



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:38 AM UTC

PDB ID : 8WA0 / pdb\_00008wa0  
EMDB ID : EMD-37387  
Title : The cryo-EM structure of the Nicotiana tabacum PEP-PAP-TEC1  
Authors : Wu, X.X.; Zhang, Y.  
Deposited on : 2023-09-06  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

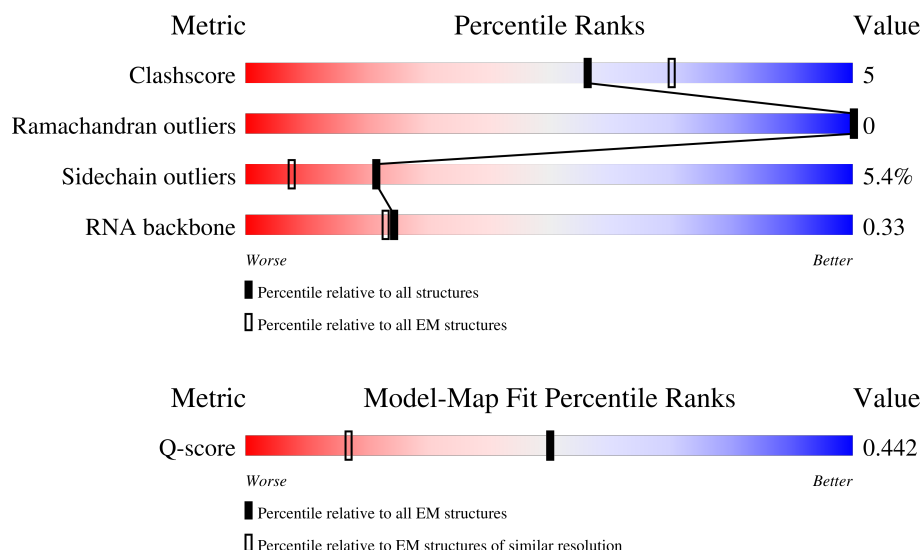
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



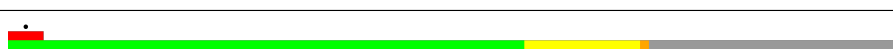
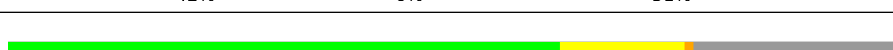
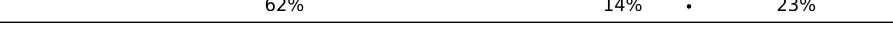
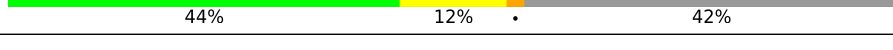
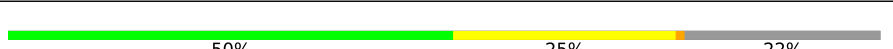
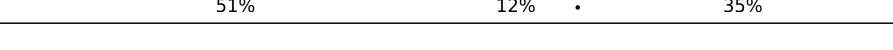
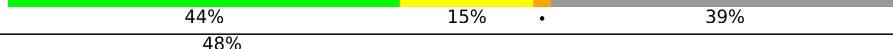
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 10327 ( 2.20 - 3.20 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 337    |                  |
| 1   | a     | 337    |                  |
| 2   | B     | 1070   |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | C     | 688    |    |
| 4   | c     | 1388   |    |
| 5   | D     | 892    |    |
| 6   | E     | 860    |    |
| 7   | F     | 682    |    |
| 8   | G     | 266    |    |
| 9   | H     | 531    |    |
| 10  | I     | 486    |    |
| 11  | i     | 648    |    |
| 12  | J     | 507    |    |
| 13  | K     | 331    |    |
| 14  | L     | 303    |    |
| 15  | M     | 178    |    |
| 15  | m     | 178    |   |
| 16  | N     | 770    |  |
| 17  | O     | 151    |  |
| 18  | P     | 143    |  |
| 19  | R     | 48     |  |
| 20  | S     | 20     |  |

## 2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 61128 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 DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2164  | 1368 | 377 | 409 | 10 |         |       |
| 1   | a     | 317      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2377  | 1515 | 410 | 442 | 10 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 973      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7296  | 4637 | 1302 | 1334 | 23 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit gamma.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 661      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4738  | 3002 | 860 | 858 | 18 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta”.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | c     | 1176     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8108  | 5081 | 1492 | 1507 | 28 |         |       |

- Molecule 5 is a protein called PAP1(pTAC3).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | D     | 645      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4772  | 3012 | 834 | 904 | 22 |         |       |

- Molecule 6 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | E     | 700      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4483  | 2784 | 816 | 862 | 21 |         |       |

- Molecule 7 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | F     | 544      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4185  | 2645 | 748 | 773 | 19 |         |       |

- Molecule 8 is a protein called superoxide dismutase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | G     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1714  | 1113 | 289 | 308 | 4 |         |       |

- Molecule 9 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | H     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2099  | 1332 | 370 | 389 | 8 |         |       |

- Molecule 10 is a protein called Fructokinase-like 1, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | I     | 376      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2924  | 1873 | 517 | 522 | 12 |         |       |

- Molecule 11 is a protein called Fructokinase-like 2, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | i     | 375      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2887  | 1837 | 496 | 540 | 14 |         |       |

- Molecule 12 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | J     | 421      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3358  | 2144 | 575 | 617 | 22 |         |       |

- Molecule 13 is a protein called PAP8(pTAC6).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | K     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1656  | 1050 | 289 | 309 | 8 |         |       |

- Molecule 14 is a protein called superoxide dismutase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | L     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1702  | 1086 | 300 | 312 | 4 |         |       |

- Molecule 15 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | M     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 931   | 594 | 150 | 180 | 7 |         |       |
| 15  | m     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 822   | 523 | 133 | 159 | 7 |         |       |

- Molecule 16 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | N     | 537      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2987  | 1818 | 579 | 584 | 6 |         |       |

- Molecule 17 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | O     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 763   | 482 | 136 | 142 | 3 |         |       |

- Molecule 18 is a protein called PAP13(pTAC18).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | P     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 761   | 489 | 133 | 137 | 2 |         |       |

- Molecule 19 is a DNA chain called DNA (48-mer).

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 19  | R     | 10       | Total | C  | N  | O  | P  | 0       | 0     |
|     |       |          | 199   | 96 | 30 | 63 | 10 |         |       |

- Molecule 20 is a RNA chain called RNA (20-mer).

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 20  | S     | 9        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 198   | 88 | 40 | 61 | 9 |         |       |

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 22  | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

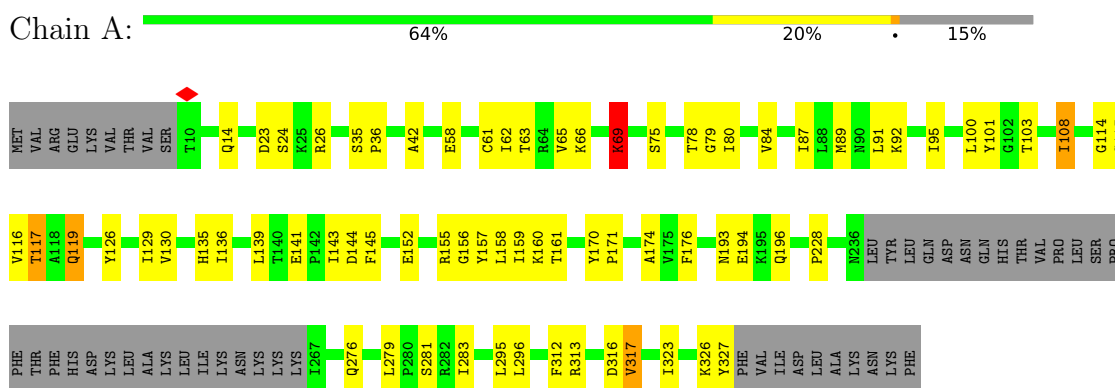
- Molecule 23 is FE (III) ION (CCD ID: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 23  | G     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 23  | L     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

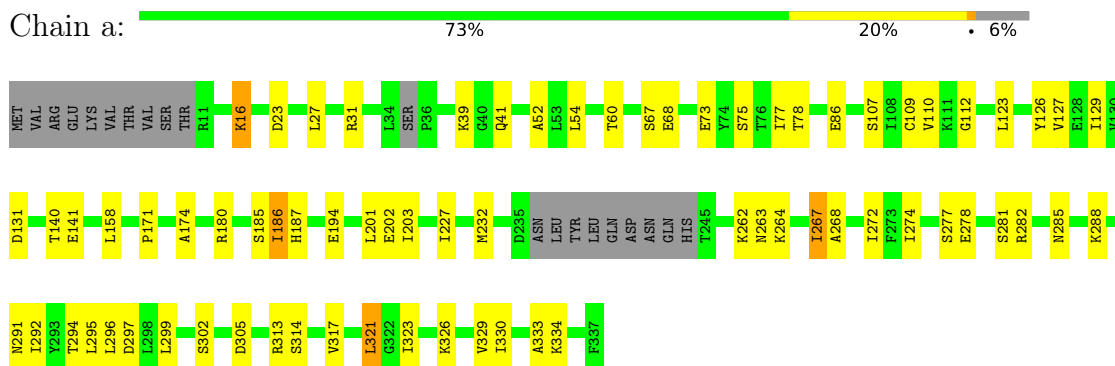
### 3 Residue-property plots

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

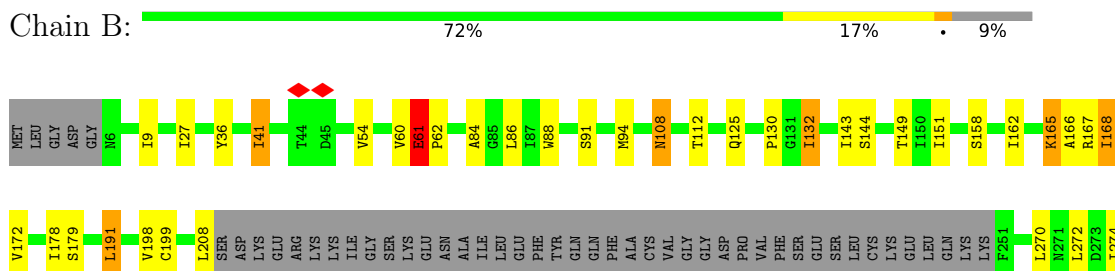
- Molecule 1: DNA-directed RNA polymerase subunit alpha

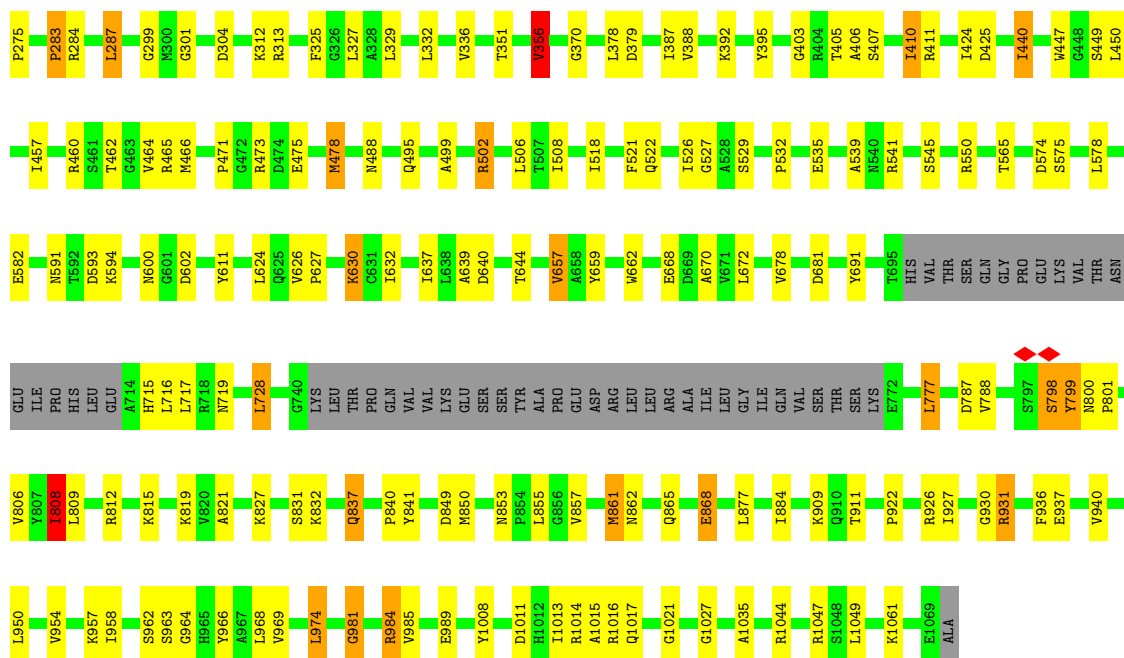


- Molecule 1: DNA-directed RNA polymerase subunit alpha

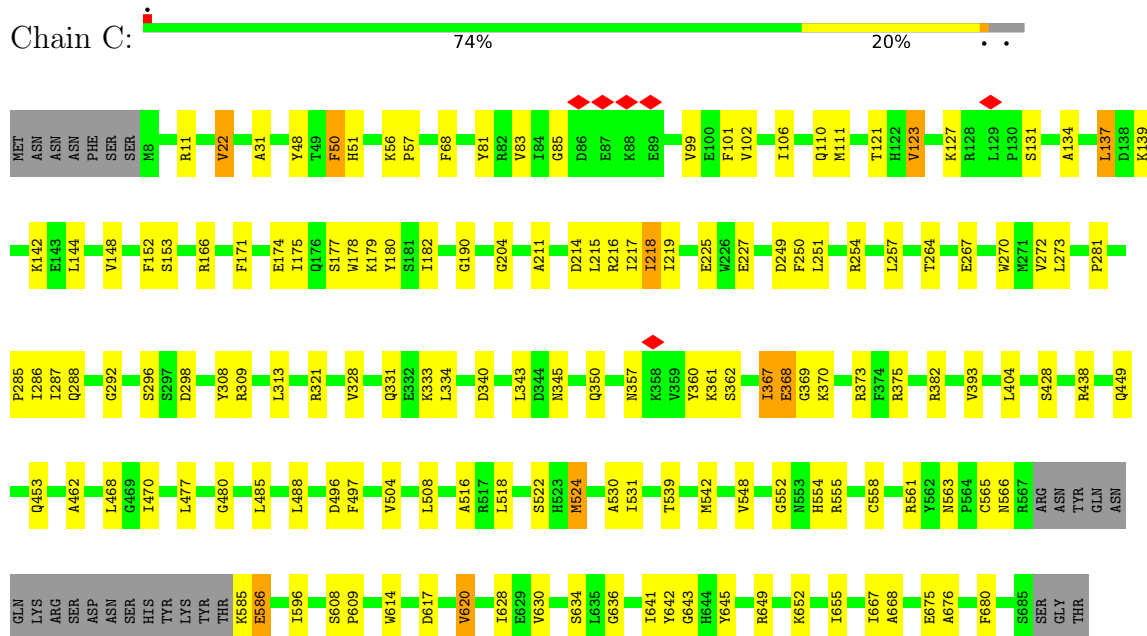


- Molecule 2: DNA-directed RNA polymerase subunit beta

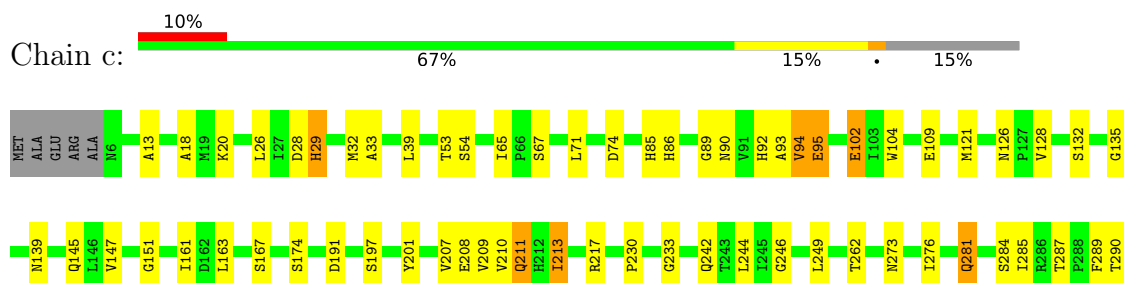


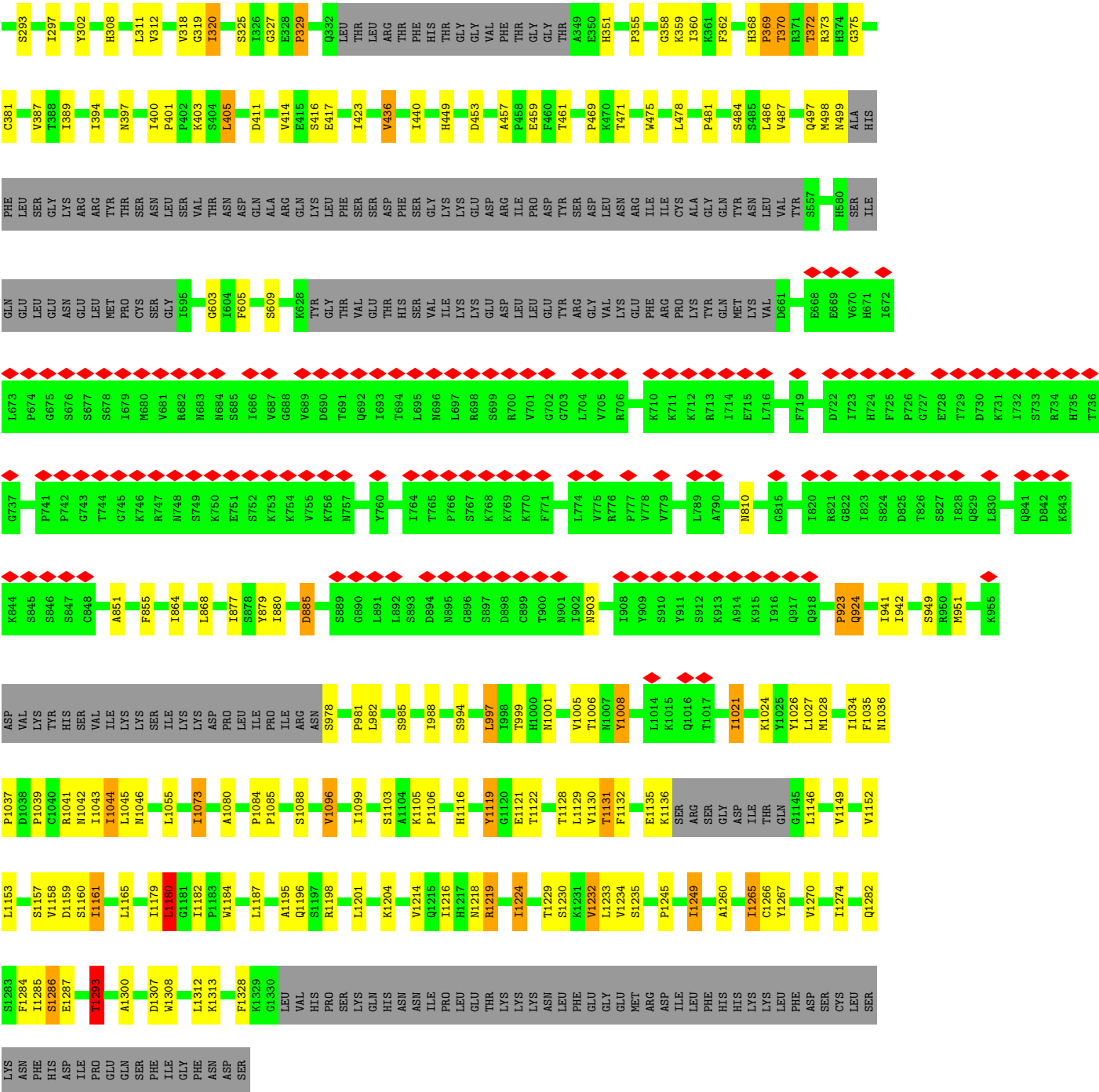


• Molecule 3: DNA-directed RNA polymerase subunit gamma



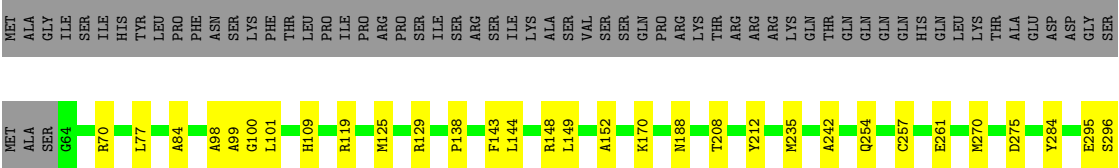
• Molecule 4: DNA-directed RNA polymerase subunit beta"





• Molecule 5: PAP1(pTAC3)

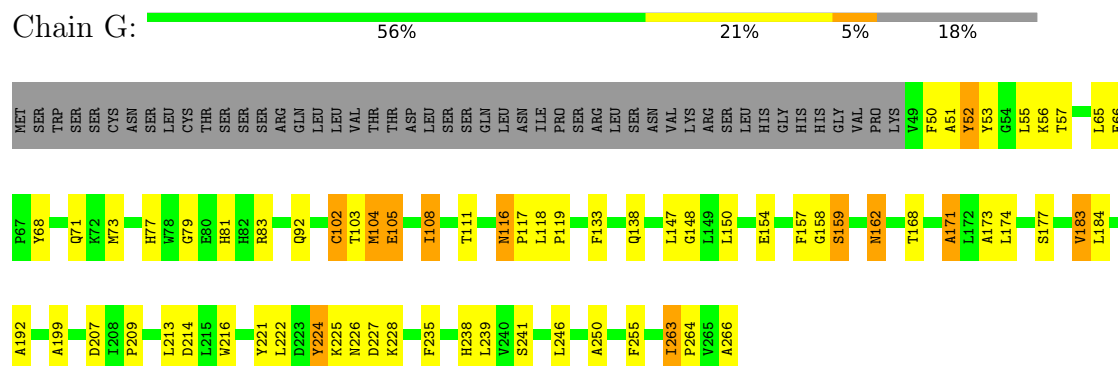
Chain D:



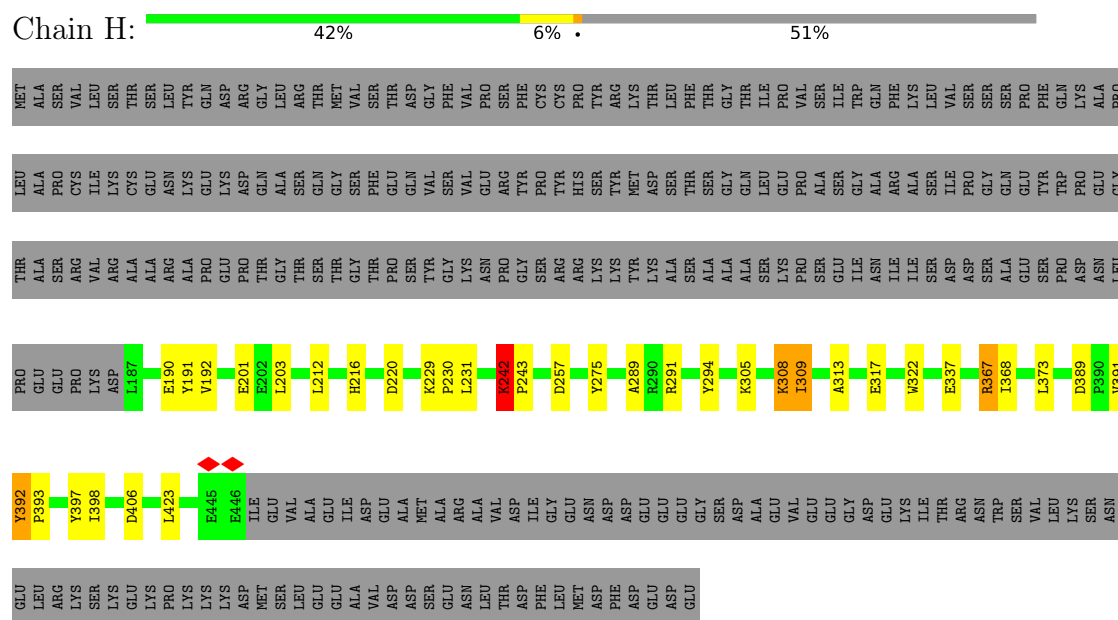




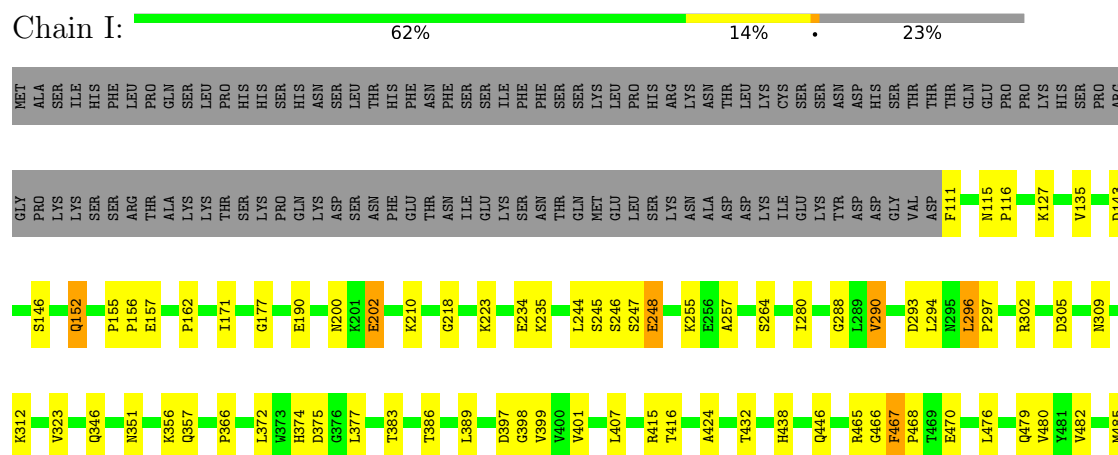
- Molecule 8: superoxide dismutase



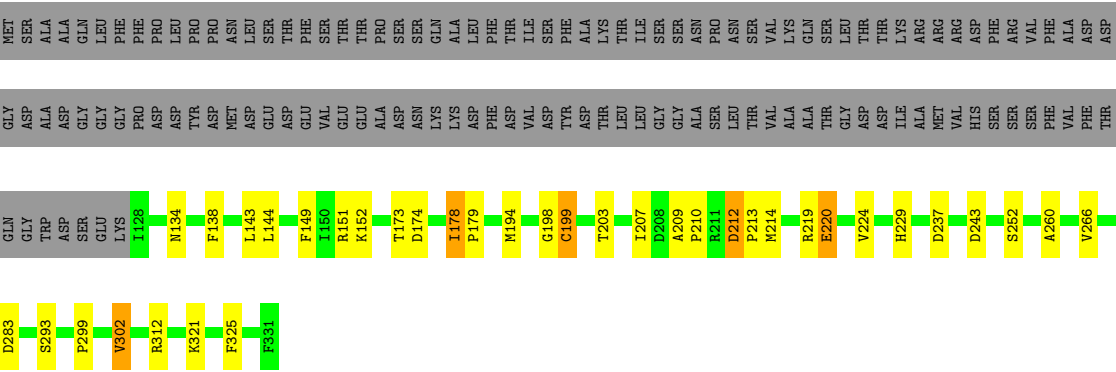
- Molecule 9: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like



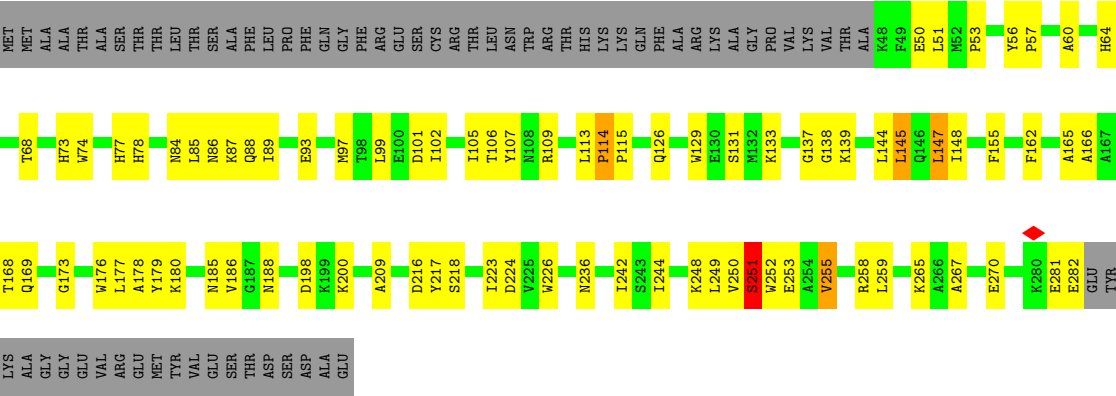
- Molecule 10: Fructokinase-like 1, chloroplastic



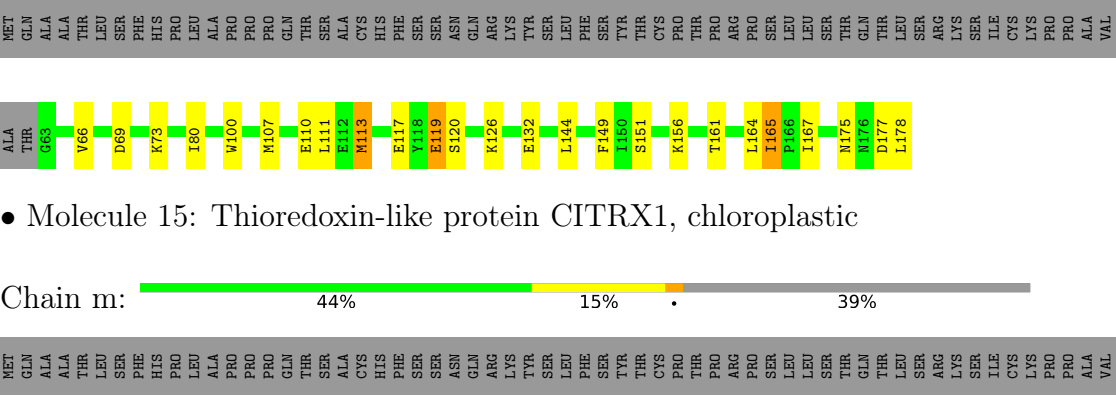




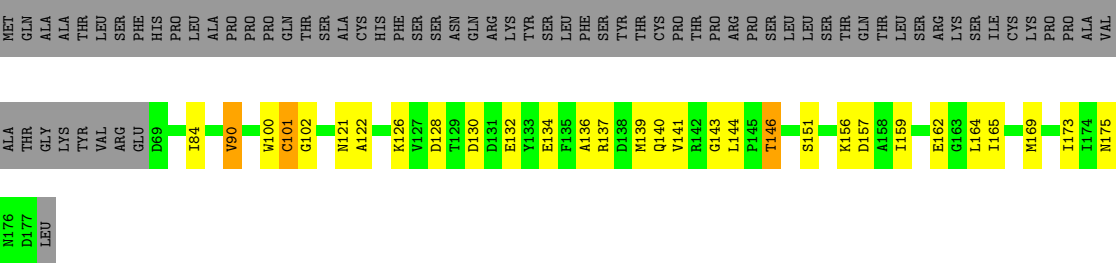
• Molecule 14: superoxide dismutase

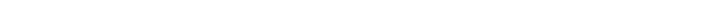


• Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic



• Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic

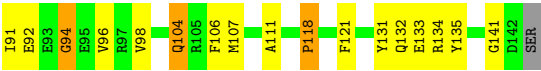
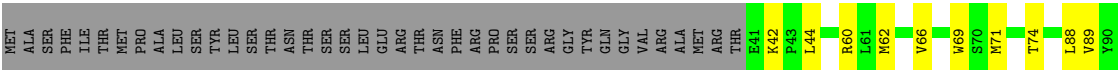


- Chain N:  48% 65% 30%

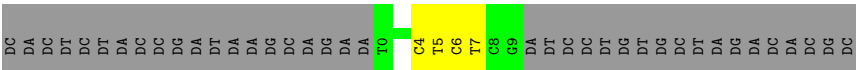




• Molecule 18: PAP13(pTAC18)



• Molecule 19: DNA (48-mer)



• Molecule 20: RNA (20-mer)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 42911                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 56                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.229                                   | Depositor |
| Minimum map value                    | -0.440                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.037                                   | Depositor |
| Recommended contour level            | 0.15                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 444.0, 444.0, 444.0                     | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.74, 0.74, 0.74                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, FE

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     | 1.04         | 0/2199          | 1.21        | 31/2982 (1.0%)   |
| 1   | a     | 1.18         | 7/2422 (0.3%)   | 1.29        | 32/3290 (1.0%)   |
| 2   | B     | 1.18         | 6/7436 (0.1%)   | 1.25        | 102/10090 (1.0%) |
| 3   | C     | 1.06         | 1/4830 (0.0%)   | 1.31        | 76/6586 (1.2%)   |
| 4   | c     | 1.21         | 10/8235 (0.1%)  | 1.23        | 106/11232 (0.9%) |
| 5   | D     | 1.20         | 6/4865 (0.1%)   | 1.20        | 58/6613 (0.9%)   |
| 6   | E     | 0.63         | 1/4549 (0.0%)   | 0.87        | 35/6214 (0.6%)   |
| 7   | F     | 1.19         | 11/4291 (0.3%)  | 1.23        | 57/5825 (1.0%)   |
| 8   | G     | 1.28         | 9/1765 (0.5%)   | 1.33        | 29/2405 (1.2%)   |
| 9   | H     | 1.42         | 5/2156 (0.2%)   | 1.23        | 17/2928 (0.6%)   |
| 10  | I     | 1.34         | 5/2999 (0.2%)   | 1.35        | 53/4063 (1.3%)   |
| 11  | i     | 1.22         | 3/2958 (0.1%)   | 1.30        | 44/4013 (1.1%)   |
| 12  | J     | 1.27         | 8/3445 (0.2%)   | 1.31        | 56/4673 (1.2%)   |
| 13  | K     | 1.33         | 5/1698 (0.3%)   | 1.29        | 21/2298 (0.9%)   |
| 14  | L     | 0.85         | 1/1749 (0.1%)   | 1.27        | 30/2391 (1.3%)   |
| 15  | M     | 1.38         | 2/947 (0.2%)    | 1.37        | 19/1280 (1.5%)   |
| 15  | m     | 1.07         | 0/834           | 1.21        | 11/1134 (1.0%)   |
| 16  | N     | 0.10         | 0/3016          | 0.24        | 0/4170           |
| 17  | O     | 1.45         | 4/776 (0.5%)    | 1.25        | 14/1046 (1.3%)   |
| 18  | P     | 0.93         | 0/784           | 1.38        | 16/1073 (1.5%)   |
| 19  | R     | 0.33         | 0/220           | 0.64        | 0/336            |
| 20  | S     | 0.41         | 0/222           | 0.66        | 0/345            |
| All | All   | 1.14         | 84/62396 (0.1%) | 1.21        | 807/84987 (0.9%) |

All (84) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 7   | F     | 545 | GLU  | CA-C  | -10.08 | 1.41        | 1.53     |
| 3   | C     | 563 | ASN  | CA-C  | -8.28  | 1.44        | 1.53     |
| 8   | G     | 57  | THR  | CA-C  | -7.82  | 1.44        | 1.53     |
| 7   | F     | 533 | ILE  | CA-C  | -7.58  | 1.43        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | I     | 246  | SER  | CA-C  | -6.99 | 1.44        | 1.52     |
| 4   | c     | 1046 | ASN  | CA-C  | -6.87 | 1.45        | 1.52     |
| 4   | c     | 1286 | SER  | CA-C  | -6.83 | 1.43        | 1.52     |
| 13  | K     | 209  | ALA  | CA-C  | -6.55 | 1.46        | 1.52     |
| 7   | F     | 173  | PRO  | CA-C  | -6.53 | 1.48        | 1.51     |
| 1   | a     | 187  | HIS  | C-O   | -6.51 | 1.15        | 1.23     |
| 5   | D     | 370  | TYR  | CA-C  | -6.50 | 1.44        | 1.52     |
| 9   | H     | 242  | LYS  | CA-C  | -6.49 | 1.46        | 1.53     |
| 8   | G     | 104  | MET  | CA-C  | -6.46 | 1.44        | 1.52     |
| 12  | J     | 418  | ALA  | CA-C  | -6.46 | 1.44        | 1.52     |
| 10  | I     | 245  | SER  | CA-C  | -6.33 | 1.44        | 1.52     |
| 4   | c     | 497  | GLN  | CA-C  | -6.20 | 1.45        | 1.52     |
| 17  | O     | 140  | LYS  | CA-C  | -6.20 | 1.46        | 1.53     |
| 4   | c     | 951  | MET  | CA-C  | -6.17 | 1.44        | 1.52     |
| 8   | G     | 105  | GLU  | N-CA  | -6.14 | 1.39        | 1.46     |
| 4   | c     | 351  | HIS  | CA-C  | -6.11 | 1.45        | 1.52     |
| 4   | c     | 26   | LEU  | C-O   | -6.10 | 1.16        | 1.24     |
| 10  | I     | 247  | SER  | CA-C  | -6.08 | 1.44        | 1.52     |
| 7   | F     | 275  | TYR  | CA-C  | -6.08 | 1.46        | 1.52     |
| 2   | B     | 855  | LEU  | CA-C  | -6.06 | 1.44        | 1.52     |
| 9   | H     | 406  | ASP  | CA-C  | -5.90 | 1.45        | 1.52     |
| 2   | B     | 125  | GLN  | C-O   | -5.89 | 1.16        | 1.23     |
| 17  | O     | 86   | ARG  | CA-C  | -5.88 | 1.45        | 1.52     |
| 7   | F     | 383  | GLN  | CA-C  | -5.84 | 1.45        | 1.53     |
| 8   | G     | 235  | PHE  | CA-C  | -5.83 | 1.45        | 1.52     |
| 4   | c     | 351  | HIS  | N-CA  | -5.76 | 1.39        | 1.46     |
| 7   | F     | 173  | PRO  | CA-CB | -5.75 | 1.48        | 1.53     |
| 7   | F     | 385  | LEU  | CA-C  | -5.74 | 1.47        | 1.53     |
| 8   | G     | 108  | ILE  | CA-CB | -5.72 | 1.47        | 1.54     |
| 15  | M     | 165  | ILE  | N-CA  | -5.72 | 1.41        | 1.46     |
| 1   | a     | 203  | ILE  | C-O   | -5.71 | 1.18        | 1.24     |
| 8   | G     | 102  | CYS  | C-O   | -5.70 | 1.16        | 1.23     |
| 1   | a     | 52   | ALA  | C-O   | -5.68 | 1.17        | 1.24     |
| 2   | B     | 639  | ALA  | CA-C  | -5.66 | 1.45        | 1.52     |
| 7   | F     | 80   | LYS  | N-CA  | -5.57 | 1.39        | 1.46     |
| 5   | D     | 376  | ARG  | CA-C  | -5.54 | 1.45        | 1.52     |
| 13  | K     | 134  | ASN  | CA-C  | -5.53 | 1.46        | 1.52     |
| 17  | O     | 78   | ARG  | CA-C  | -5.53 | 1.45        | 1.52     |
| 1   | a     | 174  | ALA  | CA-C  | -5.51 | 1.45        | 1.52     |
| 2   | B     | 659  | TYR  | CA-C  | -5.49 | 1.45        | 1.53     |
| 13  | K     | 243  | ASP  | CA-C  | -5.48 | 1.46        | 1.52     |
| 12  | J     | 349  | ALA  | CA-C  | -5.42 | 1.46        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | D     | 612  | ARG  | CA-C  | -5.40 | 1.45        | 1.52     |
| 8   | G     | 238  | HIS  | CA-CB | -5.37 | 1.46        | 1.54     |
| 12  | J     | 99   | ASP  | CA-C  | -5.34 | 1.47        | 1.53     |
| 14  | L     | 251  | SER  | CA-C  | -5.34 | 1.45        | 1.52     |
| 2   | B     | 930  | GLY  | CA-C  | -5.33 | 1.46        | 1.52     |
| 13  | K     | 237  | ASP  | CA-C  | -5.32 | 1.47        | 1.53     |
| 12  | J     | 278  | CYS  | CA-C  | -5.28 | 1.45        | 1.52     |
| 8   | G     | 171  | ALA  | CA-CB | -5.28 | 1.45        | 1.53     |
| 6   | E     | 721  | ALA  | CA-C  | -5.28 | 1.46        | 1.52     |
| 10  | I     | 146  | SER  | N-CA  | -5.27 | 1.39        | 1.46     |
| 7   | F     | 522  | SER  | CA-C  | -5.27 | 1.46        | 1.52     |
| 5   | D     | 242  | ALA  | CA-C  | -5.27 | 1.46        | 1.53     |
| 11  | i     | 456  | LEU  | CA-C  | -5.26 | 1.47        | 1.53     |
| 17  | O     | 111  | LYS  | CA-C  | -5.26 | 1.46        | 1.52     |
| 1   | a     | 75   | SER  | CA-C  | -5.25 | 1.46        | 1.53     |
| 8   | G     | 263  | ILE  | CA-C  | -5.25 | 1.48        | 1.53     |
| 12  | J     | 120  | GLU  | CA-C  | -5.19 | 1.46        | 1.52     |
| 9   | H     | 392  | TYR  | CA-C  | -5.19 | 1.47        | 1.52     |
| 2   | B     | 502  | ARG  | CA-C  | -5.18 | 1.46        | 1.53     |
| 13  | K     | 209  | ALA  | N-CA  | -5.17 | 1.41        | 1.46     |
| 9   | H     | 220  | ASP  | CA-C  | -5.14 | 1.48        | 1.53     |
| 15  | M     | 120  | SER  | CA-C  | -5.13 | 1.46        | 1.52     |
| 12  | J     | 423  | LEU  | CA-C  | -5.11 | 1.48        | 1.53     |
| 11  | i     | 319  | PHE  | CA-C  | -5.10 | 1.46        | 1.52     |
| 1   | a     | 186  | ILE  | C-O   | -5.10 | 1.18        | 1.24     |
| 4   | c     | 1131 | THR  | CA-C  | -5.08 | 1.46        | 1.52     |
| 7   | F     | 350  | ASN  | CA-C  | -5.08 | 1.46        | 1.52     |
| 1   | a     | 201  | LEU  | C-O   | -5.06 | 1.17        | 1.23     |
| 5   | D     | 109  | HIS  | CA-C  | -5.06 | 1.46        | 1.52     |
| 10  | I     | 246  | SER  | N-CA  | -5.05 | 1.40        | 1.46     |
| 11  | i     | 315  | ASP  | CA-C  | -5.04 | 1.48        | 1.52     |
| 4   | c     | 1001 | ASN  | CA-C  | -5.03 | 1.46        | 1.52     |
| 9   | H     | 192  | VAL  | CA-CB | -5.03 | 1.48        | 1.54     |
| 12  | J     | 328  | GLU  | N-CA  | -5.02 | 1.40        | 1.46     |
| 5   | D     | 284  | TYR  | CA-C  | -5.01 | 1.46        | 1.52     |
| 7   | F     | 112  | ALA  | CA-C  | -5.01 | 1.46        | 1.52     |
| 12  | J     | 329  | VAL  | CA-C  | -5.01 | 1.46        | 1.52     |
| 4   | c     | 126  | ASN  | CA-C  | -5.00 | 1.48        | 1.53     |

All (807) bond angle outliers are listed below:

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 3   | C     | 102  | VAL  | N-CA-C | 16.22  | 126.00      | 110.42   |
| 2   | B     | 1011 | ASP  | N-CA-C | 13.71  | 130.00      | 111.90   |
| 3   | C     | 393  | VAL  | N-CA-C | 13.38  | 124.27      | 110.62   |
| 3   | C     | 530  | ALA  | N-CA-C | 12.25  | 124.18      | 111.07   |
| 10  | I     | 346  | GLN  | N-CA-C | 11.90  | 124.00      | 111.14   |
| 1   | a     | 68   | GLU  | N-CA-C | 11.52  | 123.58      | 111.14   |
| 8   | G     | 57   | THR  | CA-C-N | -11.12 | 111.54      | 119.66   |
| 8   | G     | 57   | THR  | C-N-CA | -11.12 | 111.54      | 119.66   |
| 15  | M     | 119  | GLU  | N-CA-C | 11.04  | 123.06      | 111.14   |
| 15  | M     | 177  | ASP  | N-CA-C | 10.93  | 123.28      | 111.36   |
| 11  | i     | 378  | THR  | N-CA-C | 10.89  | 122.73      | 111.07   |
| 14  | L     | 107  | TYR  | N-CA-C | -10.84 | 99.47       | 111.28   |
| 2   | B     | 937  | GLU  | N-CA-C | 10.77  | 123.02      | 111.28   |
| 4   | c     | 233  | GLY  | N-CA-C | -10.68 | 91.91       | 111.14   |
| 18  | P     | 91   | ILE  | N-CA-C | 10.62  | 121.46      | 110.62   |
| 2   | B     | 911  | THR  | N-CA-C | -10.62 | 91.97       | 109.07   |
| 8   | G     | 52   | TYR  | N-CA-C | -10.52 | 98.77       | 112.24   |
| 3   | C     | 508  | LEU  | N-CA-C | 10.45  | 122.75      | 111.36   |
| 10  | I     | 127  | LYS  | N-CA-C | 10.44  | 122.42      | 111.14   |
| 1   | a     | 263  | ASN  | N-CA-C | 10.43  | 122.41      | 111.14   |
| 7   | F     | 412  | ILE  | N-CA-C | 10.41  | 121.23      | 110.72   |
| 6   | E     | 364  | ASP  | N-CA-C | -10.33 | 100.99      | 114.31   |
| 2   | B     | 91   | SER  | N-CA-C | 10.28  | 122.56      | 111.36   |
| 10  | I     | 467  | PHE  | N-CA-C | -10.22 | 96.21       | 110.31   |
| 6   | E     | 365  | GLN  | N-CA-C | -10.11 | 100.33      | 111.36   |
| 10  | I     | 115  | ASN  | N-CA-C | 9.94   | 127.28      | 113.16   |
| 1   | a     | 39   | LYS  | N-CA-C | 9.86   | 121.61      | 111.07   |
| 10  | I     | 416  | THR  | N-CA-C | 9.85   | 123.25      | 111.33   |
| 4   | c     | 988  | ILE  | N-CA-C | 9.84   | 121.94      | 108.17   |
| 11  | i     | 508  | SER  | N-CA-C | -9.66  | 100.83      | 111.36   |
| 1   | A     | 63   | THR  | N-CA-C | 9.63   | 121.86      | 111.36   |
| 5   | D     | 257  | CYS  | N-CA-C | 9.62   | 121.85      | 111.36   |
| 7   | F     | 369  | GLU  | N-CA-C | 9.60   | 121.75      | 111.28   |
| 2   | B     | 351  | THR  | N-CA-C | -9.59  | 95.83       | 110.32   |
| 1   | a     | 131  | ASP  | N-CA-C | 9.58   | 121.49      | 111.14   |
| 2   | B     | 968  | LEU  | N-CA-C | 9.48   | 121.38      | 111.14   |
| 4   | c     | 327  | GLY  | N-CA-C | 9.44   | 124.86      | 112.77   |
| 14  | L     | 198  | ASP  | N-CA-C | -9.45  | 100.98      | 111.28   |
| 3   | C     | 166  | ARG  | N-CA-C | 9.42   | 122.93      | 110.88   |
| 9   | H     | 398  | ILE  | N-CA-C | 9.36   | 121.00      | 109.30   |
| 2   | B     | 9    | ILE  | N-CA-C | -9.34  | 94.35       | 107.99   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 190 | GLY  | N-CA-C | -9.34 | 100.82      | 112.77   |
| 2   | B     | 522 | GLN  | N-CA-C | 9.32  | 121.44      | 111.28   |
| 12  | J     | 109 | ARG  | N-CA-C | -9.30 | 98.54       | 110.53   |
| 6   | E     | 304 | GLU  | N-CA-C | 9.25  | 121.44      | 111.36   |
| 3   | C     | 539 | THR  | N-CA-C | 9.19  | 124.49      | 112.72   |
| 10  | I     | 246 | SER  | N-CA-C | 9.19  | 120.91      | 111.07   |
| 2   | B     | 957 | LYS  | N-CA-C | 9.15  | 121.34      | 111.36   |
| 1   | a     | 267 | ILE  | N-CA-C | -9.12 | 104.59      | 113.53   |
| 17  | O     | 110 | ALA  | N-CA-C | -9.07 | 102.61      | 114.31   |
| 12  | J     | 347 | TYR  | N-CA-C | 9.06  | 121.16      | 111.28   |
| 2   | B     | 424 | ILE  | N-CA-C | 9.01  | 119.82      | 110.72   |
| 5   | D     | 270 | MET  | N-CA-C | 8.99  | 121.16      | 111.36   |
| 12  | J     | 382 | LEU  | N-CA-C | 8.96  | 120.82      | 111.14   |
| 2   | B     | 799 | TYR  | N-CA-C | -8.96 | 96.75       | 110.10   |
| 12  | J     | 422 | THR  | N-CA-C | 8.94  | 121.10      | 111.36   |
| 7   | F     | 177 | TRP  | CA-C-N | -8.93 | 111.18      | 120.38   |
| 7   | F     | 177 | TRP  | C-N-CA | -8.93 | 111.18      | 120.38   |
| 8   | G     | 199 | ALA  | N-CA-C | 8.92  | 121.97      | 111.71   |
| 5   | D     | 296 | SER  | N-CA-C | 8.89  | 125.78      | 114.31   |
| 3   | C     | 85  | GLY  | N-CA-C | -8.84 | 102.27      | 114.64   |
| 4   | c     | 281 | GLN  | N-CA-C | 8.83  | 124.19      | 112.35   |
| 4   | c     | 603 | GLY  | N-CA-C | -8.81 | 103.17      | 115.32   |
| 11  | i     | 349 | ASP  | N-CA-C | -8.80 | 102.09      | 112.92   |
| 11  | i     | 547 | SER  | N-CA-C | 8.72  | 120.17      | 107.88   |
| 7   | F     | 309 | ARG  | N-CA-C | 8.71  | 123.22      | 108.67   |
| 10  | I     | 312 | LYS  | N-CA-C | 8.71  | 120.39      | 111.07   |
| 12  | J     | 157 | LEU  | N-CA-C | 8.70  | 125.51      | 113.16   |
| 4   | c     | 102 | GLU  | N-CA-C | 8.68  | 120.82      | 111.36   |
| 12  | J     | 157 | LEU  | CA-C-N | -8.65 | 110.81      | 119.90   |
| 12  | J     | 157 | LEU  | C-N-CA | -8.65 | 110.81      | 119.90   |
| 10  | I     | 465 | ARG  | N-CA-C | -8.64 | 98.31       | 110.50   |
| 18  | P     | 94  | GLY  | N-CA-C | 8.61  | 121.44      | 111.36   |
| 15  | M     | 151 | SER  | N-CA-C | 8.60  | 121.88      | 110.36   |
| 5   | D     | 84  | ALA  | N-CA-C | 8.60  | 123.35      | 111.74   |
| 7   | F     | 107 | GLU  | N-CA-C | 8.59  | 120.64      | 111.28   |
| 1   | a     | 330 | ILE  | N-CA-C | 8.59  | 121.99      | 109.63   |
| 1   | A     | 193 | ASN  | N-CA-C | 8.57  | 120.62      | 111.28   |
| 2   | B     | 406 | ALA  | N-CA-C | 8.57  | 122.66      | 110.23   |
| 3   | C     | 480 | GLY  | N-CA-C | -8.57 | 103.42      | 112.08   |
| 12  | J     | 185 | SER  | N-CA-C | -8.55 | 103.28      | 114.31   |
| 11  | i     | 276 | TRP  | CA-C-N | -8.52 | 111.60      | 120.38   |
| 11  | i     | 276 | TRP  | C-N-CA | -8.52 | 111.60      | 120.38   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 100  | LEU  | N-CA-C | 8.50  | 122.56      | 110.23   |
| 1   | a     | 126  | TYR  | N-CA-C | 8.48  | 120.61      | 111.36   |
| 18  | P     | 141  | GLY  | N-CA-C | -8.38 | 96.95       | 112.37   |
| 4   | c     | 93   | ALA  | N-CA-C | 8.37  | 120.40      | 111.28   |
| 10  | I     | 235  | LYS  | N-CA-C | 8.34  | 120.45      | 111.36   |
| 6   | E     | 452  | SER  | N-CA-C | 8.32  | 120.13      | 111.14   |
| 3   | C     | 368  | GLU  | N-CA-C | 8.31  | 122.58      | 110.28   |
| 9   | H     | 337  | GLU  | N-CA-C | 8.30  | 120.41      | 111.36   |
| 8   | G     | 255  | PHE  | N-CA-C | 8.28  | 120.38      | 111.36   |
| 4   | c     | 147  | VAL  | N-CA-C | 8.26  | 120.83      | 112.90   |
| 2   | B     | 981  | GLY  | N-CA-C | 8.23  | 125.20      | 112.60   |
| 4   | c     | 1293 | THR  | N-CA-C | 8.21  | 120.23      | 111.28   |
| 11  | i     | 417  | ALA  | N-CA-C | 8.21  | 122.42      | 110.28   |
| 15  | M     | 144  | LEU  | N-CA-C | 8.21  | 127.95      | 109.81   |
| 10  | I     | 111  | PHE  | CA-C-N | -8.13 | 112.47      | 120.52   |
| 10  | I     | 111  | PHE  | C-N-CA | -8.13 | 112.47      | 120.52   |
| 1   | a     | 329  | VAL  | N-CA-C | 8.13  | 118.93      | 110.72   |
| 13  | K     | 293  | SER  | N-CA-C | 8.12  | 119.76      | 111.07   |
| 4   | c     | 461  | THR  | N-CA-C | 8.12  | 120.14      | 111.28   |
| 4   | c     | 1312 | LEU  | N-CA-C | 8.11  | 119.90      | 111.14   |
| 4   | c     | 54   | SER  | N-CA-C | 8.09  | 122.85      | 111.52   |
| 6   | E     | 720  | THR  | N-CA-C | 8.08  | 120.08      | 111.28   |
| 6   | E     | 421  | GLU  | N-CA-C | 8.07  | 119.70      | 111.07   |
| 4   | c     | 132  | SER  | N-CA-C | 8.06  | 119.85      | 111.14   |
| 5   | D     | 733  | LEU  | N-CA-C | 8.06  | 120.06      | 111.28   |
| 17  | O     | 103  | ASN  | N-CA-C | 8.05  | 120.13      | 111.36   |
| 12  | J     | 314  | PRO  | N-CA-C | 8.04  | 123.65      | 110.55   |
| 4   | c     | 244  | LEU  | N-CA-C | 8.03  | 121.13      | 111.82   |
| 10  | I     | 432  | THR  | N-CA-C | 7.96  | 120.04      | 111.36   |
| 13  | K     | 174  | ASP  | N-CA-C | 7.95  | 122.67      | 111.30   |
| 3   | C     | 175  | ILE  | N-CA-C | -7.95 | 104.82      | 112.29   |
| 3   | C     | 522  | SER  | N-CA-C | 7.94  | 119.93      | 111.28   |
| 4   | c     | 13   | ALA  | N-CA-C | 7.93  | 120.83      | 110.43   |
| 6   | E     | 294  | GLU  | N-CA-C | -7.93 | 101.36      | 113.89   |
| 9   | H     | 275  | TYR  | N-CA-C | -7.93 | 98.07       | 109.96   |
| 10  | I     | 356  | LYS  | N-CA-C | 7.91  | 123.09      | 112.88   |
| 1   | A     | 23   | ASP  | N-CA-C | 7.91  | 119.98      | 111.36   |
| 12  | J     | 378  | ALA  | N-CA-C | 7.88  | 121.65      | 110.23   |
| 6   | E     | 777  | SER  | N-CA-C | 7.84  | 121.38      | 109.62   |
| 12  | J     | 139  | ALA  | N-CA-C | 7.82  | 120.99      | 110.35   |
| 5   | D     | 346  | GLY  | N-CA-C | 7.82  | 122.78      | 112.77   |
| 4   | c     | 484  | SER  | N-CA-C | 7.81  | 122.14      | 109.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | J     | 316 | CYS  | N-CA-C  | 7.81  | 121.28      | 109.41   |
| 8   | G     | 173 | ALA  | N-CA-C  | 7.80  | 119.78      | 111.28   |
| 15  | m     | 140 | GLN  | N-CA-C  | 7.78  | 122.25      | 111.74   |
| 3   | C     | 273 | LEU  | N-CA-C  | 7.77  | 121.18      | 108.52   |
| 3   | C     | 645 | TYR  | N-CA-C  | 7.69  | 121.07      | 108.99   |
| 3   | C     | 617 | ASP  | N-CA-C  | 7.67  | 122.13      | 108.24   |
| 7   | F     | 380 | CYS  | N-CA-C  | 7.61  | 119.66      | 111.36   |
| 6   | E     | 326 | GLY  | N-CA-C  | -7.59 | 103.39      | 115.08   |
| 7   | F     | 179 | PRO  | N-CA-C  | -7.58 | 99.28       | 111.19   |
| 11  | i     | 375 | LYS  | N-CA-C  | 7.58  | 119.62      | 111.36   |
| 1   | a     | 333 | ALA  | N-CA-C  | -7.58 | 101.91      | 113.89   |
| 10  | I     | 288 | GLY  | N-CA-C  | 7.56  | 122.21      | 112.54   |
| 15  | M     | 100 | TRP  | N-CA-C  | 7.55  | 119.51      | 111.28   |
| 7   | F     | 104 | SER  | N-CA-C  | 7.54  | 119.58      | 111.36   |
| 12  | J     | 164 | ASP  | N-CA-C  | 7.54  | 121.92      | 111.74   |
| 10  | I     | 398 | GLY  | N-CA-C  | 7.54  | 120.72      | 110.69   |
| 5   | D     | 406 | ARG  | N-CA-C  | -7.53 | 97.72       | 109.25   |
| 12  | J     | 158 | PRO  | N-CA-C  | -7.53 | 99.43       | 110.80   |
| 3   | C     | 343 | LEU  | N-CA-C  | 7.52  | 119.26      | 111.14   |
| 3   | C     | 204 | GLY  | N-CA-C  | -7.52 | 103.71      | 112.73   |
| 1   | A     | 78  | THR  | CB-CA-C | -7.51 | 107.91      | 116.54   |
| 10  | I     | 157 | GLU  | N-CA-C  | 7.49  | 119.45      | 111.28   |
| 7   | F     | 103 | LYS  | N-CA-C  | 7.48  | 119.51      | 111.36   |
| 14  | L     | 186 | VAL  | N-CA-C  | 7.48  | 118.37      | 107.75   |
| 8   | G     | 108 | ILE  | CB-CA-C | -7.47 | 102.41      | 111.97   |
| 11  | i     | 606 | ASP  | N-CA-C  | 7.45  | 119.40      | 111.28   |
| 9   | H     | 294 | TYR  | N-CA-C  | 7.45  | 119.48      | 111.36   |
| 3   | C     | 123 | VAL  | N-CA-C  | 7.45  | 118.24      | 110.72   |
| 4   | c     | 319 | GLY  | N-CA-C  | 7.45  | 121.66      | 112.73   |
| 3   | C     | 642 | TYR  | N-CA-C  | -7.44 | 99.21       | 110.14   |
| 10  | I     | 115 | ASN  | CA-C-N  | -7.42 | 112.74      | 120.38   |
| 10  | I     | 115 | ASN  | C-N-CA  | -7.42 | 112.74      | 120.38   |
| 6   | E     | 715 | PRO  | N-CA-C  | 7.41  | 124.07      | 113.47   |
| 18  | P     | 104 | GLN  | N-CA-C  | -7.38 | 103.35      | 112.88   |
| 11  | i     | 374 | SER  | N-CA-C  | 7.37  | 119.10      | 111.14   |
| 7   | F     | 125 | LEU  | N-CA-C  | -7.35 | 104.30      | 113.20   |
| 6   | E     | 774 | THR  | N-CA-C  | 7.35  | 119.37      | 111.36   |
| 6   | E     | 362 | ARG  | N-CA-C  | -7.35 | 103.27      | 111.28   |
| 3   | C     | 101 | PHE  | N-CA-C  | 7.34  | 121.34      | 112.38   |
| 3   | C     | 367 | ILE  | N-CA-C  | 7.33  | 118.12      | 110.72   |
| 7   | F     | 164 | ALA  | N-CA-C  | 7.33  | 120.70      | 111.69   |
| 5   | D     | 152 | ALA  | N-CA-C  | -7.32 | 103.24      | 111.07   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 356  | VAL  | N-CA-C  | 7.31  | 118.40      | 108.17   |
| 4   | c     | 358  | GLY  | N-CA-C  | 7.31  | 121.70      | 110.88   |
| 12  | J     | 182  | GLU  | N-CA-C  | 7.30  | 120.67      | 111.69   |
| 11  | i     | 641  | TYR  | N-CA-C  | 7.30  | 119.24      | 111.28   |
| 17  | O     | 139  | PHE  | N-CA-C  | 7.29  | 121.03      | 112.72   |
| 14  | L     | 114  | PRO  | N-CA-C  | 7.28  | 119.58      | 110.70   |
| 5   | D     | 765  | GLU  | N-CA-C  | 7.27  | 119.21      | 111.28   |
| 2   | B     | 593  | ASP  | N-CA-C  | 7.27  | 119.28      | 111.36   |
| 2   | B     | 964  | GLY  | N-CA-C  | 7.26  | 125.18      | 112.83   |
| 11  | i     | 527  | LYS  | N-CA-C  | 7.24  | 119.25      | 111.36   |
| 14  | L     | 113  | LEU  | CA-C-N  | -7.24 | 112.92      | 120.38   |
| 14  | L     | 113  | LEU  | C-N-CA  | -7.24 | 112.92      | 120.38   |
| 3   | C     | 634  | SER  | N-CA-C  | 7.24  | 119.17      | 111.28   |
| 2   | B     | 849  | ASP  | N-CA-C  | 7.23  | 119.24      | 111.36   |
| 11  | i     | 580  | THR  | N-CA-C  | 7.23  | 119.24      | 111.36   |
| 14  | L     | 249  | LEU  | N-CA-C  | 7.21  | 122.82      | 109.56   |
| 7   | F     | 251  | GLN  | N-CA-C  | 7.19  | 118.90      | 111.14   |
| 4   | c     | 369  | PRO  | N-CA-C  | 7.17  | 122.32      | 111.14   |
| 3   | C     | 50   | PHE  | CB-CA-C | -7.16 | 108.33      | 116.63   |
| 11  | i     | 478  | ALA  | N-CA-C  | 7.16  | 120.91      | 109.24   |
| 6   | E     | 420  | TYR  | N-CA-C  | -7.14 | 103.58      | 111.36   |
| 2   | B     | 1035 | ALA  | CA-C-N  | -7.13 | 113.46      | 120.52   |
| 2   | B     | 1035 | ALA  | C-N-CA  | -7.13 | 113.46      | 120.52   |
| 2   | B     | 460  | ARG  | N-CA-C  | -7.13 | 98.19       | 108.60   |
| 4   | c     | 478  | LEU  | N-CA-C  | 7.12  | 121.29      | 109.46   |
| 3   | C     | 453  | GLN  | N-CA-C  | 7.10  | 119.02      | 111.28   |
| 5   | D     | 768  | ILE  | N-CA-C  | 7.09  | 117.85      | 110.62   |
| 4   | c     | 1265 | ILE  | N-CA-C  | -7.08 | 98.26       | 108.17   |
| 6   | E     | 716  | GLY  | N-CA-C  | 7.08  | 121.22      | 112.73   |
| 5   | D     | 485  | HIS  | N-CA-C  | -7.08 | 103.57      | 111.28   |
| 10  | I     | 177  | GLY  | N-CA-C  | -7.06 | 102.72      | 112.18   |
| 11  | i     | 389  | GLY  | N-CA-C  | -7.05 | 105.34      | 115.64   |
| 3   | C     | 462  | ALA  | N-CA-C  | 7.02  | 122.30      | 112.75   |
| 6   | E     | 695  | PHE  | CA-C-N  | -7.02 | 113.01      | 120.66   |
| 6   | E     | 695  | PHE  | C-N-CA  | -7.02 | 113.01      | 120.66   |
| 11  | i     | 364  | LYS  | N-CA-C  | 7.01  | 121.20      | 111.74   |
| 4   | c     | 1055 | LEU  | N-CA-C  | 7.00  | 121.53      | 112.92   |
| 12  | J     | 404  | LEU  | N-CA-C  | -6.98 | 103.43      | 112.23   |
| 7   | F     | 181  | GLY  | N-CA-C  | 6.98  | 125.27      | 115.43   |
| 11  | i     | 312  | ALA  | N-CA-C  | 6.97  | 121.87      | 112.88   |
| 15  | M     | 117  | GLU  | N-CA-C  | 6.97  | 118.95      | 111.36   |
| 7   | F     | 165  | GLY  | CA-C-N  | -6.96 | 113.52      | 120.21   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7   | F     | 165  | GLY  | C-N-CA | -6.96 | 113.52      | 120.21   |
| 2   | B     | 985  | VAL  | N-CA-C | -6.96 | 97.71       | 107.80   |
| 1   | A     | 119  | GLN  | N-CA-C | 6.91  | 121.02      | 111.90   |
| 1   | a     | 268  | ALA  | N-CA-C | -6.89 | 104.13      | 112.54   |
| 10  | I     | 466  | GLY  | N-CA-C | 6.88  | 126.15      | 113.76   |
| 3   | C     | 586  | GLU  | N-CA-C | 6.88  | 122.93      | 113.16   |
| 2   | B     | 198  | VAL  | N-CA-C | 6.88  | 118.49      | 108.58   |
| 4   | c     | 885  | ASP  | N-CA-C | 6.87  | 119.56      | 110.08   |
| 4   | c     | 375  | GLY  | N-CA-C | 6.86  | 125.10      | 115.43   |
| 4   | c     | 903  | ASN  | CA-C-N | -6.85 | 111.44      | 119.05   |
| 4   | c     | 903  | ASN  | C-N-CA | -6.85 | 111.44      | 119.05   |
| 8   | G     | 147  | LEU  | N-CA-C | 6.85  | 118.72      | 108.31   |
| 7   | F     | 395  | GLU  | N-CA-C | -6.84 | 103.83      | 111.28   |
| 2   | B     | 449  | SER  | N-CA-C | 6.83  | 119.63      | 110.35   |
| 9   | H     | 191  | TYR  | N-CA-C | 6.83  | 118.72      | 111.28   |
| 12  | J     | 377  | ASP  | N-CA-C | 6.82  | 118.80      | 111.36   |
| 4   | c     | 994  | SER  | N-CA-C | -6.82 | 105.29      | 112.93   |
| 10  | I     | 190  | GLU  | N-CA-C | 6.82  | 118.71      | 111.28   |
| 2   | B     | 370  | GLY  | N-CA-C | 6.82  | 121.50      | 112.77   |
| 3   | C     | 99   | VAL  | N-CA-C | 6.82  | 117.67      | 111.81   |
| 17  | O     | 77   | HIS  | N-CA-C | 6.81  | 118.71      | 111.28   |
| 14  | L     | 139  | LYS  | CA-C-N | -6.81 | 112.75      | 119.76   |
| 14  | L     | 139  | LYS  | C-N-CA | -6.81 | 112.75      | 119.76   |
| 2   | B     | 681  | ASP  | N-CA-C | 6.80  | 120.92      | 111.74   |
| 5   | D     | 381  | VAL  | N-CA-C | -6.79 | 103.69      | 110.62   |
| 11  | i     | 276  | TRP  | N-CA-C | 6.79  | 121.45      | 112.35   |
| 3   | C     | 31   | ALA  | N-CA-C | 6.78  | 121.21      | 112.26   |
| 12  | J     | 322  | PHE  | N-CA-C | 6.78  | 118.75      | 111.36   |
| 4   | c     | 1195 | ALA  | N-CA-C | 6.78  | 118.32      | 111.07   |
| 4   | c     | 1260 | ALA  | N-CA-C | 6.78  | 118.75      | 111.36   |
| 4   | c     | 880  | ILE  | N-CA-C | -6.77 | 103.89      | 110.72   |
| 18  | P     | 135  | TYR  | N-CA-C | 6.76  | 120.19      | 108.76   |
| 1   | a     | 264  | LYS  | N-CA-C | 6.76  | 120.55      | 109.06   |
| 5   | D     | 459  | PRO  | N-CA-C | -6.75 | 105.42      | 113.86   |
| 4   | c     | 121  | MET  | N-CA-C | 6.74  | 119.98      | 111.69   |
| 7   | F     | 555  | PHE  | N-CA-C | -6.74 | 99.86       | 109.96   |
| 4   | c     | 1080 | ALA  | N-CA-C | -6.73 | 98.77       | 108.60   |
| 5   | D     | 405  | SER  | N-CA-C | -6.73 | 103.94      | 111.28   |
| 3   | C     | 127  | LYS  | N-CA-C | 6.73  | 118.61      | 111.28   |
| 1   | A     | 130  | VAL  | N-CA-C | 6.72  | 117.50      | 110.72   |
| 10  | I     | 155  | PRO  | N-CA-C | 6.72  | 118.89      | 110.70   |
| 14  | L     | 93   | GLU  | N-CA-C | -6.71 | 104.04      | 111.82   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8   | G     | 238  | HIS  | N-CA-C | 6.71  | 123.44      | 114.12   |
| 2   | B     | 594  | LYS  | N-CA-C | 6.70  | 119.36      | 109.24   |
| 10  | I     | 372  | LEU  | N-CA-C | 6.69  | 121.60      | 113.17   |
| 8   | G     | 183  | VAL  | N-CA-C | 6.69  | 116.98      | 108.82   |
| 2   | B     | 270  | LEU  | N-CA-C | -6.69 | 97.62       | 108.52   |
| 4   | c     | 423  | ILE  | N-CA-C | 6.68  | 116.81      | 110.53   |
| 2   | B     | 922  | PRO  | N-CA-C | 6.67  | 121.30      | 111.03   |
| 4   | c     | 151  | GLY  | N-CA-C | 6.66  | 124.15      | 112.83   |
| 4   | c     | 401  | PRO  | N-CA-C | 6.66  | 118.83      | 110.70   |
| 13  | K     | 212  | ASP  | N-CA-C | 6.66  | 117.26      | 109.60   |
| 12  | J     | 326  | MET  | N-CA-C | 6.65  | 120.01      | 109.50   |
| 4   | c     | 951  | MET  | N-CA-C | 6.64  | 118.52      | 111.28   |
| 4   | c     | 308  | HIS  | N-CA-C | 6.63  | 120.98      | 113.02   |
| 3   | C     | 369  | GLY  | N-CA-C | 6.62  | 124.76      | 112.77   |
| 11  | i     | 273  | SER  | N-CA-C | 6.62  | 123.55      | 113.61   |
| 12  | J     | 367  | ASN  | N-CA-C | -6.62 | 98.09       | 109.15   |
| 5   | D     | 410  | THR  | N-CA-C | -6.62 | 98.67       | 108.79   |
| 7   | F     | 410  | TRP  | N-CA-C | -6.61 | 104.07      | 111.28   |
| 7   | F     | 545  | GLU  | CA-C-N | -6.61 | 111.57      | 119.84   |
| 7   | F     | 545  | GLU  | C-N-CA | -6.61 | 111.57      | 119.84   |
| 8   | G     | 104  | MET  | N-CA-C | -6.61 | 104.08      | 111.28   |
| 7   | F     | 543  | LEU  | N-CA-C | 6.59  | 118.55      | 111.36   |
| 4   | c     | 211  | GLN  | N-CA-C | -6.57 | 105.27      | 113.55   |
| 5   | D     | 170  | LYS  | N-CA-C | 6.57  | 120.23      | 111.30   |
| 5   | D     | 383  | LEU  | N-CA-C | -6.56 | 104.12      | 111.28   |
| 3   | C     | 298  | ASP  | N-CA-C | -6.56 | 104.54      | 112.54   |
| 4   | c     | 1096 | VAL  | N-CA-C | 6.55  | 117.30      | 110.62   |
| 13  | K     | 220  | GLU  | N-CA-C | 6.55  | 120.28      | 111.24   |
| 17  | O     | 83   | GLU  | N-CA-C | 6.54  | 119.81      | 108.76   |
| 8   | G     | 148  | GLY  | N-CA-C | 6.54  | 120.57      | 112.73   |
| 11  | i     | 456  | LEU  | CA-C-N | -6.54 | 113.99      | 120.98   |
| 11  | i     | 456  | LEU  | C-N-CA | -6.54 | 113.99      | 120.98   |
| 7   | F     | 308  | LYS  | N-CA-C | 6.51  | 120.13      | 109.06   |
| 6   | E     | 277  | VAL  | N-CA-C | 6.51  | 116.76      | 111.62   |
| 4   | c     | 877  | ILE  | N-CA-C | 6.50  | 117.29      | 110.72   |
| 2   | B     | 518  | ILE  | N-CA-C | 6.50  | 121.03      | 113.42   |
| 7   | F     | 533  | ILE  | N-CA-C | -6.50 | 104.18      | 110.42   |
| 2   | B     | 403  | GLY  | N-CA-C | 6.50  | 120.53      | 112.73   |
| 9   | H     | 397  | TYR  | N-CA-C | 6.48  | 118.42      | 111.36   |
| 4   | c     | 161  | ILE  | N-CA-C | 6.46  | 121.86      | 113.07   |
| 11  | i     | 460  | LEU  | N-CA-C | 6.46  | 120.84      | 113.15   |
| 2   | B     | 143  | ILE  | N-CA-C | 6.46  | 117.91      | 109.58   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 11  | i     | 506  | ASP  | N-CA-C | 6.45  | 123.29      | 113.61   |
| 15  | m     | 144  | LEU  | N-CA-C | 6.45  | 122.31      | 113.16   |
| 5   | D     | 254  | GLN  | N-CA-C | 6.44  | 118.38      | 111.36   |
| 5   | D     | 455  | THR  | N-CA-C | -6.44 | 99.09       | 109.40   |
| 10  | I     | 480  | VAL  | N-CA-C | 6.44  | 117.22      | 110.72   |
| 8   | G     | 105  | GLU  | N-CA-C | -6.43 | 104.28      | 111.28   |
| 4   | c     | 1285 | ILE  | N-CA-C | 6.42  | 117.10      | 110.36   |
| 8   | G     | 116  | ASN  | CA-C-N | -6.42 | 113.35      | 119.90   |
| 8   | G     | 116  | ASN  | C-N-CA | -6.42 | 113.35      | 119.90   |
| 12  | J     | 423  | LEU  | CA-C-N | -6.42 | 113.34      | 119.76   |
| 12  | J     | 423  | LEU  | C-N-CA | -6.42 | 113.34      | 119.76   |
| 1   | a     | 112  | GLY  | CA-C-N | -6.42 | 113.34      | 119.76   |
| 1   | a     | 112  | GLY  | C-N-CA | -6.42 | 113.34      | 119.76   |
| 15  | M     | 126  | LYS  | N-CA-C | 6.41  | 119.85      | 109.40   |
| 13  | K     | 283  | ASP  | N-CA-C | 6.41  | 120.49      | 111.52   |
| 13  | K     | 178  | ILE  | N-CA-C | 6.40  | 114.13      | 108.63   |
| 1   | a     | 313  | ARG  | N-CA-C | 6.39  | 118.39      | 109.31   |
| 5   | D     | 497  | GLY  | N-CA-C | 6.38  | 125.35      | 112.34   |
| 8   | G     | 55   | LEU  | N-CA-C | -6.38 | 98.80       | 109.07   |
| 2   | B     | 962  | SER  | N-CA-C | -6.38 | 98.22       | 109.06   |
| 10  | I     | 255  | LYS  | N-CA-C | 6.37  | 118.23      | 111.28   |
| 12  | J     | 323  | LYS  | N-CA-C | 6.37  | 118.22      | 111.28   |
| 2   | B     | 1013 | ILE  | N-CA-C | 6.37  | 116.53      | 110.42   |
| 10  | I     | 143  | ASP  | N-CA-C | 6.35  | 121.15      | 113.41   |
| 2   | B     | 984  | ARG  | N-CA-C | 6.34  | 119.84      | 109.76   |
| 4   | c     | 924  | GLN  | N-CA-C | 6.34  | 120.14      | 111.39   |
| 4   | c     | 1308 | TRP  | N-CA-C | -6.33 | 98.95       | 109.46   |
| 5   | D     | 814  | ALA  | N-CA-C | -6.33 | 99.27       | 109.40   |
| 2   | B     | 272  | LEU  | N-CA-C | -6.33 | 99.11       | 108.79   |
| 2   | B     | 624  | LEU  | N-CA-C | 6.33  | 119.40      | 110.23   |
| 12  | J     | 415  | ALA  | N-CA-C | 6.33  | 118.25      | 111.36   |
| 3   | C     | 137  | LEU  | N-CA-C | 6.32  | 118.25      | 111.36   |
| 5   | D     | 295  | GLU  | N-CA-C | 6.32  | 121.14      | 113.17   |
| 14  | L     | 50   | GLU  | N-CA-C | 6.32  | 118.88      | 109.59   |
| 4   | c     | 139  | ASN  | N-CA-C | -6.32 | 99.70       | 109.24   |
| 1   | A     | 158  | LEU  | N-CA-C | 6.32  | 118.17      | 111.28   |
| 14  | L     | 169  | GLN  | N-CA-C | 6.32  | 117.83      | 111.07   |
| 14  | L     | 177  | LEU  | N-CA-C | -6.32 | 99.10       | 109.40   |
| 7   | F     | 254  | TYR  | CA-C-N | -6.32 | 113.25      | 119.76   |
| 7   | F     | 254  | TYR  | C-N-CA | -6.32 | 113.25      | 119.76   |
| 2   | B     | 868  | GLU  | N-CA-C | 6.31  | 118.24      | 111.36   |
| 4   | c     | 281  | GLN  | CA-C-N | -6.31 | 111.95      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | c     | 281  | GLN  | C-N-CA  | -6.31 | 111.95      | 119.84   |
| 17  | O     | 108  | TYR  | N-CA-C  | 6.31  | 119.06      | 110.55   |
| 12  | J     | 360  | TYR  | N-CA-C  | 6.30  | 122.89      | 114.12   |
| 2   | B     | 473  | ARG  | N-CA-C  | 6.30  | 118.95      | 111.33   |
| 17  | O     | 105  | ARG  | N-CA-C  | 6.30  | 118.15      | 111.28   |
| 2   | B     | 545  | SER  | N-CA-C  | 6.29  | 118.14      | 111.28   |
| 5   | D     | 275  | ASP  | N-CA-C  | 6.29  | 118.14      | 111.28   |
| 8   | G     | 66   | GLU  | N-CA-C  | 6.29  | 122.09      | 113.16   |
| 10  | I     | 305  | ASP  | N-CA-C  | 6.29  | 118.22      | 111.36   |
| 9   | H     | 289  | ALA  | N-CA-C  | 6.29  | 118.22      | 111.36   |
| 1   | A     | 42   | ALA  | N-CA-C  | 6.28  | 118.13      | 111.28   |
| 10  | I     | 290  | VAL  | N-CA-C  | 6.28  | 117.63      | 108.58   |
| 9   | H     | 313  | ALA  | N-CA-C  | 6.28  | 118.20      | 111.36   |
| 11  | i     | 521  | LEU  | N-CA-C  | 6.28  | 120.94      | 113.16   |
| 2   | B     | 464  | VAL  | CB-CA-C | -6.27 | 103.09      | 111.80   |
| 5   | D     | 188  | ASN  | N-CA-C  | 6.26  | 120.19      | 111.74   |
| 4   | c     | 1230 | SER  | N-CA-C  | 6.25  | 121.05      | 113.17   |
| 12  | J     | 221  | LEU  | N-CA-C  | -6.25 | 104.47      | 111.28   |
| 4   | c     | 985  | SER  | N-CA-C  | 6.25  | 118.85      | 110.35   |
| 7   | F     | 579  | GLU  | N-CA-C  | -6.24 | 104.53      | 111.71   |
| 15  | M     | 144  | LEU  | CA-C-N  | -6.24 | 112.04      | 119.84   |
| 15  | M     | 144  | LEU  | C-N-CA  | -6.24 | 112.04      | 119.84   |
| 2   | B     | 787  | ASP  | N-CA-C  | 6.24  | 118.33      | 108.79   |
| 5   | D     | 70   | ARG  | N-CA-C  | -6.23 | 104.48      | 111.28   |
| 11  | i     | 350  | ASP  | N-CA-C  | -6.23 | 102.49      | 110.53   |
| 1   | A     | 69   | LYS  | N-CA-C  | 6.22  | 118.06      | 111.28   |
| 1   | A     | 161  | THR  | CA-C-N  | -6.21 | 113.38      | 119.90   |
| 1   | A     | 161  | THR  | C-N-CA  | -6.21 | 113.38      | 119.90   |
| 7   | F     | 354  | LEU  | N-CA-C  | 6.20  | 120.68      | 113.18   |
| 1   | A     | 75   | SER  | N-CA-C  | 6.20  | 118.51      | 108.41   |
| 1   | a     | 314  | SER  | N-CA-C  | -6.20 | 105.85      | 113.41   |
| 12  | J     | 257  | SER  | N-CA-C  | 6.20  | 118.04      | 111.28   |
| 2   | B     | 392  | LYS  | N-CA-C  | 6.19  | 119.23      | 110.50   |
| 12  | J     | 162  | PHE  | N-CA-C  | 6.18  | 123.47      | 109.81   |
| 5   | D     | 414  | SER  | N-CA-C  | 6.18  | 118.02      | 111.28   |
| 7   | F     | 305  | VAL  | N-CA-C  | -6.18 | 101.16      | 107.89   |
| 9   | H     | 216  | HIS  | N-CA-C  | 6.18  | 113.78      | 108.22   |
| 4   | c     | 1182 | ILE  | CB-CA-C | -6.17 | 107.81      | 114.35   |
| 12  | J     | 95   | LEU  | N-CA-C  | 6.16  | 118.48      | 110.53   |
| 13  | K     | 198  | GLY  | N-CA-C  | 6.16  | 119.48      | 110.80   |
| 12  | J     | 137  | ARG  | N-CA-C  | 6.16  | 118.07      | 111.36   |
| 2   | B     | 165  | LYS  | N-CA-C  | -6.15 | 99.63       | 109.96   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 160  | LYS  | N-CA-C  | -6.15 | 100.84      | 109.69   |
| 1   | A     | 135  | HIS  | N-CA-C  | 6.14  | 118.80      | 107.99   |
| 1   | A     | 276  | GLN  | N-CA-C  | 6.14  | 118.05      | 111.36   |
| 2   | B     | 304  | ASP  | N-CA-C  | 6.14  | 118.63      | 110.53   |
| 3   | C     | 565  | CYS  | N-CA-C  | 6.14  | 117.97      | 111.28   |
| 4   | c     | 997  | LEU  | N-CA-C  | -6.13 | 100.76      | 109.96   |
| 3   | C     | 102  | VAL  | CB-CA-C | -6.13 | 104.12      | 111.97   |
| 3   | C     | 586  | GLU  | CA-C-N  | -6.12 | 113.46      | 119.76   |
| 3   | C     | 586  | GLU  | C-N-CA  | -6.12 | 113.46      | 119.76   |
| 1   | A     | 24   | SER  | N-CA-C  | -6.12 | 100.30      | 108.74   |
| 4   | c     | 457  | ALA  | N-CA-C  | 6.11  | 117.35      | 109.65   |
| 7   | F     | 556  | GLY  | N-CA-C  | 6.11  | 120.59      | 111.18   |
| 2   | B     | 539  | ALA  | N-CA-C  | 6.11  | 118.73      | 111.71   |
| 5   | D     | 492  | THR  | N-CA-C  | -6.11 | 104.62      | 111.28   |
| 7   | F     | 186  | LYS  | N-CA-C  | 6.10  | 117.93      | 111.28   |
| 2   | B     | 1027 | GLY  | N-CA-C  | 6.09  | 121.55      | 112.41   |
| 1   | A     | 101  | TYR  | N-CA-C  | -6.09 | 98.48       | 108.41   |
| 3   | C     | 83   | VAL  | N-CA-C  | 6.09  | 116.28      | 108.12   |
| 7   | F     | 459  | LYS  | N-CA-C  | -6.09 | 104.58      | 112.68   |
| 15  | m     | 175  | ASN  | N-CA-C  | 6.09  | 118.00      | 111.36   |
| 5   | D     | 505  | SER  | N-CA-C  | 6.09  | 117.91      | 111.28   |
| 5   | D     | 780  | TRP  | N-CA-C  | -6.07 | 104.66      | 111.28   |
| 7   | F     | 177  | TRP  | N-CA-CB | 6.07  | 119.34      | 110.30   |
| 11  | i     | 333  | ALA  | N-CA-C  | 6.07  | 117.89      | 111.28   |
| 5   | D     | 417  | GLU  | CA-C-N  | -6.06 | 113.53      | 119.90   |
| 5   | D     | 417  | GLU  | C-N-CA  | -6.06 | 113.53      | 119.90   |
| 13  | K     | 151  | ARG  | N-CA-C  | 6.06  | 119.25      | 110.28   |
| 17  | O     | 59   | GLU  | N-CA-C  | 6.06  | 118.39      | 111.11   |
| 4   | c     | 1235 | SER  | N-CA-C  | 6.06  | 119.75      | 110.36   |
| 7   | F     | 157  | GLU  | CA-C-N  | -6.06 | 114.03      | 120.03   |
| 7   | F     | 157  | GLU  | C-N-CA  | -6.06 | 114.03      | 120.03   |
| 14  | L     | 217  | TYR  | N-CA-C  | -6.05 | 99.37       | 109.24   |
| 14  | L     | 176  | TRP  | N-CA-C  | 6.05  | 119.06      | 109.50   |
| 10  | I     | 357  | GLN  | N-CA-C  | 6.05  | 119.59      | 111.24   |
| 10  | I     | 424  | ALA  | N-CA-C  | 6.04  | 117.53      | 111.07   |
| 4   | c     | 208  | GLU  | N-CA-C  | 6.03  | 117.86      | 111.28   |
| 11  | i     | 534  | GLY  | N-CA-C  | -6.03 | 103.14      | 111.76   |
| 12  | J     | 163  | PRO  | N-CA-C  | -6.03 | 106.33      | 113.86   |
| 2   | B     | 909  | LYS  | N-CA-C  | 6.01  | 117.91      | 111.36   |
| 1   | A     | 116  | VAL  | N-CA-C  | -6.00 | 96.86       | 109.34   |
| 5   | D     | 242  | ALA  | N-CA-C  | 6.00  | 118.45      | 110.53   |
| 11  | i     | 630  | ASP  | N-CA-C  | 6.00  | 117.01      | 108.74   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | M     | 167  | ILE  | N-CA-C  | 5.99  | 116.73      | 110.62   |
| 4   | c     | 370  | THR  | N-CA-C  | 5.99  | 117.35      | 108.60   |
| 1   | a     | 281  | SER  | N-CA-C  | 5.99  | 117.80      | 111.28   |
| 2   | B     | 108  | ASN  | N-CA-C  | -5.99 | 102.47      | 110.55   |
| 4   | c     | 1224 | ILE  | N-CA-C  | 5.98  | 116.76      | 110.72   |
| 2   | B     | 611  | TYR  | N-CA-C  | 5.97  | 119.64      | 111.39   |
| 4   | c     | 1103 | SER  | N-CA-C  | 5.97  | 119.12      | 110.28   |
| 18  | P     | 92   | GLU  | CB-CA-C | -5.97 | 109.11      | 117.23   |
| 6   | E     | 721  | ALA  | N-CA-C  | -5.97 | 104.86      | 111.36   |
| 11  | i     | 528  | VAL  | N-CA-C  | 5.96  | 116.94      | 108.42   |
| 4   | c     | 1218 | ASN  | N-CA-C  | 5.95  | 118.73      | 111.82   |
| 2   | B     | 777  | LEU  | N-CA-C  | 5.95  | 117.39      | 109.83   |
| 4   | c     | 28   | ASP  | N-CA-C  | 5.95  | 117.44      | 111.07   |
| 4   | c     | 1008 | TYR  | N-CA-C  | 5.95  | 117.85      | 111.36   |
| 15  | M     | 110  | GLU  | N-CA-C  | 5.94  | 117.76      | 111.28   |
| 12  | J     | 166  | ILE  | N-CA-C  | 5.93  | 114.76      | 108.95   |
| 12  | J     | 310  | HIS  | N-CA-C  | 5.92  | 118.85      | 110.50   |
| 11  | i     | 456  | LEU  | N-CA-C  | 5.92  | 118.00      | 109.48   |
| 7   | F     | 348  | ASP  | CA-C-N  | -5.92 | 112.44      | 119.84   |
| 7   | F     | 348  | ASP  | C-N-CA  | -5.92 | 112.44      | 119.84   |
| 12  | J     | 110  | SER  | N-CA-C  | 5.92  | 119.87      | 110.70   |
| 15  | M     | 156  | LYS  | N-CA-C  | 5.92  | 119.23      | 110.48   |
| 2   | B     | 411  | ARG  | N-CA-C  | 5.91  | 119.46      | 112.72   |
| 1   | a     | 291  | ASN  | N-CA-C  | 5.91  | 119.58      | 111.54   |
| 7   | F     | 604  | MET  | N-CA-C  | 5.91  | 118.27      | 108.99   |
| 5   | D     | 829  | SER  | N-CA-C  | -5.91 | 104.84      | 111.28   |
| 2   | B     | 940  | VAL  | N-CA-C  | 5.90  | 117.94      | 108.85   |
| 6   | E     | 698  | LEU  | N-CA-C  | -5.90 | 106.04      | 113.18   |
| 12  | J     | 150  | MET  | N-CA-C  | 5.90  | 118.14      | 110.53   |
| 10  | I     | 264  | SER  | N-CA-C  | 5.90  | 120.09      | 113.01   |
| 11  | i     | 274  | TYR  | N-CA-C  | 5.90  | 117.58      | 111.03   |
| 11  | i     | 620  | GLU  | N-CA-C  | -5.90 | 99.17       | 108.14   |
| 17  | O     | 111  | LYS  | N-CA-C  | -5.89 | 99.59       | 109.07   |
| 5   | D     | 769  | LYS  | N-CA-C  | 5.89  | 117.70      | 111.28   |
| 1   | A     | 62   | ILE  | N-CA-C  | 5.88  | 115.72      | 107.37   |
| 9   | H     | 367  | ARG  | N-CA-C  | 5.88  | 117.77      | 111.36   |
| 4   | c     | 95   | GLU  | N-CA-C  | 5.87  | 117.68      | 111.28   |
| 5   | D     | 468  | ASN  | CA-C-N  | -5.87 | 113.92      | 119.85   |
| 5   | D     | 468  | ASN  | C-N-CA  | -5.87 | 113.92      | 119.85   |
| 9   | H     | 201  | GLU  | N-CA-C  | 5.87  | 118.46      | 108.02   |
| 4   | c     | 1184 | TRP  | N-CA-C  | 5.86  | 120.71      | 113.50   |
| 3   | C     | 152  | PHE  | N-CA-C  | -5.85 | 99.81       | 108.99   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | c     | 1165 | LEU  | N-CA-C | 5.84  | 117.73      | 111.36   |
| 7   | F     | 271  | LEU  | N-CA-C | 5.84  | 122.71      | 109.81   |
| 3   | C     | 292  | GLY  | N-CA-C | -5.83 | 105.43      | 112.49   |
| 5   | D     | 143  | PHE  | N-CA-C | -5.83 | 104.92      | 111.28   |
| 1   | A     | 79   | GLY  | N-CA-C | 5.83  | 119.73      | 112.73   |
| 4   | c     | 453  | ASP  | N-CA-C | 5.82  | 120.33      | 113.23   |
| 4   | c     | 89   | GLY  | N-CA-C | 5.82  | 123.64      | 115.43   |
| 13  | K     | 213  | PRO  | N-CA-C | 5.81  | 119.98      | 111.03   |
| 1   | a     | 109  | CYS  | N-CA-C | 5.81  | 117.26      | 110.41   |
| 2   | B     | 575  | SER  | N-CA-C | 5.80  | 117.69      | 111.36   |
| 18  | P     | 111  | ALA  | N-CA-C | 5.80  | 116.59      | 108.00   |
| 10  | I     | 135  | VAL  | N-CA-C | 5.80  | 117.68      | 108.87   |
| 18  | P     | 42   | LYS  | CA-C-N | -5.80 | 113.81      | 119.78   |
| 18  | P     | 42   | LYS  | C-N-CA | -5.80 | 113.81      | 119.78   |
| 2   | B     | 283  | PRO  | N-CA-C | 5.79  | 121.47      | 113.65   |
| 13  | K     | 214  | MET  | N-CA-C | 5.79  | 118.53      | 111.82   |
| 9   | H     | 309  | ILE  | N-CA-C | 5.79  | 116.56      | 110.72   |
| 3   | C     | 555  | ARG  | N-CA-C | 5.79  | 120.37      | 112.68   |
| 4   | c     | 29   | HIS  | N-CA-C | 5.79  | 117.67      | 111.36   |
| 5   | D     | 352  | GLY  | N-CA-C | -5.79 | 107.19      | 115.64   |
| 2   | B     | 808  | ILE  | N-CA-C | 5.78  | 116.21      | 108.11   |
| 2   | B     | 884  | ILE  | N-CA-C | 5.78  | 116.17      | 107.80   |
| 4   | c     | 33   | ALA  | N-CA-C | 5.78  | 117.38      | 111.14   |
| 13  | K     | 252  | SER  | N-CA-C | 5.78  | 117.66      | 111.36   |
| 2   | B     | 84   | ALA  | N-CA-C | 5.77  | 117.96      | 109.24   |
| 3   | C     | 81   | TYR  | N-CA-C | 5.77  | 117.81      | 108.41   |
| 3   | C     | 516  | ALA  | N-CA-C | 5.77  | 117.24      | 111.07   |
| 5   | D     | 316  | ARG  | N-CA-C | 5.77  | 117.65      | 111.36   |
| 14  | L     | 242  | ILE  | N-CA-C | 5.77  | 115.89      | 110.30   |
| 15  | m     | 100  | TRP  | N-CA-C | 5.77  | 117.57      | 111.28   |
| 3   | C     | 22   | VAL  | N-CA-C | 5.76  | 117.73      | 108.85   |
| 7   | F     | 273  | PHE  | N-CA-C | 5.76  | 117.56      | 111.28   |
| 18  | P     | 132  | GLN  | N-CA-C | -5.76 | 100.58      | 109.52   |
| 4   | c     | 1245 | PRO  | N-CA-C | 5.76  | 121.54      | 113.53   |
| 6   | E     | 434  | ASP  | N-CA-C | -5.76 | 105.00      | 111.28   |
| 8   | G     | 158  | GLY  | N-CA-C | 5.76  | 121.88      | 110.77   |
| 5   | D     | 362  | LYS  | N-CA-C | 5.74  | 117.53      | 111.28   |
| 15  | m     | 126  | LYS  | N-CA-C | 5.74  | 118.82      | 109.24   |
| 4   | c     | 1282 | GLN  | N-CA-C | 5.73  | 120.00      | 112.89   |
| 10  | I     | 479  | GLN  | N-CA-C | 5.73  | 117.61      | 111.36   |
| 12  | J     | 141  | VAL  | N-CA-C | 5.72  | 116.45      | 108.89   |
| 4   | c     | 86   | HIS  | N-CA-C | -5.72 | 105.05      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 6   | E     | 336  | ARG  | N-CA-C | -5.72 | 105.05      | 111.28   |
| 14  | L     | 216  | ASP  | N-CA-C | 5.72  | 119.46      | 111.74   |
| 6   | E     | 329  | LYS  | N-CA-C | -5.71 | 105.05      | 111.28   |
| 8   | G     | 68   | TYR  | N-CA-C | 5.71  | 117.59      | 111.36   |
| 13  | K     | 219  | ARG  | N-CA-C | 5.71  | 117.59      | 111.36   |
| 2   | B     | 637  | ILE  | N-CA-C | 5.71  | 116.95      | 109.58   |
| 4   | c     | 1119 | TYR  | N-CA-C | 5.71  | 117.50      | 111.28   |
| 9   | H     | 317  | GLU  | N-CA-C | -5.71 | 105.06      | 111.28   |
| 3   | C     | 552  | GLY  | N-CA-C | 5.70  | 117.32      | 111.56   |
| 14  | L     | 173  | GLY  | N-CA-C | 5.70  | 118.27      | 110.69   |
| 12  | J     | 330  | MET  | N-CA-C | 5.70  | 118.75      | 109.24   |
| 4   | c     | 1300 | ALA  | N-CA-C | 5.69  | 117.57      | 111.36   |
| 4   | c     | 242  | GLN  | N-CA-C | 5.69  | 118.22      | 111.33   |
| 8   | G     | 92   | GLN  | N-CA-C | -5.69 | 105.08      | 111.28   |
| 3   | C     | 518  | LEU  | N-CA-C | 5.69  | 119.94      | 112.89   |
| 1   | A     | 281  | SER  | N-CA-C | 5.69  | 117.48      | 111.28   |
| 2   | B     | 719  | ASN  | N-CA-C | 5.68  | 118.41      | 111.82   |
| 5   | D     | 504  | ILE  | N-CA-C | -5.67 | 106.96      | 112.29   |
| 2   | B     | 407  | SER  | N-CA-C | 5.67  | 118.01      | 110.53   |
| 1   | a     | 317  | VAL  | N-CA-C | -5.66 | 104.84      | 110.62   |
| 1   | a     | 52   | ALA  | N-CA-C | 5.66  | 117.53      | 111.36   |
| 4   | c     | 191  | ASP  | N-CA-C | 5.66  | 117.45      | 111.28   |
| 2   | B     | 931  | ARG  | N-CA-C | 5.65  | 117.52      | 111.36   |
| 15  | M     | 151  | SER  | CA-C-N | -5.65 | 113.86      | 119.56   |
| 15  | M     | 151  | SER  | C-N-CA | -5.65 | 113.86      | 119.56   |
| 17  | O     | 84   | ASP  | N-CA-C | 5.65  | 117.51      | 111.36   |
| 10  | I     | 375  | ASP  | N-CA-C | 5.64  | 117.43      | 111.28   |
| 15  | M     | 175  | ASN  | N-CA-C | 5.64  | 117.51      | 111.36   |
| 6   | E     | 766  | ALA  | N-CA-C | 5.64  | 120.30      | 113.41   |
| 8   | G     | 162  | ASN  | N-CA-C | -5.64 | 105.14      | 111.28   |
| 18  | P     | 62   | MET  | N-CA-C | -5.62 | 105.15      | 111.28   |
| 11  | i     | 599  | ALA  | N-CA-C | 5.62  | 117.41      | 111.28   |
| 11  | i     | 321  | ARG  | N-CA-C | 5.62  | 118.06      | 108.90   |
| 10  | I     | 257  | ALA  | N-CA-C | 5.61  | 118.46      | 110.10   |
| 12  | J     | 216  | GLU  | N-CA-C | 5.61  | 119.82      | 112.92   |
| 15  | m     | 101  | CYS  | N-CA-C | 5.61  | 118.37      | 109.96   |
| 2   | B     | 144  | SER  | N-CA-C | 5.60  | 118.57      | 110.28   |
| 12  | J     | 116  | ILE  | N-CA-C | 5.60  | 117.88      | 108.81   |
| 2   | B     | 94   | MET  | N-CA-C | 5.60  | 118.03      | 108.90   |
| 4   | c     | 864  | ILE  | N-CA-C | 5.60  | 116.36      | 108.36   |
| 7   | F     | 264  | TYR  | N-CA-C | 5.60  | 118.26      | 108.52   |
| 10  | I     | 438  | HIS  | N-CA-C | 5.60  | 120.26      | 113.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | F     | 258 | ARG  | N-CA-C  | 5.59  | 118.44      | 110.10   |
| 15  | m     | 151 | SER  | N-CA-C  | 5.58  | 118.81      | 109.09   |
| 1   | a     | 140 | THR  | CB-CA-C | -5.58 | 101.99      | 111.02   |
| 3   | C     | 404 | LEU  | CA-C-N  | -5.57 | 114.02      | 119.76   |
| 3   | C     | 404 | LEU  | C-N-CA  | -5.57 | 114.02      | 119.76   |
| 7   | F     | 151 | ILE  | N-CA-C  | 5.57  | 115.81      | 107.51   |
| 14  | L     | 85  | LEU  | N-CA-C  | -5.57 | 105.20      | 111.28   |
| 6   | E     | 338 | MET  | N-CA-C  | -5.57 | 105.21      | 111.28   |
| 8   | G     | 238 | HIS  | N-CA-CB | -5.57 | 103.19      | 110.88   |
| 6   | E     | 324 | HIS  | N-CA-C  | -5.57 | 105.21      | 111.28   |
| 2   | B     | 405 | THR  | N-CA-C  | 5.57  | 117.43      | 111.36   |
| 17  | O     | 56  | PRO  | N-CA-C  | 5.56  | 121.26      | 113.53   |
| 6   | E     | 406 | HIS  | N-CA-C  | -5.56 | 105.22      | 111.28   |
| 4   | c     | 67  | SER  | N-CA-C  | 5.56  | 119.69      | 113.02   |
| 1   | a     | 262 | LYS  | N-CA-C  | 5.55  | 117.41      | 111.36   |
| 2   | B     | 950 | LEU  | N-CA-C  | 5.55  | 118.74      | 110.52   |
| 10  | I     | 401 | VAL  | N-CA-C  | 5.55  | 116.74      | 109.58   |
| 14  | L     | 168 | THR  | N-CA-C  | 5.55  | 118.26      | 111.82   |
| 2   | B     | 440 | ILE  | N-CA-C  | 5.54  | 115.74      | 110.42   |
| 9   | H     | 190 | GLU  | N-CA-C  | -5.54 | 105.62      | 112.38   |
| 1   | A     | 157 | TYR  | N-CA-C  | -5.54 | 99.49       | 108.41   |
| 3   | C     | 148 | VAL  | N-CA-C  | 5.53  | 116.26      | 110.62   |
| 2   | B     | 963 | SER  | CB-CA-C | -5.53 | 110.21      | 116.63   |
| 2   | B     | 809 | LEU  | N-CA-C  | 5.53  | 117.97      | 109.07   |
| 3   | C     | 668 | ALA  | N-CA-C  | 5.53  | 117.31      | 111.28   |
| 3   | C     | 321 | ARG  | N-CA-C  | -5.53 | 105.25      | 111.28   |
| 12  | J     | 298 | ALA  | N-CA-C  | 5.52  | 117.37      | 109.14   |
| 3   | C     | 462 | ALA  | CA-C-N  | -5.52 | 112.94      | 119.84   |
| 3   | C     | 462 | ALA  | C-N-CA  | -5.52 | 112.94      | 119.84   |
| 2   | B     | 387 | ILE  | N-CA-C  | 5.52  | 116.30      | 110.72   |
| 3   | C     | 308 | TYR  | N-CA-C  | 5.52  | 117.10      | 111.14   |
| 3   | C     | 643 | GLY  | N-CA-C  | 5.51  | 119.34      | 112.73   |
| 4   | c     | 459 | GLU  | N-CA-C  | 5.51  | 117.29      | 111.28   |
| 5   | D     | 743 | ARG  | N-CA-C  | 5.51  | 117.36      | 111.36   |
| 10  | I     | 386 | THR  | N-CA-C  | -5.51 | 106.23      | 113.17   |
| 11  | i     | 544 | GLU  | N-CA-C  | 5.50  | 120.15      | 113.38   |
| 18  | P     | 98  | VAL  | CB-CA-C | -5.50 | 102.93      | 110.96   |
| 4   | c     | 486 | LEU  | N-CA-C  | -5.50 | 105.39      | 111.71   |
| 11  | i     | 311 | ASP  | N-CA-C  | 5.49  | 117.27      | 111.28   |
| 3   | C     | 620 | VAL  | N-CA-C  | 5.49  | 116.08      | 108.84   |
| 4   | c     | 197 | SER  | N-CA-C  | 5.49  | 117.26      | 111.28   |
| 13  | K     | 229 | HIS  | N-CA-C  | -5.49 | 102.77      | 110.50   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | c     | 1180 | LEU  | N-CA-C  | 5.48  | 118.01      | 109.52   |
| 6   | E     | 316  | ASN  | N-CA-C  | 5.48  | 117.25      | 111.28   |
| 2   | B     | 301  | GLY  | N-CA-C  | 5.47  | 119.64      | 110.56   |
| 11  | i     | 585  | LEU  | N-CA-C  | 5.47  | 119.48      | 112.26   |
| 7   | F     | 514  | TYR  | N-CA-C  | -5.46 | 105.40      | 111.36   |
| 10  | I     | 351  | ASN  | N-CA-C  | -5.46 | 100.76      | 109.07   |
| 10  | I     | 302  | ARG  | N-CA-C  | 5.46  | 117.04      | 111.14   |
| 14  | L     | 178  | ALA  | N-CA-C  | 5.46  | 117.10      | 108.96   |
| 3   | C     | 438  | ARG  | N-CA-C  | 5.46  | 118.15      | 111.82   |
| 10  | I     | 116  | PRO  | N-CA-C  | -5.46 | 104.04      | 110.70   |
| 10  | I     | 248  | GLU  | CA-C-N  | -5.46 | 115.40      | 123.05   |
| 10  | I     | 248  | GLU  | C-N-CA  | -5.46 | 115.40      | 123.05   |
| 1   | a     | 41   | GLN  | N-CA-C  | 5.46  | 117.23      | 111.28   |
| 4   | c     | 372  | THR  | N-CA-C  | 5.46  | 117.57      | 110.53   |
| 12  | J     | 505  | ILE  | N-CA-C  | -5.46 | 105.06      | 110.62   |
| 2   | B     | 857  | VAL  | CB-CA-C | -5.45 | 108.57      | 114.35   |
| 3   | C     | 180  | TYR  | N-CA-C  | 5.45  | 117.03      | 111.14   |
| 1   | a     | 140  | THR  | N-CA-C  | 5.45  | 119.49      | 112.41   |
| 2   | B     | 715  | HIS  | N-CA-C  | -5.45 | 105.44      | 111.71   |
| 15  | m     | 157  | ASP  | N-CA-C  | 5.45  | 118.80      | 110.36   |
| 5   | D     | 464  | PHE  | N-CA-C  | -5.44 | 100.83      | 109.59   |
| 11  | i     | 277  | PRO  | N-CA-C  | -5.44 | 104.06      | 110.70   |
| 2   | B     | 678  | VAL  | N-CA-C  | 5.44  | 116.22      | 110.72   |
| 2   | B     | 1061 | LYS  | N-CA-C  | 5.44  | 117.01      | 111.14   |
| 2   | B     | 861  | MET  | N-CA-C  | 5.44  | 119.08      | 111.74   |
| 12  | J     | 411  | PHE  | CA-C-N  | -5.44 | 114.19      | 121.80   |
| 12  | J     | 411  | PHE  | C-N-CA  | -5.44 | 114.19      | 121.80   |
| 7   | F     | 334  | ASP  | N-CA-C  | 5.43  | 116.73      | 109.83   |
| 12  | J     | 371  | VAL  | N-CA-C  | 5.42  | 115.70      | 108.11   |
| 10  | I     | 234  | GLU  | N-CA-C  | 5.42  | 117.47      | 108.20   |
| 1   | A     | 66   | LYS  | N-CA-C  | 5.42  | 118.30      | 107.62   |
| 4   | c     | 1182 | ILE  | CA-C-N  | -5.42 | 113.04      | 119.05   |
| 4   | c     | 1182 | ILE  | C-N-CA  | -5.42 | 113.04      | 119.05   |
| 5   | D     | 798  | THR  | CA-C-N  | -5.42 | 114.18      | 119.76   |
| 5   | D     | 798  | THR  | C-N-CA  | -5.42 | 114.18      | 119.76   |
| 11  | i     | 509  | LYS  | N-CA-C  | -5.42 | 103.54      | 110.53   |
| 1   | A     | 141  | GLU  | CA-C-N  | -5.41 | 113.98      | 119.83   |
| 1   | A     | 141  | GLU  | C-N-CA  | -5.41 | 113.98      | 119.83   |
| 2   | B     | 798  | SER  | N-CA-C  | -5.39 | 103.57      | 110.53   |
| 13  | K     | 173  | THR  | O-C-N   | -5.39 | 116.65      | 123.17   |
| 5   | D     | 101  | LEU  | N-CA-C  | -5.39 | 102.41      | 110.23   |
| 5   | D     | 138  | PRO  | N-CA-C  | 5.38  | 119.77      | 111.21   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | m     | 165  | ILE  | CA-C-N  | -5.38 | 114.71      | 120.03   |
| 15  | m     | 165  | ILE  | C-N-CA  | -5.38 | 114.71      | 120.03   |
| 3   | C     | 250  | PHE  | N-CA-C  | -5.38 | 104.87      | 111.75   |
| 6   | E     | 718  | ALA  | N-CA-C  | -5.38 | 105.42      | 111.28   |
| 5   | D     | 417  | GLU  | N-CA-C  | 5.37  | 120.05      | 112.75   |
| 1   | a     | 171  | PRO  | CA-C-O  | -5.37 | 115.53      | 122.13   |
| 4   | c     | 32   | MET  | N-CA-C  | 5.37  | 117.88      | 111.71   |
| 7   | F     | 282  | GLY  | N-CA-C  | 5.37  | 121.08      | 110.83   |
| 4   | c     | 85   | HIS  | N-CA-C  | 5.36  | 118.03      | 111.82   |
| 15  | M     | 73   | LYS  | N-CA-C  | 5.35  | 118.21      | 109.59   |
| 6   | E     | 768  | TYR  | N-CA-C  | -5.35 | 105.45      | 111.28   |
| 5   | D     | 336  | VAL  | N-CA-C  | -5.34 | 98.23       | 109.34   |
| 4   | c     | 109  | GLU  | N-CA-C  | 5.34  | 118.01      | 111.82   |
| 2   | B     | 1049 | LEU  | N-CA-C  | -5.33 | 106.64      | 112.72   |
| 12  | J     | 305  | ALA  | N-CA-C  | -5.33 | 106.16      | 113.30   |
| 7   | F     | 574  | GLU  | N-CA-C  | 5.33  | 117.92      | 109.40   |
| 2   | B     | 61   | GLU  | N-CA-C  | 5.33  | 117.87      | 110.20   |
| 2   | B     | 626  | VAL  | N-CA-C  | 5.32  | 113.94      | 107.61   |
| 1   | a     | 107  | SER  | N-CA-C  | 5.32  | 117.27      | 109.24   |
| 5   | D     | 747  | ILE  | N-CA-C  | 5.32  | 116.05      | 110.62   |
| 3   | C     | 428  | SER  | N-CA-C  | 5.32  | 118.23      | 111.69   |
| 4   | c     | 18   | ALA  | N-CA-C  | 5.31  | 117.07      | 111.28   |
| 10  | I     | 293  | ASP  | N-CA-C  | -5.31 | 99.86       | 108.41   |
| 12  | J     | 302  | VAL  | N-CA-C  | 5.31  | 113.93      | 107.61   |
| 7   | F     | 542  | PRO  | N-CA-C  | 5.30  | 119.20      | 110.55   |
| 5   | D     | 261  | GLU  | N-CA-C  | 5.30  | 117.06      | 111.28   |
| 3   | C     | 561  | ARG  | N-CA-C  | 5.30  | 117.13      | 111.36   |
| 14  | L     | 155  | PHE  | N-CA-C  | -5.30 | 105.51      | 111.28   |
| 4   | c     | 325  | SER  | N-CA-C  | 5.29  | 117.05      | 111.28   |
| 3   | C     | 360  | TYR  | N-CA-C  | 5.29  | 117.96      | 110.50   |
| 3   | C     | 182  | ILE  | CB-CA-C | -5.28 | 108.76      | 114.35   |
| 3   | C     | 357  | ASN  | N-CA-C  | 5.28  | 117.67      | 110.55   |
| 3   | C     | 630  | VAL  | N-CA-C  | -5.28 | 100.72      | 108.11   |
| 3   | C     | 56   | LYS  | N-CA-C  | -5.27 | 100.25      | 109.48   |
| 2   | B     | 179  | SER  | N-CA-C  | 5.27  | 117.32      | 108.73   |
| 6   | E     | 382  | ALA  | N-CA-C  | -5.26 | 104.96      | 111.33   |
| 18  | P     | 60   | ARG  | N-CA-C  | -5.26 | 105.55      | 111.28   |
| 17  | O     | 113  | ALA  | N-CA-C  | 5.26  | 117.01      | 111.28   |
| 10  | I     | 156  | PRO  | N-CA-C  | -5.25 | 102.86      | 111.21   |
| 4   | c     | 284  | SER  | N-CA-C  | 5.25  | 117.29      | 108.73   |
| 8   | G     | 147  | LEU  | CB-CA-C | -5.25 | 110.50      | 116.54   |
| 10  | I     | 468  | PRO  | N-CA-C  | 5.25  | 119.29      | 111.41   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | P     | 118 | PRO  | N-CA-C  | 5.25  | 119.55      | 111.57   |
| 6   | E     | 728 | ASP  | N-CA-C  | -5.24 | 105.57      | 111.28   |
| 14  | L     | 226 | TRP  | N-CA-C  | -5.24 | 102.53      | 110.24   |
| 8   | G     | 50  | PHE  | N-CA-C  | 5.24  | 117.62      | 108.76   |
| 12  | J     | 183 | THR  | N-CA-C  | 5.24  | 119.67      | 113.12   |
| 2   | B     | 199 | CYS  | N-CA-C  | -5.24 | 103.78      | 110.53   |
| 12  | J     | 344 | THR  | N-CA-C  | 5.23  | 117.77      | 109.50   |
| 1   | A     | 78  | THR  | N-CA-C  | 5.23  | 116.26      | 108.31   |
| 3   | C     | 179 | LYS  | N-CA-C  | -5.23 | 106.22      | 113.18   |
| 10  | I     | 296 | LEU  | N-CA-C  | 5.23  | 117.01      | 109.48   |
| 14  | L     | 109 | ARG  | CB-CA-C | -5.23 | 110.56      | 116.63   |
| 7   | F     | 476 | LEU  | N-CA-C  | 5.23  | 116.98      | 111.28   |
| 18  | P     | 106 | PHE  | N-CA-C  | 5.23  | 117.36      | 109.41   |
| 4   | c     | 167 | SER  | N-CA-C  | 5.23  | 117.62      | 109.52   |
| 13  | K     | 266 | VAL  | CA-C-N  | -5.23 | 114.33      | 119.92   |
| 13  | K     | 266 | VAL  | C-N-CA  | -5.23 | 114.33      | 119.92   |
| 4   | c     | 923 | PRO  | N-CA-C  | 5.22  | 122.22      | 114.80   |
| 12  | J     | 155 | LYS  | N-CA-C  | 5.22  | 117.05      | 111.36   |
| 8   | G     | 159 | SER  | N-CA-C  | -5.22 | 101.47      | 109.41   |
| 15  | M     | 165 | ILE  | N-CA-C  | -5.22 | 102.19      | 108.45   |
| 6   | E     | 296 | VAL  | N-CA-C  | 5.22  | 115.43      | 110.42   |
| 7   | F     | 570 | ASP  | N-CA-C  | -5.22 | 103.80      | 110.53   |
| 10  | I     | 399 | VAL  | N-CA-C  | 5.21  | 116.22      | 108.46   |
| 13  | K     | 194 | MET  | N-CA-C  | 5.21  | 117.98      | 109.59   |
| 15  | m     | 121 | ASN  | N-CA-C  | -5.21 | 106.51      | 112.92   |
| 2   | B     | 191 | LEU  | N-CA-C  | -5.21 | 105.61      | 111.28   |
| 4   | c     | 74  | ASP  | N-CA-C  | 5.21  | 117.03      | 111.36   |
| 7   | F     | 392 | VAL  | N-CA-C  | 5.21  | 116.72      | 109.80   |
| 2   | B     | 41  | ILE  | N-CA-C  | 5.20  | 115.45      | 108.17   |
| 13  | K     | 152 | LYS  | N-CA-C  | 5.20  | 119.04      | 109.10   |
| 6   | E     | 321 | ALA  | N-CA-C  | -5.20 | 105.79      | 111.82   |
| 2   | B     | 574 | ASP  | N-CA-C  | 5.20  | 119.62      | 113.28   |
| 3   | C     | 350 | GLN  | CA-C-N  | -5.20 | 113.34      | 119.84   |
| 3   | C     | 350 | GLN  | C-N-CA  | -5.20 | 113.34      | 119.84   |
| 5   | D     | 759 | ALA  | N-CA-C  | 5.20  | 117.03      | 111.36   |
| 1   | a     | 67  | SER  | N-CA-C  | -5.19 | 100.78      | 109.24   |
| 11  | i     | 297 | SER  | N-CA-C  | 5.19  | 115.90      | 108.74   |
| 5   | D     | 418 | PRO  | N-CA-C  | -5.18 | 102.97      | 110.80   |
| 14  | L     | 60  | ALA  | N-CA-C  | -5.18 | 106.54      | 112.92   |
| 5   | D     | 299 | ARG  | N-CA-C  | 5.18  | 118.35      | 111.30   |
| 12  | J     | 178 | SER  | CB-CA-C | -5.18 | 104.04      | 111.91   |
| 1   | A     | 194 | GLU  | N-CA-C  | 5.17  | 117.05      | 109.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | E     | 414 | GLU  | N-CA-C  | 5.17  | 117.22      | 110.08   |
| 7   | F     | 254 | TYR  | N-CA-C  | -5.17 | 100.48      | 108.55   |
| 2   | B     | 526 | ILE  | N-CA-C  | 5.17  | 115.90      | 110.62   |
| 4   | c     | 285 | ILE  | N-CA-C  | 5.17  | 115.93      | 108.48   |
| 13  | K     | 325 | PHE  | N-CA-C  | 5.17  | 116.92      | 111.28   |
| 2   | B     | 299 | GLY  | N-CA-C  | 5.17  | 122.56      | 115.27   |
| 12  | J     | 283 | ARG  | N-CA-C  | 5.17  | 119.55      | 112.88   |
| 4   | c     | 469 | PRO  | N-CA-C  | 5.16  | 120.32      | 113.40   |
| 8   | G     | 207 | ASP  | N-CA-C  | -5.16 | 101.56      | 109.41   |
| 3   | C     | 211 | ALA  | N-CA-C  | 5.16  | 116.91      | 111.28   |
| 5   | D     | 836 | SER  | N-CA-C  | 5.16  | 120.49      | 113.16   |
| 1   | A     | 159 | ILE  | N-CA-C  | 5.16  | 120.07      | 109.34   |
| 3   | C     | 361 | LYS  | N-CA-C  | 5.16  | 117.10      | 108.23   |
| 8   | G     | 66  | GLU  | CA-C-N  | -5.15 | 113.61      | 118.97   |
| 8   | G     | 66  | GLU  | C-N-CA  | -5.15 | 113.61      | 118.97   |
| 7   | F     | 583 | GLN  | N-CA-C  | -5.15 | 107.55      | 113.88   |
| 4   | c     | 471 | THR  | N-CA-C  | 5.15  | 117.68      | 109.96   |
| 17  | O     | 126 | GLY  | N-CA-C  | 5.15  | 123.16      | 115.64   |
| 11  | i     | 369 | SER  | N-CA-C  | 5.14  | 118.81      | 112.54   |
| 9   | H     | 308 | LYS  | N-CA-C  | 5.14  | 116.69      | 111.14   |
| 12  | J     | 359 | ARG  | N-CA-C  | 5.14  | 118.01      | 111.69   |
| 2   | B     | 178 | ILE  | N-CA-C  | -5.14 | 100.49      | 108.81   |
| 14  | L     | 105 | ILE  | N-CA-C  | 5.13  | 115.86      | 110.62   |
| 13  | K     | 199 | CYS  | N-CA-C  | 5.13  | 117.43      | 108.76   |
| 5   | D     | 474 | PHE  | N-CA-C  | -5.13 | 105.69      | 111.28   |
| 6   | E     | 778 | SER  | N-CA-C  | -5.13 | 105.77      | 111.36   |
| 10  | I     | 248 | GLU  | N-CA-C  | -5.13 | 106.80      | 113.16   |
| 2   | B     | 954 | VAL  | CB-CA-C | -5.12 | 105.22      | 112.14   |
| 12  | J     | 269 | ASP  | CA-C-N  | -5.12 | 114.47      | 119.64   |
| 12  | J     | 269 | ASP  | C-N-CA  | -5.12 | 114.47      | 119.64   |
| 2   | B     | 425 | ASP  | N-CA-C  | 5.11  | 117.89      | 109.76   |
| 10  | I     | 146 | SER  | N-CA-C  | -5.11 | 106.82      | 113.16   |
| 14  | L     | 53  | PRO  | N-CA-C  | -5.11 | 104.46      | 110.70   |
| 11  | i     | 532 | THR  | N-CA-C  | 5.11  | 117.23      | 108.90   |
| 1   | A     | 114 | GLY  | N-CA-C  | -5.11 | 101.07      | 113.18   |
| 7   | F     | 79  | ARG  | N-CA-C  | 5.11  | 116.85      | 111.28   |
| 4   | c     | 246 | GLY  | N-CA-C  | 5.11  | 122.63      | 115.43   |
| 2   | B     | 958 | ILE  | N-CA-C  | 5.10  | 116.98      | 109.63   |
| 14  | L     | 51  | LEU  | N-CA-C  | -5.10 | 101.97      | 109.62   |
| 15  | M     | 113 | MET  | N-CA-C  | 5.10  | 116.92      | 111.36   |
| 3   | C     | 264 | THR  | N-CA-C  | 5.09  | 120.34      | 113.72   |
| 1   | a     | 141 | GLU  | CA-C-N  | -5.09 | 113.48      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | a     | 141  | GLU  | C-N-CA  | -5.09 | 113.48      | 119.84   |
| 3   | C     | 11   | ARG  | N-CA-C  | -5.09 | 101.67      | 109.76   |
| 4   | c     | 1073 | ILE  | N-CA-C  | 5.08  | 115.17      | 107.80   |
| 18  | P     | 66   | VAL  | CB-CA-C | -5.08 | 108.96      | 114.35   |
| 4   | c     | 1034 | ILE  | N-CA-C  | 5.08  | 115.66      | 107.73   |
| 1   | a     | 23   | ASP  | N-CA-C  | 5.08  | 116.90      | 111.36   |
| 1   | A     | 80   | ILE  | N-CA-C  | 5.08  | 115.95      | 109.30   |
| 4   | c     | 394  | ILE  | N-CA-C  | 5.08  | 116.31      | 108.44   |
| 2   | B     | 821  | ALA  | N-CA-C  | 5.08  | 116.79      | 109.07   |
| 4   | c     | 135  | GLY  | N-CA-C  | -5.08 | 108.11      | 115.27   |
| 3   | C     | 174  | GLU  | N-CA-C  | 5.08  | 117.02      | 109.25   |
| 3   | C     | 488  | LEU  | N-CA-C  | 5.07  | 119.34      | 113.20   |
| 2   | B     | 447  | TRP  | N-CA-C  | -5.07 | 102.50      | 110.36   |
| 4   | c     | 981  | PRO  | CB-CA-C | -5.07 | 107.61      | 111.87   |
| 4   | c     | 949  | SER  | N-CA-C  | 5.07  | 117.08      | 109.23   |
| 15  | M     | 69   | ASP  | N-CA-C  | 5.07  | 116.88      | 111.36   |
| 2   | B     | 1021 | GLY  | N-CA-C  | 5.06  | 118.38      | 112.50   |
| 11  | i     | 454  | VAL  | N-CA-C  | -5.06 | 101.05      | 108.54   |
| 2   | B     | 841  | TYR  | N-CA-C  | 5.06  | 117.50      | 109.50   |
| 12  | J     | 351  | GLN  | N-CA-C  | 5.06  | 117.99      | 109.95   |
| 7   | F     | 397  | GLU  | CA-C-N  | -5.06 | 114.74      | 119.85   |
| 7   | F     | 397  | GLU  | C-N-CA  | -5.06 | 114.74      | 119.85   |
| 11  | i     | 348  | GLY  | O-C-N   | 5.06  | 129.28      | 122.70   |
| 13  | K     | 260  | ALA  | N-CA-C  | 5.06  | 117.38      | 110.55   |
| 2   | B     | 600  | ASN  | N-CA-C  | 5.06  | 118.30      | 111.17   |
| 9   | H     | 389  | ASP  | N-CA-C  | 5.06  | 116.25      | 109.83   |
| 1   | a     | 277  | SER  | N-CA-C  | -5.04 | 99.55       | 108.23   |
| 7   | F     | 177  | TRP  | CB-CA-C | -5.04 | 103.38      | 112.76   |
| 5   | D     | 99   | ALA  | N-CA-C  | -5.04 | 106.23      | 112.38   |
| 1   | a     | 180  | ARG  | N-CA-C  | 5.04  | 116.85      | 111.36   |
| 4   | c     | 1106 | PRO  | N-CA-C  | 5.04  | 119.39      | 111.38   |
| 14  | L     | 185  | ASN  | N-CA-C  | 5.04  | 119.52      | 113.17   |
| 2   | B     | 591  | ASN  | N-CA-C  | -5.03 | 101.64      | 109.24   |
| 9   | H     | 257  | ASP  | N-CA-C  | 5.03  | 116.49      | 108.79   |
| 14  | L     | 209  | ALA  | N-CA-C  | 5.03  | 117.17      | 109.62   |
| 2   | B     | 532  | PRO  | CA-C-O  | -5.03 | 115.45      | 121.48   |
| 4   | c     | 1328 | PHE  | N-CA-C  | -5.03 | 102.61      | 110.10   |
| 4   | c     | 1135 | GLU  | N-CA-C  | 5.03  | 116.79      | 108.20   |
| 12  | J     | 315  | ASN  | N-CA-C  | 5.03  | 116.84      | 111.36   |
| 2   | B     | 88   | TRP  | N-CA-C  | -5.02 | 102.95      | 110.23   |
| 2   | B     | 853  | ASN  | CA-C-N  | -5.02 | 114.96      | 121.04   |
| 2   | B     | 853  | ASN  | C-N-CA  | -5.02 | 114.96      | 121.04   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | D     | 77  | LEU  | N-CA-C | -5.02 | 105.81      | 111.28   |
| 8   | G     | 71  | GLN  | N-CA-C | -5.02 | 105.80      | 111.28   |
| 2   | B     | 527 | GLY  | N-CA-C | 5.02  | 118.75      | 112.73   |
| 17  | O     | 106 | ASP  | N-CA-C | 5.02  | 119.25      | 113.18   |
| 3   | C     | 636 | GLY  | N-CA-C | 5.02  | 125.07      | 113.18   |
| 4   | c     | 104 | TRP  | N-CA-C | 5.01  | 116.83      | 111.36   |
| 3   | C     | 48  | TYR  | N-CA-C | 5.01  | 117.50      | 110.23   |
| 2   | B     | 639 | ALA  | O-C-N  | -5.01 | 117.67      | 123.33   |
| 10  | I     | 309 | ASN  | N-CA-C | 5.01  | 116.82      | 111.36   |
| 10  | I     | 470 | GLU  | N-CA-C | 5.01  | 116.74      | 111.28   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2164  | 0        | 2058     | 21      | 0            |
| 1   | a     | 2377  | 0        | 2264     | 17      | 0            |
| 2   | B     | 7296  | 0        | 6975     | 59      | 0            |
| 3   | C     | 4738  | 0        | 4243     | 46      | 0            |
| 4   | c     | 8108  | 0        | 7049     | 87      | 0            |
| 5   | D     | 4772  | 0        | 4333     | 47      | 0            |
| 6   | E     | 4483  | 0        | 3445     | 71      | 0            |
| 7   | F     | 4185  | 0        | 3724     | 47      | 0            |
| 8   | G     | 1714  | 0        | 1606     | 37      | 0            |
| 9   | H     | 2099  | 0        | 1951     | 10      | 0            |
| 10  | I     | 2924  | 0        | 2773     | 15      | 0            |
| 11  | i     | 2887  | 0        | 2764     | 33      | 0            |
| 12  | J     | 3358  | 0        | 3198     | 32      | 0            |
| 13  | K     | 1656  | 0        | 1580     | 11      | 0            |
| 14  | L     | 1702  | 0        | 1456     | 30      | 0            |
| 15  | M     | 931   | 0        | 920      | 8       | 0            |
| 15  | m     | 822   | 0        | 790      | 10      | 0            |
| 16  | N     | 2987  | 0        | 1863     | 20      | 0            |
| 17  | O     | 763   | 0        | 728      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | P     | 761   | 0        | 612      | 8       | 0            |
| 19  | R     | 199   | 0        | 115      | 3       | 0            |
| 20  | S     | 198   | 0        | 99       | 2       | 0            |
| 21  | B     | 1     | 0        | 0        | 0       | 0            |
| 22  | C     | 1     | 0        | 0        | 0       | 0            |
| 23  | G     | 1     | 0        | 0        | 1       | 0            |
| 23  | L     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 61128 | 0        | 54546    | 565     | 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 5.

All (565) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:541:ARG:HG3   | 2:B:862:ASN:HD21  | 0.95                     | 1.10              |
| 4:c:436:VAL:HG21  | 4:c:1136:LYS:HE3  | 1.40                     | 1.02              |
| 2:B:541:ARG:HG3   | 2:B:862:ASN:ND2   | 1.75                     | 1.00              |
| 6:E:466:ALA:HB2   | 6:E:712:ARG:HD3   | 1.45                     | 0.97              |
| 7:F:409:LEU:HA    | 7:F:412:ILE:HG12  | 1.55                     | 0.88              |
| 8:G:157:PHE:HZ    | 8:G:192:ALA:HA    | 1.37                     | 0.86              |
| 6:E:715:PRO:HG3   | 6:E:763:VAL:HA    | 1.59                     | 0.84              |
| 4:c:436:VAL:HG21  | 4:c:1136:LYS:CE   | 2.08                     | 0.83              |
| 11:i:419:MET:HE3  | 11:i:576:ILE:HG23 | 1.63                     | 0.81              |
| 5:D:435:TYR:CD2   | 16:N:632:PRO:HG3  | 2.16                     | 0.81              |
| 5:D:100:GLY:HA3   | 6:E:788:ARG:HD2   | 1.63                     | 0.79              |
| 5:D:734:ASP:HB2   | 5:D:737:GLU:HG2   | 1.64                     | 0.78              |
| 5:D:450:PRO:HG2   | 16:N:676:LEU:HD12 | 1.67                     | 0.76              |
| 3:C:309:ARG:HD3   | 3:C:334:LEU:HB3   | 1.66                     | 0.76              |
| 15:M:149:PHE:HB3  | 15:M:178:LEU:HD11 | 1.66                     | 0.76              |
| 4:c:329:PRO:HG2   | 4:c:1216:ILE:HD11 | 1.66                     | 0.76              |
| 6:E:674:TRP:CD1   | 6:E:720:THR:HG22  | 2.22                     | 0.75              |
| 6:E:683:ALA:HB2   | 6:E:720:THR:HB    | 1.68                     | 0.75              |
| 12:J:171:PRO:HB2  | 12:J:263:ILE:HD11 | 1.68                     | 0.75              |
| 5:D:493:LEU:HA    | 5:D:497:GLY:HA3   | 1.68                     | 0.75              |
| 11:i:380:ILE:HG23 | 15:m:159:ILE:HG23 | 1.71                     | 0.73              |
| 1:A:117:THR:HG22  | 1:A:136:ILE:HB    | 1.72                     | 0.72              |
| 4:c:855:PHE:O     | 7:F:464:LYS:HA    | 1.90                     | 0.72              |
| 2:B:541:ARG:CG    | 2:B:862:ASN:HD21  | 1.89                     | 0.71              |
| 2:B:1008:TYR:CE1  | 2:B:1015:ALA:HB1  | 2.25                     | 0.71              |
| 4:c:297:ILE:HD11  | 4:c:318:VAL:HG21  | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:52:TYR:OH     | 8:G:104:MET:N     | 2.25                     | 0.70              |
| 8:G:157:PHE:CZ    | 8:G:192:ALA:HA    | 2.24                     | 0.70              |
| 11:i:346:LYS:HE2  | 11:i:373:ASP:HB2  | 1.73                     | 0.68              |
| 3:C:286:ILE:HA    | 3:C:296:SER:HA    | 1.74                     | 0.68              |
| 6:E:502:LEU:HD22  | 6:E:505:GLU:H     | 1.59                     | 0.68              |
| 12:J:439:ARG:NH1  | 12:J:502:GLN:HB3  | 2.09                     | 0.68              |
| 4:c:230:PRO:HD2   | 4:c:281:GLN:HG3   | 1.76                     | 0.68              |
| 18:P:118:PRO:HG2  | 18:P:121:PHE:HB2  | 1.76                     | 0.68              |
| 2:B:627:PRO:HD2   | 2:B:630:LYS:HD2   | 1.75                     | 0.68              |
| 1:a:123:LEU:HD11  | 1:a:129:ILE:HG23  | 1.76                     | 0.67              |
| 6:E:655:ASN:HB3   | 6:E:692:ARG:HH21  | 1.58                     | 0.67              |
| 8:G:214:ASP:OD2   | 23:G:2001:FE:FE   | 1.47                     | 0.67              |
| 4:c:609:SER:HA    | 7:F:590:HIS:HE1   | 1.60                     | 0.66              |
| 14:L:224:ASP:OD2  | 23:L:2001:FE:FE   | 1.46                     | 0.66              |
| 4:c:436:VAL:HG21  | 4:c:1136:LYS:CD   | 2.25                     | 0.66              |
| 6:E:428:GLY:HA2   | 6:E:461:ALA:HB2   | 1.76                     | 0.66              |
| 13:K:207:ILE:HG23 | 13:K:212:ASP:HB3  | 1.77                     | 0.66              |
| 3:C:345:ASN:H     | 3:C:362:SER:HB3   | 1.60                     | 0.66              |
| 3:C:548:VAL:HG11  | 4:c:53:THR:HG21   | 1.77                     | 0.66              |
| 11:i:299:ARG:HG3  | 11:i:553:GLU:HB3  | 1.77                     | 0.65              |
| 15:M:107:MET:HE1  | 15:M:164:LEU:HA   | 1.78                     | 0.65              |
| 3:C:106:ILE:HG13  | 3:C:110:GLN:HB2   | 1.78                     | 0.65              |
| 1:A:14:GLN:H      | 1:A:35:SER:HB2    | 1.60                     | 0.65              |
| 12:J:360:TYR:N    | 12:J:360:TYR:CD1  | 2.65                     | 0.64              |
| 15:M:161:THR:HG21 | 15:M:165:ILE:HD13 | 1.80                     | 0.64              |
| 6:E:498:ALA:O     | 6:E:534:GLN:NE2   | 2.31                     | 0.64              |
| 8:G:225:LYS:H     | 8:G:225:LYS:HD2   | 1.63                     | 0.64              |
| 14:L:144:LEU:HD23 | 14:L:259:LEU:HD22 | 1.80                     | 0.63              |
| 2:B:984:ARG:HB2   | 3:C:382:ARG:HH11  | 1.62                     | 0.63              |
| 7:F:348:ASP:HB3   | 7:F:349:PRO:HD3   | 1.78                     | 0.63              |
| 7:F:365:PHE:HB3   | 7:F:367:ARG:HD2   | 1.79                     | 0.63              |
| 5:D:119:ARG:HA    | 5:D:149:LEU:HD11  | 1.81                     | 0.62              |
| 5:D:144:LEU:HG    | 5:D:148:ARG:HH12  | 1.64                     | 0.62              |
| 4:c:1039:PRO:HB3  | 7:F:212:VAL:HG11  | 1.82                     | 0.62              |
| 10:I:383:THR:HG22 | 10:I:389:LEU:HD13 | 1.80                     | 0.62              |
| 1:A:26:ARG:HG3    | 1:A:95:ILE:HD13   | 1.81                     | 0.62              |
| 3:C:214:ASP:HB3   | 3:C:217:ILE:HB    | 1.79                     | 0.62              |
| 7:F:173:PRO:HD2   | 7:F:195:THR:HG21  | 1.80                     | 0.62              |
| 1:a:186:ILE:HD12  | 9:H:367:ARG:HD3   | 1.82                     | 0.61              |
| 6:E:456:THR:HG23  | 6:E:492:SER:HB2   | 1.82                     | 0.61              |
| 10:I:171:ILE:HG23 | 10:I:202:GLU:HG2  | 1.81                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:58:GLU:HG2    | 1:A:155:ARG:HB3   | 1.81                     | 0.61              |
| 14:L:88:GLN:NE2   | 14:L:115:PRO:HB3  | 2.15                     | 0.61              |
| 4:c:1028:MET:HE1  | 7:F:203:VAL:HG11  | 1.82                     | 0.61              |
| 11:i:346:LYS:CE   | 11:i:373:ASP:HB2  | 2.30                     | 0.61              |
| 14:L:179:TYR:HB3  | 14:L:218:SER:HB2  | 1.82                     | 0.61              |
| 12:J:310:HIS:CE1  | 12:J:347:TYR:H    | 2.19                     | 0.60              |
| 4:c:982:LEU:HD22  | 4:c:1044:ILE:HG12 | 1.82                     | 0.60              |
| 4:c:1179:ILE:HG13 | 5:D:735:ILE:HD12  | 1.83                     | 0.60              |
| 6:E:568:CYS:SG    | 6:E:569:PHE:N     | 2.75                     | 0.60              |
| 10:I:482:VAL:HG22 | 10:I:485:MET:HE2  | 1.84                     | 0.60              |
| 8:G:183:VAL:HG12  | 8:G:209:PRO:HA    | 1.84                     | 0.60              |
| 16:N:303:VAL:HA   | 16:N:321:ILE:HA   | 1.83                     | 0.60              |
| 4:c:1198:ARG:HE   | 4:c:1229:THR:HG21 | 1.66                     | 0.60              |
| 11:i:428:LEU:HD21 | 11:i:460:LEU:HD11 | 1.84                     | 0.59              |
| 2:B:657:VAL:HG22  | 2:B:850:MET:HB2   | 1.85                     | 0.59              |
| 11:i:457:PRO:HD2  | 11:i:460:LEU:HD13 | 1.84                     | 0.59              |
| 12:J:213:SER:H    | 12:J:216:GLU:HG3  | 1.68                     | 0.59              |
| 2:B:989:GLU:HG3   | 3:C:470:ILE:HD11  | 1.85                     | 0.59              |
| 2:B:578:LEU:HD11  | 2:B:644:THR:HG21  | 1.84                     | 0.59              |
| 6:E:568:CYS:HB2   | 6:E:601:ILE:HD11  | 1.85                     | 0.58              |
| 3:C:675:GLU:HB2   | 17:O:58:LEU:HD11  | 1.85                     | 0.58              |
| 9:H:391:VAL:HG11  | 10:I:476:LEU:HD13 | 1.86                     | 0.58              |
| 15:M:107:MET:HG3  | 15:M:111:LEU:HD23 | 1.85                     | 0.58              |
| 3:C:50:PHE:HA     | 3:C:57:PRO:HA     | 1.85                     | 0.58              |
| 4:c:1265:ILE:HG12 | 4:c:1267:TYR:HD2  | 1.69                     | 0.57              |
| 11:i:278:PRO:HB3  | 11:i:418:LYS:HD3  | 1.85                     | 0.57              |
| 12:J:481:ILE:HA   | 12:J:484:ARG:HD3  | 1.85                     | 0.57              |
| 18:P:69:TRP:HB2   | 18:P:134:ARG:HB3  | 1.86                     | 0.57              |
| 12:J:359:ARG:CB   | 12:J:360:TYR:CD1  | 2.87                     | 0.57              |
| 14:L:131:SER:HA   | 14:L:258:ARG:HH22 | 1.70                     | 0.57              |
| 12:J:374:PHE:CD2  | 12:J:424:PRO:HD3  | 2.39                     | 0.57              |
| 6:E:746:VAL:HG13  | 6:E:788:ARG:HH21  | 1.68                     | 0.57              |
| 8:G:77:HIS:HA     | 8:G:81:HIS:HD2    | 1.70                     | 0.57              |
| 12:J:439:ARG:CZ   | 12:J:502:GLN:HB3  | 2.34                     | 0.57              |
| 2:B:325:PHE:O     | 2:B:329:LEU:HG    | 2.05                     | 0.56              |
| 2:B:149:THR:HA    | 2:B:158:SER:O     | 2.06                     | 0.56              |
| 6:E:678:GLN:NE2   | 6:E:680:GLU:OE1   | 2.39                     | 0.56              |
| 4:c:1157:SER:HB2  | 4:c:1160:SER:HB3  | 1.87                     | 0.56              |
| 12:J:359:ARG:HB3  | 12:J:360:TYR:CE1  | 2.39                     | 0.56              |
| 6:E:424:ILE:HG21  | 6:E:454:VAL:HA    | 1.87                     | 0.56              |
| 12:J:359:ARG:HB3  | 12:J:360:TYR:CD1  | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:L:126:GLN:HA   | 14:L:129:TRP:CD1  | 2.41                     | 0.56              |
| 5:D:368:SER:O     | 5:D:372:ARG:HG2   | 2.06                     | 0.56              |
| 6:E:651:PHE:O     | 6:E:692:ARG:NH1   | 2.37                     | 0.56              |
| 11:i:540:TYR:HE2  | 11:i:545:HIS:HD2  | 1.52                     | 0.56              |
| 4:c:1037:PRO:HB2  | 4:c:1043:ILE:HD12 | 1.88                     | 0.56              |
| 6:E:633:MET:O     | 6:E:681:ARG:NH1   | 2.34                     | 0.56              |
| 2:B:861:MET:HE1   | 4:c:145:GLN:HB2   | 1.88                     | 0.55              |
| 6:E:709:ASP:HA    | 6:E:746:VAL:HB    | 1.88                     | 0.55              |
| 6:E:628:GLN:O     | 6:E:632:GLN:NE2   | 2.40                     | 0.55              |
| 7:F:490:ARG:HD2   | 7:F:500:TYR:HB3   | 1.88                     | 0.55              |
| 1:A:156:GLY:HA2   | 1:A:176:PHE:HB2   | 1.87                     | 0.55              |
| 7:F:565:PRO:HB2   | 7:F:567:TYR:HD1   | 1.72                     | 0.55              |
| 2:B:284:ARG:HH21  | 2:B:287:LEU:HB3   | 1.71                     | 0.55              |
| 16:N:595:ALA:HB2  | 16:N:604:LEU:HD12 | 1.88                     | 0.55              |
| 3:C:566:ASN:HD22  | 9:H:212:LEU:HD22  | 1.72                     | 0.54              |
| 6:E:604:LYS:HA    | 6:E:675:TRP:HE1   | 1.71                     | 0.54              |
| 2:B:862:ASN:HB2   | 2:B:865:GLN:HE21  | 1.73                     | 0.54              |
| 4:c:475:TRP:HZ3   | 4:c:1088:SER:HB3  | 1.72                     | 0.54              |
| 6:E:499:LYS:HG3   | 6:E:712:ARG:HD2   | 1.89                     | 0.54              |
| 1:A:69:LYS:HZ1    | 1:A:145:PHE:HA    | 1.71                     | 0.54              |
| 16:N:589:GLY:HA3  | 16:N:715:ILE:HG22 | 1.88                     | 0.54              |
| 17:O:149:GLU:O    | 17:O:150:LEU:C    | 2.50                     | 0.54              |
| 4:c:810:ASN:O     | 7:F:601:TRP:N     | 2.40                     | 0.54              |
| 8:G:224:TYR:HB3   | 8:G:227:ASP:HB2   | 1.88                     | 0.54              |
| 4:c:923:PRO:HG2   | 4:c:942:ILE:HD12  | 1.89                     | 0.54              |
| 4:c:1116:HIS:HE1  | 4:c:1131:THR:HG23 | 1.73                     | 0.54              |
| 10:I:294:LEU:HD12 | 10:I:323:VAL:HG12 | 1.89                     | 0.54              |
| 4:c:609:SER:HA    | 7:F:590:HIS:CE1   | 2.42                     | 0.53              |
| 5:D:100:GLY:HA3   | 6:E:788:ARG:CD    | 2.37                     | 0.53              |
| 7:F:284:VAL:HG12  | 7:F:321:VAL:HA    | 1.89                     | 0.53              |
| 10:I:244:LEU:O    | 10:I:248:GLU:HB2  | 2.08                     | 0.53              |
| 1:a:321:LEU:HG    | 1:a:334:LYS:HE2   | 1.89                     | 0.53              |
| 5:D:840:ASP:HB2   | 5:D:873:THR:HG21  | 1.88                     | 0.53              |
| 11:i:584:HIS:H    | 11:i:584:HIS:CD2  | 2.25                     | 0.53              |
| 13:K:138:PHE:CD2  | 13:K:149:PHE:HB3  | 2.42                     | 0.53              |
| 18:P:94:GLY:HA2   | 18:P:131:TYR:HA   | 1.91                     | 0.53              |
| 3:C:628:ILE:HD11  | 13:K:302:VAL:HG23 | 1.89                     | 0.53              |
| 7:F:88:ALA:HB2    | 7:F:310:ASN:OD1   | 2.09                     | 0.53              |
| 4:c:360:ILE:HD11  | 4:c:414:VAL:HG21  | 1.89                     | 0.53              |
| 6:E:497:PHE:HD2   | 6:E:509:ILE:HD13  | 1.74                     | 0.53              |
| 4:c:95:GLU:HG2    | 4:c:373:ARG:O     | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:c:436:VAL:CG2   | 4:c:1136:LYS:HE3  | 2.27                     | 0.53              |
| 5:D:450:PRO:HG3   | 16:N:673:GLN:HG2  | 1.91                     | 0.53              |
| 8:G:159:SER:H     | 8:G:162:ASN:HB3   | 1.74                     | 0.53              |
| 6:E:683:ALA:HB2   | 6:E:720:THR:CB    | 2.38                     | 0.53              |
| 3:C:554:HIS:HB3   | 3:C:558:CYS:HB2   | 1.92                     | 0.52              |
| 6:E:572:LEU:HB3   | 6:E:575:GLU:HB2   | 1.91                     | 0.52              |
| 2:B:1044:ARG:HA   | 2:B:1047:ARG:HG2  | 1.91                     | 0.52              |
| 6:E:592:ILE:HD11  | 6:E:627:HIS:HA    | 1.90                     | 0.52              |
| 7:F:175:ARG:NH2   | 8:G:102:CYS:H     | 2.07                     | 0.52              |
| 8:G:79:GLY:HA2    | 8:G:83:ARG:HH21   | 1.73                     | 0.52              |
| 2:B:529:SER:O     | 2:B:565:THR:HG21  | 2.09                     | 0.52              |
| 14:L:144:LEU:O    | 14:L:148:ILE:HG12 | 2.09                     | 0.52              |
| 2:B:332:LEU:HD11  | 2:B:356:VAL:HG23  | 1.91                     | 0.52              |
| 4:c:1073:ILE:O    | 4:c:1088:SER:HA   | 2.10                     | 0.52              |
| 4:c:1232:VAL:HG12 | 4:c:1249:ILE:HG13 | 1.92                     | 0.52              |
| 7:F:177:TRP:CE2   | 7:F:179:PRO:HD3   | 2.45                     | 0.52              |
| 18:P:89:VAL:HG13  | 18:P:133:GLU:HG3  | 1.92                     | 0.52              |
| 3:C:216:ARG:O     | 3:C:219:ILE:HG12  | 2.09                     | 0.52              |
| 14:L:133:LYS:HD3  | 14:L:251:SER:HB3  | 1.91                     | 0.52              |
| 3:C:649:ARG:HG2   | 3:C:655:ILE:HA    | 1.92                     | 0.52              |
| 4:c:1021:ILE:HD12 | 4:c:1024:LYS:HE2  | 1.91                     | 0.52              |
| 6:E:684:ARG:HH11  | 6:E:687:ASN:HB2   | 1.75                     | 0.52              |
| 3:C:267:GLU:HB2   | 3:C:270:TRP:CE2   | 2.45                     | 0.52              |
| 8:G:105:GLU:HA    | 8:G:108:ILE:HD12  | 1.93                     | 0.52              |
| 5:D:381:VAL:HA    | 5:D:384:LEU:HD12  | 1.91                     | 0.51              |
| 19:R:6:DC:H2'     | 19:R:7:DT:C6      | 2.44                     | 0.51              |
| 12:J:374:PHE:HD2  | 12:J:424:PRO:HD3  | 1.74                     | 0.51              |
| 6:E:639:ASP:HA    | 6:E:644:TRP:HB2   | 1.91                     | 0.51              |
| 2:B:162:ILE:HG12  | 2:B:168:ILE:H     | 1.76                     | 0.51              |
| 3:C:137:LEU:HB3   | 3:C:139:LYS:HG2   | 1.91                     | 0.51              |
| 10:I:280:ILE:HG23 | 10:I:290:VAL:HG21 | 1.93                     | 0.51              |
| 12:J:146:PRO:HA   | 12:J:326:MET:HG2  | 1.93                     | 0.51              |
| 6:E:525:PHE:HB3   | 6:E:548:MET:HE2   | 1.91                     | 0.51              |
| 12:J:310:HIS:CE1  | 12:J:347:TYR:N    | 2.79                     | 0.51              |
| 6:E:702:ASN:OD1   | 6:E:703:LYS:N     | 2.41                     | 0.51              |
| 1:A:103:THR:HG22  | 1:A:152:GLU:HG2   | 1.92                     | 0.51              |
| 1:A:108:ILE:HD11  | 1:A:117:THR:HG23  | 1.92                     | 0.51              |
| 4:c:92:HIS:CD2    | 4:c:94:VAL:HG13   | 2.46                     | 0.51              |
| 4:c:1198:ARG:HE   | 4:c:1229:THR:CG2  | 2.23                     | 0.51              |
| 14:L:86:ASN:HA    | 14:L:89:ILE:HG12  | 1.92                     | 0.51              |
| 2:B:112:THR:HG21  | 2:B:378:LEU:HD22  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:221:TYR:O     | 8:G:222:LEU:C     | 2.54                     | 0.51              |
| 11:i:375:LYS:HG3  | 11:i:376:LYS:HD2  | 1.93                     | 0.51              |
| 1:A:312:PHE:HE2   | 1:A:317:VAL:HG12  | 1.75                     | 0.50              |
| 7:F:134:ILE:CD1   | 7:F:144:TYR:HB2   | 2.41                     | 0.50              |
| 8:G:52:TYR:OH     | 8:G:103:THR:HA    | 2.10                     | 0.50              |
| 8:G:133:PHE:HE1   | 8:G:213:LEU:HD12  | 1.76                     | 0.50              |
| 2:B:462:THR:HG21  | 2:B:465:ARG:HH21  | 1.76                     | 0.50              |
| 7:F:519:TRP:HZ2   | 14:L:188:ASN:O    | 1.93                     | 0.50              |
| 13:K:138:PHE:HD2  | 13:K:149:PHE:HB3  | 1.75                     | 0.50              |
| 5:D:129:ARG:NH1   | 6:E:477:THR:HG22  | 2.26                     | 0.50              |
| 6:E:577:GLU:OE2   | 6:E:602:TYR:OH    | 2.24                     | 0.50              |
| 7:F:545:GLU:HB3   | 7:F:548:ARG:HB2   | 1.93                     | 0.50              |
| 2:B:191:LEU:HD11  | 2:B:208:LEU:HD21  | 1.94                     | 0.50              |
| 6:E:707:SER:OG    | 6:E:708:VAL:N     | 2.45                     | 0.49              |
| 11:i:290:PHE:CZ   | 15:m:143:GLY:HA3  | 2.47                     | 0.49              |
| 4:c:1024:LYS:HB3  | 4:c:1026:TYR:CE2  | 2.46                     | 0.49              |
| 5:D:391:ALA:C     | 5:D:393:ASP:N     | 2.69                     | 0.49              |
| 7:F:454:LYS:HA    | 7:F:462:LEU:O     | 2.12                     | 0.49              |
| 4:c:355:PRO:HD2   | 4:c:389:ILE:HD12  | 1.94                     | 0.49              |
| 4:c:997:LEU:HD11  | 8:G:250:ALA:HB1   | 1.93                     | 0.49              |
| 5:D:381:VAL:O     | 5:D:384:LEU:HB2   | 2.12                     | 0.49              |
| 6:E:491:ASN:HA    | 6:E:494:ILE:HG22  | 1.94                     | 0.49              |
| 6:E:706:TRP:HB3   | 6:E:740:PRO:HG3   | 1.94                     | 0.49              |
| 2:B:388:VAL:HG21  | 2:B:550:ARG:HD3   | 1.94                     | 0.49              |
| 3:C:68:PHE:HB3    | 3:C:281:PRO:HG3   | 1.95                     | 0.49              |
| 7:F:192:ILE:O     | 7:F:195:THR:HG22  | 2.12                     | 0.49              |
| 19:R:5:DT:H2'     | 19:R:6:DC:C6      | 2.48                     | 0.49              |
| 4:c:1149:VAL:HA   | 4:c:1152:VAL:HG12 | 1.94                     | 0.49              |
| 12:J:419:ALA:O    | 12:J:423:LEU:HG   | 2.13                     | 0.49              |
| 16:N:737:ASP:OD1  | 16:N:737:ASP:N    | 2.44                     | 0.49              |
| 19:R:4:DC:H2'     | 19:R:5:DT:C6      | 2.48                     | 0.49              |
| 2:B:798:SER:O     | 2:B:799:TYR:C     | 2.56                     | 0.49              |
| 2:B:1008:TYR:CD1  | 2:B:1015:ALA:HB1  | 2.47                     | 0.49              |
| 4:c:1161:ILE:HD12 | 4:c:1201:LEU:HD21 | 1.94                     | 0.49              |
| 6:E:720:THR:OG1   | 6:E:721:ALA:N     | 2.44                     | 0.48              |
| 12:J:359:ARG:CB   | 12:J:360:TYR:CE1  | 2.96                     | 0.48              |
| 2:B:662:TRP:CZ3   | 2:B:840:PRO:HG3   | 2.47                     | 0.48              |
| 4:c:481:PRO:HB3   | 4:c:1122:THR:HG21 | 1.95                     | 0.48              |
| 5:D:423:ALA:HB2   | 5:D:806:VAL:HG23  | 1.95                     | 0.48              |
| 13:K:143:LEU:HD11 | 13:K:224:VAL:HG23 | 1.95                     | 0.48              |
| 2:B:312:LYS:HE2   | 2:B:395:TYR:HE1   | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:J:379:LYS:HG2  | 12:J:424:PRO:HB2  | 1.94                     | 0.48              |
| 2:B:450:LEU:O     | 2:B:471:PRO:HD3   | 2.13                     | 0.48              |
| 4:c:1036:ASN:O    | 7:F:214:MET:HA    | 2.14                     | 0.48              |
| 8:G:52:TYR:OH     | 8:G:103:THR:C     | 2.56                     | 0.48              |
| 4:c:362:PHE:HB3   | 4:c:387:VAL:HG12  | 1.96                     | 0.48              |
| 5:D:777:SER:OG    | 5:D:780:TRP:HB2   | 2.14                     | 0.48              |
| 7:F:177:TRP:O     | 7:F:178:PRO:C     | 2.55                     | 0.48              |
| 11:i:392:ARG:HG3  | 15:m:139:MET:HG3  | 1.95                     | 0.48              |
| 1:A:115:SER:HB2   | 1:A:139:LEU:H     | 1.78                     | 0.48              |
| 6:E:609:ASN:HA    | 6:E:612:HIS:HD2   | 1.78                     | 0.48              |
| 14:L:106:THR:HG21 | 14:L:115:PRO:HB2  | 1.95                     | 0.48              |
| 16:N:595:ALA:HB3  | 16:N:719:ALA:HB1  | 1.95                     | 0.48              |
| 2:B:716:LEU:O     | 2:B:717:LEU:HB2   | 2.13                     | 0.48              |
| 4:c:29:HIS:HA     | 13:K:210:PRO:O    | 2.13                     | 0.48              |
| 4:c:359:LYS:HE3   | 4:c:411:ASP:OD1   | 2.13                     | 0.48              |
| 5:D:391:ALA:C     | 5:D:393:ASP:H     | 2.22                     | 0.48              |
| 12:J:116:ILE:CD1  | 12:J:143:MET:HG2  | 2.44                     | 0.48              |
| 2:B:440:ILE:HD12  | 2:B:521:PHE:HB3   | 1.96                     | 0.48              |
| 6:E:488:GLU:HA    | 6:E:491:ASN:HD21  | 1.79                     | 0.47              |
| 1:a:274:ILE:HD11  | 1:a:292:ILE:HG22  | 1.95                     | 0.47              |
| 3:C:313:LEU:HG    | 3:C:331:GLN:HE21  | 1.79                     | 0.47              |
| 3:C:585:LYS:HG2   | 3:C:586:GLU:H     | 1.79                     | 0.47              |
| 6:E:711:HIS:CE1   | 6:E:749:ARG:H     | 2.32                     | 0.47              |
| 4:c:210:VAL:HG23  | 4:c:213:ILE:HG13  | 1.97                     | 0.47              |
| 5:D:387:LEU:HB3   | 5:D:791:LYS:HD3   | 1.96                     | 0.47              |
| 6:E:717:GLY:HA2   | 6:E:720:THR:HG23  | 1.95                     | 0.47              |
| 8:G:73:MET:HA     | 8:G:222:LEU:HD12  | 1.97                     | 0.47              |
| 10:I:162:PRO:HD2  | 10:I:415:ARG:O    | 2.14                     | 0.47              |
| 3:C:676:ALA:HA    | 17:O:61:GLN:HE22  | 1.78                     | 0.47              |
| 5:D:476:GLN:O     | 5:D:479:LEU:HG    | 2.15                     | 0.47              |
| 3:C:285:PRO:O     | 3:C:286:ILE:C     | 2.58                     | 0.47              |
| 7:F:200:SER:HA    | 8:G:56:LYS:HE2    | 1.96                     | 0.47              |
| 12:J:235:LYS:HB3  | 12:J:235:LYS:HE3  | 1.75                     | 0.47              |
| 14:L:147:LEU:HD12 | 14:L:147:LEU:HA   | 1.69                     | 0.47              |
| 1:a:285:ASN:CB    | 11:i:273:SER:HB2  | 2.45                     | 0.47              |
| 2:B:630:LYS:HB2   | 2:B:630:LYS:HE3   | 1.38                     | 0.47              |
| 3:C:249:ASP:C     | 3:C:251:LEU:N     | 2.65                     | 0.47              |
| 3:C:652:LYS:H     | 3:C:652:LYS:HG2   | 1.44                     | 0.47              |
| 4:c:209:VAL:HG21  | 4:c:1274:ILE:HD12 | 1.96                     | 0.47              |
| 4:c:370:THR:HG21  | 4:c:405:LEU:HD11  | 1.96                     | 0.47              |
| 5:D:810:ALA:HA    | 5:D:813:ARG:HE    | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:262:LYS:HB2   | 7:F:262:LYS:HE2   | 1.78                     | 0.47              |
| 12:J:360:TYR:N    | 12:J:360:TYR:HD1  | 2.10                     | 0.47              |
| 11:i:346:LYS:HG3  | 11:i:371:ARG:O    | 2.15                     | 0.47              |
| 1:A:295:LEU:O     | 1:A:296:LEU:C     | 2.57                     | 0.47              |
| 4:c:440:ILE:HD11  | 4:c:1132:PHE:HE2  | 1.80                     | 0.47              |
| 7:F:249:TYR:HB3   | 7:F:367:ARG:NH1   | 2.30                     | 0.47              |
| 14:L:97:MET:HB3   | 14:L:101:ASP:HB2  | 1.97                     | 0.47              |
| 2:B:691:TYR:HE2   | 2:B:808:ILE:HG12  | 1.80                     | 0.47              |
| 2:B:788:VAL:HG12  | 2:B:806:VAL:HG12  | 1.97                     | 0.47              |
| 8:G:111:THR:HA    | 8:G:118:LEU:HD12  | 1.96                     | 0.47              |
| 7:F:388:LYS:CE    | 7:F:552:PRO:HB3   | 2.45                     | 0.46              |
| 8:G:157:PHE:HZ    | 8:G:192:ALA:CA    | 2.19                     | 0.46              |
| 8:G:159:SER:H     | 8:G:162:ASN:CB    | 2.28                     | 0.46              |
| 15:m:134:GLU:HA   | 15:m:137:ARG:HG2  | 1.98                     | 0.46              |
| 4:c:329:PRO:HB3   | 4:c:1214:VAL:HG11 | 1.97                     | 0.46              |
| 5:D:826:THR:O     | 5:D:829:SER:HB2   | 2.16                     | 0.46              |
| 6:E:544:ALA:O     | 6:E:548:MET:HG3   | 2.14                     | 0.46              |
| 6:E:717:GLY:HA2   | 6:E:720:THR:CG2   | 2.46                     | 0.46              |
| 7:F:133:LYS:HD2   | 7:F:133:LYS:HA    | 1.72                     | 0.46              |
| 10:I:374:HIS:CE1  | 10:I:377:LEU:HD13 | 2.50                     | 0.46              |
| 4:c:605:PHE:HB2   | 4:c:851:ALA:HB3   | 1.98                     | 0.46              |
| 7:F:504:LYS:HG3   | 7:F:508:ASN:HB2   | 1.97                     | 0.46              |
| 11:i:475:TRP:HZ2  | 11:i:521:LEU:HD13 | 1.80                     | 0.46              |
| 2:B:672:LEU:HD12  | 2:B:832:LYS:HB3   | 1.97                     | 0.46              |
| 6:E:475:PHE:CD1   | 6:E:493:LEU:HD11  | 2.50                     | 0.46              |
| 11:i:518:ILE:O    | 11:i:521:LEU:HG   | 2.16                     | 0.46              |
| 1:a:54:LEU:O      | 2:B:837:GLN:HG2   | 2.16                     | 0.46              |
| 2:B:130:PRO:HA    | 2:B:151:ILE:HB    | 1.98                     | 0.46              |
| 4:c:416:SER:O     | 4:c:417:GLU:HG2   | 2.16                     | 0.46              |
| 6:E:701:ARG:NH1   | 6:E:702:ASN:O     | 2.49                     | 0.46              |
| 7:F:529:MET:O     | 7:F:533:ILE:HG12  | 2.15                     | 0.46              |
| 14:L:265:LYS:HA   | 14:L:265:LYS:HD3  | 1.68                     | 0.46              |
| 4:c:405:LEU:HD12  | 4:c:405:LEU:HA    | 1.78                     | 0.46              |
| 12:J:230:GLU:O    | 12:J:484:ARG:HD2  | 2.15                     | 0.46              |
| 4:c:1179:ILE:HG22 | 4:c:1180:LEU:HD12 | 1.98                     | 0.46              |
| 4:c:1196:GLN:HE21 | 5:D:731:PHE:HD1   | 1.64                     | 0.46              |
| 7:F:93:ILE:HG21   | 7:F:149:PHE:CE1   | 2.50                     | 0.46              |
| 11:i:348:GLY:O    | 11:i:353:GLY:HA3  | 2.16                     | 0.46              |
| 16:N:728:ILE:HA   | 16:N:733:LYS:HA   | 1.97                     | 0.46              |
| 5:D:412:VAL:HG12  | 5:D:788:VAL:HG12  | 1.98                     | 0.45              |
| 7:F:365:PHE:CB    | 7:F:367:ARG:HD2   | 2.46                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:i:612:ARG:HA  | 11:i:612:ARG:HD3  | 1.66                     | 0.45              |
| 4:c:209:VAL:HG21 | 4:c:1274:ILE:HG23 | 1.99                     | 0.45              |
| 2:B:668:GLU:HB2  | 3:C:497:PHE:HD2   | 1.81                     | 0.45              |
| 5:D:505:SER:HB2  | 5:D:509:TYR:CZ    | 2.51                     | 0.45              |
| 5:D:809:ARG:O    | 5:D:812:VAL:HG22  | 2.17                     | 0.45              |
| 8:G:52:TYR:CZ    | 8:G:104:MET:N     | 2.85                     | 0.45              |
| 14:L:78:HIS:CE1  | 14:L:129:TRP:HE1  | 2.34                     | 0.45              |
| 16:N:656:ASP:N   | 16:N:656:ASP:OD1  | 2.48                     | 0.45              |
| 4:c:287:THR:HG23 | 4:c:289:PHE:H     | 1.82                     | 0.45              |
| 6:E:456:THR:HG23 | 6:E:492:SER:CB    | 2.45                     | 0.45              |
| 16:N:686:PRO:HB3 | 16:N:692:ARG:HE   | 1.82                     | 0.45              |
| 4:c:20:LYS:HB2   | 4:c:20:LYS:HE3    | 1.72                     | 0.45              |
| 4:c:1286:SER:O   | 4:c:1287:GLU:C    | 2.59                     | 0.45              |
| 12:J:384:THR:O   | 12:J:388:VAL:HG12 | 2.17                     | 0.45              |
| 14:L:138:GLY:H   | 14:L:252:TRP:CD1  | 2.35                     | 0.45              |
| 3:C:333:LYS:HA   | 3:C:333:LYS:HD3   | 1.51                     | 0.45              |
| 1:a:294:THR:O    | 1:a:297:ASP:HB2   | 2.17                     | 0.45              |
| 4:c:436:VAL:CG2  | 4:c:1136:LYS:HG3  | 2.47                     | 0.45              |
| 4:c:605:PHE:N    | 4:c:851:ALA:O     | 2.50                     | 0.45              |
| 6:E:250:SER:O    | 6:E:251:ALA:C     | 2.60                     | 0.45              |
| 9:H:229:LYS:HA   | 9:H:230:PRO:HD3   | 1.75                     | 0.45              |
| 9:H:392:TYR:HA   | 9:H:393:PRO:HD3   | 1.79                     | 0.45              |
| 7:F:134:ILE:HD12 | 7:F:144:TYR:HB2   | 1.99                     | 0.45              |
| 16:N:608:VAL:O   | 16:N:612:GLY:N    | 2.31                     | 0.45              |
| 2:B:728:LEU:HD12 | 2:B:788:VAL:HG22  | 1.99                     | 0.45              |
| 4:c:368:HIS:HA   | 4:c:369:PRO:HD3   | 1.86                     | 0.45              |
| 6:E:424:ILE:HG21 | 6:E:454:VAL:HG13  | 1.98                     | 0.45              |
| 8:G:263:ILE:HA   | 8:G:264:PRO:HD3   | 1.88                     | 0.45              |
| 1:a:16:LYS:HB3   | 1:a:16:LYS:HE2    | 1.85                     | 0.44              |
| 2:B:283:PRO:HB2  | 7:F:566:LEU:HD23  | 1.99                     | 0.44              |
| 2:B:815:LYS:HB2  | 2:B:815:LYS:HE2   | 1.74                     | 0.44              |
| 5:D:98:ALA:HA    | 6:E:746:VAL:HG21  | 1.99                     | 0.44              |
| 6:E:747:VAL:HG12 | 6:E:788:ARG:HA    | 1.99                     | 0.44              |
| 3:C:111:MET:HE3  | 3:C:111:MET:HB3   | 1.83                     | 0.44              |
| 8:G:51:ALA:C     | 8:G:53:TYR:N      | 2.66                     | 0.44              |
| 16:N:654:THR:H   | 16:N:730:GLY:HA2  | 1.82                     | 0.44              |
| 4:c:499:ASN:HB2  | 4:c:924:GLN:HG3   | 2.00                     | 0.44              |
| 6:E:562:ALA:O    | 6:E:566:VAL:HG23  | 2.17                     | 0.44              |
| 9:H:242:LYS:HA   | 9:H:243:PRO:HD3   | 1.88                     | 0.44              |
| 9:H:308:LYS:HE2  | 9:H:308:LYS:HB3   | 1.79                     | 0.44              |
| 1:A:65:VAL:HG21  | 1:A:91:LEU:HD13   | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:153:SER:O     | 3:C:171:PHE:HA    | 2.17                     | 0.44              |
| 5:D:448:TRP:HB2   | 16:N:671:SER:HB2  | 1.99                     | 0.44              |
| 18:P:71:MET:HA    | 18:P:133:GLU:O    | 2.18                     | 0.44              |
| 4:c:302:TYR:O     | 4:c:1219:ARG:HD2  | 2.17                     | 0.44              |
| 16:N:240:ALA:HB2  | 16:N:257:LEU:H    | 1.83                     | 0.44              |
| 1:A:279:LEU:HD22  | 1:A:283:ILE:HD11  | 2.00                     | 0.44              |
| 1:A:326:LYS:O     | 1:A:327:TYR:C     | 2.61                     | 0.44              |
| 4:c:436:VAL:HG21  | 4:c:1136:LYS:HG3  | 1.99                     | 0.44              |
| 6:E:522:ARG:NH2   | 6:E:554:ASP:O     | 2.49                     | 0.44              |
| 8:G:52:TYR:HH     | 8:G:103:THR:HA    | 1.81                     | 0.44              |
| 11:i:445:LYS:HE2  | 11:i:445:LYS:HB3  | 1.82                     | 0.44              |
| 11:i:518:ILE:H    | 11:i:518:ILE:HG12 | 1.61                     | 0.44              |
| 12:J:310:HIS:CE1  | 12:J:346:ASP:HA   | 2.53                     | 0.44              |
| 2:B:478:MET:SD    | 2:B:508:ILE:HD13  | 2.58                     | 0.44              |
| 4:c:92:HIS:HD2    | 4:c:94:VAL:HG13   | 1.82                     | 0.44              |
| 5:D:510:ILE:H     | 5:D:510:ILE:HG13  | 1.61                     | 0.44              |
| 7:F:367:ARG:HE    | 7:F:367:ARG:HB3   | 1.55                     | 0.44              |
| 1:a:31:ARG:HG3    | 1:a:202:GLU:HG2   | 2.00                     | 0.44              |
| 6:E:742:LEU:HD11  | 6:E:790:VAL:HB    | 2.00                     | 0.44              |
| 12:J:155:LYS:HE2  | 12:J:155:LYS:HB3  | 1.67                     | 0.44              |
| 1:A:61:CYS:SG     | 1:A:174:ALA:HB1   | 2.58                     | 0.43              |
| 1:A:156:GLY:CA    | 1:A:176:PHE:HB2   | 2.48                     | 0.43              |
| 2:B:167:ARG:O     | 2:B:168:ILE:C     | 2.61                     | 0.43              |
| 2:B:466:MET:HE3   | 2:B:466:MET:HB3   | 1.91                     | 0.43              |
| 13:K:178:ILE:HA   | 13:K:179:PRO:HD3  | 1.80                     | 0.43              |
| 6:E:619:MET:O     | 6:E:628:GLN:NE2   | 2.40                     | 0.43              |
| 7:F:388:LYS:HE3   | 7:F:552:PRO:HB3   | 1.99                     | 0.43              |
| 11:i:506:ASP:O    | 11:i:507:ARG:HB2  | 2.18                     | 0.43              |
| 11:i:540:TYR:CE1  | 11:i:547:SER:HB3  | 2.53                     | 0.43              |
| 11:i:610:GLN:HG3  | 11:i:613:ARG:HH11 | 1.83                     | 0.43              |
| 11:i:634:LYS:HE3  | 11:i:634:LYS:HB2  | 1.85                     | 0.43              |
| 15:M:113:MET:HE3  | 15:M:113:MET:HB3  | 1.91                     | 0.43              |
| 1:a:302:SER:HB3   | 1:a:305:ASP:CG    | 2.43                     | 0.43              |
| 4:c:318:VAL:H     | 4:c:318:VAL:HG22  | 1.46                     | 0.43              |
| 11:i:361:ASN:HD22 | 11:i:361:ASN:HA   | 1.70                     | 0.43              |
| 14:L:244:ILE:HG23 | 14:L:248:LYS:HE2  | 2.00                     | 0.43              |
| 15:m:136:ALA:HB1  | 15:m:141:VAL:HG11 | 2.00                     | 0.43              |
| 1:A:36:PRO:HB3    | 1:A:196:GLN:HB3   | 1.99                     | 0.43              |
| 2:B:966:TYR:CZ    | 2:B:1016:ARG:HD3  | 2.54                     | 0.43              |
| 5:D:482:TRP:HZ3   | 5:D:773:PRO:C     | 2.26                     | 0.43              |
| 6:E:573:VAL:HG13  | 6:E:601:ILE:HG22  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:177:SER:HB3   | 8:G:216:TRP:CD2   | 2.53                     | 0.43              |
| 10:I:210:LYS:HD3  | 10:I:210:LYS:HA   | 1.73                     | 0.43              |
| 12:J:186:ASP:HB2  | 12:J:277:MET:HE3  | 2.00                     | 0.43              |
| 20:S:-2:U:H2'     | 20:S:-1:A:C8      | 2.53                     | 0.43              |
| 6:E:670:ILE:HD11  | 6:E:685:VAL:HB    | 2.00                     | 0.43              |
| 6:E:724:VAL:HA    | 6:E:727:ASN:ND2   | 2.34                     | 0.43              |
| 16:N:305:SER:HA   | 16:N:323:GLU:HA   | 2.00                     | 0.43              |
| 6:E:600:ALA:HB2   | 6:E:672:ALA:HA    | 2.01                     | 0.43              |
| 13:K:144:LEU:HD13 | 13:K:220:GLU:HG3  | 1.99                     | 0.43              |
| 4:c:381:CYS:O     | 4:c:403:LYS:HA    | 2.19                     | 0.43              |
| 5:D:129:ARG:NH1   | 6:E:477:THR:CG2   | 2.81                     | 0.43              |
| 5:D:824:LEU:HD21  | 5:D:858:ILE:HD12  | 2.00                     | 0.43              |
| 6:E:747:VAL:HG13  | 6:E:748:VAL:HG12  | 1.99                     | 0.43              |
| 14:L:74:TRP:O     | 14:L:78:HIS:HB2   | 2.18                     | 0.43              |
| 18:P:74:THR:H     | 18:P:131:TYR:HB3  | 1.83                     | 0.43              |
| 2:B:275:PRO:HD3   | 7:F:559:GLN:HG3   | 2.00                     | 0.43              |
| 3:C:131:SER:HB2   | 3:C:134:ALA:HB3   | 2.01                     | 0.43              |
| 12:J:359:ARG:HB2  | 12:J:360:TYR:CD1  | 2.54                     | 0.43              |
| 16:N:346:LEU:HA   | 16:N:417:VAL:HA   | 1.99                     | 0.43              |
| 2:B:1014:ARG:O    | 2:B:1017:GLN:HG2  | 2.19                     | 0.43              |
| 4:c:1005:VAL:HA   | 4:c:1008:TYR:CZ   | 2.54                     | 0.43              |
| 5:D:125:MET:O     | 5:D:129:ARG:HG3   | 2.19                     | 0.43              |
| 5:D:745:ARG:O     | 5:D:746:ASN:HB2   | 2.18                     | 0.43              |
| 7:F:337:ARG:HA    | 7:F:337:ARG:HD3   | 1.87                     | 0.43              |
| 14:L:145:LEU:HD23 | 14:L:145:LEU:HA   | 1.67                     | 0.43              |
| 14:L:73:HIS:O     | 14:L:77:HIS:HB2   | 2.19                     | 0.43              |
| 3:C:50:PHE:HB3    | 3:C:51:HIS:H      | 1.51                     | 0.42              |
| 3:C:485:LEU:HD23  | 3:C:485:LEU:HA    | 1.86                     | 0.42              |
| 5:D:782:VAL:HG21  | 5:D:816:MET:HG2   | 2.01                     | 0.42              |
| 7:F:565:PRO:O     | 7:F:566:LEU:HB2   | 2.19                     | 0.42              |
| 3:C:370:LYS:HA    | 3:C:375:ARG:HE    | 1.83                     | 0.42              |
| 4:c:411:ASP:HB3   | 9:H:231:LEU:HG    | 2.00                     | 0.42              |
| 1:a:295:LEU:O     | 1:a:296:LEU:C     | 2.60                     | 0.42              |
| 1:a:326:LYS:HE2   | 1:a:326:LYS:HB3   | 1.75                     | 0.42              |
| 2:B:800:ASN:O     | 2:B:801:PRO:C     | 2.62                     | 0.42              |
| 3:C:368:GLU:HA    | 4:c:1293:THR:HG21 | 2.02                     | 0.42              |
| 4:c:1035:PHE:CE1  | 7:F:213:LYS:HD2   | 2.54                     | 0.42              |
| 5:D:148:ARG:HH11  | 5:D:148:ARG:HB2   | 1.84                     | 0.42              |
| 14:L:99:LEU:HD12  | 14:L:99:LEU:HA    | 1.84                     | 0.42              |
| 14:L:137:GLY:HA2  | 14:L:252:TRP:HD1  | 1.84                     | 0.42              |
| 17:O:58:LEU:HD12  | 17:O:58:LEU:HA    | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:927:ILE:HG13  | 2:B:936:PHE:HD2   | 1.84                     | 0.42              |
| 6:E:543:LYS:O     | 6:E:546:VAL:HG12  | 2.19                     | 0.42              |
| 8:G:246:LEU:HD12  | 8:G:246:LEU:HA    | 1.82                     | 0.42              |
| 18:P:88:LEU:HA    | 18:P:88:LEU:HD23  | 1.78                     | 0.42              |
| 3:C:218:ILE:HD12  | 3:C:254:ARG:HH22  | 1.84                     | 0.42              |
| 7:F:283:LYS:HE3   | 7:F:283:LYS:HB2   | 1.81                     | 0.42              |
| 10:I:218:GLY:O    | 15:M:161:THR:HA   | 2.19                     | 0.42              |
| 12:J:317:PHE:CZ   | 12:J:330:MET:HE3  | 2.55                     | 0.42              |
| 15:m:146:THR:HG22 | 15:m:162:GLU:HG2  | 2.01                     | 0.42              |
| 3:C:137:LEU:HD12  | 3:C:144:LEU:HD22  | 2.00                     | 0.42              |
| 3:C:142:LYS:HE2   | 3:C:142:LYS:HB2   | 1.76                     | 0.42              |
| 4:c:273:ASN:O     | 4:c:276:ILE:HG12  | 2.18                     | 0.42              |
| 4:c:1084:PRO:HA   | 4:c:1085:PRO:HD3  | 1.87                     | 0.42              |
| 4:c:1286:SER:OG   | 4:c:1313:LYS:HB3  | 2.19                     | 0.42              |
| 5:D:235:MET:HE3   | 5:D:235:MET:HB2   | 1.83                     | 0.42              |
| 8:G:168:THR:O     | 8:G:171:ALA:HB3   | 2.18                     | 0.42              |
| 10:I:296:LEU:HA   | 10:I:297:PRO:HD3  | 1.80                     | 0.42              |
| 4:c:163:LEU:HD12  | 4:c:163:LEU:HA    | 1.90                     | 0.42              |
| 11:i:560:TYR:O    | 15:m:102:GLY:HA3  | 2.20                     | 0.42              |
| 14:L:84:ASN:HD22  | 14:L:87:LYS:HD2   | 1.85                     | 0.42              |
| 2:B:499:ALA:O     | 2:B:506:LEU:HD23  | 2.19                     | 0.42              |
| 4:c:1036:ASN:HD22 | 4:c:1039:PRO:HA   | 1.84                     | 0.42              |
| 6:E:565:SER:HA    | 6:E:568:CYS:HB3   | 2.02                     | 0.42              |
| 7:F:353:HIS:CD2   | 7:F:354:LEU:HG    | 2.54                     | 0.42              |
| 10:I:366:PRO:HG3  | 10:I:397:ASP:OD2  | 2.20                     | 0.42              |
| 16:N:600:ALA:HA   | 16:N:603:ARG:HG2  | 2.01                     | 0.42              |
| 5:D:854:ALA:O     | 5:D:858:ILE:HG12  | 2.19                     | 0.42              |
| 6:E:484:ARG:HA    | 6:E:485:PRO:HD3   | 1.89                     | 0.42              |
| 8:G:222:LEU:HA    | 8:G:222:LEU:HD23  | 1.83                     | 0.42              |
| 1:A:170:TYR:HA    | 1:A:171:PRO:HD3   | 1.94                     | 0.42              |
| 1:a:296:LEU:HD12  | 1:a:296:LEU:HA    | 1.94                     | 0.42              |
| 3:C:177:SER:O     | 3:C:178:TRP:C     | 2.62                     | 0.42              |
| 3:C:641:ILE:HG21  | 13:K:302:VAL:CG2  | 2.50                     | 0.42              |
| 4:c:1204:LYS:HB3  | 4:c:1204:LYS:HE3  | 1.85                     | 0.42              |
| 4:c:1284:PHE:CE2  | 4:c:1307:ASP:HB2  | 2.55                     | 0.42              |
| 5:D:500:ILE:HD12  | 5:D:500:ILE:HA    | 1.90                     | 0.42              |
| 6:E:722:ILE:HD13  | 6:E:771:LEU:HD21  | 2.02                     | 0.42              |
| 8:G:116:ASN:O     | 8:G:117:PRO:C     | 2.59                     | 0.42              |
| 14:L:180:LYS:HB2  | 14:L:200:LYS:H    | 1.84                     | 0.42              |
| 11:i:346:LYS:HB2  | 11:i:404:LEU:HD13 | 2.02                     | 0.41              |
| 2:B:36:TYR:HA     | 2:B:54:VAL:HG11   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:410:ILE:H     | 2:B:410:ILE:HG12  | 1.62                     | 0.41              |
| 3:C:524:MET:HE3   | 17:O:77:HIS:NE2   | 2.35                     | 0.41              |
| 3:C:608:SER:HA    | 3:C:609:PRO:HD3   | 1.93                     | 0.41              |
| 6:E:490:PHE:CD2   | 6:E:518:VAL:HG21  | 2.55                     | 0.41              |
| 8:G:138:GLN:CB    | 8:G:241:SER:HB2   | 2.50                     | 0.41              |
| 14:L:252:TRP:O    | 14:L:255:VAL:HG22 | 2.20                     | 0.41              |
| 4:c:449:HIS:HD2   | 4:c:1119:TYR:OH   | 2.02                     | 0.41              |
| 4:c:997:LEU:HD11  | 8:G:250:ALA:CB    | 2.50                     | 0.41              |
| 6:E:556:ASP:N     | 6:E:559:THR:OG1   | 2.54                     | 0.41              |
| 8:G:52:TYR:OH     | 8:G:103:THR:CA    | 2.68                     | 0.41              |
| 10:I:152:GLN:HE21 | 10:I:152:GLN:HB2  | 1.71                     | 0.41              |
| 2:B:132:ILE:HA    | 2:B:149:THR:O     | 2.20                     | 0.41              |
| 2:B:819:LYS:HD2   | 2:B:827:LYS:HD2   | 2.02                     | 0.41              |
| 4:c:211:GLN:HG3   | 4:c:320:ILE:HD11  | 2.02                     | 0.41              |
| 9:H:242:LYS:HE3   | 9:H:242:LYS:HB3   | 1.86                     | 0.41              |
| 12:J:324:ASP:OD2  | 17:O:81:LEU:HD13  | 2.20                     | 0.41              |
| 12:J:453:LEU:HD12 | 12:J:453:LEU:HA   | 1.87                     | 0.41              |
| 14:L:165:ALA:O    | 14:L:166:ALA:C    | 2.63                     | 0.41              |
| 1:A:89:MET:O      | 1:A:92:LYS:HG2    | 2.21                     | 0.41              |
| 2:B:27:ILE:HD13   | 2:B:27:ILE:HA     | 1.92                     | 0.41              |
| 2:B:165:LYS:O     | 2:B:166:ALA:C     | 2.63                     | 0.41              |
| 5:D:359:ASN:HD22  | 5:D:363:TYR:HE2   | 1.68                     | 0.41              |
| 20:S:-9:C:H2'     | 20:S:-8:G:C8      | 2.56                     | 0.41              |
| 1:a:285:ASN:HB3   | 11:i:273:SER:HB2  | 2.03                     | 0.41              |
| 2:B:974:LEU:O     | 2:B:981:GLY:HA3   | 2.20                     | 0.41              |
| 14:L:114:PRO:HB2  | 14:L:115:PRO:HD3  | 2.02                     | 0.41              |
| 14:L:162:PHE:HE2  | 14:L:223:ILE:HD11 | 1.86                     | 0.41              |
| 3:C:345:ASN:H     | 3:C:362:SER:CB    | 2.30                     | 0.41              |
| 4:c:372:THR:HG22  | 4:c:373:ARG:H     | 1.85                     | 0.41              |
| 4:c:498:MET:HE2   | 4:c:498:MET:HB3   | 1.94                     | 0.41              |
| 5:D:822:ASN:O     | 5:D:825:GLN:HB3   | 2.21                     | 0.41              |
| 6:E:416:ASN:H     | 6:E:419:THR:CB    | 2.34                     | 0.41              |
| 6:E:560:LEU:HB3   | 6:E:583:ILE:HD11  | 2.03                     | 0.41              |
| 7:F:78:ARG:NH1    | 8:G:266:ALA:H     | 2.18                     | 0.41              |
| 10:I:223:LYS:HB2  | 10:I:223:LYS:HE3  | 1.84                     | 0.41              |
| 5:D:212:TYR:HB3   | 5:D:235:MET:HE2   | 2.03                     | 0.41              |
| 5:D:732:PRO:HB2   | 5:D:737:GLU:HG3   | 2.02                     | 0.41              |
| 11:i:428:LEU:HA   | 11:i:428:LEU:HD23 | 1.81                     | 0.41              |
| 14:L:56:TYR:O     | 14:L:57:PRO:C     | 2.60                     | 0.41              |
| 1:A:84:VAL:O      | 1:A:87:ILE:HG12   | 2.21                     | 0.41              |
| 1:A:313:ARG:O     | 1:A:316:ASP:HB2   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:670:ALA:HB1   | 2:B:831:SER:OG    | 2.21                     | 0.41              |
| 3:C:477:LEU:HD12  | 3:C:477:LEU:HA    | 1.96                     | 0.41              |
| 3:C:585:LYS:HB2   | 3:C:609:PRO:HB2   | 2.02                     | 0.41              |
| 4:c:855:PHE:HA    | 4:c:868:LEU:CB    | 2.50                     | 0.41              |
| 4:c:879:TYR:HB3   | 4:c:885:ASP:HA    | 2.02                     | 0.41              |
| 4:c:1024:LYS:HB3  | 4:c:1026:TYR:HE2  | 1.85                     | 0.41              |
| 6:E:521:ASN:O     | 6:E:524:SER:OG    | 2.39                     | 0.41              |
| 7:F:389:ASP:HA    | 7:F:390:PRO:HD3   | 1.79                     | 0.41              |
| 8:G:118:LEU:HB3   | 8:G:119:PRO:HD2   | 2.03                     | 0.41              |
| 11:i:627:VAL:O    | 11:i:628:PRO:C    | 2.62                     | 0.41              |
| 12:J:381:HIS:CE1  | 12:J:427:SER:HA   | 2.56                     | 0.41              |
| 13:K:321:LYS:HB3  | 13:K:321:LYS:HE2  | 1.78                     | 0.41              |
| 14:L:267:ALA:O    | 14:L:270:GLU:HG3  | 2.21                     | 0.41              |
| 15:m:84:ILE:HD12  | 15:m:84:ILE:HA    | 1.93                     | 0.41              |
| 18:P:44:LEU:HB3   | 18:P:107:MET:HE2  | 2.03                     | 0.41              |
| 1:a:282:ARG:HE    | 1:a:282:ARG:HB3   | 1.72                     | 0.41              |
| 16:N:657:PRO:HB2  | 16:N:658:LEU:HD12 | 2.02                     | 0.41              |
| 2:B:313:ARG:HE    | 2:B:313:ARG:HB3   | 1.57                     | 0.40              |
| 4:c:436:VAL:HG21  | 4:c:1136:LYS:CG   | 2.51                     | 0.40              |
| 4:c:1027:LEU:HD12 | 7:F:169:VAL:O     | 2.21                     | 0.40              |
| 4:c:1096:VAL:H    | 4:c:1096:VAL:HG22 | 1.63                     | 0.40              |
| 12:J:439:ARG:NH2  | 12:J:502:GLN:HA   | 2.36                     | 0.40              |
| 15:M:107:MET:HE2  | 15:M:107:MET:HB2  | 1.80                     | 0.40              |
| 1:a:267:ILE:HD13  | 1:a:267:ILE:HA    | 1.82                     | 0.40              |
| 3:C:287:ILE:O     | 3:C:288:GLN:C     | 2.64                     | 0.40              |
| 3:C:542:MET:H     | 3:C:542:MET:HG3   | 1.69                     | 0.40              |
| 5:D:98:ALA:HA     | 6:E:746:VAL:CG2   | 2.51                     | 0.40              |
| 5:D:765:GLU:O     | 5:D:766:LYS:C     | 2.64                     | 0.40              |
| 8:G:52:TYR:HH     | 8:G:103:THR:CA    | 2.34                     | 0.40              |
| 11:i:513:TYR:HA   | 11:i:514:PRO:HD3  | 1.91                     | 0.40              |
| 12:J:166:ILE:HA   | 12:J:167:PRO:HD3  | 1.87                     | 0.40              |
| 15:m:90:VAL:HB    | 15:m:122:ALA:HA   | 2.03                     | 0.40              |
| 6:E:625:ASP:N     | 6:E:625:ASP:OD1   | 2.55                     | 0.40              |
| 13:K:299:PRO:O    | 13:K:302:VAL:HG22 | 2.21                     | 0.40              |
| 1:a:296:LEU:HA    | 1:a:299:LEU:HD12  | 2.04                     | 0.40              |
| 2:B:61:GLU:HA     | 2:B:62:PRO:HD3    | 1.94                     | 0.40              |
| 3:C:218:ILE:HD12  | 3:C:254:ARG:NH2   | 2.36                     | 0.40              |
| 7:F:195:THR:HB    | 7:F:223:ARG:HD2   | 2.04                     | 0.40              |
| 7:F:362:ALA:HA    | 7:F:363:PRO:HD3   | 1.93                     | 0.40              |
| 9:H:305:LYS:HE2   | 9:H:305:LYS:HB3   | 1.90                     | 0.40              |
| 11:i:344:MET:HG3  | 11:i:369:SER:HB2  | 2.03                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:M:80:ILE:HD13  | 15:M:80:ILE:HA   | 1.90                     | 0.40              |
| 15:m:173:ILE:HD13 | 15:m:173:ILE:HA  | 1.92                     | 0.40              |
| 2:B:475:GLU:HG2   | 2:B:502:ARG:HA   | 2.04                     | 0.40              |
| 4:c:1146:LEU:HD23 | 4:c:1146:LEU:HA  | 1.95                     | 0.40              |
| 5:D:435:TYR:CE2   | 16:N:632:PRO:HG3 | 2.55                     | 0.40              |
| 6:E:630:ILE:HD13  | 6:E:665:PHE:HZ   | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 284/337 (84%)   | 275 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 1   | a     | 311/337 (92%)   | 297 (96%)  | 14 (4%) | 0        | 100         | 100 |
| 2   | B     | 965/1070 (90%)  | 939 (97%)  | 26 (3%) | 0        | 100         | 100 |
| 3   | C     | 657/688 (96%)   | 633 (96%)  | 24 (4%) | 0        | 100         | 100 |
| 4   | c     | 1162/1388 (84%) | 1136 (98%) | 26 (2%) | 0        | 100         | 100 |
| 5   | D     | 639/892 (72%)   | 625 (98%)  | 14 (2%) | 0        | 100         | 100 |
| 6   | E     | 698/860 (81%)   | 679 (97%)  | 19 (3%) | 0        | 100         | 100 |
| 7   | F     | 542/682 (80%)   | 532 (98%)  | 10 (2%) | 0        | 100         | 100 |
| 8   | G     | 216/266 (81%)   | 213 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 9   | H     | 258/531 (49%)   | 253 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 10  | I     | 374/486 (77%)   | 365 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 11  | i     | 373/648 (58%)   | 361 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 12  | J     | 419/507 (83%)   | 413 (99%)  | 6 (1%)  | 0        | 100         | 100 |
| 13  | K     | 202/331 (61%)   | 198 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 14  | L     | 233/303 (77%)   | 222 (95%)  | 11 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 15  | M     | 114/178 (64%)    | 108 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 15  | m     | 107/178 (60%)    | 103 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 16  | N     | 535/770 (70%)    | 521 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 17  | O     | 95/151 (63%)     | 92 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 18  | P     | 100/143 (70%)    | 92 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| All | All   | 8284/10746 (77%) | 8057 (97%) | 227 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 219/308 (71%)  | 208 (95%) | 11 (5%)  | 22          | 48 |
| 1   | a     | 240/308 (78%)  | 221 (92%) | 19 (8%)  | 11          | 28 |
| 2   | B     | 712/924 (77%)  | 675 (95%) | 37 (5%)  | 21          | 47 |
| 3   | C     | 414/612 (68%)  | 390 (94%) | 24 (6%)  | 18          | 42 |
| 4   | c     | 680/1238 (55%) | 625 (92%) | 55 (8%)  | 11          | 27 |
| 5   | D     | 435/770 (56%)  | 417 (96%) | 18 (4%)  | 27          | 56 |
| 6   | E     | 289/741 (39%)  | 279 (96%) | 10 (4%)  | 32          | 61 |
| 7   | F     | 382/615 (62%)  | 363 (95%) | 19 (5%)  | 22          | 48 |
| 8   | G     | 167/232 (72%)  | 158 (95%) | 9 (5%)   | 20          | 45 |
| 9   | H     | 208/472 (44%)  | 200 (96%) | 8 (4%)   | 29          | 58 |
| 10  | I     | 289/437 (66%)  | 282 (98%) | 7 (2%)   | 43          | 72 |
| 11  | i     | 299/567 (53%)  | 284 (95%) | 15 (5%)  | 22          | 48 |
| 12  | J     | 350/449 (78%)  | 330 (94%) | 20 (6%)  | 18          | 43 |
| 13  | K     | 177/300 (59%)  | 173 (98%) | 4 (2%)   | 44          | 73 |
| 14  | L     | 142/258 (55%)  | 130 (92%) | 12 (8%)  | 10          | 25 |
| 15  | M     | 101/160 (63%)  | 98 (97%)  | 3 (3%)   | 36          | 66 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 15  | m     | 85/160 (53%)    | 76 (89%)   | 9 (11%)  | 6           | 17 |
| 16  | N     | 97/659 (15%)    | 92 (95%)   | 5 (5%)   | 21          | 47 |
| 17  | O     | 75/130 (58%)    | 70 (93%)   | 5 (7%)   | 15          | 36 |
| 18  | P     | 61/129 (47%)    | 59 (97%)   | 2 (3%)   | 33          | 63 |
| All | All   | 5422/9469 (57%) | 5130 (95%) | 292 (5%) | 21          | 45 |

All (292) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 69  | LYS  |
| 1   | A     | 108 | ILE  |
| 1   | A     | 117 | THR  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 126 | TYR  |
| 1   | A     | 129 | ILE  |
| 1   | A     | 143 | ILE  |
| 1   | A     | 144 | ASP  |
| 1   | A     | 228 | PRO  |
| 1   | A     | 317 | VAL  |
| 1   | A     | 323 | ILE  |
| 1   | a     | 16  | LYS  |
| 1   | a     | 27  | LEU  |
| 1   | a     | 60  | THR  |
| 1   | a     | 73  | GLU  |
| 1   | a     | 77  | ILE  |
| 1   | a     | 78  | THR  |
| 1   | a     | 86  | GLU  |
| 1   | a     | 110 | VAL  |
| 1   | a     | 127 | VAL  |
| 1   | a     | 158 | LEU  |
| 1   | a     | 185 | SER  |
| 1   | a     | 194 | GLU  |
| 1   | a     | 227 | ILE  |
| 1   | a     | 232 | MET  |
| 1   | a     | 272 | ILE  |
| 1   | a     | 278 | GLU  |
| 1   | a     | 288 | LYS  |
| 1   | a     | 321 | LEU  |
| 1   | a     | 323 | ILE  |
| 2   | B     | 41  | ILE  |
| 2   | B     | 60  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 61  | GLU  |
| 2   | B     | 86  | LEU  |
| 2   | B     | 108 | ASN  |
| 2   | B     | 132 | ILE  |
| 2   | B     | 168 | ILE  |
| 2   | B     | 172 | VAL  |
| 2   | B     | 274 | ILE  |
| 2   | B     | 287 | LEU  |
| 2   | B     | 327 | LEU  |
| 2   | B     | 336 | VAL  |
| 2   | B     | 356 | VAL  |
| 2   | B     | 379 | ASP  |
| 2   | B     | 410 | ILE  |
| 2   | B     | 457 | ILE  |
| 2   | B     | 478 | MET  |
| 2   | B     | 488 | ASN  |
| 2   | B     | 495 | GLN  |
| 2   | B     | 535 | GLU  |
| 2   | B     | 582 | GLU  |
| 2   | B     | 602 | ASP  |
| 2   | B     | 630 | LYS  |
| 2   | B     | 632 | ILE  |
| 2   | B     | 640 | ASP  |
| 2   | B     | 657 | VAL  |
| 2   | B     | 728 | LEU  |
| 2   | B     | 777 | LEU  |
| 2   | B     | 808 | ILE  |
| 2   | B     | 812 | ARG  |
| 2   | B     | 837 | GLN  |
| 2   | B     | 868 | GLU  |
| 2   | B     | 877 | LEU  |
| 2   | B     | 926 | ARG  |
| 2   | B     | 931 | ARG  |
| 2   | B     | 969 | VAL  |
| 2   | B     | 974 | LEU  |
| 3   | C     | 22  | VAL  |
| 3   | C     | 121 | THR  |
| 3   | C     | 123 | VAL  |
| 3   | C     | 215 | LEU  |
| 3   | C     | 218 | ILE  |
| 3   | C     | 225 | GLU  |
| 3   | C     | 227 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 257 | LEU  |
| 3   | C     | 272 | VAL  |
| 3   | C     | 328 | VAL  |
| 3   | C     | 340 | ASP  |
| 3   | C     | 367 | ILE  |
| 3   | C     | 373 | ARG  |
| 3   | C     | 449 | GLN  |
| 3   | C     | 468 | LEU  |
| 3   | C     | 496 | ASP  |
| 3   | C     | 504 | VAL  |
| 3   | C     | 524 | MET  |
| 3   | C     | 531 | ILE  |
| 3   | C     | 596 | ILE  |
| 3   | C     | 614 | TRP  |
| 3   | C     | 620 | VAL  |
| 3   | C     | 667 | ILE  |
| 3   | C     | 680 | PHE  |
| 4   | c     | 39  | LEU  |
| 4   | c     | 65  | ILE  |
| 4   | c     | 71  | LEU  |
| 4   | c     | 90  | ASN  |
| 4   | c     | 94  | VAL  |
| 4   | c     | 102 | GLU  |
| 4   | c     | 128 | VAL  |
| 4   | c     | 174 | SER  |
| 4   | c     | 201 | TYR  |
| 4   | c     | 207 | VAL  |
| 4   | c     | 213 | ILE  |
| 4   | c     | 217 | ARG  |
| 4   | c     | 249 | LEU  |
| 4   | c     | 262 | THR  |
| 4   | c     | 290 | THR  |
| 4   | c     | 293 | SER  |
| 4   | c     | 311 | LEU  |
| 4   | c     | 312 | VAL  |
| 4   | c     | 320 | ILE  |
| 4   | c     | 329 | PRO  |
| 4   | c     | 397 | ASN  |
| 4   | c     | 400 | ILE  |
| 4   | c     | 405 | LEU  |
| 4   | c     | 436 | VAL  |
| 4   | c     | 487 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | c     | 941  | ILE  |
| 4   | c     | 978  | SER  |
| 4   | c     | 999  | THR  |
| 4   | c     | 1006 | THR  |
| 4   | c     | 1021 | ILE  |
| 4   | c     | 1041 | ARG  |
| 4   | c     | 1042 | ASN  |
| 4   | c     | 1044 | ILE  |
| 4   | c     | 1045 | LEU  |
| 4   | c     | 1099 | ILE  |
| 4   | c     | 1105 | LYS  |
| 4   | c     | 1121 | GLU  |
| 4   | c     | 1128 | THR  |
| 4   | c     | 1129 | LEU  |
| 4   | c     | 1130 | VAL  |
| 4   | c     | 1153 | LEU  |
| 4   | c     | 1158 | VAL  |
| 4   | c     | 1159 | ASP  |
| 4   | c     | 1161 | ILE  |
| 4   | c     | 1180 | LEU  |
| 4   | c     | 1187 | LEU  |
| 4   | c     | 1219 | ARG  |
| 4   | c     | 1224 | ILE  |
| 4   | c     | 1232 | VAL  |
| 4   | c     | 1233 | LEU  |
| 4   | c     | 1234 | VAL  |
| 4   | c     | 1249 | ILE  |
| 4   | c     | 1266 | CYS  |
| 4   | c     | 1270 | VAL  |
| 4   | c     | 1293 | THR  |
| 5   | D     | 208  | THR  |
| 5   | D     | 339  | GLU  |
| 5   | D     | 432  | ILE  |
| 5   | D     | 442  | THR  |
| 5   | D     | 496  | GLU  |
| 5   | D     | 516  | LEU  |
| 5   | D     | 735  | ILE  |
| 5   | D     | 736  | GLN  |
| 5   | D     | 740  | VAL  |
| 5   | D     | 755  | THR  |
| 5   | D     | 756  | ILE  |
| 5   | D     | 795  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D     | 798 | THR  |
| 5   | D     | 803 | ASP  |
| 5   | D     | 806 | VAL  |
| 5   | D     | 812 | VAL  |
| 5   | D     | 822 | ASN  |
| 5   | D     | 843 | ILE  |
| 6   | E     | 424 | ILE  |
| 6   | E     | 502 | LEU  |
| 6   | E     | 588 | ILE  |
| 6   | E     | 634 | ILE  |
| 6   | E     | 653 | LYS  |
| 6   | E     | 673 | LEU  |
| 6   | E     | 676 | LEU  |
| 6   | E     | 708 | VAL  |
| 6   | E     | 720 | THR  |
| 6   | E     | 763 | VAL  |
| 7   | F     | 134 | ILE  |
| 7   | F     | 155 | ILE  |
| 7   | F     | 159 | LEU  |
| 7   | F     | 168 | VAL  |
| 7   | F     | 174 | PRO  |
| 7   | F     | 176 | ASP  |
| 7   | F     | 184 | VAL  |
| 7   | F     | 255 | PRO  |
| 7   | F     | 257 | ARG  |
| 7   | F     | 284 | VAL  |
| 7   | F     | 319 | ILE  |
| 7   | F     | 347 | ILE  |
| 7   | F     | 367 | ARG  |
| 7   | F     | 371 | THR  |
| 7   | F     | 494 | GLN  |
| 7   | F     | 517 | ILE  |
| 7   | F     | 589 | VAL  |
| 7   | F     | 595 | VAL  |
| 7   | F     | 600 | VAL  |
| 8   | G     | 65  | LEU  |
| 8   | G     | 150 | LEU  |
| 8   | G     | 154 | GLU  |
| 8   | G     | 174 | LEU  |
| 8   | G     | 184 | LEU  |
| 8   | G     | 224 | TYR  |
| 8   | G     | 226 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 228 | LYS  |
| 8   | G     | 239 | LEU  |
| 9   | H     | 203 | LEU  |
| 9   | H     | 242 | LYS  |
| 9   | H     | 291 | ARG  |
| 9   | H     | 309 | ILE  |
| 9   | H     | 322 | TRP  |
| 9   | H     | 368 | ILE  |
| 9   | H     | 373 | LEU  |
| 9   | H     | 423 | LEU  |
| 10  | I     | 152 | GLN  |
| 10  | I     | 200 | ASN  |
| 10  | I     | 202 | GLU  |
| 10  | I     | 407 | LEU  |
| 10  | I     | 446 | GLN  |
| 10  | I     | 467 | PHE  |
| 10  | I     | 486 | TRP  |
| 11  | i     | 361 | ASN  |
| 11  | i     | 472 | GLN  |
| 11  | i     | 483 | VAL  |
| 11  | i     | 501 | ASP  |
| 11  | i     | 518 | ILE  |
| 11  | i     | 546 | ASN  |
| 11  | i     | 557 | LEU  |
| 11  | i     | 563 | ASP  |
| 11  | i     | 578 | MET  |
| 11  | i     | 581 | VAL  |
| 11  | i     | 596 | LEU  |
| 11  | i     | 612 | ARG  |
| 11  | i     | 620 | GLU  |
| 11  | i     | 629 | ASP  |
| 11  | i     | 638 | GLU  |
| 12  | J     | 90  | THR  |
| 12  | J     | 134 | GLU  |
| 12  | J     | 183 | THR  |
| 12  | J     | 186 | ASP  |
| 12  | J     | 189 | LEU  |
| 12  | J     | 229 | LEU  |
| 12  | J     | 295 | VAL  |
| 12  | J     | 302 | VAL  |
| 12  | J     | 325 | ARG  |
| 12  | J     | 348 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | J     | 360 | TYR  |
| 12  | J     | 366 | VAL  |
| 12  | J     | 372 | ILE  |
| 12  | J     | 388 | VAL  |
| 12  | J     | 392 | SER  |
| 12  | J     | 412 | VAL  |
| 12  | J     | 437 | LEU  |
| 12  | J     | 489 | LEU  |
| 12  | J     | 503 | ASP  |
| 12  | J     | 506 | LEU  |
| 13  | K     | 199 | CYS  |
| 13  | K     | 203 | THR  |
| 13  | K     | 302 | VAL  |
| 13  | K     | 312 | ARG  |
| 14  | L     | 64  | HIS  |
| 14  | L     | 68  | THR  |
| 14  | L     | 102 | ILE  |
| 14  | L     | 145 | LEU  |
| 14  | L     | 147 | LEU  |
| 14  | L     | 236 | ASN  |
| 14  | L     | 250 | VAL  |
| 14  | L     | 251 | SER  |
| 14  | L     | 253 | GLU  |
| 14  | L     | 255 | VAL  |
| 14  | L     | 281 | GLU  |
| 14  | L     | 282 | GLU  |
| 15  | M     | 66  | VAL  |
| 15  | M     | 119 | GLU  |
| 15  | M     | 132 | GLU  |
| 15  | m     | 90  | VAL  |
| 15  | m     | 101 | CYS  |
| 15  | m     | 128 | ASP  |
| 15  | m     | 130 | ASP  |
| 15  | m     | 132 | GLU  |
| 15  | m     | 146 | THR  |
| 15  | m     | 156 | LYS  |
| 15  | m     | 164 | LEU  |
| 15  | m     | 169 | MET  |
| 16  | N     | 619 | VAL  |
| 16  | N     | 654 | THR  |
| 16  | N     | 661 | LEU  |
| 16  | N     | 701 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | N     | 759 | THR  |
| 17  | O     | 55  | ILE  |
| 17  | O     | 58  | LEU  |
| 17  | O     | 60  | GLU  |
| 17  | O     | 83  | GLU  |
| 17  | O     | 102 | GLU  |
| 18  | P     | 96  | VAL  |
| 18  | P     | 104 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | GLN  |
| 1   | A     | 196 | GLN  |
| 1   | A     | 276 | GLN  |
| 1   | A     | 285 | ASN  |
| 1   | a     | 41  | GLN  |
| 1   | a     | 99  | ASN  |
| 1   | a     | 119 | GLN  |
| 1   | a     | 187 | HIS  |
| 1   | a     | 196 | GLN  |
| 1   | a     | 221 | ASN  |
| 1   | a     | 231 | HIS  |
| 1   | a     | 263 | ASN  |
| 1   | a     | 276 | GLN  |
| 1   | a     | 285 | ASN  |
| 2   | B     | 58  | GLN  |
| 2   | B     | 124 | ASN  |
| 2   | B     | 128 | GLN  |
| 2   | B     | 267 | ASN  |
| 2   | B     | 276 | GLN  |
| 2   | B     | 278 | ASN  |
| 2   | B     | 307 | ASN  |
| 2   | B     | 322 | GLN  |
| 2   | B     | 334 | ASN  |
| 2   | B     | 372 | HIS  |
| 2   | B     | 386 | GLN  |
| 2   | B     | 389 | HIS  |
| 2   | B     | 483 | ASN  |
| 2   | B     | 488 | ASN  |
| 2   | B     | 503 | GLN  |
| 2   | B     | 522 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 615  | ASN  |
| 2   | B     | 621  | HIS  |
| 2   | B     | 636  | GLN  |
| 2   | B     | 862  | ASN  |
| 2   | B     | 865  | GLN  |
| 2   | B     | 881  | HIS  |
| 2   | B     | 910  | GLN  |
| 2   | B     | 913  | ASN  |
| 2   | B     | 934  | ASN  |
| 2   | B     | 938  | GLN  |
| 2   | B     | 953  | GLN  |
| 2   | B     | 971  | GLN  |
| 2   | B     | 980  | GLN  |
| 2   | B     | 1064 | GLN  |
| 3   | C     | 135  | ASN  |
| 3   | C     | 221  | ASN  |
| 3   | C     | 331  | GLN  |
| 3   | C     | 336  | GLN  |
| 3   | C     | 453  | GLN  |
| 3   | C     | 471  | GLN  |
| 3   | C     | 513  | GLN  |
| 3   | C     | 523  | HIS  |
| 3   | C     | 525  | ASN  |
| 3   | C     | 553  | ASN  |
| 3   | C     | 591  | ASN  |
| 3   | C     | 605  | ASN  |
| 3   | C     | 666  | HIS  |
| 4   | c     | 37   | HIS  |
| 4   | c     | 41   | GLN  |
| 4   | c     | 49   | GLN  |
| 4   | c     | 73   | GLN  |
| 4   | c     | 77   | GLN  |
| 4   | c     | 92   | HIS  |
| 4   | c     | 118  | ASN  |
| 4   | c     | 351  | HIS  |
| 4   | c     | 374  | HIS  |
| 4   | c     | 397  | ASN  |
| 4   | c     | 449  | HIS  |
| 4   | c     | 492  | HIS  |
| 4   | c     | 497  | GLN  |
| 4   | c     | 924  | GLN  |
| 4   | c     | 947  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | c     | 1007 | ASN  |
| 4   | c     | 1031 | ASN  |
| 4   | c     | 1051 | ASN  |
| 4   | c     | 1076 | ASN  |
| 4   | c     | 1095 | GLN  |
| 4   | c     | 1116 | HIS  |
| 4   | c     | 1196 | GLN  |
| 4   | c     | 1206 | GLN  |
| 4   | c     | 1207 | GLN  |
| 4   | c     | 1212 | GLN  |
| 5   | D     | 175  | GLN  |
| 5   | D     | 188  | ASN  |
| 5   | D     | 194  | ASN  |
| 5   | D     | 225  | HIS  |
| 5   | D     | 227  | ASN  |
| 5   | D     | 254  | GLN  |
| 5   | D     | 394  | ASN  |
| 5   | D     | 420  | GLN  |
| 5   | D     | 468  | ASN  |
| 5   | D     | 822  | ASN  |
| 5   | D     | 882  | GLN  |
| 6   | E     | 476  | ASN  |
| 6   | E     | 491  | ASN  |
| 6   | E     | 579  | GLN  |
| 6   | E     | 612  | HIS  |
| 6   | E     | 643  | ASN  |
| 6   | E     | 711  | HIS  |
| 6   | E     | 792  | GLN  |
| 7   | F     | 81   | ASN  |
| 7   | F     | 128  | ASN  |
| 7   | F     | 148  | GLN  |
| 7   | F     | 251  | GLN  |
| 7   | F     | 278  | GLN  |
| 7   | F     | 288  | HIS  |
| 7   | F     | 301  | HIS  |
| 7   | F     | 324  | HIS  |
| 7   | F     | 366  | HIS  |
| 7   | F     | 402  | ASN  |
| 7   | F     | 417  | GLN  |
| 7   | F     | 494  | GLN  |
| 7   | F     | 559  | GLN  |
| 7   | F     | 590  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | F     | 591 | ASN  |
| 8   | G     | 81  | HIS  |
| 8   | G     | 92  | GLN  |
| 8   | G     | 116 | ASN  |
| 8   | G     | 151 | GLN  |
| 8   | G     | 226 | ASN  |
| 8   | G     | 253 | GLN  |
| 9   | H     | 195 | GLN  |
| 9   | H     | 216 | HIS  |
| 9   | H     | 247 | GLN  |
| 9   | H     | 271 | GLN  |
| 9   | H     | 300 | GLN  |
| 9   | H     | 320 | GLN  |
| 9   | H     | 332 | GLN  |
| 9   | H     | 334 | HIS  |
| 9   | H     | 353 | GLN  |
| 9   | H     | 399 | GLN  |
| 10  | I     | 139 | GLN  |
| 10  | I     | 152 | GLN  |
| 10  | I     | 193 | GLN  |
| 10  | I     | 200 | ASN  |
| 10  | I     | 261 | HIS  |
| 10  | I     | 317 | GLN  |
| 10  | I     | 346 | GLN  |
| 10  | I     | 440 | GLN  |
| 11  | i     | 287 | GLN  |
| 11  | i     | 288 | HIS  |
| 11  | i     | 354 | GLN  |
| 11  | i     | 361 | ASN  |
| 11  | i     | 363 | ASN  |
| 11  | i     | 545 | HIS  |
| 11  | i     | 584 | HIS  |
| 11  | i     | 607 | GLN  |
| 12  | J     | 244 | GLN  |
| 12  | J     | 281 | GLN  |
| 12  | J     | 288 | GLN  |
| 12  | J     | 299 | ASN  |
| 12  | J     | 313 | GLN  |
| 12  | J     | 319 | HIS  |
| 12  | J     | 367 | ASN  |
| 12  | J     | 373 | HIS  |
| 12  | J     | 446 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | J     | 496 | GLN  |
| 14  | L     | 64  | HIS  |
| 14  | L     | 84  | ASN  |
| 14  | L     | 86  | ASN  |
| 14  | L     | 125 | HIS  |
| 14  | L     | 188 | ASN  |
| 14  | L     | 236 | ASN  |
| 15  | M     | 121 | ASN  |
| 15  | m     | 121 | ASN  |
| 15  | m     | 176 | ASN  |
| 16  | N     | 673 | GLN  |
| 16  | N     | 691 | HIS  |
| 17  | O     | 61  | GLN  |
| 17  | O     | 82  | ASN  |
| 17  | O     | 99  | GLN  |
| 17  | O     | 104 | ASN  |
| 17  | O     | 116 | HIS  |
| 17  | O     | 120 | ASN  |
| 18  | P     | 104 | GLN  |
| 18  | P     | 132 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 20  | S     | 8/20 (40%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

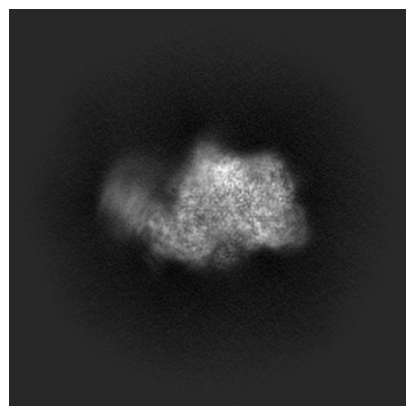
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37387. These allow visual inspection of the internal detail of the map and identification of artifacts.

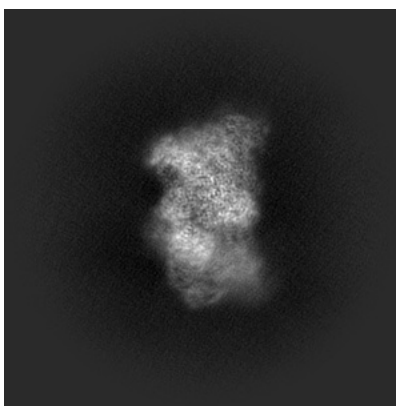
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

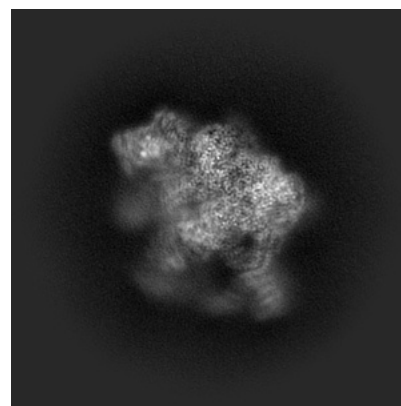
#### 6.1.1 Primary map



X

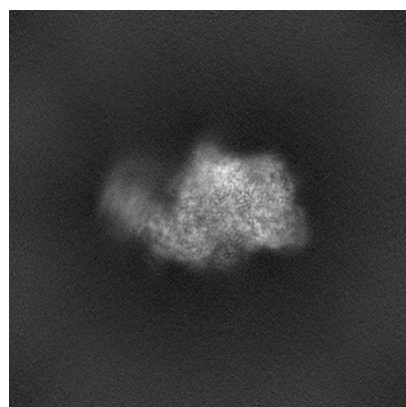


Y

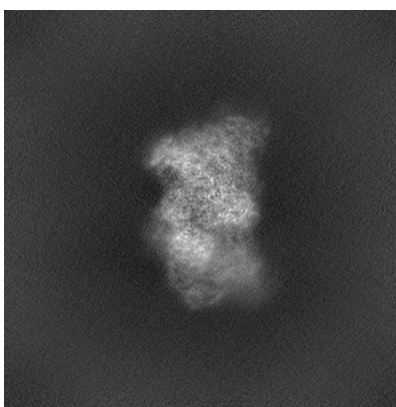


Z

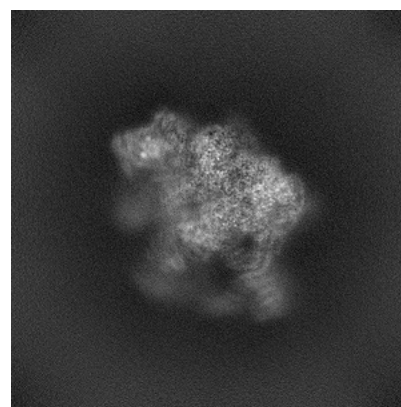
#### 6.1.2 Raw map



X



Y

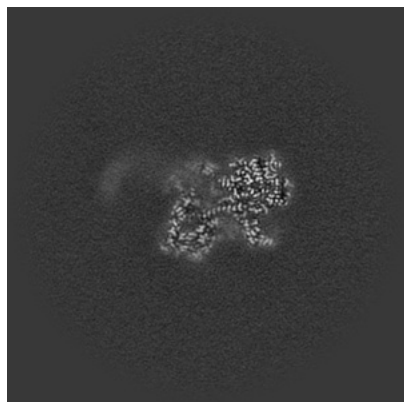


Z

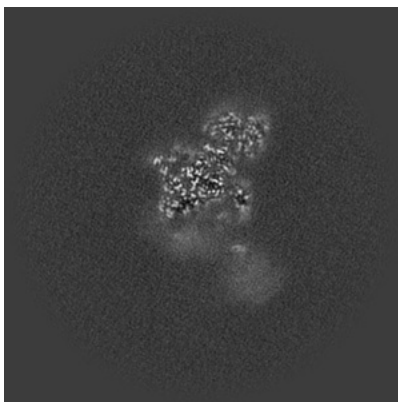
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

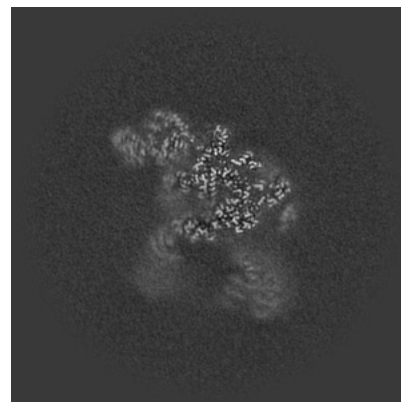
### 6.2.1 Primary map



X Index: 300

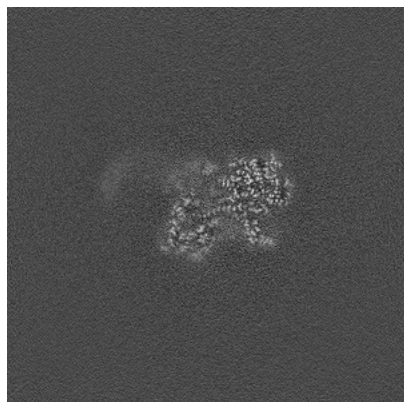


Y Index: 300

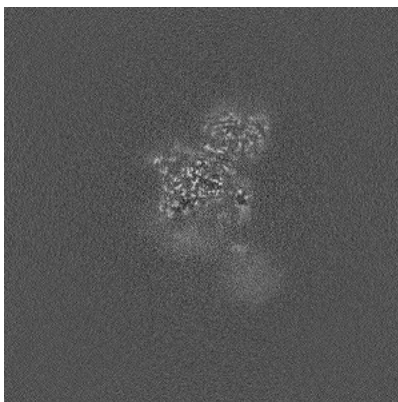


Z Index: 300

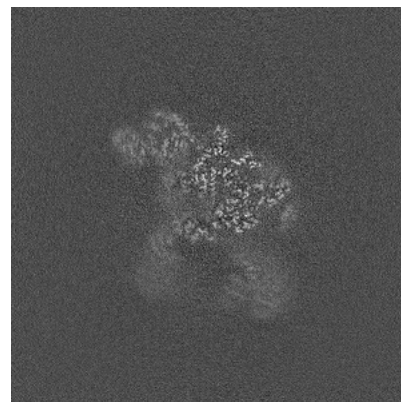
### 6.2.2 Raw map



X Index: 300



Y Index: 300

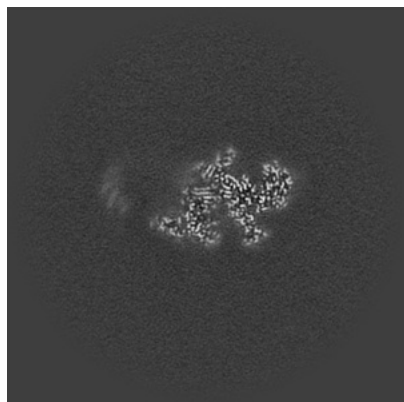


Z Index: 300

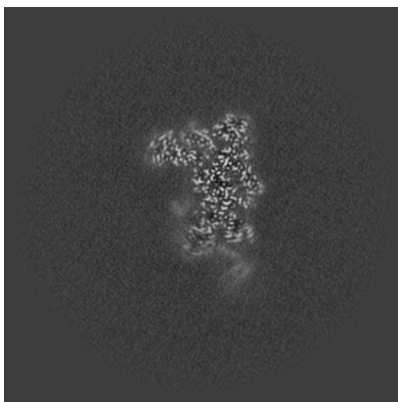
The images above show central slices of the map in three orthogonal directions.

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

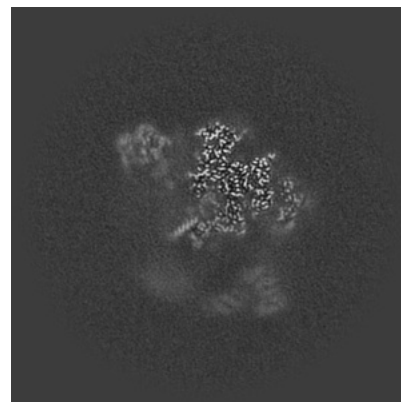
### 6.3.1 Primary map



X Index: 323

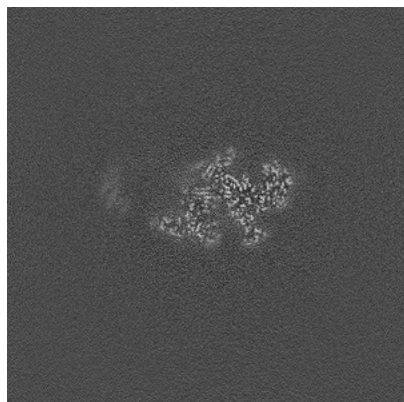


Y Index: 335

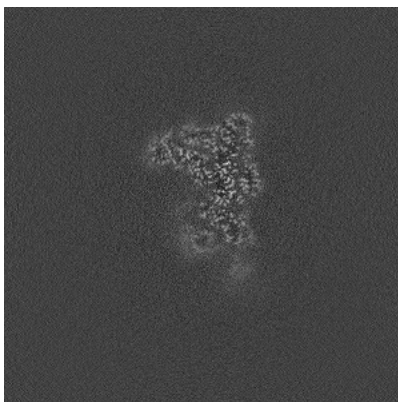


Z Index: 322

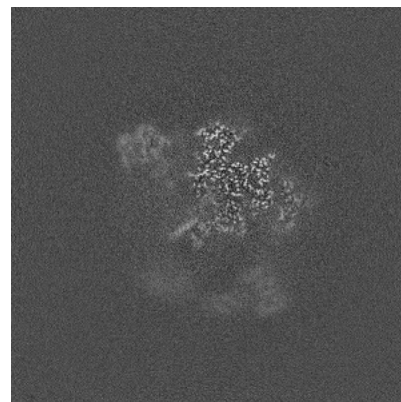
### 6.3.2 Raw map



X Index: 323



Y Index: 329

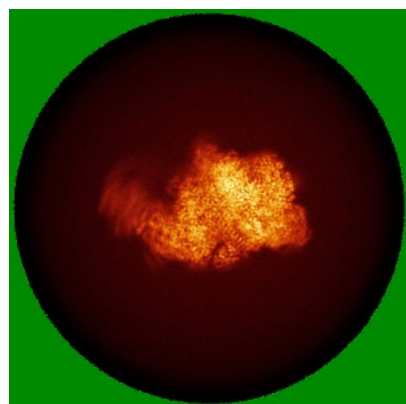


Z Index: 322

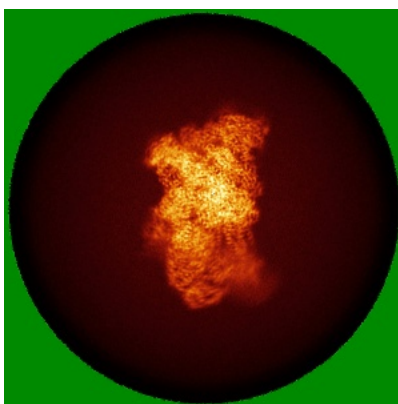
The images above show the largest variance slices of the map in three orthogonal directions.

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

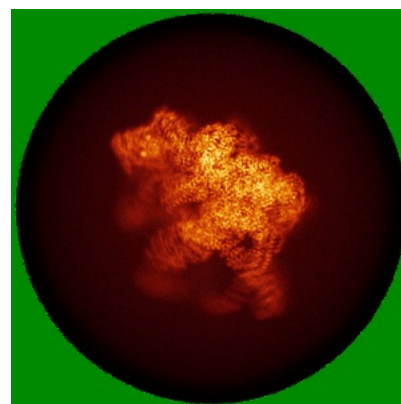
### 6.4.1 Primary map



X

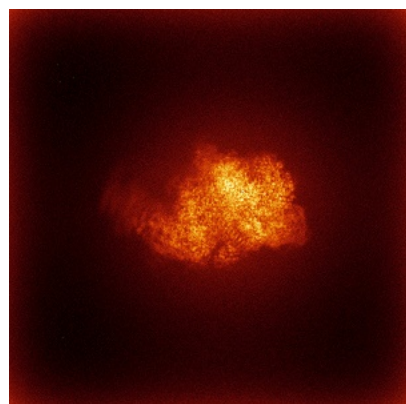


Y

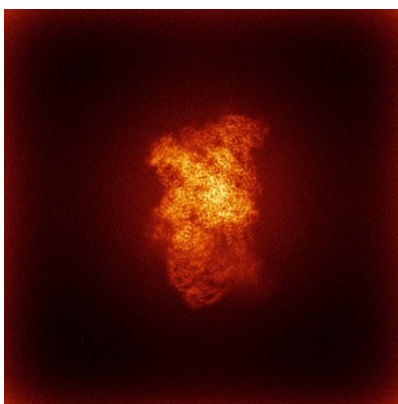


Z

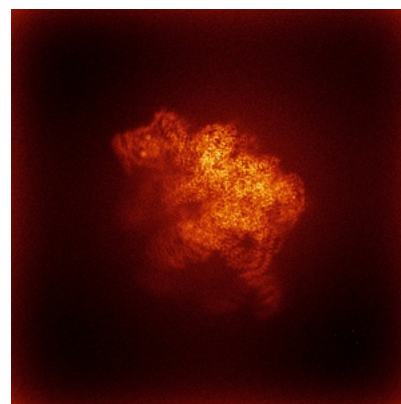
### 6.4.2 Raw map



X



Y

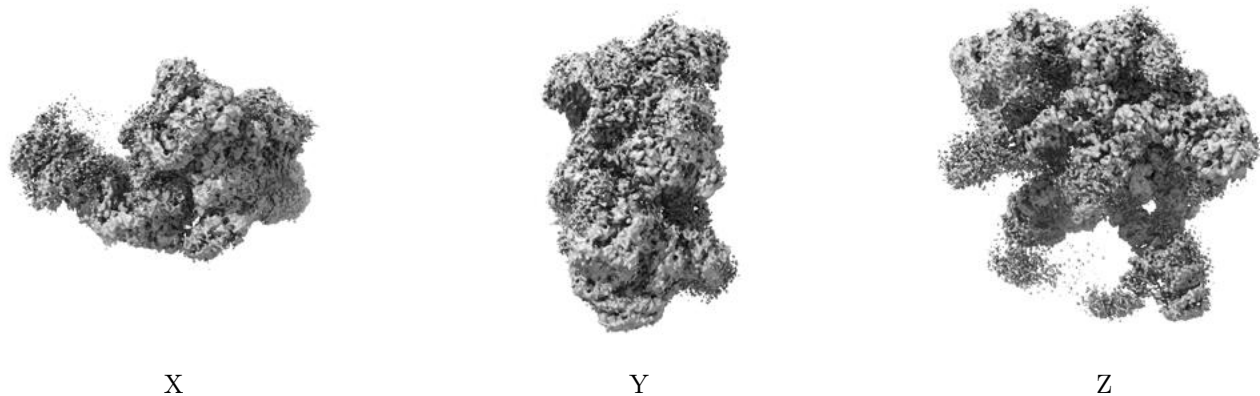


Z

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

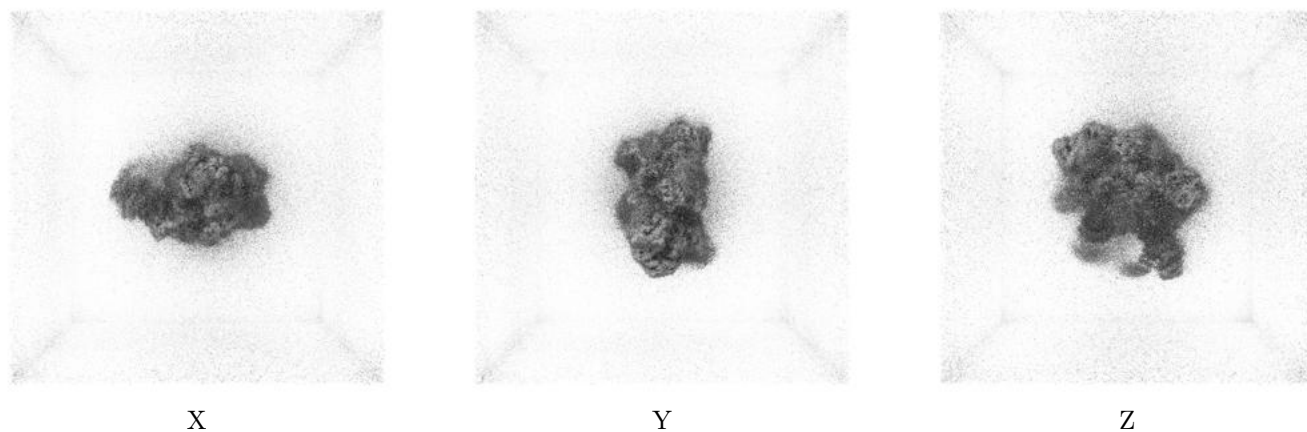
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

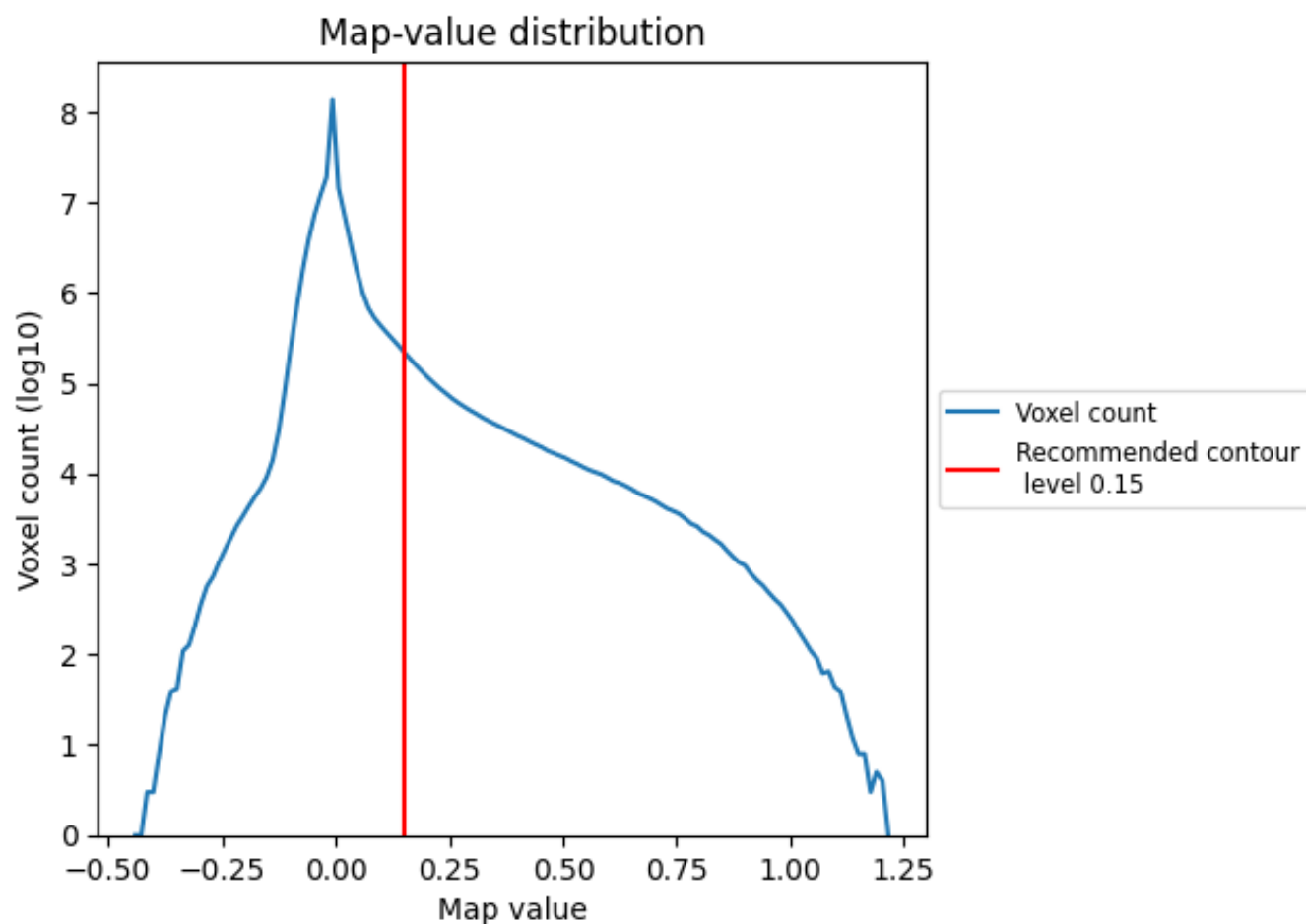
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

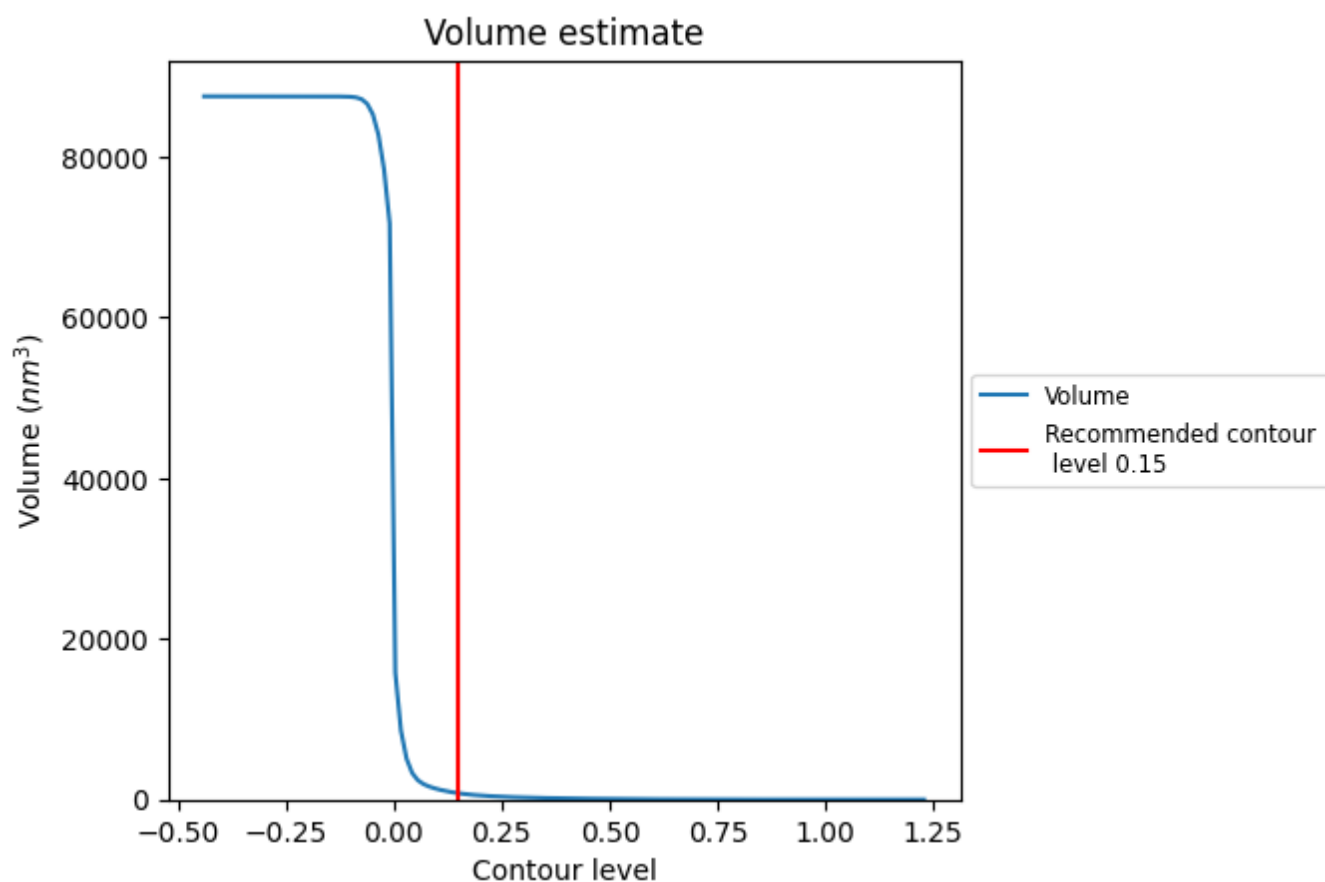
This section contains the results of statistical analysis of the map.

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



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

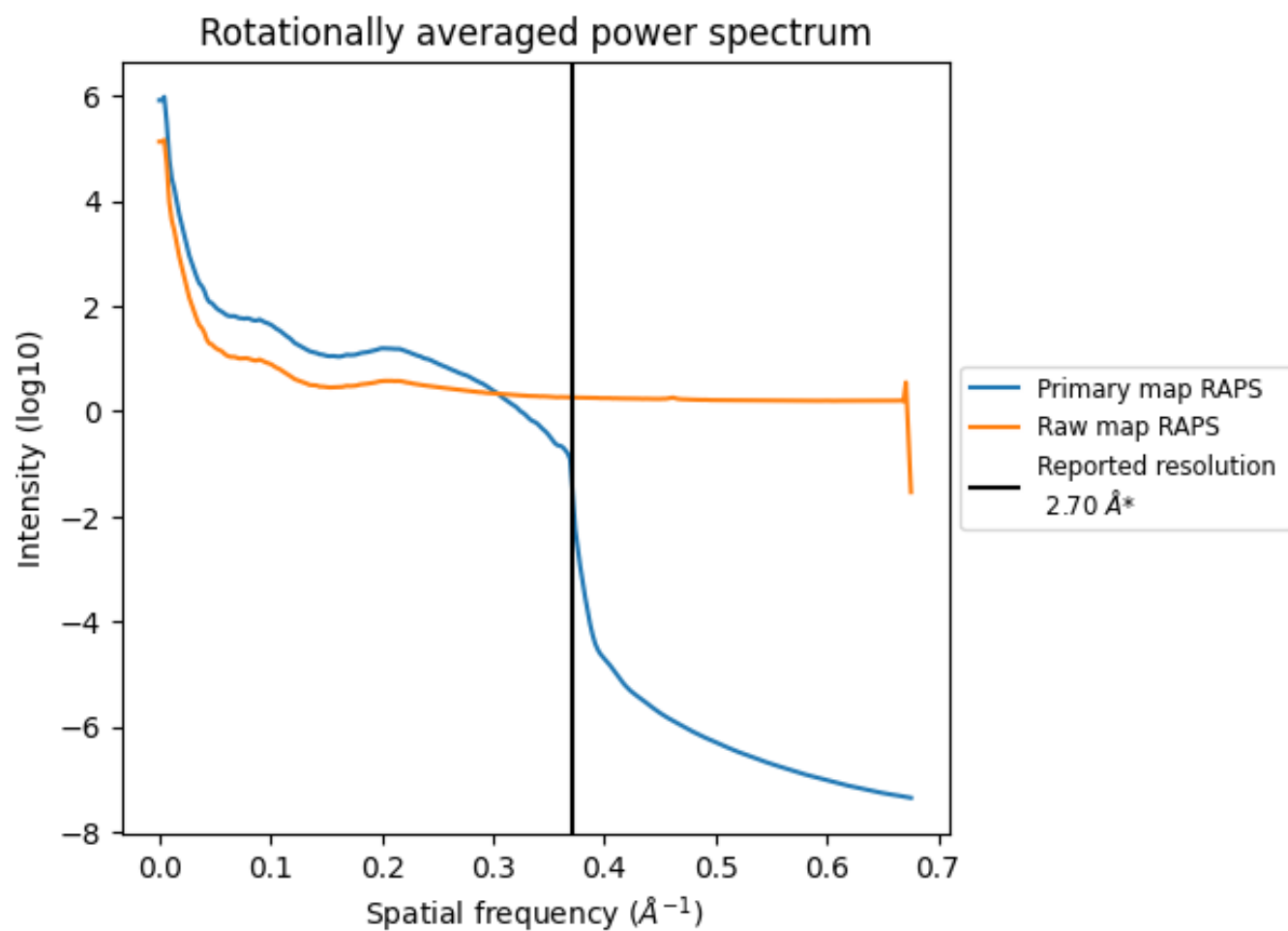
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 787  $\text{nm}^3$ ; this corresponds to an approximate mass of 711 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 ⓘ

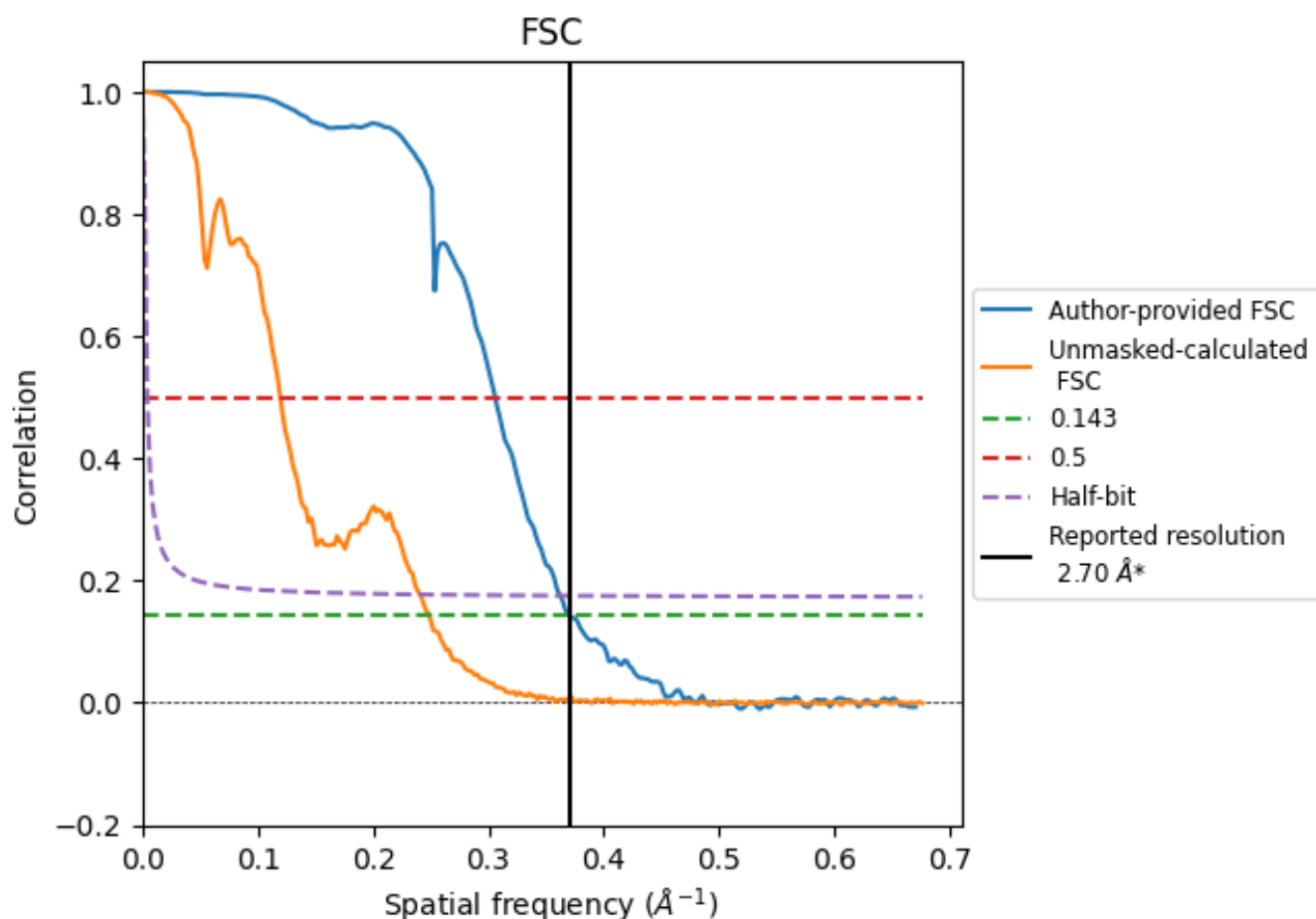


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

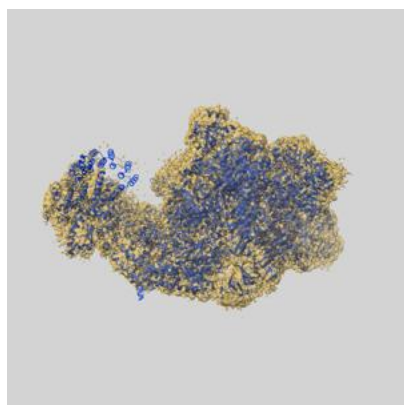
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.70                               | -    | -        |
| Author-provided FSC curve | 2.70                               | 3.27 | 2.76     |
| Unmasked-calculated*      | 4.02                               | 8.37 | 4.15     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.7 by more than 10 %

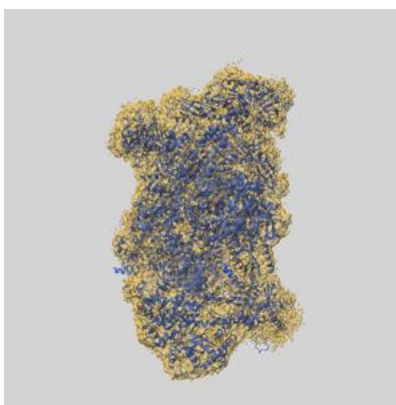
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37387 and PDB model 8WA0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

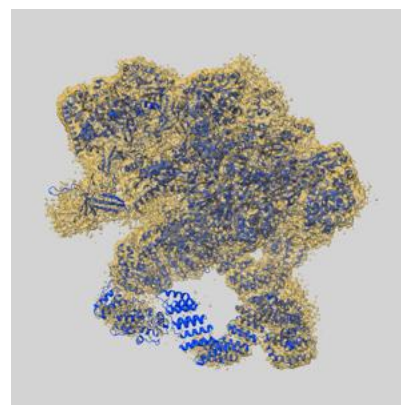
### 9.1 Map-model overlay [i](#)



X



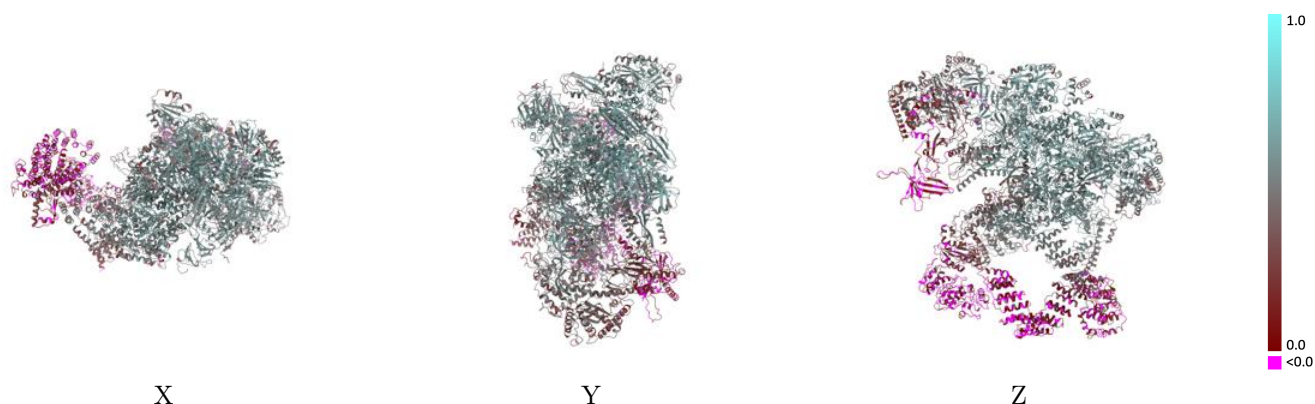
Y



Z

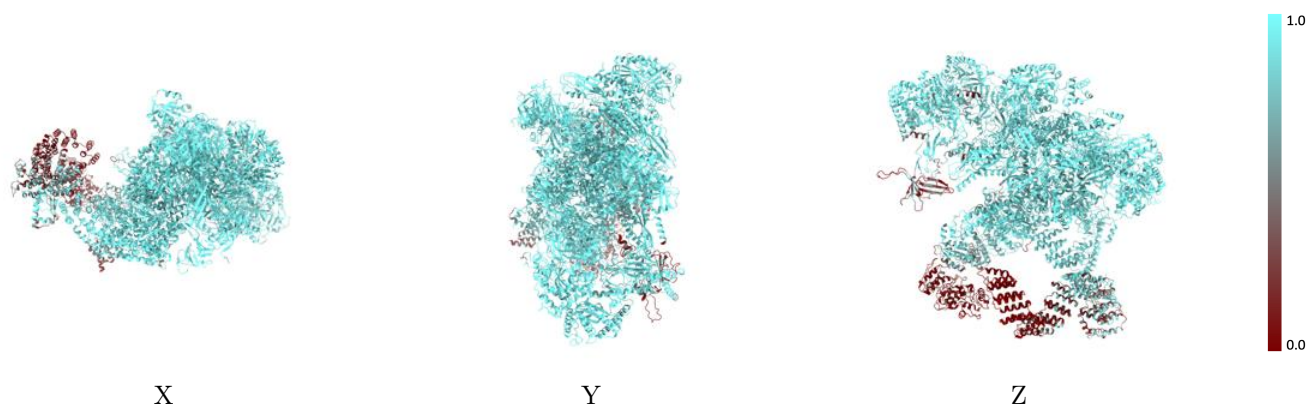
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



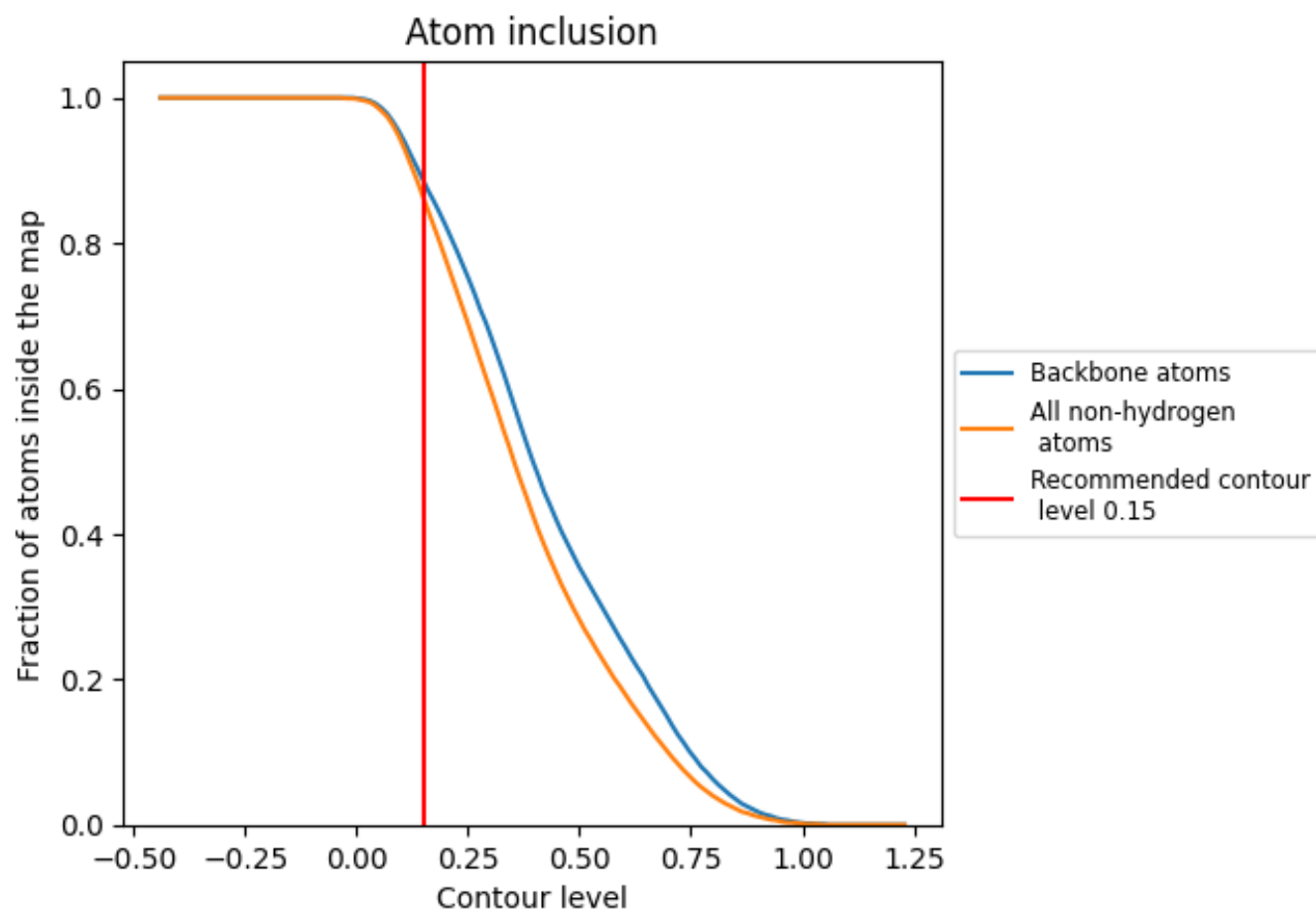
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8620   |  0.4420   |
| A     |  0.9500   |  0.5240   |
| B     |  0.9580   |  0.5500   |
| C     |  0.9410   |  0.4980   |
| D     |  0.8630   |  0.4180   |
| E     |  0.3940   |  0.0810   |
| F     |  0.9130   |  0.4170   |
| G     |  0.9450   |  0.4510   |
| H     |  0.9550   |  0.5580   |
| I     |  0.9750   |  0.5820   |
| J     |  0.9610   |  0.5210   |
| K     |  0.9590   |  0.5320   |
| L     |  0.9380   |  0.3450   |
| M     |  0.9610   |  0.5700   |
| N     |  0.3370  |  0.0790  |
| O     |  0.9490 |  0.5610 |
| P     |  0.9610 |  0.4330 |
| R     |  0.8790 |  0.4550 |
| S     |  0.8890 |  0.4290 |
| a     |  0.9680 |  0.5450 |
| c     |  0.8730 |  0.4480 |
| i     |  0.9580 |  0.5310 |
| m     |  0.9260 |  0.4910 |

