| 4:S:64:VAL:CG1   | 4:S:68:PHE:CD1   | 2.98                     | 0.46              |
| 4:S:243:THR:O    | 4:S:245:LEU:CD1  | 2.64                     | 0.46              |
| 1:A:218:PHE:CD1  | 1:A:278:HIS:HB3  | 2.51                     | 0.46              |
| 1:A:52:ILE:HG21  | 1:A:56:TYR:OH    | 2.15                     | 0.46              |
| 2:B:231:ALA:HB3  | 2:B:275:SER:HA   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:49:ILE:O     | 3:D:53:MET:HB2   | 2.16                     | 0.46              |
| 1:A:74:ILE:HD11  | 1:A:88:ILE:CD1   | 2.45                     | 0.46              |
| 1:A:143:SER:HB2  | 1:A:233:TYR:CE2  | 2.51                     | 0.46              |
| 1:A:171:CYS:C    | 1:A:174:VAL:HG22 | 2.41                     | 0.46              |
| 1:A:198:CYS:O    | 1:A:199:MET:HE2  | 2.15                     | 0.46              |
| 1:A:227:LEU:HD12 | 1:A:228:ILE:N    | 2.30                     | 0.46              |
| 3:D:312:ASN:HB2  | 3:D:320:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:270:PHE:HD1  | 1:A:274:TRP:HE3  | 1.62                     | 0.46              |
| 2:B:18:ILE:CG2   | 2:B:259:GLN:HE22 | 2.28                     | 0.46              |
| 3:D:329:ASP:C    | 3:D:331:LYS:H    | 2.24                     | 0.46              |
| 1:A:307:GLY:O    | 1:A:310:ASN:CG   | 2.59                     | 0.45              |
| 2:B:217:MET:HE3  | 2:B:219:ARG:NH2  | 2.31                     | 0.45              |
| 1:A:250:LYS:HD2  | 1:A:250:LYS:N    | 2.30                     | 0.45              |
| 2:B:165:THR:HG23 | 2:B:180:PHE:O    | 2.16                     | 0.45              |
| 2:B:254:ASP:O    | 2:B:257:ALA:O    | 2.35                     | 0.45              |
| 4:S:70:ILE:CD1   | 4:S:81:LEU:HB2   | 2.47                     | 0.45              |
| 4:S:138:ILE:HB   | 4:S:231:GLN:CD   | 2.39                     | 0.45              |
| 1:A:72:PHE:HA    | 1:A:75:VAL:CG2   | 2.47                     | 0.45              |
| 1:A:256:LEU:C    | 1:A:256:LEU:HD23 | 2.41                     | 0.45              |
| 2:B:22:ARG:O     | 2:B:26:ALA:HB3   | 2.16                     | 0.45              |
| 2:B:39:PRO:HG3   | 2:B:301:LYS:HZ1  | 1.81                     | 0.45              |
| 4:S:188:LEU:HA   | 4:S:199:VAL:HG11 | 1.99                     | 0.45              |
| 1:A:299:ALA:C    | 1:A:301:HIS:N    | 2.71                     | 0.45              |
| 4:S:2:VAL:HA     | 4:S:26:GLY:HA3   | 1.98                     | 0.45              |
| 4:S:161:SER:H    | 4:S:210:THR:HG23 | 1.81                     | 0.45              |
| 1:A:119:LEU:O    | 1:A:122:LYS:HG2  | 2.17                     | 0.45              |
| 5:C:14:LYS:O     | 5:C:17:GLU:CB    | 2.62                     | 0.45              |
| 5:C:9:ILE:C      | 5:C:12:ALA:HB3   | 2.41                     | 0.45              |
| 2:B:18:ILE:HG13  | 5:C:27:ARG:CD    | 2.47                     | 0.45              |
| 3:D:208:GLU:OE2  | 3:D:210:LYS:NZ   | 2.41                     | 0.45              |
| 5:C:10:ALA:C     | 5:C:14:LYS:H     | 2.23                     | 0.45              |
| 2:B:3:GLU:C      | 2:B:3:GLU:CD     | 2.85                     | 0.45              |
| 2:B:51:LEU:N     | 2:B:336:LEU:O    | 2.38                     | 0.45              |
| 4:S:149:VAL:HG11 | 4:S:219:LEU:HD13 | 1.99                     | 0.45              |
| 4:S:175:TYR:HD1  | 4:S:190:TYR:HA   | 1.81                     | 0.45              |
| 4:S:244:LYS:HZ2  | 4:S:246:GLU:HG3  | 1.82                     | 0.45              |
| 1:A:46:LEU:O     | 1:A:49:ALA:HB3   | 2.17                     | 0.45              |
| 1:A:273:CYS:O    | 1:A:276:PRO:HD2  | 2.17                     | 0.45              |
| 2:B:48:ARG:HA    | 2:B:48:ARG:HD3   | 1.65                     | 0.45              |
| 2:B:293:ASN:HB2  | 2:B:309:ALA:HB2  | 1.99                     | 0.45              |
| 3:D:189:HIS:CG   | 3:D:198:LYS:CG   | 3.00                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:93:MET:HE3   | 4:S:116:THR:CG2  | 2.46                     | 0.45              |
| 1:A:54:ALA:CA    | 1:A:57:SER:HB3   | 2.46                     | 0.44              |
| 2:B:233:CYS:SG   | 2:B:276:VAL:O    | 2.66                     | 0.44              |
| 2:B:235:PHE:CB   | 2:B:240:ALA:HB3  | 2.47                     | 0.44              |
| 4:S:64:VAL:HG13  | 4:S:68:PHE:CZ    | 2.53                     | 0.44              |
| 1:A:146:ARG:HH11 | 3:D:354:LEU:CD1  | 2.27                     | 0.44              |
| 3:D:43:GLU:O     | 3:D:243:ARG:NH2  | 2.49                     | 0.44              |
| 1:A:119:LEU:HD12 | 1:A:122:LYS:HZ1  | 1.82                     | 0.44              |
| 2:B:22:ARG:HA    | 5:C:30:VAL:CG1   | 2.32                     | 0.44              |
| 2:B:200:VAL:CG2  | 2:B:210:LEU:HD12 | 2.46                     | 0.44              |
| 3:D:231:TYR:CE1  | 3:D:275:PHE:CE1  | 3.05                     | 0.44              |
| 4:S:73:ASP:OD1   | 4:S:76:LYS:HG2   | 2.18                     | 0.44              |
| 1:A:240:LEU:HD21 | 1:A:246:LEU:HD22 | 2.00                     | 0.44              |
| 1:A:311:SER:OG   | 1:A:312:SER:N    | 2.50                     | 0.44              |
| 2:B:243:THR:HG22 | 2:B:251:ARG:O    | 2.16                     | 0.44              |
| 2:B:254:ASP:HB3  | 2:B:261:LEU:HD11 | 1.99                     | 0.44              |
| 3:D:189:HIS:ND1  | 3:D:198:LYS:CG   | 2.80                     | 0.44              |
| 3:D:248:MET:HE2  | 3:D:288:PHE:HZ   | 1.82                     | 0.44              |
| 3:D:276:GLU:HG2  | 3:D:297:TYR:HB2  | 1.99                     | 0.44              |
| 3:D:291:TYR:OH   | 3:D:299:GLU:HG2  | 2.17                     | 0.44              |
| 5:C:17:GLU:HA    | 5:C:20:LYS:HB2   | 1.98                     | 0.44              |
| 5:C:17:GLU:O     | 5:C:20:LYS:HB2   | 2.18                     | 0.44              |
| 1:A:56:TYR:O     | 1:A:59:VAL:CG1   | 2.66                     | 0.44              |
| 1:A:56:TYR:OH    | 1:A:301:HIS:O    | 2.28                     | 0.44              |
| 1:A:130:TYR:HE1  | 1:A:177:SER:CA   | 2.30                     | 0.44              |
| 1:A:239:ARG:O    | 1:A:243:VAL:HG23 | 2.17                     | 0.44              |
| 2:B:168:LEU:O    | 2:B:169:TRP:CG   | 2.70                     | 0.44              |
| 2:B:3:GLU:O      | 2:B:4:LEU:C      | 2.61                     | 0.44              |
| 2:B:4:LEU:HG     | 2:B:5:ASP:N      | 2.32                     | 0.44              |
| 4:S:88:SER:HA    | 4:S:119:VAL:HB   | 1.99                     | 0.44              |
| 1:A:56:TYR:HH    | 1:A:301:HIS:C    | 2.22                     | 0.44              |
| 1:A:294:PRO:HG2  | 1:A:295:LEU:CD1  | 2.48                     | 0.44              |
| 1:A:255:SER:O    | 1:A:256:LEU:C    | 2.61                     | 0.44              |
| 1:A:292:ARG:HD2  | 1:A:292:ARG:O    | 2.17                     | 0.44              |
| 1:A:238:LEU:O    | 1:A:241:ARG:HB3  | 2.17                     | 0.44              |
| 2:B:289:TYR:O    | 2:B:315:VAL:HG22 | 2.17                     | 0.44              |
| 3:D:348:ASN:HA   | 3:D:351:ASP:OD1  | 2.17                     | 0.44              |
| 4:S:235:TYR:HB2  | 4:S:236:PRO:HD3  | 2.00                     | 0.44              |
| 2:B:82:TRP:HB2   | 2:B:88:ASN:C     | 2.43                     | 0.43              |
| 2:B:22:ARG:NH2   | 2:B:259:GLN:CD   | 2.76                     | 0.43              |
| 2:B:277:SER:OG   | 2:B:320:VAL:HG12 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:188:THR:CG2   | 3:D:199:MET:HE3   | 2.48                     | 0.43              |
| 1:A:224:VAL:O     | 1:A:227:LEU:HG    | 2.18                     | 0.43              |
| 2:B:28:ALA:O      | 2:B:29:THR:C      | 2.61                     | 0.43              |
| 2:B:139:LEU:HD12  | 2:B:139:LEU:N     | 2.32                     | 0.43              |
| 3:D:49:ILE:CD1    | 3:D:268:PHE:HD2   | 2.31                     | 0.43              |
| 4:S:50:TYR:O      | 4:S:58:ILE:HA     | 2.18                     | 0.43              |
| 1:A:217:VAL:O     | 1:A:221:ALA:HB3   | 2.18                     | 0.43              |
| 2:B:274:THR:O     | 2:B:274:THR:OG1   | 2.33                     | 0.43              |
| 3:D:284:LEU:CD1   | 3:D:300:ALA:HB1   | 2.48                     | 0.43              |
| 1:A:139:LEU:C     | 1:A:139:LEU:HD23  | 2.43                     | 0.43              |
| 1:A:262:MET:C     | 1:A:264:LEU:N     | 2.66                     | 0.43              |
| 3:D:49:ILE:CD1    | 3:D:268:PHE:CD2   | 3.02                     | 0.43              |
| 1:A:254:ARG:O     | 1:A:257:ARG:HB3   | 2.19                     | 0.43              |
| 6:A:401:A1LXY:C08 | 6:A:401:A1LXY:O16 | 2.67                     | 0.43              |
| 1:A:283:VAL:HA    | 1:A:286:LEU:HB2   | 2.01                     | 0.43              |
| 2:B:279:SER:HB2   | 5:C:50:LEU:HD12   | 2.01                     | 0.43              |
| 2:B:33:ILE:O      | 2:B:33:ILE:CG2    | 2.67                     | 0.43              |
| 2:B:111:TYR:CD2   | 2:B:155:ASN:HB2   | 2.54                     | 0.43              |
| 2:B:253:PHE:CD1   | 2:B:260:GLU:HA    | 2.48                     | 0.43              |
| 2:B:313:ASN:C     | 2:B:331:SER:OG    | 2.61                     | 0.43              |
| 3:D:231:TYR:OH    | 3:D:279:ILE:HG22  | 2.19                     | 0.43              |
| 1:A:146:ARG:NH1   | 3:D:354:LEU:HD21  | 2.34                     | 0.43              |
| 2:B:10:GLU:O      | 2:B:13:GLN:HB3    | 2.18                     | 0.43              |
| 2:B:163:ASP:CG    | 2:B:164:THR:N     | 2.77                     | 0.43              |
| 3:D:283:PRO:HA    | 3:D:295:ASN:HD21  | 1.83                     | 0.42              |
| 4:S:69:THR:HG22   | 4:S:82:GLN:O      | 2.19                     | 0.42              |
| 2:B:215:GLU:CG    | 2:B:217:MET:HG2   | 2.48                     | 0.42              |
| 4:S:70:ILE:HD12   | 4:S:81:LEU:HD13   | 1.91                     | 0.42              |
| 4:S:165:LEU:HD12  | 4:S:212:PHE:CE2   | 2.54                     | 0.42              |
| 1:A:56:TYR:O      | 1:A:59:VAL:HG12   | 2.20                     | 0.42              |
| 1:A:282:ILE:O     | 1:A:286:LEU:N     | 2.52                     | 0.42              |
| 2:B:200:VAL:HG23  | 2:B:234:PHE:HZ    | 1.82                     | 0.42              |
| 2:B:229:ILE:HD13  | 2:B:244:GLY:O     | 2.19                     | 0.42              |
| 3:D:188:THR:O     | 3:D:198:LYS:CA    | 2.61                     | 0.42              |
| 1:A:69:LEU:O      | 1:A:72:PHE:N      | 2.52                     | 0.42              |
| 1:A:262:MET:C     | 1:A:262:MET:SD    | 3.02                     | 0.42              |
| 4:S:204:SER:O     | 4:S:214:LEU:HD12  | 2.18                     | 0.42              |
| 1:A:77:TYR:O      | 1:A:79:LYS:HB2    | 2.20                     | 0.42              |
| 1:A:114:TRP:CH2   | 1:A:121:CYS:HA    | 2.55                     | 0.42              |
| 2:B:119:ASN:HA    | 2:B:144:GLY:O     | 2.18                     | 0.42              |
| 2:B:205:ASP:OD1   | 2:B:205:ASP:N     | 2.51                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:7:ALA:N      | 5:C:10:ALA:HB3   | 2.35                     | 0.42              |
| 3:D:50:VAL:O     | 3:D:51:LYS:C     | 2.62                     | 0.42              |
| 4:S:70:ILE:HG13  | 4:S:81:LEU:CA    | 2.50                     | 0.42              |
| 1:A:108:LYS:C    | 1:A:110:LEU:N    | 2.74                     | 0.42              |
| 1:A:141:MET:HE2  | 1:A:168:ILE:HG21 | 2.02                     | 0.42              |
| 1:A:170:ILE:O    | 1:A:174:VAL:CG1  | 2.67                     | 0.42              |
| 2:B:153:ASP:CG   | 2:B:196:THR:CG2  | 2.92                     | 0.42              |
| 2:B:314:ARG:C    | 2:B:331:SER:OG   | 2.62                     | 0.42              |
| 4:S:73:ASP:N     | 4:S:78:THR:O     | 2.29                     | 0.42              |
| 1:A:78:THR:HG23  | 1:A:85:ASN:ND2   | 2.35                     | 0.41              |
| 2:B:80:ILE:HD11  | 3:D:23:LEU:CD1   | 2.50                     | 0.41              |
| 1:A:224:VAL:CA   | 1:A:227:LEU:HG   | 2.44                     | 0.41              |
| 2:B:94:PRO:C     | 2:B:95:LEU:HD12  | 2.46                     | 0.41              |
| 3:D:53:MET:HG2   | 3:D:190:PHE:CE2  | 2.55                     | 0.41              |
| 4:S:178:LEU:HD21 | 4:S:180:ARG:HH11 | 1.85                     | 0.41              |
| 1:A:139:LEU:HD23 | 1:A:229:ILE:HD12 | 2.01                     | 0.41              |
| 4:S:3:GLN:O      | 4:S:25:SER:O     | 2.39                     | 0.41              |
| 1:A:116:PHE:CG   | 1:A:120:LEU:HD12 | 2.55                     | 0.41              |
| 1:A:222:PHE:O    | 1:A:226:ILE:CD1  | 2.68                     | 0.41              |
| 3:D:41:ALA:HB2   | 3:D:250:LEU:HD13 | 2.02                     | 0.41              |
| 3:D:48:THR:C     | 3:D:51:LYS:N     | 2.78                     | 0.41              |
| 1:A:306:LEU:C    | 1:A:309:ALA:HB3  | 2.44                     | 0.41              |
| 2:B:208:ALA:O    | 2:B:222:PHE:N    | 2.39                     | 0.41              |
| 2:B:313:ASN:HB3  | 2:B:331:SER:OG   | 2.20                     | 0.41              |
| 3:D:257:ASN:OD1  | 3:D:258:LYS:N    | 2.53                     | 0.41              |
| 4:S:106:SER:OG   | 4:S:109:ASP:OD2  | 2.37                     | 0.41              |
| 2:B:298:ASP:OD2  | 2:B:301:LYS:HB2  | 2.20                     | 0.41              |
| 5:C:8:SER:O      | 5:C:12:ALA:CA    | 2.57                     | 0.41              |
| 1:A:53:THR:O     | 1:A:57:SER:HB2   | 2.21                     | 0.41              |
| 2:B:60:ALA:HB3   | 2:B:73:ALA:CB    | 2.47                     | 0.41              |
| 2:B:314:ARG:HD3  | 2:B:332:TRP:CZ3  | 2.56                     | 0.41              |
| 3:D:189:HIS:HE2  | 3:D:196:HIS:HB3  | 1.85                     | 0.41              |
| 4:S:4:LEU:HD11   | 4:S:27:PHE:CE1   | 2.56                     | 0.41              |
| 1:A:102:LEU:HD23 | 1:A:102:LEU:H    | 1.84                     | 0.41              |
| 1:A:146:ARG:CG   | 3:D:354:LEU:HD11 | 2.50                     | 0.41              |
| 1:A:295:LEU:HD12 | 1:A:295:LEU:N    | 2.36                     | 0.41              |
| 1:A:304:ILE:HG13 | 1:A:304:ILE:H    | 1.73                     | 0.41              |
| 2:B:22:ARG:NH2   | 2:B:259:GLN:HG3  | 2.36                     | 0.41              |
| 2:B:197:ARG:NE   | 2:B:214:ARG:NH2  | 2.47                     | 0.41              |
| 2:B:271:CYS:HB2  | 2:B:291:ASP:OD1  | 2.21                     | 0.41              |
| 4:S:14:PRO:C     | 4:S:16:GLY:H     | 2.29                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:14:LYS:O     | 5:C:17:GLU:CA    | 2.68                     | 0.41              |
| 2:B:13:GLN:HA    | 2:B:16:ASN:HB2   | 2.03                     | 0.41              |
| 2:B:15:LYS:O     | 2:B:19:ARG:N     | 2.49                     | 0.41              |
| 4:S:12:VAL:CG1   | 4:S:13:GLN:H     | 2.32                     | 0.41              |
| 1:A:56:TYR:CA    | 1:A:59:VAL:CG1   | 2.85                     | 0.40              |
| 1:A:146:ARG:HD2  | 3:D:354:LEU:HD11 | 2.00                     | 0.40              |
| 1:A:299:ALA:O    | 1:A:302:LEU:CB   | 2.69                     | 0.40              |
| 2:B:18:ILE:HG22  | 2:B:259:GLN:HE22 | 1.85                     | 0.40              |
| 2:B:130:GLU:O    | 4:S:27:PHE:HB2   | 2.21                     | 0.40              |
| 2:B:239:ASN:HB3  | 2:B:256:ARG:NH2  | 2.36                     | 0.40              |
| 4:S:93:MET:HE2   | 4:S:114:GLY:C    | 2.47                     | 0.40              |
| 1:A:71:MET:C     | 1:A:71:MET:SD    | 3.04                     | 0.40              |
| 2:B:62:HIS:O     | 2:B:70:LEU:HD12  | 2.22                     | 0.40              |
| 2:B:279:SER:OG   | 5:C:50:LEU:HD12  | 2.22                     | 0.40              |
| 1:A:53:THR:OG1   | 1:A:54:ALA:N     | 2.55                     | 0.40              |
| 2:B:199:PHE:O    | 2:B:211:TRP:N    | 2.22                     | 0.40              |
| 2:B:283:ARG:HE   | 2:B:300:LEU:HB2  | 1.87                     | 0.40              |
| 3:D:48:THR:O     | 3:D:49:ILE:C     | 2.60                     | 0.40              |
| 3:D:291:TYR:CD1  | 3:D:303:TYR:CD2  | 3.09                     | 0.40              |
| 1:A:85:ASN:O     | 1:A:88:ILE:HG22  | 2.21                     | 0.40              |
| 1:A:147:TYR:HD1  | 1:A:151:CYS:HG   | 1.65                     | 0.40              |
| 2:B:168:LEU:C    | 2:B:169:TRP:CG   | 3.00                     | 0.40              |
| 1:A:107:ALA:O    | 1:A:110:LEU:HB3  | 2.21                     | 0.40              |
| 1:A:283:VAL:O    | 1:A:286:LEU:N    | 2.53                     | 0.40              |
| 2:B:150:ARG:O    | 2:B:158:VAL:CG2  | 2.70                     | 0.40              |
| 2:B:163:ASP:CG   | 2:B:164:THR:H    | 2.29                     | 0.40              |
| 2:B:270:ILE:HD12 | 2:B:270:ILE:HA   | 1.82                     | 0.40              |
| 3:D:18:MET:HE2   | 3:D:18:MET:HB3   | 1.97                     | 0.40              |
| 5:C:7:ALA:O      | 5:C:10:ALA:HB3   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 284/325 (87%)   | 245 (86%)  | 38 (13%)  | 1 (0%)   | 30          | 62  |
| 2   | B     | 338/358 (94%)   | 300 (89%)  | 38 (11%)  | 0        | 100         | 100 |
| 3   | D     | 219/355 (62%)   | 199 (91%)  | 20 (9%)   | 0        | 100         | 100 |
| 4   | S     | 228/266 (86%)   | 207 (91%)  | 21 (9%)   | 0        | 100         | 100 |
| 5   | C     | 55/71 (78%)     | 54 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| All | All   | 1124/1375 (82%) | 1005 (89%) | 118 (10%) | 1 (0%)   | 49          | 79  |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 78  | THR  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 247/278 (89%)  | 245 (99%)  | 2 (1%)   | 73          | 77  |
| 2   | B     | 279/298 (94%)  | 268 (96%)  | 11 (4%)  | 28          | 56  |
| 3   | D     | 195/309 (63%)  | 195 (100%) | 0        | 100         | 100 |
| 4   | S     | 193/215 (90%)  | 188 (97%)  | 5 (3%)   | 40          | 64  |
| 5   | C     | 46/58 (79%)    | 46 (100%)  | 0        | 100         | 100 |
| All | All   | 960/1158 (83%) | 942 (98%)  | 18 (2%)  | 49          | 68  |

All (18) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 71  | MET  |
| 1   | A     | 274 | TRP  |
| 2   | B     | 3   | GLU  |
| 2   | B     | 4   | LEU  |
| 2   | B     | 6   | GLN  |
| 2   | B     | 79  | LEU  |
| 2   | B     | 165 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 187 | VAL  |
| 2   | B     | 200 | VAL  |
| 2   | B     | 247 | ASP  |
| 2   | B     | 258 | ASP  |
| 2   | B     | 259 | GLN  |
| 2   | B     | 270 | ILE  |
| 4   | S     | 57  | THR  |
| 4   | S     | 59  | TYR  |
| 4   | S     | 87  | ARG  |
| 4   | S     | 88  | SER  |
| 4   | S     | 234 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | ASN  |
| 1   | A     | 301 | HIS  |
| 1   | A     | 314 | ASN  |
| 2   | B     | 9   | GLN  |
| 2   | B     | 32  | GLN  |
| 2   | B     | 91  | HIS  |
| 2   | B     | 110 | ASN  |
| 2   | B     | 237 | ASN  |
| 2   | B     | 259 | GLN  |
| 2   | B     | 311 | HIS  |
| 2   | B     | 340 | ASN  |
| 3   | D     | 47  | ASN  |
| 3   | D     | 205 | GLN  |
| 4   | S     | 35  | HIS  |
| 4   | S     | 194 | ASN  |
| 4   | S     | 231 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type  | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|-------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |       |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 6   | A1LXY | A     | 401 | -    | 31,32,32     | 2.20 | 7 (22%)     | 38,46,46    | 2.13 | 13 (34%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type  | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|-------|-------|-----|------|---------|------------|---------|
| 6   | A1LXY | A     | 401 | -    | -       | 5/16/40/40 | 1/4/4/4 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type  | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|-------|---------|------|-------------|----------|
| 6   | A     | 401 | A1LXY | C10-C09 | 6.26 | 1.40        | 1.34     |
| 6   | A     | 401 | A1LXY | C04-N03 | 5.74 | 1.46        | 1.34     |
| 6   | A     | 401 | A1LXY | C24-C11 | 5.36 | 1.59        | 1.52     |
| 6   | A     | 401 | A1LXY | C14-C15 | 3.58 | 1.47        | 1.41     |
| 6   | A     | 401 | A1LXY | C19-C13 | 3.09 | 1.45        | 1.39     |
| 6   | A     | 401 | A1LXY | C26-C25 | 2.32 | 1.42        | 1.38     |
| 6   | A     | 401 | A1LXY | C05-C04 | 2.10 | 1.53        | 1.50     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|-------|-------------|-------|-------------|----------|
| 6   | A     | 401 | A1LXY | C24-C11-C20 | -6.01 | 103.30      | 109.63   |
| 6   | A     | 401 | A1LXY | C23-C24-C11 | 4.15  | 115.40      | 111.96   |

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| Mol | Chain | Res | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|-------|-------------|-------|-------------|----------|
| 6   | A     | 401 | A1LXY | C08-C09-C10 | 3.48  | 124.39      | 120.00   |
| 6   | A     | 401 | A1LXY | O12-C13-C19 | 3.45  | 121.82      | 116.60   |
| 6   | A     | 401 | A1LXY | C14-C09-C10 | -3.35 | 115.33      | 118.25   |
| 6   | A     | 401 | A1LXY | O12-C11-C10 | -3.35 | 104.98      | 109.85   |
| 6   | A     | 401 | A1LXY | C21-C20-C11 | 3.01  | 114.45      | 111.96   |
| 6   | A     | 401 | A1LXY | C05-C04-N03 | 2.97  | 122.37      | 118.66   |
| 6   | A     | 401 | A1LXY | C25-C08-C09 | 2.62  | 124.27      | 120.98   |
| 6   | A     | 401 | A1LXY | O27-C04-N03 | -2.45 | 118.50      | 122.35   |
| 6   | A     | 401 | A1LXY | C25-C08-C07 | -2.43 | 115.48      | 118.57   |
| 6   | A     | 401 | A1LXY | C17-C15-C14 | 2.37  | 123.17      | 120.15   |
| 6   | A     | 401 | A1LXY | C14-C09-C08 | -2.22 | 118.80      | 122.97   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type  | Atoms           |
|-----|-------|-----|-------|-----------------|
| 6   | A     | 401 | A1LXY | C01-C02-N03-C04 |
| 6   | A     | 401 | A1LXY | C01-C02-N03-C28 |
| 6   | A     | 401 | A1LXY | C07-C08-C09-C10 |
| 6   | A     | 401 | A1LXY | C25-C08-C09-C10 |
| 6   | A     | 401 | A1LXY | C25-C08-C09-C14 |

All (1) ring outliers are listed below:

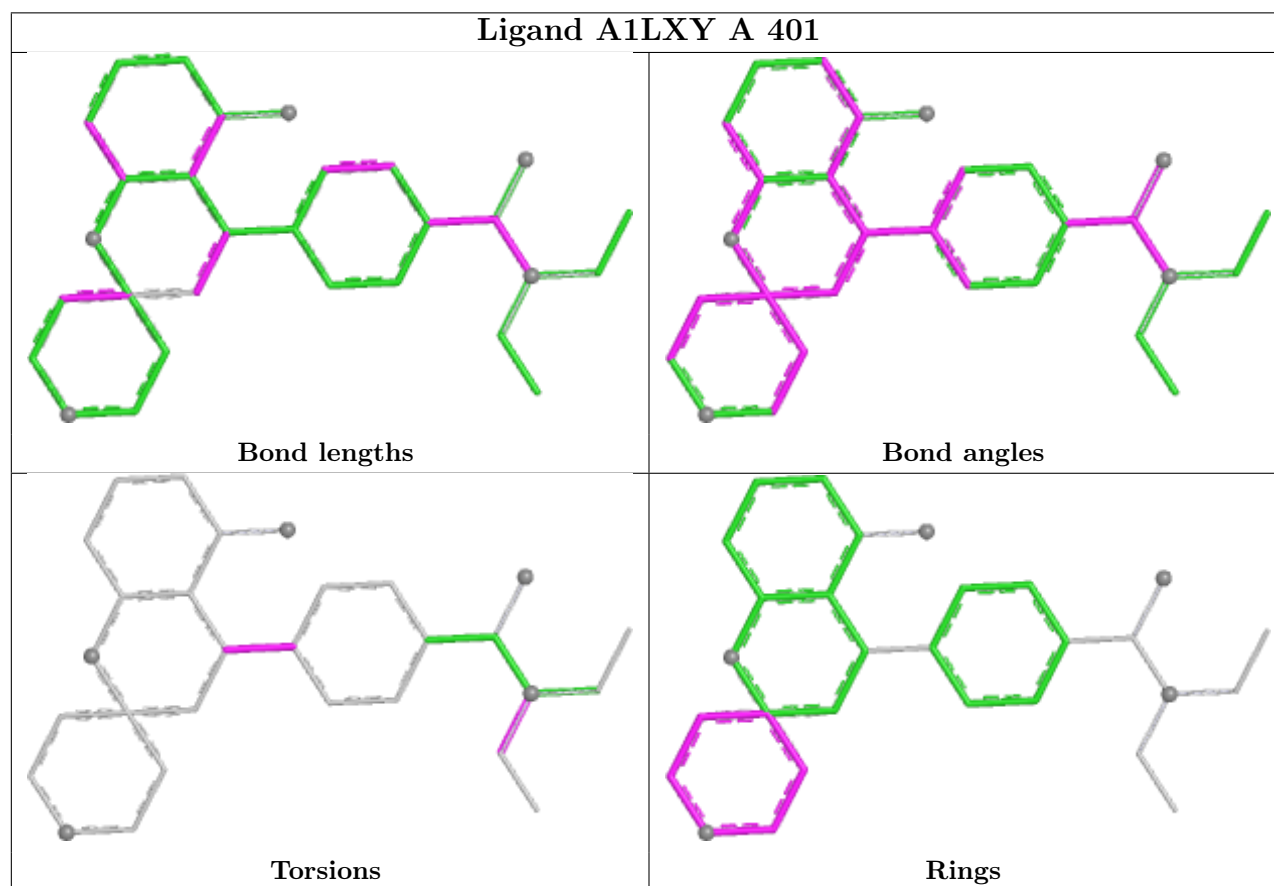
| Mol | Chain | Res | Type  | Atoms                   |
|-----|-------|-----|-------|-------------------------|
| 6   | A     | 401 | A1LXY | C11-C20-C21-C23-C24-N22 |

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type  | Clashes | Symm-Clashes |
|-----|-------|-----|-------|---------|--------------|
| 6   | A     | 401 | A1LXY | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

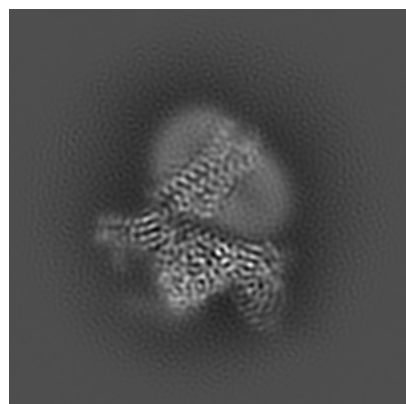
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38909. These allow visual inspection of the internal detail of the map and identification of artifacts.

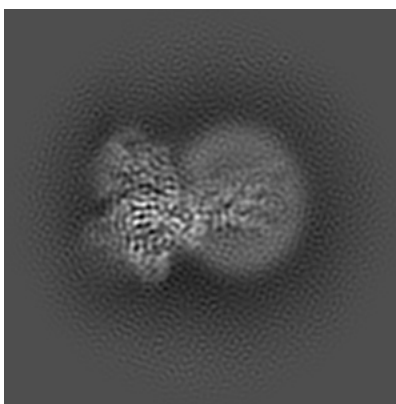
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

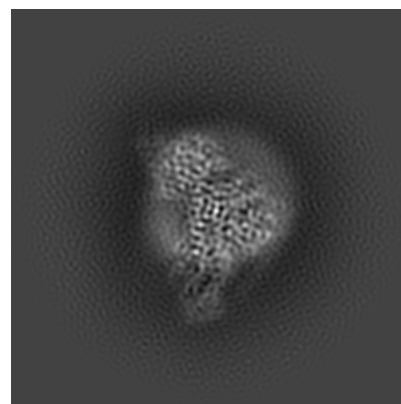
#### 6.1.1 Primary map



X

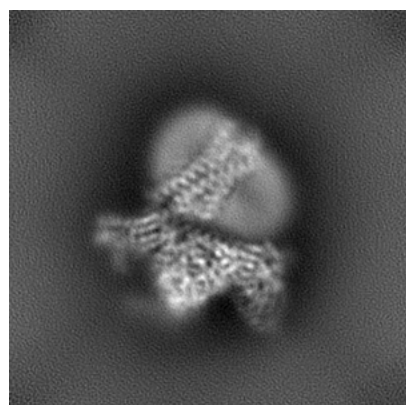


Y

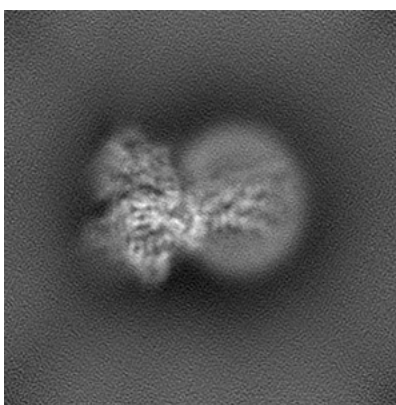


Z

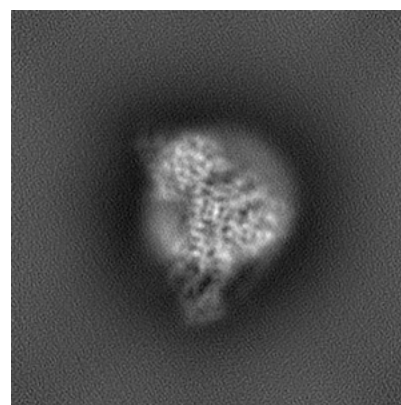
#### 6.1.2 Raw map



X



Y

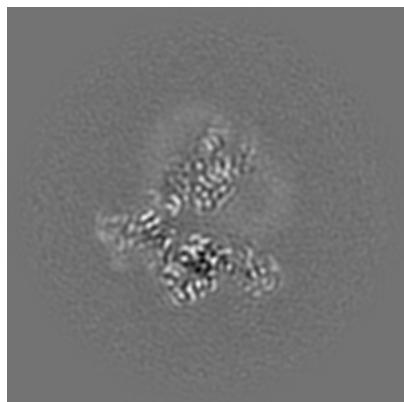


Z

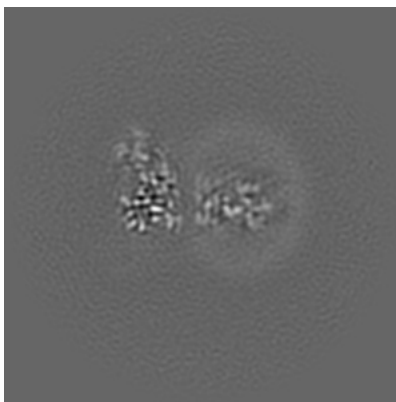
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

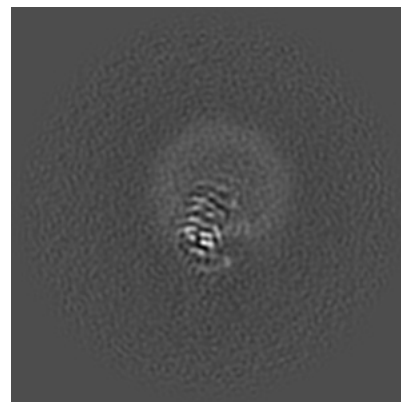
### 6.2.1 Primary map



X Index: 128

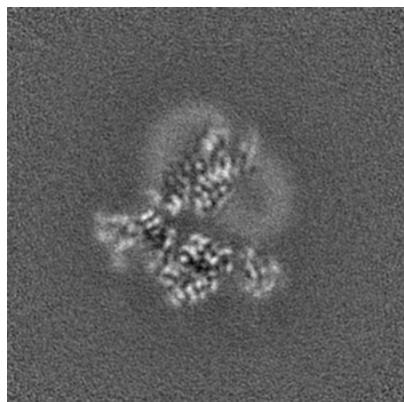


Y Index: 128

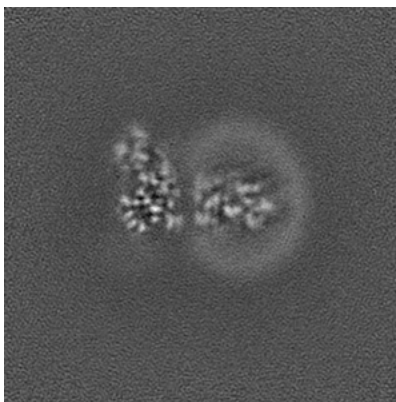


Z Index: 128

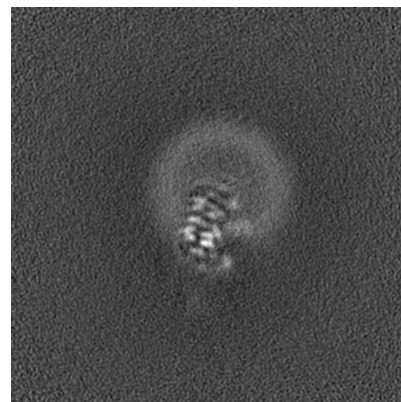
### 6.2.2 Raw map



X Index: 128



Y Index: 128

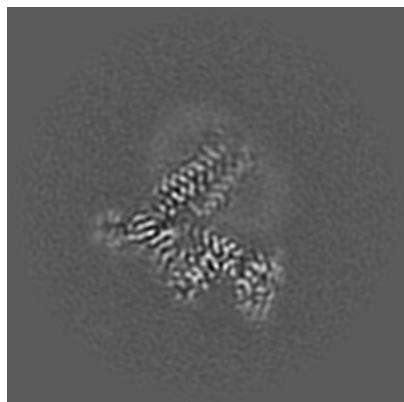


Z Index: 128

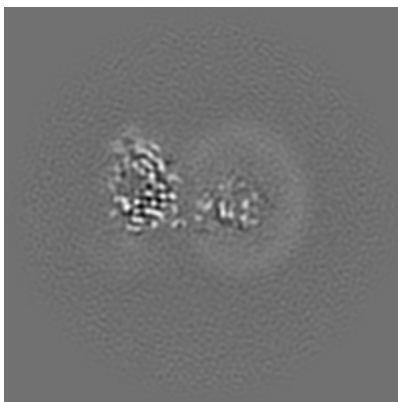
The images above show central slices of the map in three orthogonal directions.

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

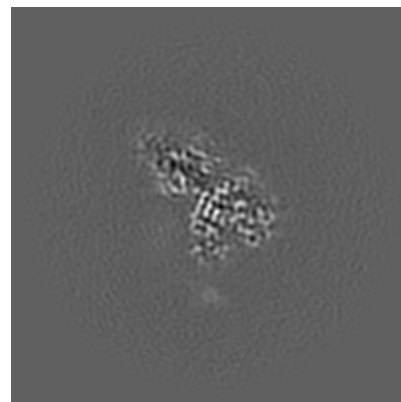
### 6.3.1 Primary map



X Index: 120

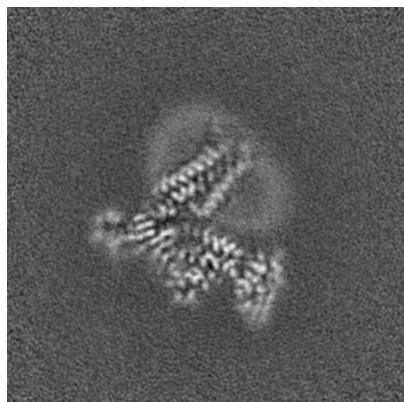


Y Index: 122

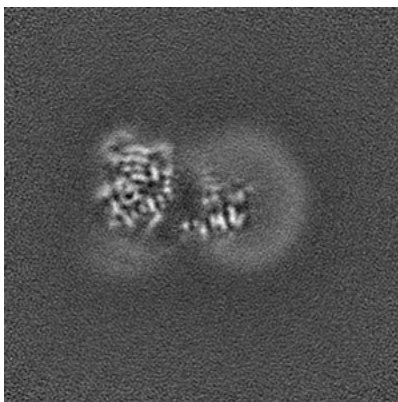


Z Index: 95

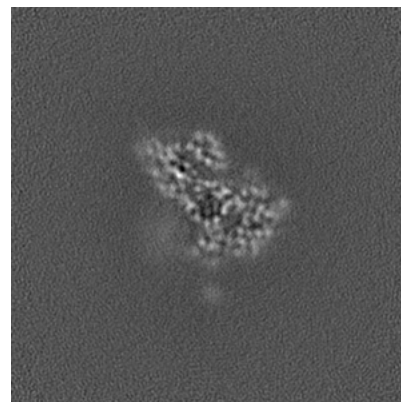
### 6.3.2 Raw map



X Index: 120



Y Index: 112

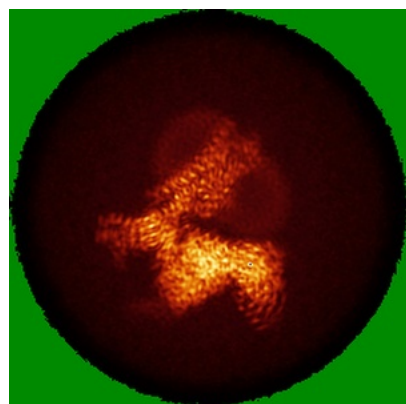


Z Index: 88

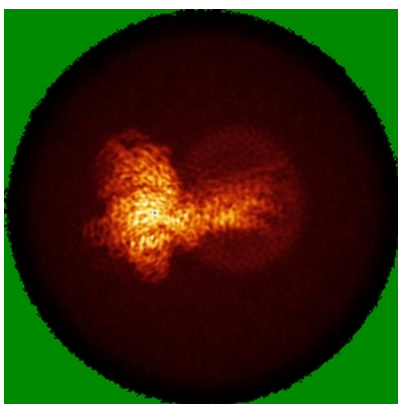
The images above show the largest variance slices of the map in three orthogonal directions.

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

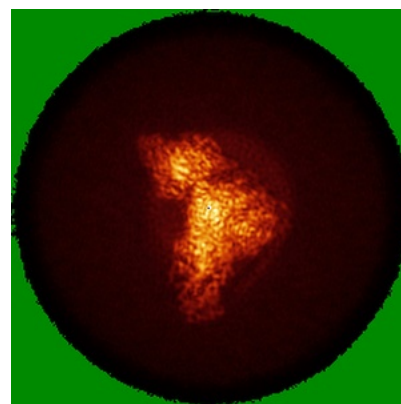
### 6.4.1 Primary map



X

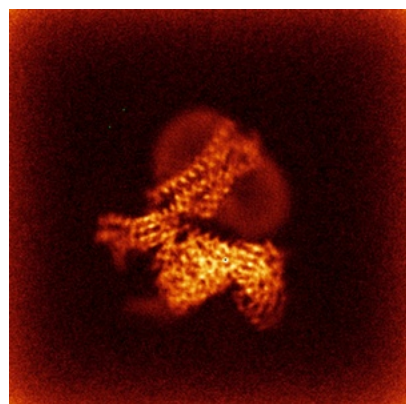


Y

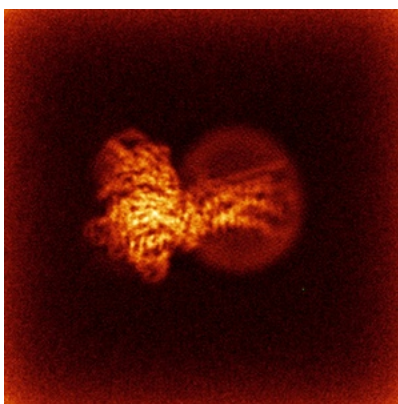


Z

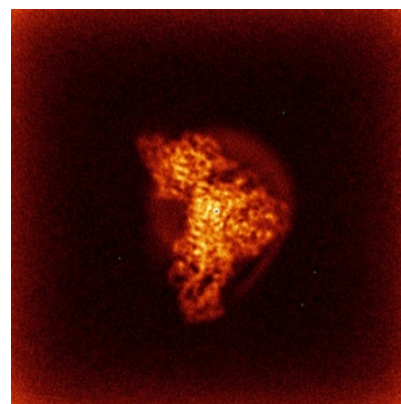
### 6.4.2 Raw map



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](#)

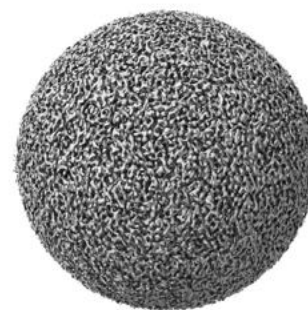
### 6.5.1 Primary map



X



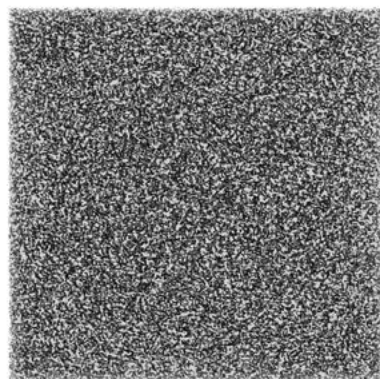
Y



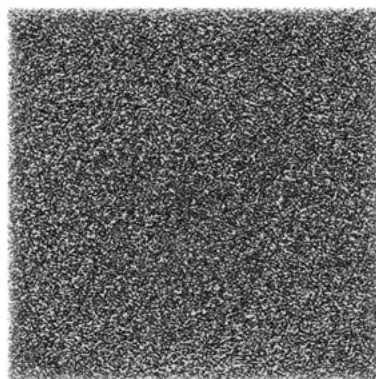
Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

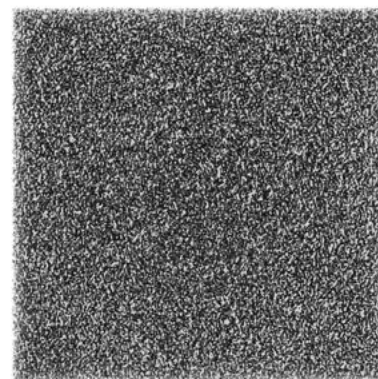
### 6.5.2 Raw map



X



Y



Z

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.

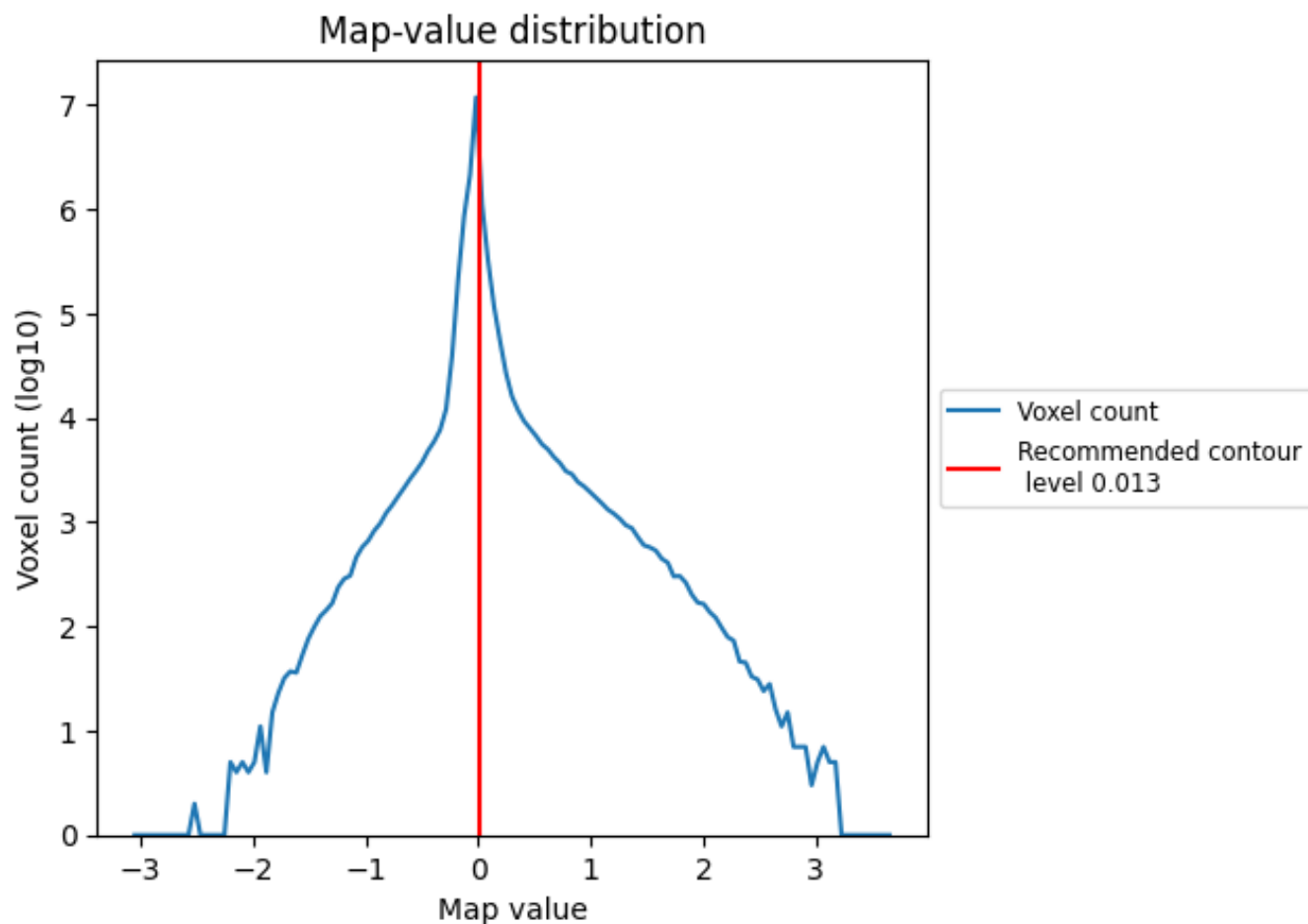
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

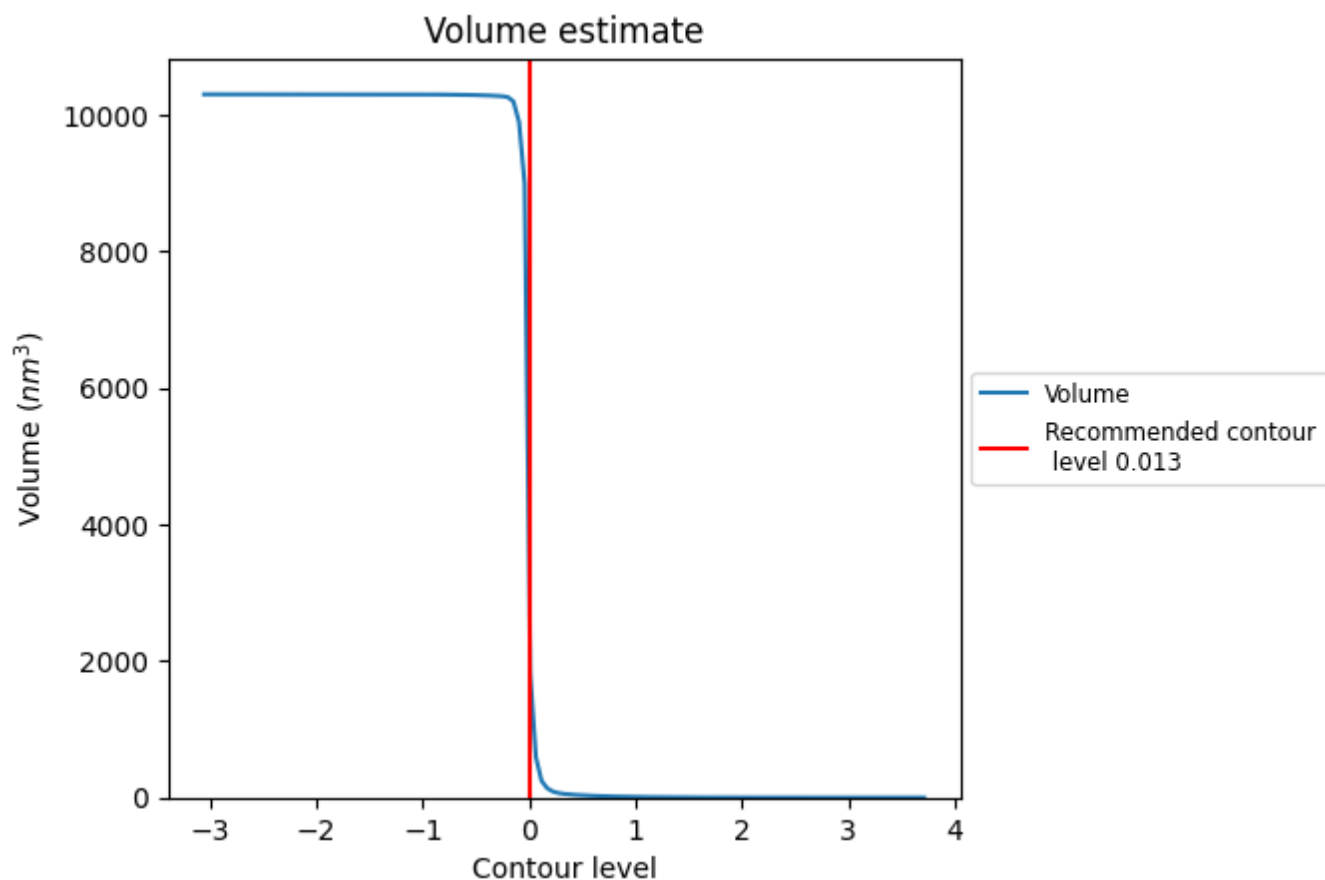
This section contains the results of statistical analysis of the map.

### 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.

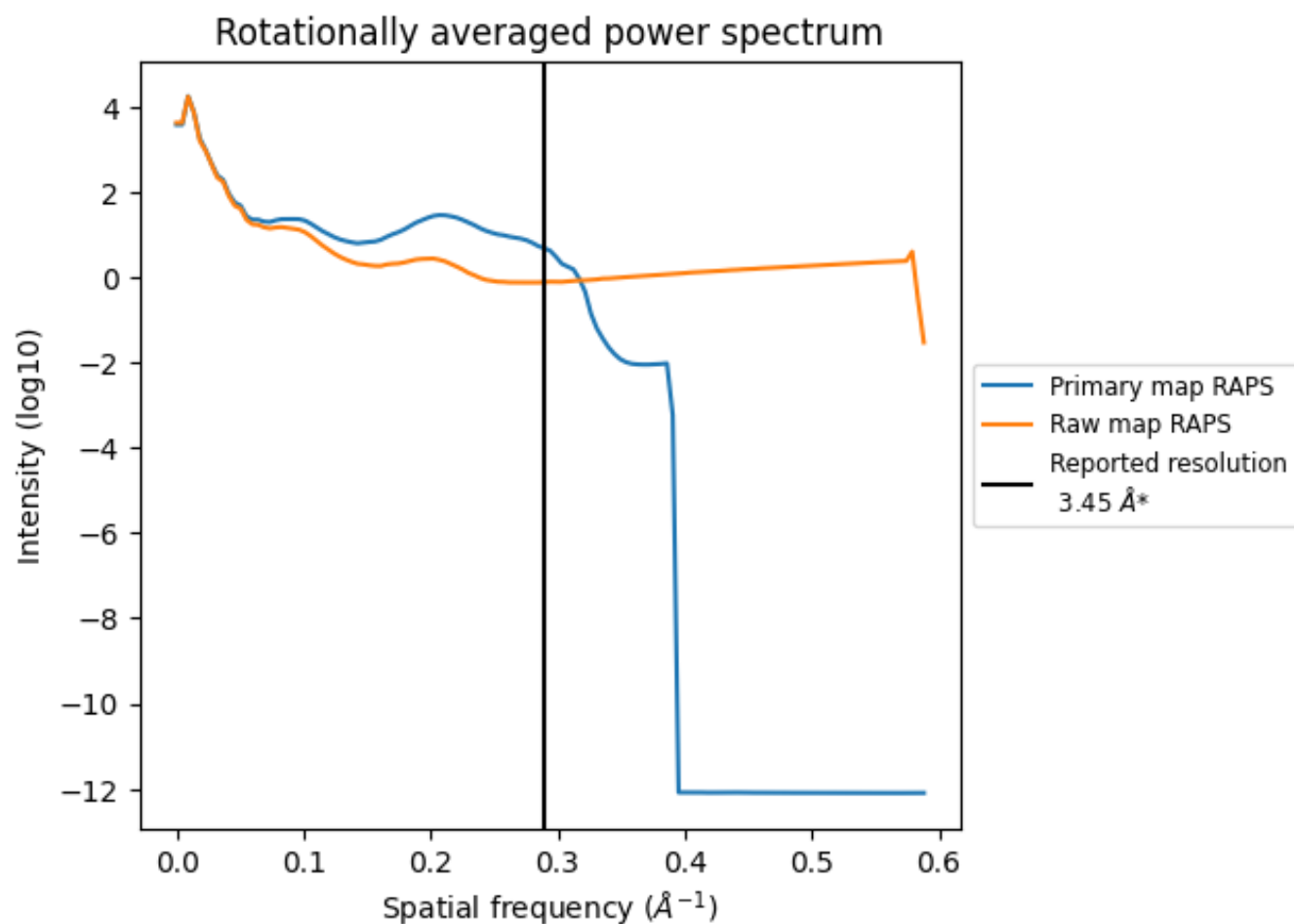
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1715 nm<sup>3</sup>; this corresponds to an approximate mass of 1549 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 ⓘ

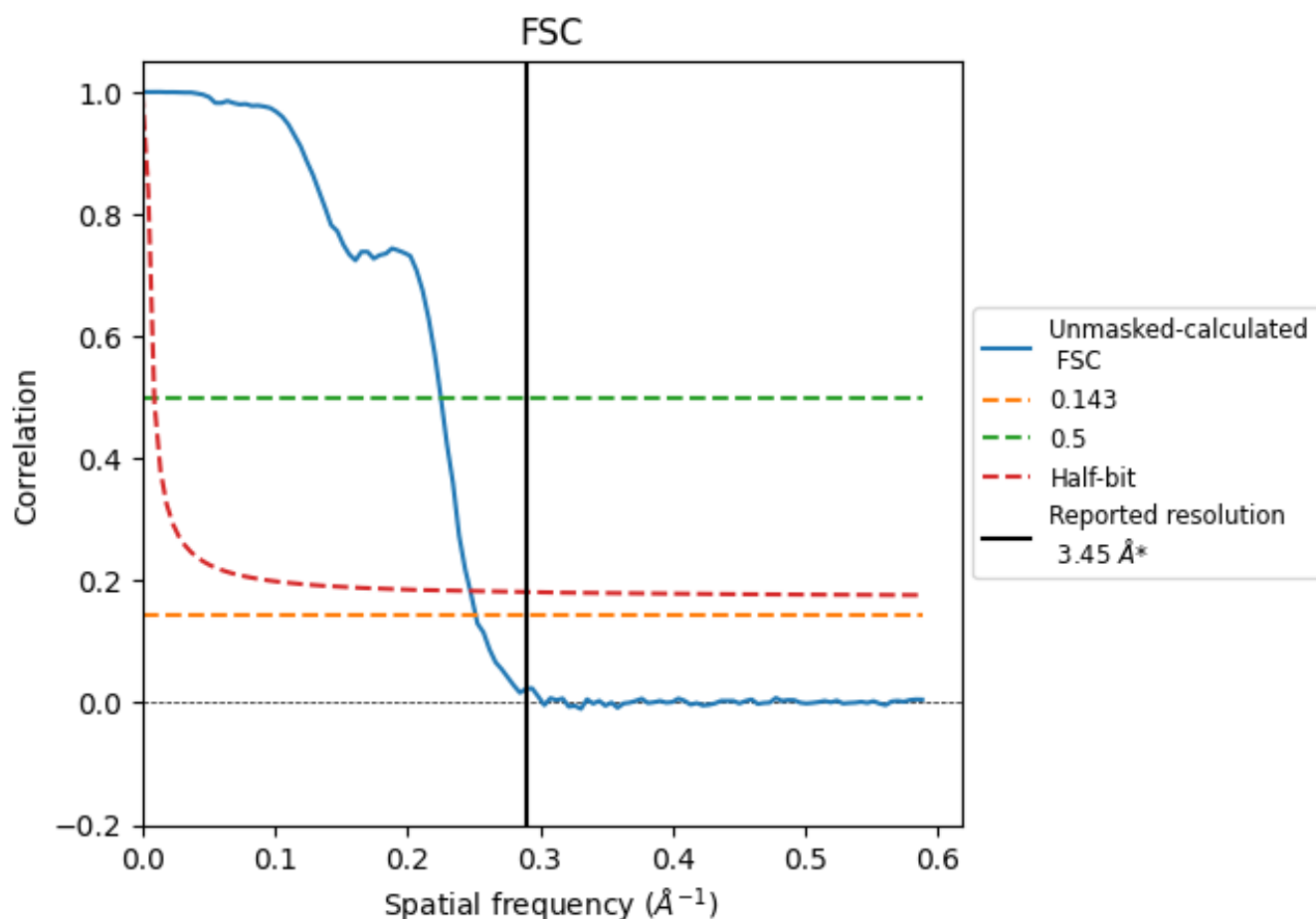


\*Reported resolution corresponds to spatial frequency of 0.290 Å<sup>-1</sup>

## 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  $0.290 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.45                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.98                               | 4.44 | 4.04     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.45 by more than 10 %

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

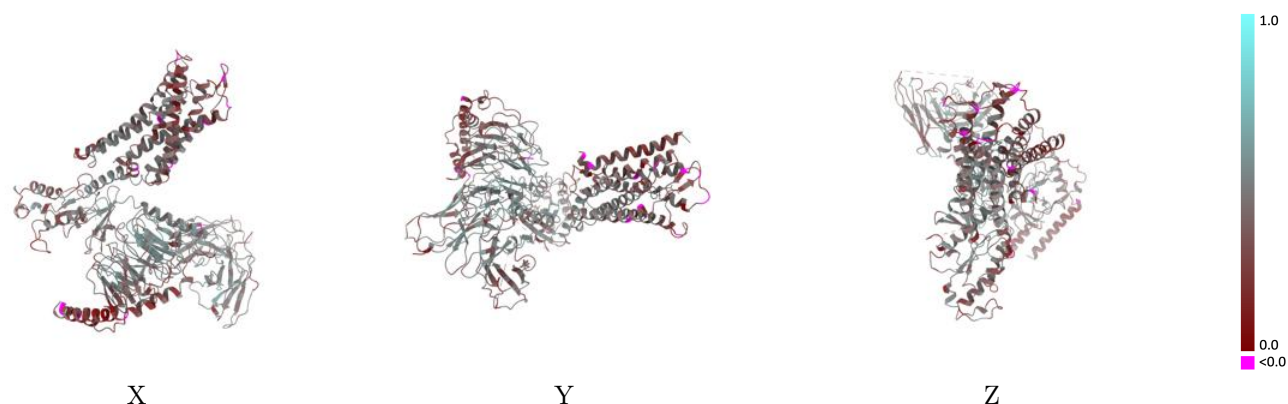
This section contains information regarding the fit between EMDB map EMD-38909 and PDB model 8Y45. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



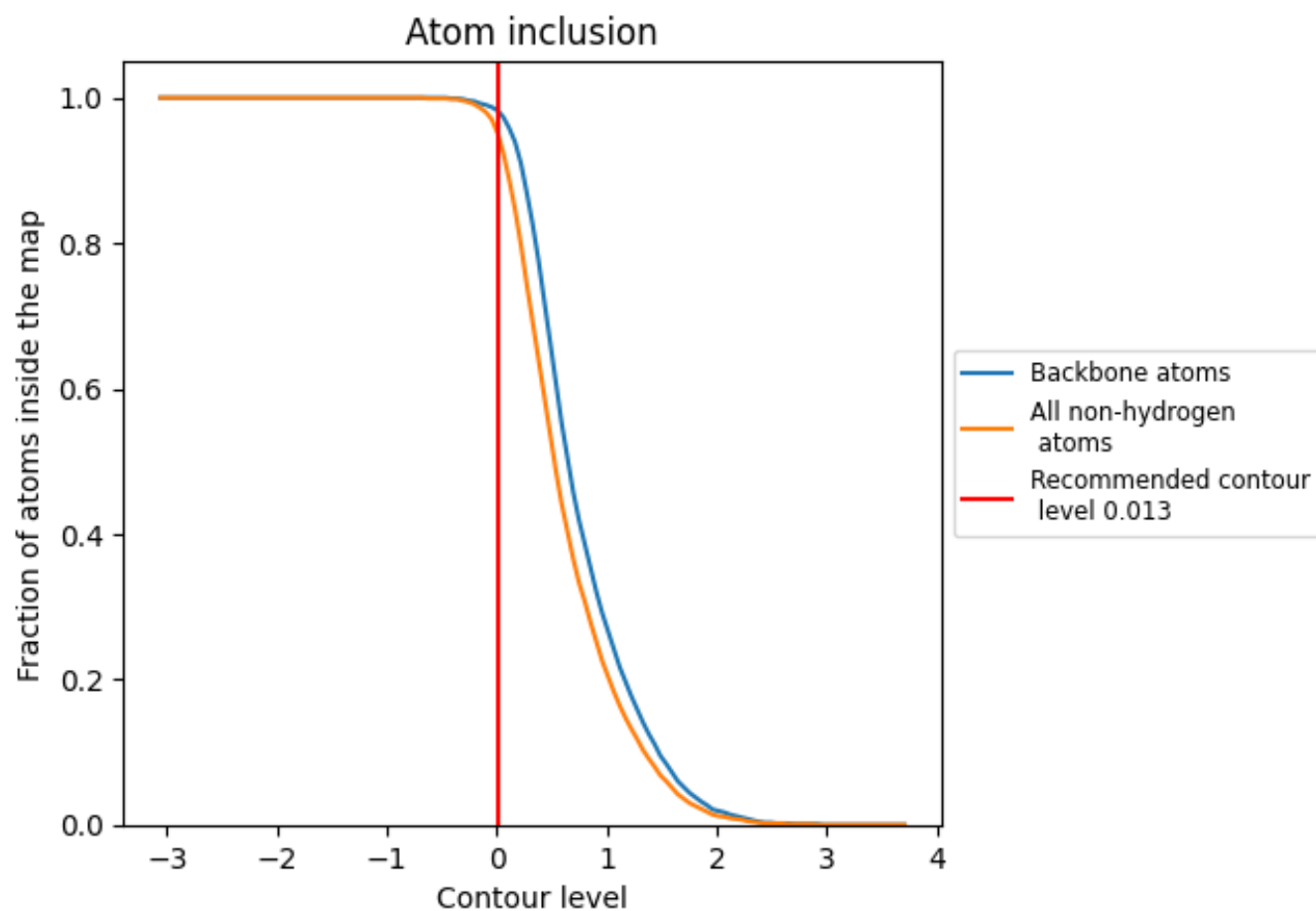
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9500 | <div></div> 0.4070 |
| A     | <div></div> 0.9370 | <div></div> 0.3520 |
| B     | <div></div> 0.9600 | <div></div> 0.4430 |
| C     | <div></div> 0.9120 | <div></div> 0.2650 |
| D     | <div></div> 0.9490 | <div></div> 0.4180 |
| S     | <div></div> 0.9640 | <div></div> 0.4480 |

