



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:43 PM UTC

PDB ID : 5Y5Z / pdb\_00005y5z  
EMDB ID : EMD-6812  
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 2  
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.  
Deposited on : 2017-08-10  
Resolution : 6.70 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:

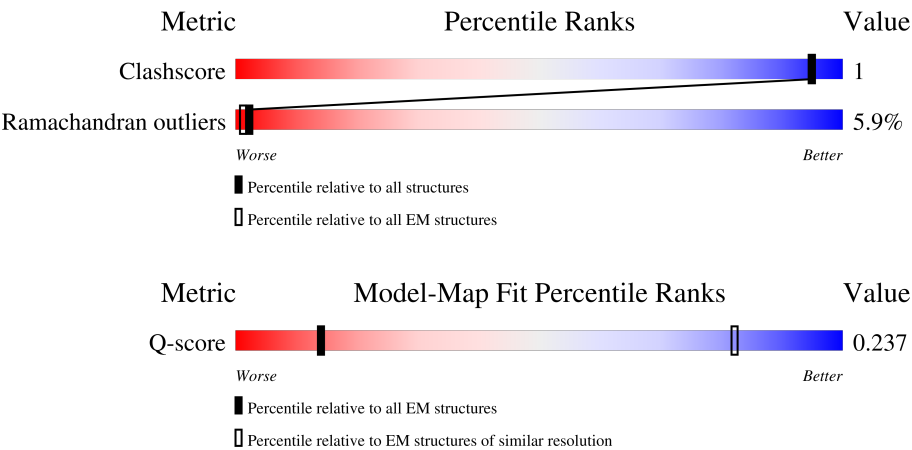
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 6.70 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.



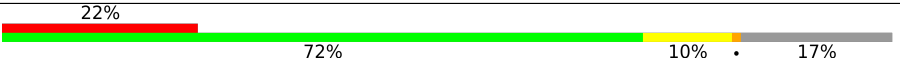
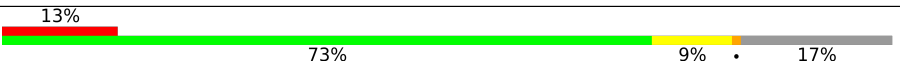
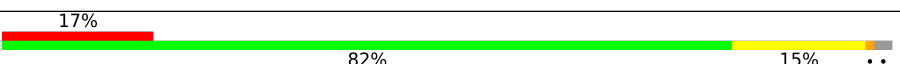
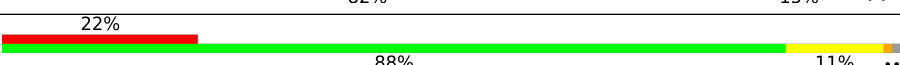
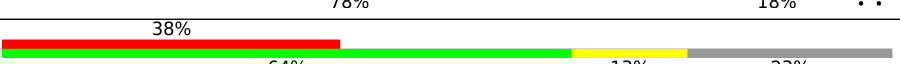
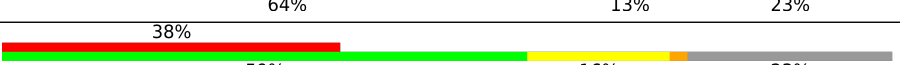
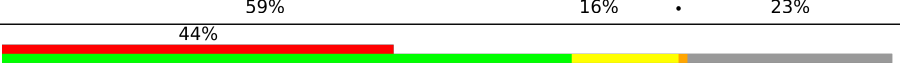
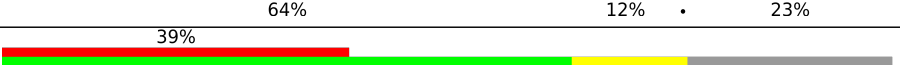
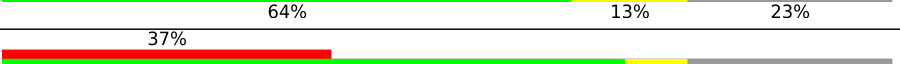
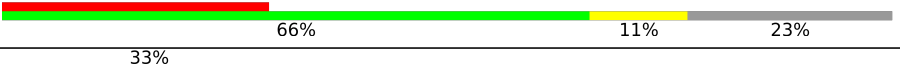
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Q-score               | -                           | 25397                       | 523 ( 6.20 - 7.20 )                                      |

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     | 578    | <div><div>7%</div><div>70%</div><div>27%</div><div>.</div></div>             |
| 1   | B     | 578    | <div><div>.</div><div>69%</div><div>29%</div><div>.</div></div>              |
| 1   | C     | 578    | <div><div>.</div><div>69%</div><div>28%</div><div>.</div></div>              |
| 2   | D     | 478    | <div><div>7%</div><div>65%</div><div>29%</div><div>.</div><div>.</div></div> |
| 2   | E     | 478    | <div><div>5%</div><div>62%</div><div>31%</div><div>.</div><div>.</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | F     | 478    |    |
| 3   | G     | 223    |    |
| 4   | H     | 104    |    |
| 5   | I     | 120    |    |
| 5   | K     | 120    |    |
| 6   | J     | 188    |    |
| 6   | L     | 188    |    |
| 7   | M     | 323    |    |
| 8   | N     | 652    |    |
| 9   | O     | 99     |    |
| 9   | P     | 99     |    |
| 9   | Q     | 99     |    |
| 9   | R     | 99     |   |
| 9   | S     | 99     |  |
| 9   | T     | 99     |  |
| 9   | U     | 99     |  |
| 9   | V     | 99     |  |
| 9   | W     | 99     |  |
| 9   | X     | 99     |  |
| 9   | Y     | 99     |  |
| 9   | Z     | 99     |  |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23433 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 V-type ATP synthase alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 1   | A     | 577      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2307  | 1154 | 577 | 576 |         |       |
| 1   | B     | 577      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2307  | 1154 | 577 | 576 |         |       |
| 1   | C     | 577      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2307  | 1154 | 577 | 576 |         |       |

- Molecule 2 is a protein called V-type ATP synthase beta chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | D     | 459      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1835  | 918 | 459 | 458 |         |       |
| 2   | E     | 459      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1835  | 918 | 459 | 458 |         |       |
| 2   | F     | 459      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1835  | 918 | 459 | 458 |         |       |

- Molecule 3 is a protein called V-type ATP synthase subunit D.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | G     | 210      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 839   | 420 | 210 | 209 |         |       |

- Molecule 4 is a protein called V-type ATP synthase subunit F.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 4   | H     | 100      | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 399   | 200 | 100 | 99 |         |       |

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 5   | I     | 100      | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 399   | 200 | 100 | 99 |         |       |
| 5   | K     | 100      | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 399   | 200 | 100 | 99 |         |       |

- Molecule 6 is a protein called V-type ATP synthase subunit E.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | J     | 185      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 738   | 370 | 185 | 183 |         |       |
| 6   | L     | 185      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 738   | 370 | 185 | 183 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| J     | 134     | MET      | LEU    | conflict | UNP P74901 |
| J     | 171     | MET      | LEU    | conflict | UNP P74901 |
| J     | 178     | MET      | LEU    | conflict | UNP P74901 |
| L     | 134     | MET      | LEU    | conflict | UNP P74901 |
| L     | 171     | MET      | LEU    | conflict | UNP P74901 |
| L     | 178     | MET      | LEU    | conflict | UNP P74901 |

- Molecule 7 is a protein called V-type ATP synthase subunit C.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | M     | 320      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1279  | 640 | 320 | 319 |         |       |

- Molecule 8 is a protein called V-type ATP synthase subunit I.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 8   | N     | 632      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2526  | 1264 | 632 | 630 |         |       |

- Molecule 9 is a protein called V-type ATP synthase, subunit K.

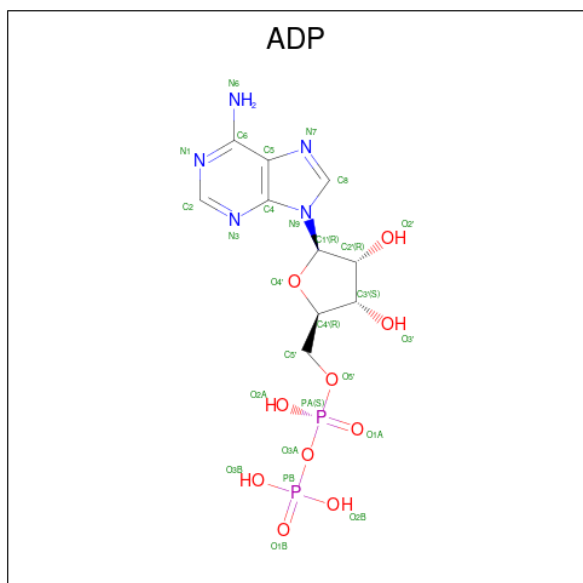
| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | O     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | P     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | Q     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | R     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | S     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | T     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | U     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | V     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | W     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | X     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | Y     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |
| 9   | Z     | 76       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 152 | 76 | 75 |         |       |

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 10  | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

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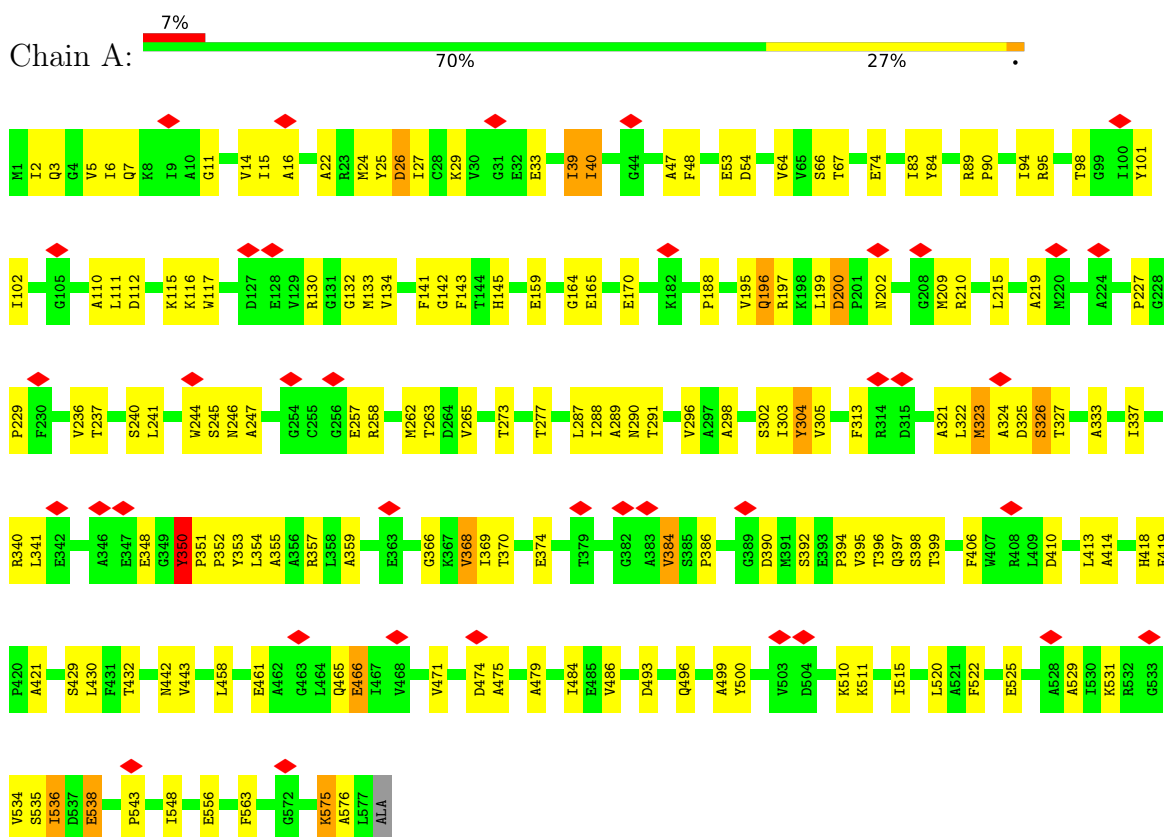
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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 10  | C     | 1        | 27    | 10 | 5 | 10 | 2 | 0       |

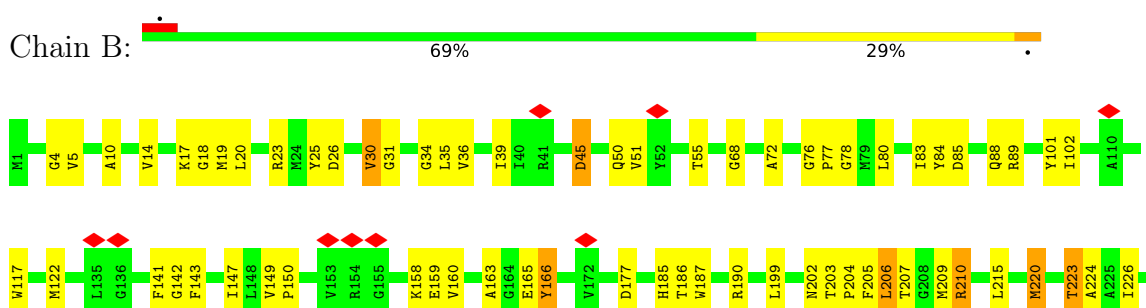
### 3 Residue-property plots

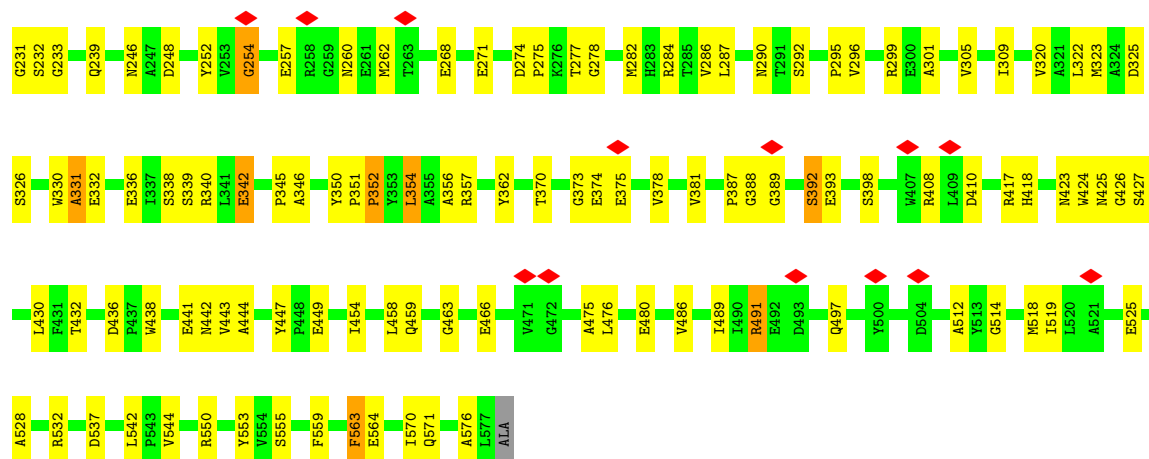
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: V-type ATP synthase alpha chain

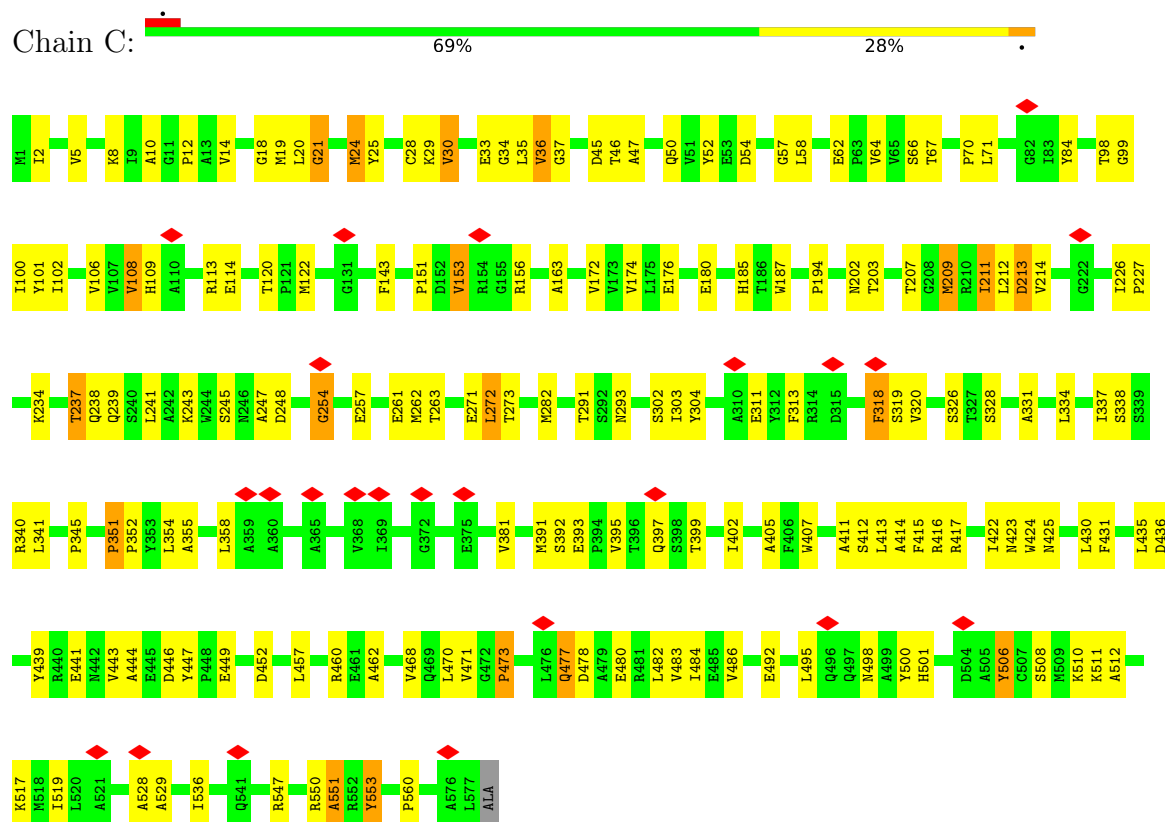


- Molecule 1: V-type ATP synthase alpha chain

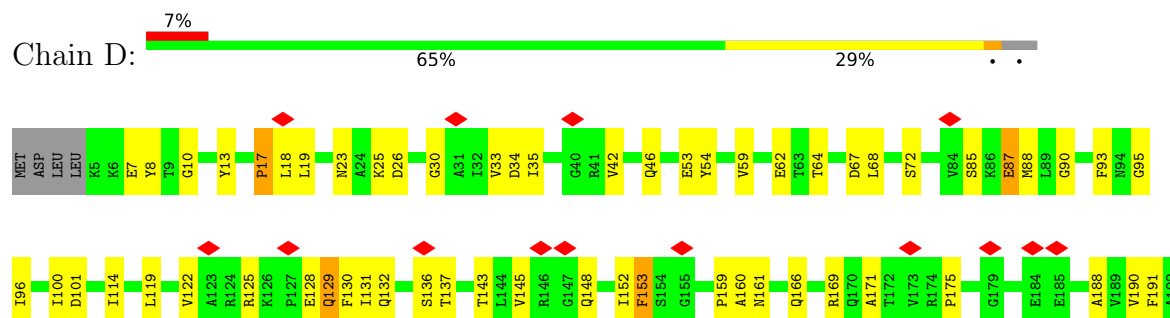


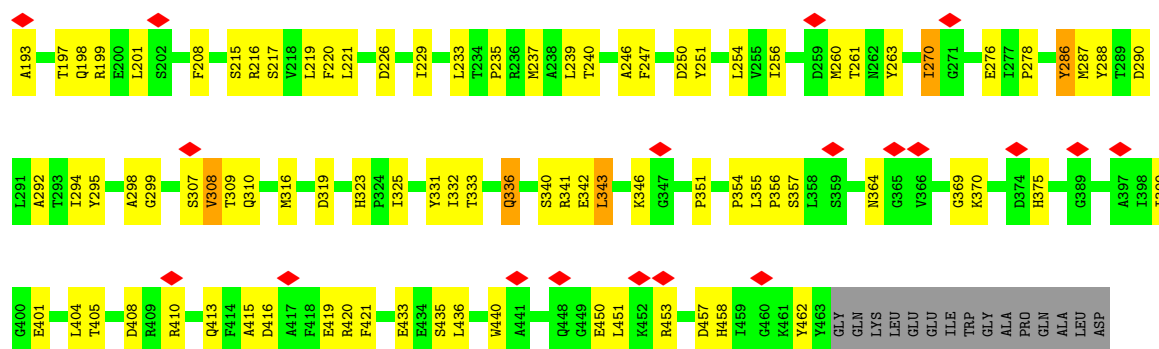


• Molecule 1: V-type ATP synthase alpha chain

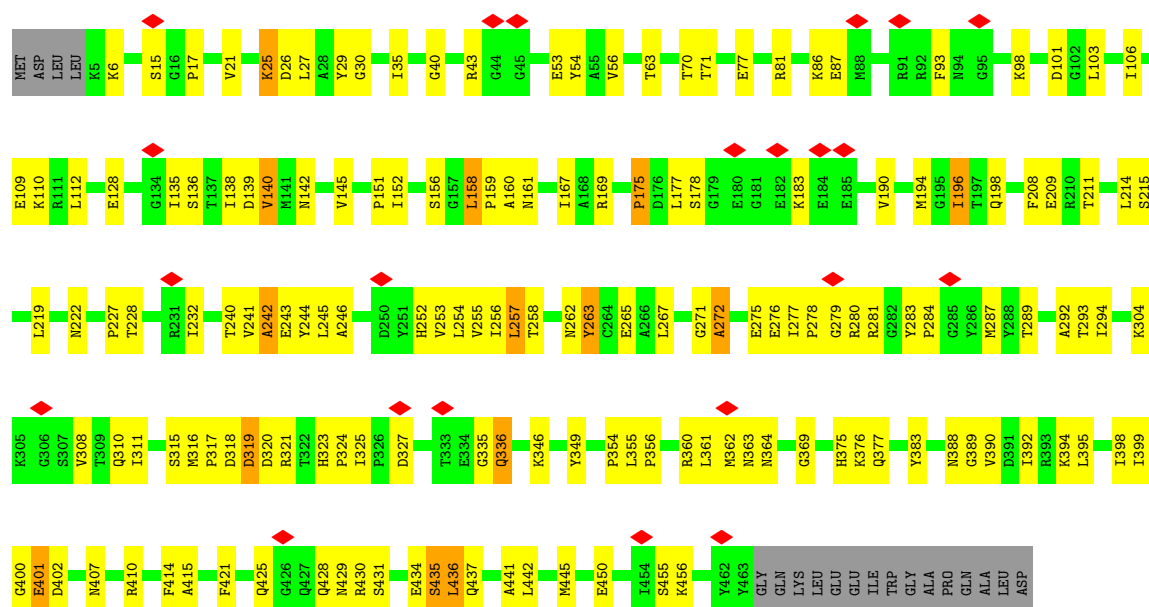


• Molecule 2: V-type ATP synthase beta chain

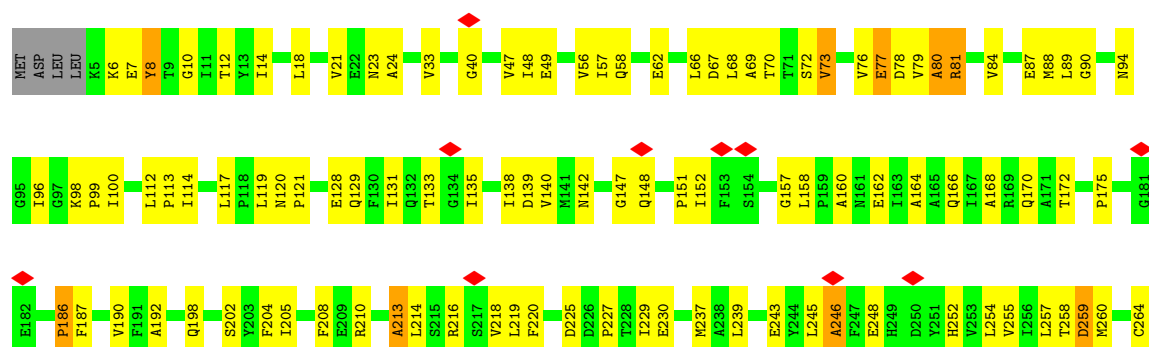


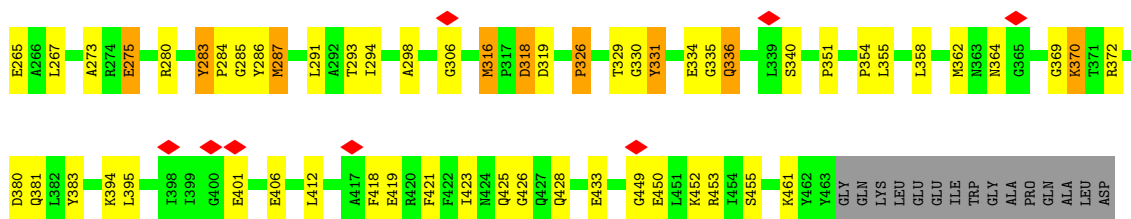


• Molecule 2: V-type ATP synthase beta chain

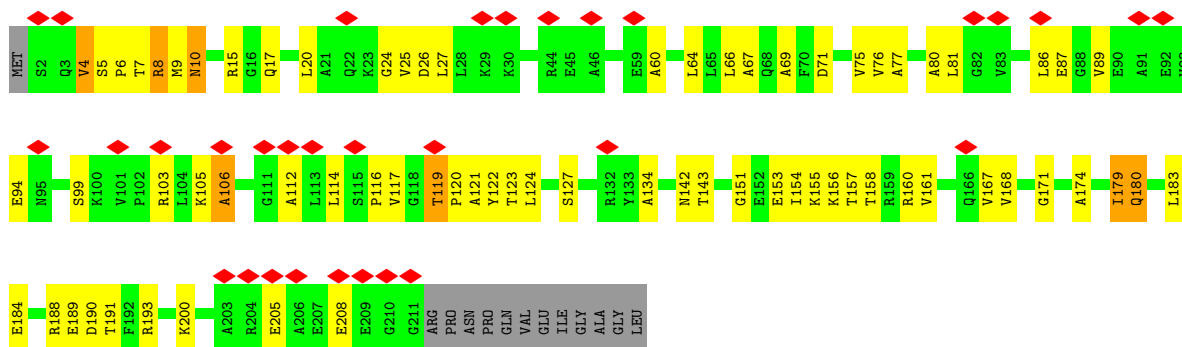


• Molecule 2: V-type ATP synthase beta chain

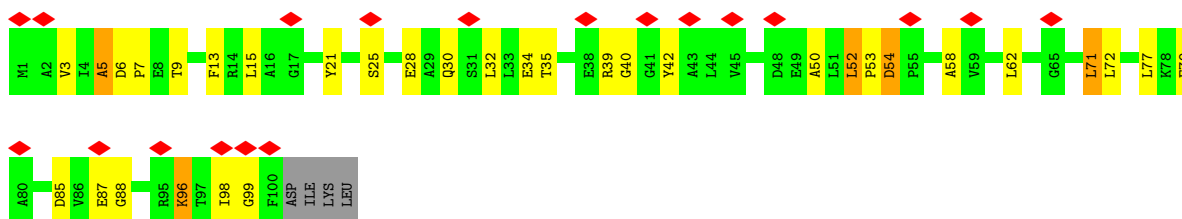




• Molecule 3: V-type ATP synthase subunit D



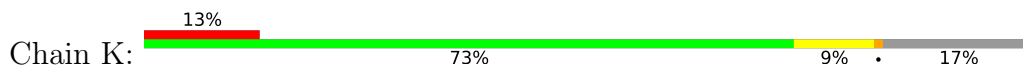
• Molecule 4: V-type ATP synthase subunit F

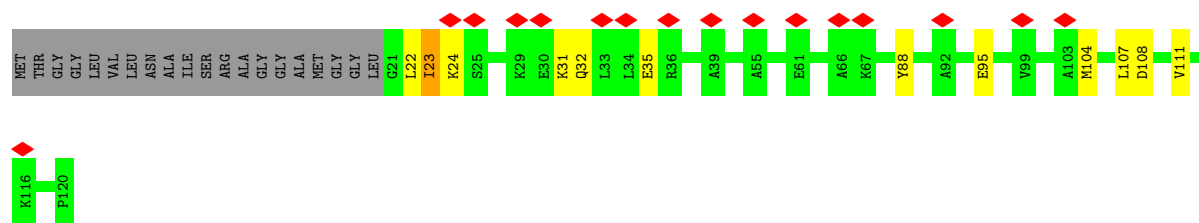


• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

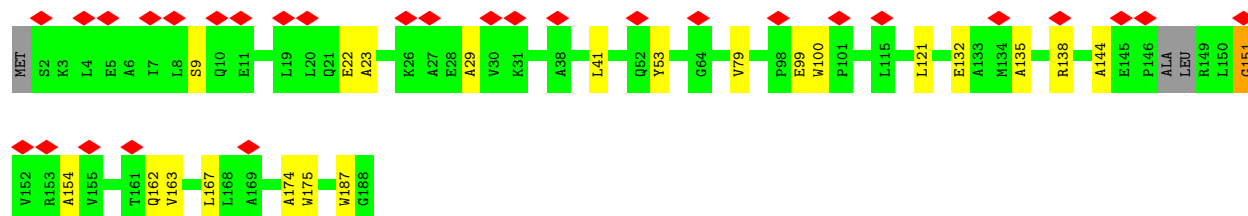
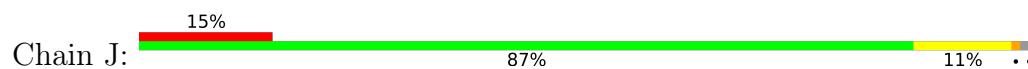


• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

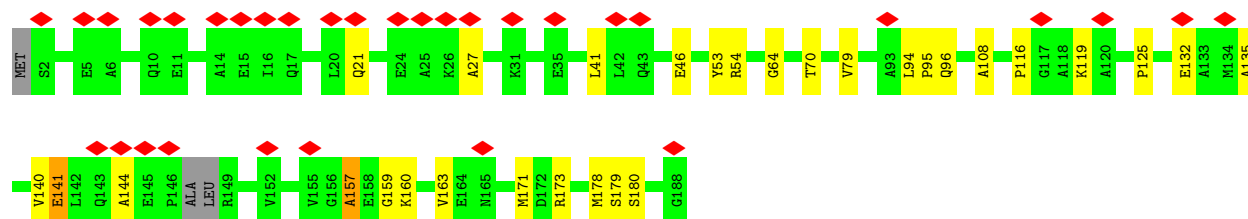
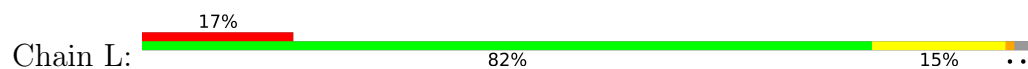




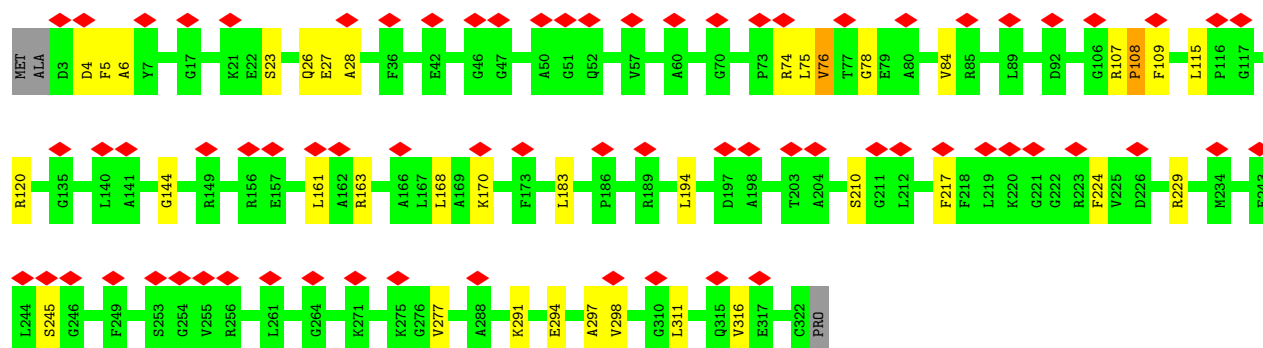
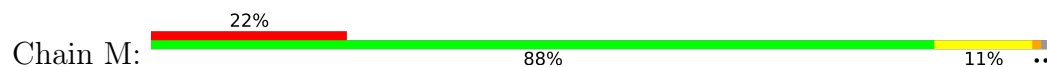
• Molecule 6: V-type ATP synthase subunit E



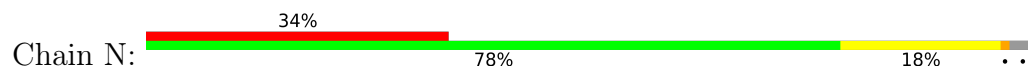
• Molecule 6: V-type ATP synthase subunit E

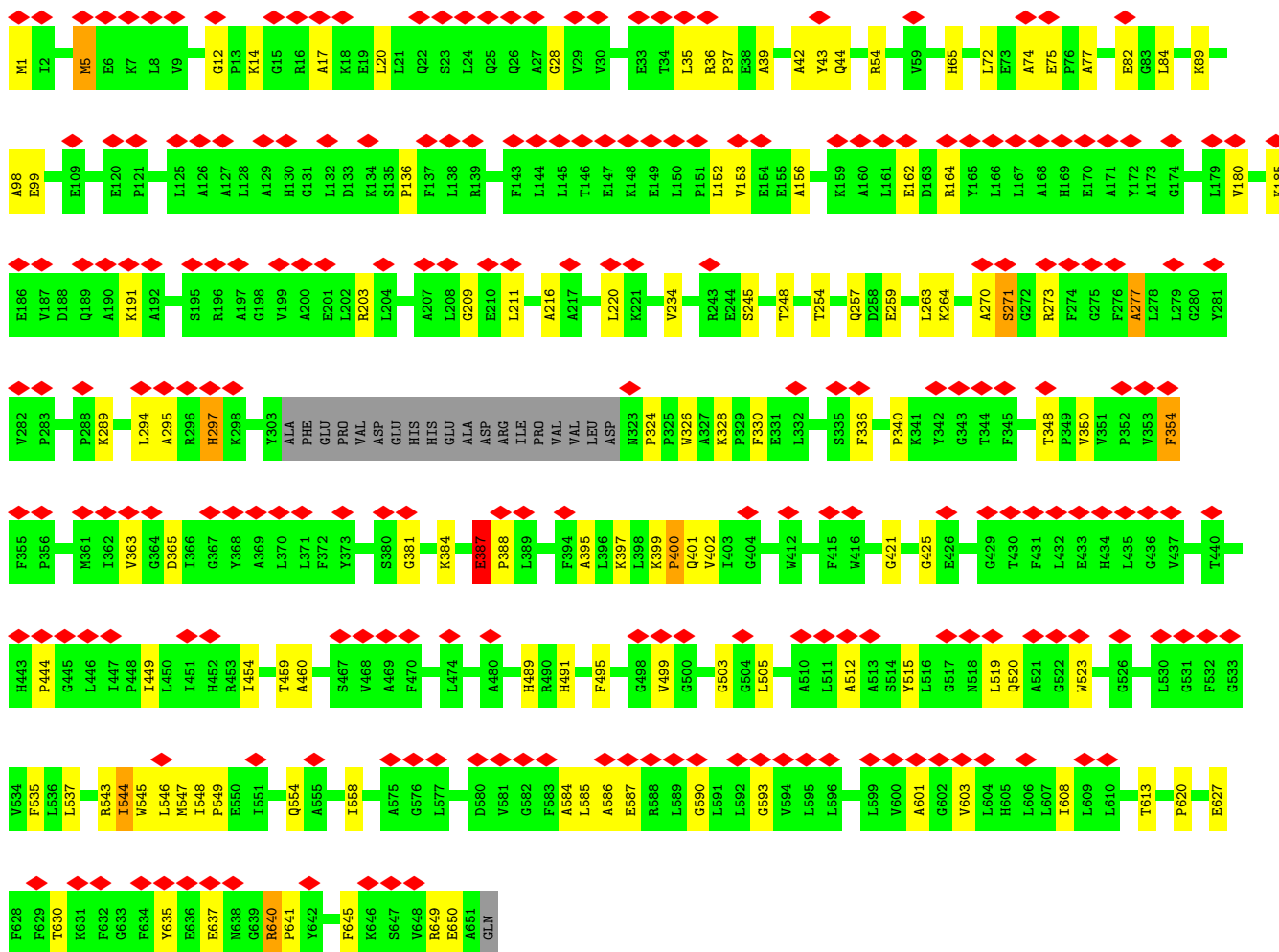


• Molecule 7: V-type ATP synthase subunit C

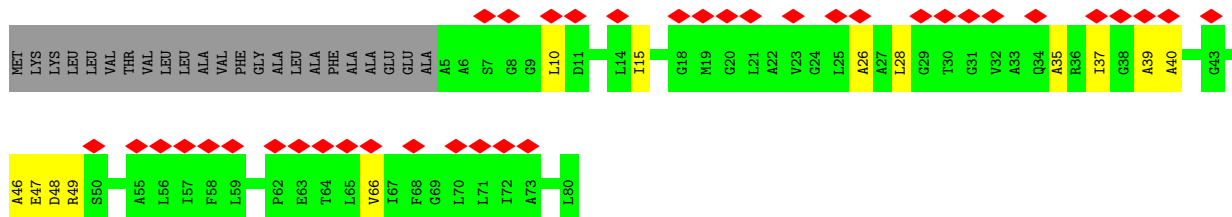
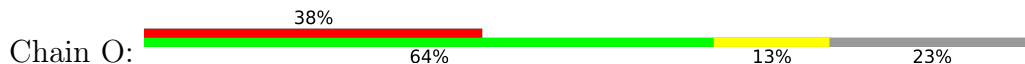


• Molecule 8: V-type ATP synthase subunit I

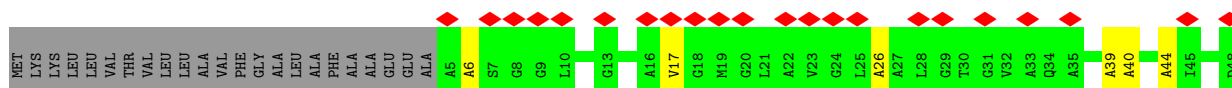


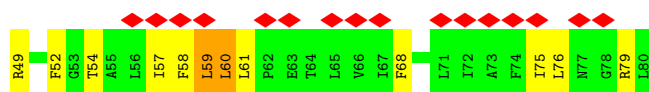


• Molecule 9: V-type ATP synthase, subunit K

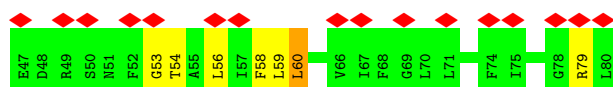
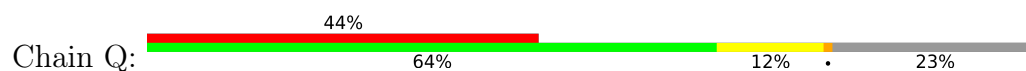


• Molecule 9: V-type ATP synthase, subunit K

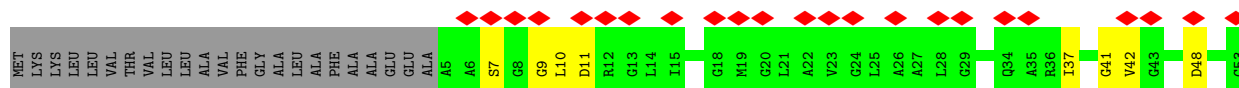
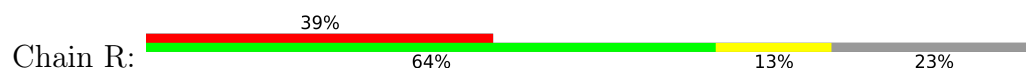




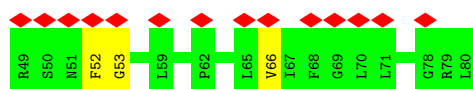
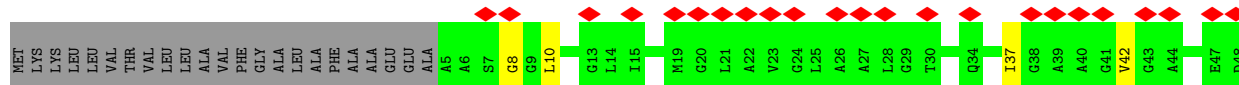
- Molecule 9: V-type ATP synthase, subunit K



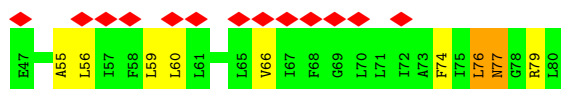
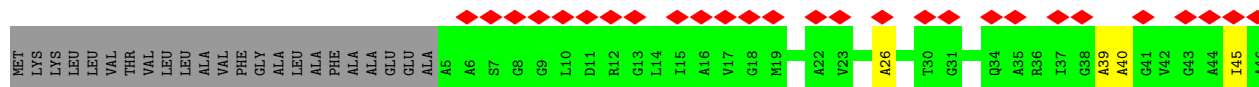
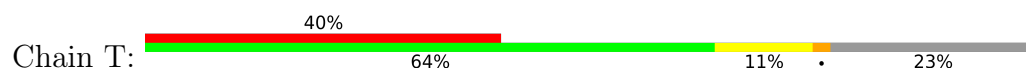
- Molecule 9: V-type ATP synthase, subunit K



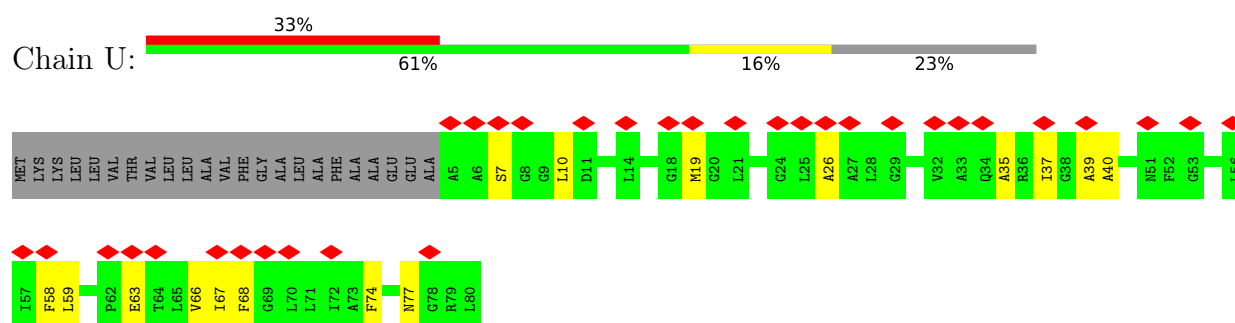
- Molecule 9: V-type ATP synthase, subunit K



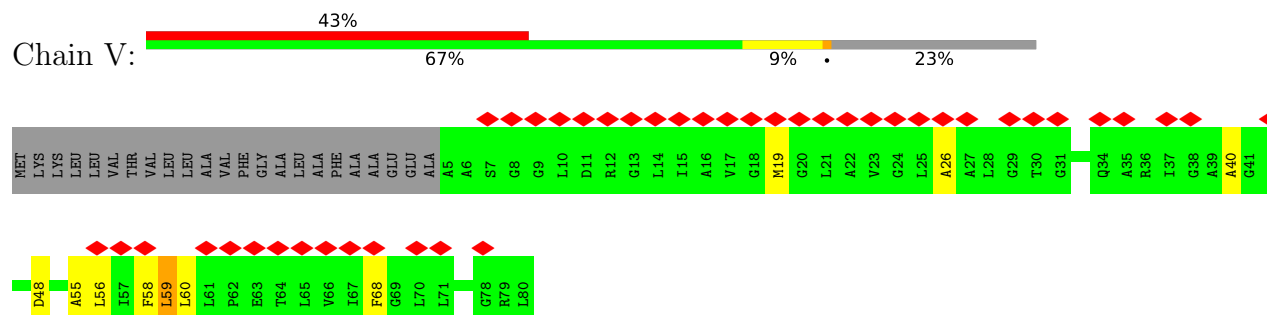
- Molecule 9: V-type ATP synthase, subunit K



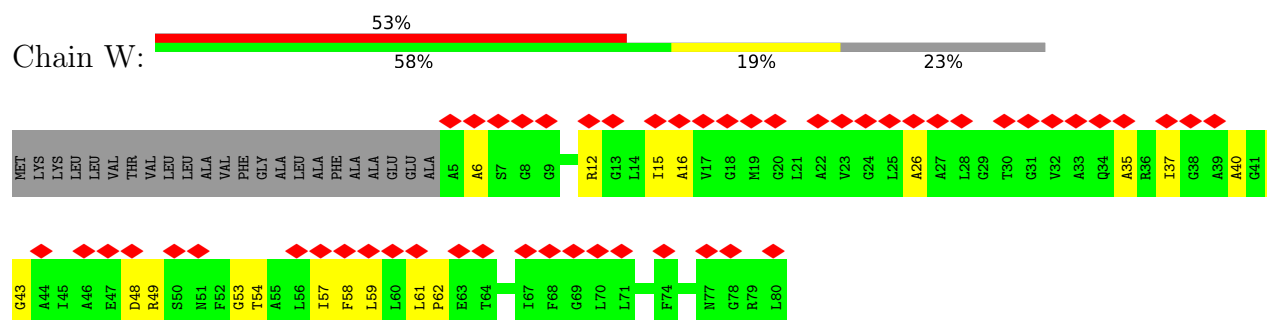
- Molecule 9: V-type ATP synthase, subunit K



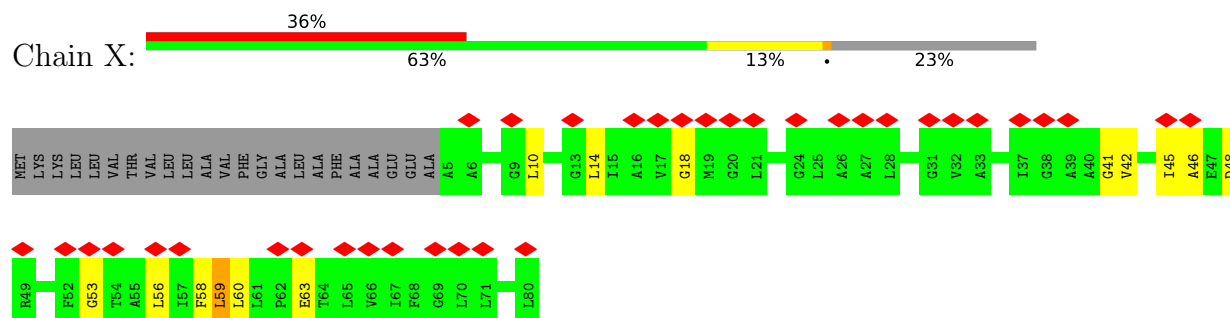
- Molecule 9: V-type ATP synthase, subunit K



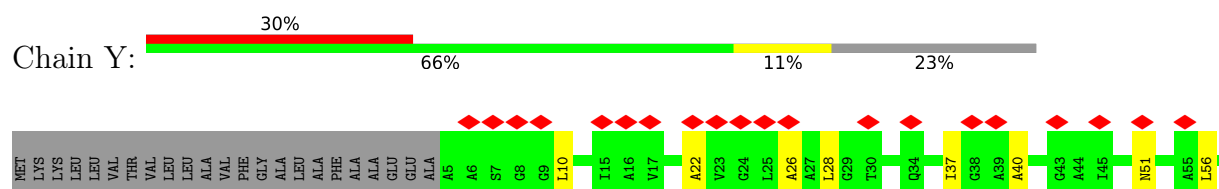
- Molecule 9: V-type ATP synthase, subunit K

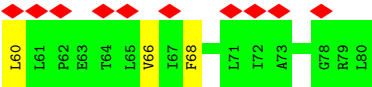


- Molecule 9: V-type ATP synthase, subunit K

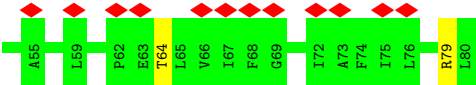


- Molecule 9: V-type ATP synthase, subunit K





• Molecule 9: V-type ATP synthase, subunit K



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 30802                                   | 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 ( $e^-/\text{\AA}^2$ ) | 26                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.518                                   | Depositor |
| Minimum map value                    | -0.322                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.026                                   | Depositor |
| Recommended contour level            | 0.1                                     | Depositor |
| Map size (Å)                         | 330.4, 330.4, 330.4                     | wwPDB     |
| Map dimensions                       | 236, 236, 236                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.4, 1.4, 1.4                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 1   | A     | 2.29         | 71/2306 (3.1%)   | 2.22        | 93/2881 (3.2%)    |
| 1   | B     | 2.37         | 75/2306 (3.3%)   | 2.25        | 115/2881 (4.0%)   |
| 1   | C     | 2.32         | 66/2306 (2.9%)   | 2.23        | 111/2881 (3.9%)   |
| 2   | D     | 2.26         | 47/1834 (2.6%)   | 2.24        | 89/2291 (3.9%)    |
| 2   | E     | 2.42         | 65/1834 (3.5%)   | 2.24        | 92/2291 (4.0%)    |
| 2   | F     | 2.44         | 69/1834 (3.8%)   | 2.27        | 92/2291 (4.0%)    |
| 3   | G     | 2.27         | 16/838 (1.9%)    | 2.46        | 60/1046 (5.7%)    |
| 4   | H     | 2.04         | 6/398 (1.5%)     | 2.24        | 22/496 (4.4%)     |
| 5   | I     | 1.66         | 0/398            | 2.32        | 22/496 (4.4%)     |
| 5   | K     | 1.87         | 1/398 (0.3%)     | 2.32        | 20/496 (4.0%)     |
| 6   | J     | 1.87         | 3/736 (0.4%)     | 2.14        | 20/917 (2.2%)     |
| 6   | L     | 1.89         | 2/736 (0.3%)     | 2.16        | 26/917 (2.8%)     |
| 7   | M     | 1.86         | 4/1278 (0.3%)    | 2.09        | 40/1596 (2.5%)    |
| 8   | N     | 1.81         | 12/2524 (0.5%)   | 2.26        | 127/3152 (4.0%)   |
| 9   | O     | 1.40         | 0/302            | 2.44        | 20/376 (5.3%)     |
| 9   | P     | 1.46         | 0/302            | 2.55        | 26/376 (6.9%)     |
| 9   | Q     | 1.43         | 0/302            | 2.35        | 22/376 (5.9%)     |
| 9   | R     | 1.42         | 0/302            | 2.36        | 15/376 (4.0%)     |
| 9   | S     | 1.42         | 0/302            | 2.38        | 11/376 (2.9%)     |
| 9   | T     | 1.32         | 0/302            | 2.41        | 20/376 (5.3%)     |
| 9   | U     | 1.36         | 0/302            | 2.52        | 25/376 (6.6%)     |
| 9   | V     | 1.37         | 0/302            | 2.30        | 16/376 (4.3%)     |
| 9   | W     | 1.33         | 0/302            | 2.63        | 32/376 (8.5%)     |
| 9   | X     | 1.40         | 0/302            | 2.52        | 22/376 (5.9%)     |
| 9   | Y     | 1.41         | 0/302            | 2.41        | 21/376 (5.6%)     |
| 9   | Z     | 1.44         | 0/302            | 2.12        | 13/376 (3.5%)     |
| All | All   | 2.09         | 437/23350 (1.9%) | 2.27        | 1172/29144 (4.0%) |

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

sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 14                  |
| 1   | B     | 0                   | 15                  |
| 1   | C     | 0                   | 21                  |
| 2   | D     | 0                   | 10                  |
| 2   | E     | 0                   | 17                  |
| 2   | F     | 0                   | 16                  |
| 3   | G     | 0                   | 7                   |
| 4   | H     | 0                   | 5                   |
| 6   | J     | 0                   | 1                   |
| 6   | L     | 0                   | 6                   |
| 7   | M     | 0                   | 4                   |
| 8   | N     | 0                   | 14                  |
| 9   | O     | 0                   | 2                   |
| 9   | P     | 0                   | 2                   |
| 9   | Q     | 0                   | 1                   |
| 9   | R     | 0                   | 2                   |
| 9   | T     | 0                   | 2                   |
| 9   | V     | 0                   | 3                   |
| 9   | X     | 0                   | 2                   |
| All | All   | 0                   | 144                 |

All (437) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | C     | 52  | TYR  | CA-C  | -11.67 | 1.46        | 1.52     |
| 1   | B     | 442 | ASN  | CA-C  | -10.68 | 1.43        | 1.52     |
| 2   | E     | 255 | VAL  | CA-C  | -9.27  | 1.41        | 1.52     |
| 1   | A     | 461 | GLU  | CA-C  | -8.42  | 1.44        | 1.52     |
| 2   | D     | 93  | PHE  | CA-C  | -8.28  | 1.45        | 1.53     |
| 2   | D     | 323 | HIS  | CA-C  | -7.87  | 1.45        | 1.52     |
| 1   | C     | 84  | TYR  | CA-C  | -7.69  | 1.43        | 1.52     |
| 3   | G     | 190 | ASP  | CA-C  | -7.69  | 1.43        | 1.52     |
| 2   | F     | 425 | GLN  | N-CA  | -7.50  | 1.40        | 1.47     |
| 1   | A     | 353 | TYR  | CA-C  | -7.46  | 1.43        | 1.52     |
| 2   | D     | 290 | ASP  | CA-C  | -7.42  | 1.43        | 1.52     |
| 2   | F     | 81  | ARG  | CA-C  | -7.34  | 1.43        | 1.52     |
| 2   | D     | 233 | LEU  | CA-C  | -7.33  | 1.44        | 1.52     |
| 2   | E     | 394 | LYS  | CA-C  | -7.30  | 1.45        | 1.53     |
| 2   | E     | 311 | ILE  | CA-C  | -7.28  | 1.45        | 1.52     |
| 2   | E     | 277 | ILE  | CA-C  | -7.27  | 1.45        | 1.52     |
| 2   | E     | 292 | ALA  | CA-C  | -7.27  | 1.44        | 1.52     |
| 2   | E     | 152 | ILE  | CA-C  | -7.24  | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 538 | GLU  | CA-C  | -7.22 | 1.46        | 1.52     |
| 2   | F     | 208 | PHE  | CA-C  | -7.20 | 1.43        | 1.52     |
| 2   | F     | 129 | GLN  | CA-C  | -7.16 | 1.43        | 1.52     |
| 1   | C     | 358 | LEU  | CA-C  | -7.14 | 1.45        | 1.53     |
| 2   | F     | 220 | PHE  | CA-C  | -7.09 | 1.43        | 1.52     |
| 1   | B     | 459 | GLN  | CA-C  | -7.08 | 1.44        | 1.52     |
| 1   | C     | 29  | LYS  | CA-C  | -7.03 | 1.44        | 1.52     |
| 1   | B     | 72  | ALA  | N-CA  | -7.01 | 1.38        | 1.46     |
| 1   | B     | 370 | THR  | CA-C  | -6.97 | 1.43        | 1.53     |
| 1   | A     | 341 | LEU  | CA-C  | -6.96 | 1.44        | 1.52     |
| 2   | F     | 204 | PHE  | CA-C  | -6.96 | 1.43        | 1.52     |
| 1   | A     | 287 | LEU  | CA-C  | -6.94 | 1.44        | 1.52     |
| 1   | C     | 5   | VAL  | CA-C  | -6.89 | 1.46        | 1.52     |
| 1   | B     | 491 | ARG  | CA-C  | -6.88 | 1.43        | 1.52     |
| 1   | C     | 98  | THR  | CA-C  | -6.88 | 1.47        | 1.52     |
| 1   | B     | 374 | GLU  | CA-C  | -6.86 | 1.44        | 1.52     |
| 2   | F     | 334 | GLU  | CA-C  | -6.86 | 1.47        | 1.53     |
| 1   | A     | 39  | ILE  | CA-C  | -6.84 | 1.44        | 1.52     |
| 2   | F     | 255 | VAL  | CA-C  | -6.83 | 1.44        | 1.52     |
| 2   | E     | 252 | HIS  | CA-C  | -6.83 | 1.45        | 1.53     |
| 1   | B     | 143 | PHE  | CA-C  | -6.81 | 1.44        | 1.52     |
| 2   | E     | 26  | ASP  | CA-C  | -6.79 | 1.46        | 1.52     |
| 1   | B     | 423 | ASN  | CA-C  | -6.79 | 1.44        | 1.53     |
| 1   | B     | 226 | ILE  | CA-C  | -6.77 | 1.47        | 1.53     |
| 2   | F     | 254 | LEU  | CA-C  | -6.77 | 1.44        | 1.52     |
| 1   | A     | 442 | ASN  | CA-C  | -6.75 | 1.44        | 1.53     |
| 1   | B     | 449 | GLU  | CA-C  | -6.71 | 1.47        | 1.52     |
| 2   | F     | 239 | LEU  | CA-C  | -6.71 | 1.44        | 1.52     |
| 2   | F     | 287 | MET  | N-CA  | -6.70 | 1.38        | 1.46     |
| 2   | D     | 175 | PRO  | CA-C  | -6.67 | 1.45        | 1.52     |
| 2   | E     | 256 | ILE  | CA-C  | -6.66 | 1.44        | 1.52     |
| 2   | F     | 412 | LEU  | CA-C  | -6.64 | 1.45        | 1.53     |
| 1   | B     | 441 | GLU  | CA-C  | -6.62 | 1.44        | 1.52     |
| 2   | F     | 140 | VAL  | CA-C  | -6.61 | 1.44        | 1.52     |
| 6   | J     | 53  | TYR  | CA-C  | -6.60 | 1.46        | 1.52     |
| 2   | D     | 208 | PHE  | CA-C  | -6.60 | 1.45        | 1.52     |
| 1   | A     | 291 | THR  | CA-C  | -6.60 | 1.44        | 1.52     |
| 2   | F     | 273 | ALA  | CA-C  | -6.60 | 1.45        | 1.52     |
| 1   | C     | 8   | LYS  | CA-C  | -6.58 | 1.45        | 1.52     |
| 2   | E     | 26  | ASP  | N-CA  | -6.56 | 1.41        | 1.47     |
| 1   | A     | 241 | LEU  | CA-C  | -6.54 | 1.44        | 1.52     |
| 1   | C     | 334 | LEU  | CA-C  | -6.54 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | F     | 12  | THR  | CA-C  | -6.54 | 1.44        | 1.52     |
| 2   | E     | 254 | LEU  | CA-C  | -6.53 | 1.44        | 1.52     |
| 4   | H     | 72  | LEU  | CA-C  | -6.53 | 1.47        | 1.52     |
| 1   | B     | 559 | PHE  | N-CA  | -6.52 | 1.41        | 1.46     |
| 1   | B     | 351 | PRO  | C-N   | -6.51 | 1.27        | 1.33     |
| 2   | E     | 138 | ILE  | CA-C  | -6.49 | 1.45        | 1.52     |
| 2   | E     | 161 | ASN  | CA-C  | -6.49 | 1.44        | 1.53     |
| 2   | E     | 272 | ALA  | CA-C  | -6.48 | 1.44        | 1.52     |
| 2   | F     | 245 | LEU  | CA-C  | -6.48 | 1.46        | 1.53     |
| 1   | C     | 399 | THR  | CA-C  | -6.48 | 1.44        | 1.52     |
| 8   | N     | 259 | GLU  | CA-C  | -6.42 | 1.44        | 1.52     |
| 1   | C     | 19  | MET  | CA-C  | -6.41 | 1.45        | 1.52     |
| 1   | C     | 272 | LEU  | CA-C  | -6.41 | 1.44        | 1.52     |
| 6   | J     | 151 | GLY  | CA-C  | -6.39 | 1.45        | 1.51     |
| 1   | B     | 454 | ILE  | CA-C  | -6.38 | 1.46        | 1.52     |
| 2   | D     | 276 | GLU  | CA-C  | -6.38 | 1.44        | 1.52     |
| 1   | A     | 419 | PHE  | CA-C  | -6.38 | 1.47        | 1.52     |
| 1   | A     | 290 | ASN  | CA-C  | -6.33 | 1.44        | 1.52     |
| 2   | D     | 246 | ALA  | CA-C  | -6.32 | 1.45        | 1.52     |
| 2   | F     | 246 | ALA  | CA-C  | -6.32 | 1.44        | 1.52     |
| 3   | G     | 183 | LEU  | CA-C  | -6.32 | 1.44        | 1.52     |
| 2   | E     | 280 | ARG  | CA-C  | -6.30 | 1.44        | 1.52     |
| 3   | G     | 157 | THR  | CA-C  | -6.29 | 1.45        | 1.52     |
| 2   | D     | 129 | GLN  | CA-C  | -6.27 | 1.45        | 1.52     |
| 8   | N     | 257 | GLN  | CA-C  | -6.25 | 1.44        | 1.52     |
| 1   | B     | 339 | SER  | CA-C  | -6.24 | 1.44        | 1.52     |
| 2   | F     | 58  | GLN  | CA-C  | -6.24 | 1.45        | 1.53     |
| 2   | F     | 219 | LEU  | CA-C  | -6.24 | 1.44        | 1.52     |
| 1   | B     | 83  | ILE  | CA-C  | -6.23 | 1.44        | 1.52     |
| 1   | A     | 143 | PHE  | CA-C  | -6.23 | 1.45        | 1.52     |
| 1   | C     | 498 | ASN  | CA-C  | -6.23 | 1.45        | 1.52     |
| 2   | F     | 267 | LEU  | CA-C  | -6.21 | 1.45        | 1.52     |
| 2   | E     | 317 | PRO  | CA-C  | -6.21 | 1.44        | 1.52     |
| 1   | C     | 211 | ILE  | CA-C  | -6.20 | 1.44        | 1.52     |
| 2   | E     | 308 | VAL  | CA-C  | -6.19 | 1.46        | 1.53     |
| 2   | F     | 336 | GLN  | CA-C  | -6.17 | 1.44        | 1.52     |
| 2   | D     | 125 | ARG  | CA-C  | -6.17 | 1.45        | 1.52     |
| 2   | F     | 162 | GLU  | CA-C  | -6.14 | 1.46        | 1.53     |
| 3   | G     | 75  | VAL  | CA-C  | -6.13 | 1.44        | 1.52     |
| 1   | B     | 39  | ILE  | CA-C  | -6.11 | 1.46        | 1.53     |
| 2   | F     | 319 | ASP  | CA-C  | -6.10 | 1.44        | 1.52     |
| 2   | F     | 423 | ILE  | CA-C  | -6.09 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 84  | TYR  | CA-C  | -6.09 | 1.45        | 1.52     |
| 1   | B     | 309 | ILE  | CA-C  | -6.09 | 1.44        | 1.52     |
| 2   | F     | 190 | VAL  | CA-C  | -6.08 | 1.45        | 1.52     |
| 2   | D     | 270 | ILE  | CA-C  | -6.08 | 1.45        | 1.52     |
| 2   | D     | 188 | ALA  | CA-C  | -6.07 | 1.45        | 1.52     |
| 1   | B     | 322 | LEU  | CA-C  | -6.07 | 1.45        | 1.52     |
| 1   | C     | 519 | ILE  | CA-C  | -6.07 | 1.45        | 1.52     |
| 2   | E     | 281 | ARG  | CA-C  | -6.07 | 1.45        | 1.53     |
| 2   | F     | 57  | ILE  | CA-C  | -6.06 | 1.45        | 1.52     |
| 1   | A     | 273 | THR  | CA-C  | -6.06 | 1.45        | 1.52     |
| 2   | D     | 130 | PHE  | CA-C  | -6.06 | 1.45        | 1.52     |
| 2   | E     | 35  | ILE  | N-CA  | -6.06 | 1.38        | 1.46     |
| 6   | L     | 53  | TYR  | CA-C  | -6.05 | 1.47        | 1.52     |
| 1   | B     | 354 | LEU  | CA-C  | -6.05 | 1.44        | 1.52     |
| 2   | F     | 280 | ARG  | CA-C  | -6.04 | 1.44        | 1.52     |
| 2   | F     | 421 | PHE  | CA-C  | -6.04 | 1.45        | 1.52     |
| 2   | E     | 361 | LEU  | CA-C  | -6.03 | 1.45        | 1.52     |
| 3   | G     | 106 | ALA  | CA-C  | -6.03 | 1.46        | 1.53     |
| 1   | B     | 226 | ILE  | N-CA  | -6.02 | 1.41        | 1.46     |
| 8   | N     | 245 | SER  | CA-C  | -6.02 | 1.44        | 1.52     |
| 1   | C     | 303 | ILE  | CA-C  | -6.01 | 1.45        | 1.52     |
| 1   | C     | 439 | TYR  | CA-C  | -6.01 | 1.45        | 1.52     |
| 2   | E     | 262 | ASN  | CA-C  | -6.00 | 1.44        | 1.52     |
| 1   | B     | 564 | GLU  | CA-C  | -6.00 | 1.45        | 1.52     |
| 1   | A     | 575 | LYS  | CA-C  | -5.99 | 1.47        | 1.53     |
| 2   | E     | 392 | ILE  | CA-C  | -5.99 | 1.45        | 1.52     |
| 2   | F     | 47  | VAL  | CA-C  | -5.99 | 1.46        | 1.52     |
| 1   | B     | 268 | GLU  | CA-C  | -5.99 | 1.45        | 1.52     |
| 2   | E     | 219 | LEU  | CA-C  | -5.98 | 1.46        | 1.52     |
| 2   | E     | 284 | PRO  | CA-C  | -5.98 | 1.45        | 1.52     |
| 2   | D     | 436 | LEU  | CA-C  | -5.96 | 1.45        | 1.52     |
| 1   | A     | 337 | ILE  | CA-C  | -5.96 | 1.45        | 1.52     |
| 2   | F     | 425 | GLN  | CA-C  | -5.95 | 1.47        | 1.52     |
| 1   | A     | 7   | GLN  | CA-C  | -5.95 | 1.46        | 1.52     |
| 1   | A     | 327 | THR  | CA-C  | -5.94 | 1.45        | 1.52     |
| 2   | E     | 267 | LEU  | CA-C  | -5.94 | 1.45        | 1.52     |
| 1   | A     | 188 | PRO  | CA-C  | -5.93 | 1.45        | 1.52     |
| 2   | F     | 186 | PRO  | CA-C  | -5.93 | 1.46        | 1.52     |
| 1   | A     | 145 | HIS  | CA-C  | -5.93 | 1.45        | 1.52     |
| 1   | B     | 459 | GLN  | N-CA  | -5.93 | 1.39        | 1.46     |
| 3   | G     | 71  | ASP  | CA-C  | -5.92 | 1.44        | 1.52     |
| 2   | D     | 119 | LEU  | CA-C  | -5.92 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 165 | GLU  | CA-C  | -5.92 | 1.45        | 1.52     |
| 2   | E     | 336 | GLN  | CA-C  | -5.92 | 1.44        | 1.52     |
| 2   | F     | 33  | VAL  | CA-C  | -5.92 | 1.45        | 1.52     |
| 1   | A     | 493 | ASP  | CA-C  | -5.91 | 1.47        | 1.52     |
| 1   | A     | 115 | LYS  | CA-C  | -5.91 | 1.45        | 1.53     |
| 1   | A     | 101 | TYR  | CA-C  | -5.91 | 1.44        | 1.53     |
| 1   | C     | 209 | MET  | CA-C  | -5.89 | 1.45        | 1.52     |
| 4   | H     | 32  | LEU  | CA-C  | -5.88 | 1.47        | 1.53     |
| 2   | D     | 251 | TYR  | N-CA  | -5.88 | 1.39        | 1.45     |
| 2   | F     | 264 | CYS  | CA-C  | -5.88 | 1.45        | 1.52     |
| 1   | A     | 333 | ALA  | CA-C  | -5.87 | 1.45        | 1.52     |
| 2   | E     | 265 | GLU  | CA-C  | -5.87 | 1.45        | 1.52     |
| 1   | A     | 399 | THR  | CA-C  | -5.86 | 1.45        | 1.52     |
| 2   | D     | 33  | VAL  | CA-C  | -5.86 | 1.45        | 1.52     |
| 2   | E     | 289 | THR  | CA-C  | -5.85 | 1.45        | 1.52     |
| 1   | B     | 296 | VAL  | N-CA  | -5.85 | 1.39        | 1.46     |
| 1   | A     | 321 | ALA  | CA-C  | -5.84 | 1.47        | 1.53     |
| 2   | E     | 320 | ASP  | CA-C  | -5.84 | 1.45        | 1.52     |
| 2   | F     | 229 | ILE  | N-CA  | -5.83 | 1.39        | 1.46     |
| 2   | F     | 257 | LEU  | CA-C  | -5.83 | 1.45        | 1.52     |
| 1   | B     | 351 | PRO  | CA-C  | -5.83 | 1.46        | 1.52     |
| 2   | D     | 295 | TYR  | CA-C  | -5.81 | 1.45        | 1.52     |
| 2   | E     | 81  | ARG  | CA-C  | -5.81 | 1.45        | 1.52     |
| 1   | C     | 447 | TYR  | N-CA  | -5.80 | 1.41        | 1.46     |
| 2   | F     | 112 | LEU  | CA-C  | -5.79 | 1.46        | 1.52     |
| 1   | B     | 205 | PHE  | CA-C  | -5.79 | 1.45        | 1.52     |
| 1   | A     | 313 | PHE  | CA-C  | -5.79 | 1.45        | 1.52     |
| 2   | D     | 263 | TYR  | CA-C  | -5.79 | 1.45        | 1.52     |
| 7   | M     | 298 | VAL  | CA-C  | -5.78 | 1.45        | 1.52     |
| 1   | A     | 215 | LEU  | CA-C  | -5.77 | 1.45        | 1.53     |
| 2   | F     | 162 | GLU  | N-CA  | -5.77 | 1.40        | 1.46     |
| 3   | G     | 64  | LEU  | CA-C  | -5.77 | 1.45        | 1.52     |
| 1   | C     | 156 | ARG  | CA-C  | -5.76 | 1.45        | 1.52     |
| 2   | D     | 336 | GLN  | CA-C  | -5.76 | 1.45        | 1.52     |
| 2   | F     | 326 | PRO  | CA-C  | -5.76 | 1.44        | 1.52     |
| 3   | G     | 188 | ARG  | CA-C  | -5.76 | 1.45        | 1.52     |
| 1   | C     | 226 | ILE  | N-CA  | -5.75 | 1.41        | 1.46     |
| 1   | C     | 257 | GLU  | CA-C  | -5.75 | 1.45        | 1.52     |
| 1   | A     | 263 | THR  | CA-C  | -5.75 | 1.44        | 1.52     |
| 3   | G     | 158 | THR  | CA-C  | -5.75 | 1.45        | 1.52     |
| 2   | E     | 376 | LYS  | CA-C  | -5.74 | 1.45        | 1.52     |
| 1   | C     | 508 | SER  | CA-C  | -5.74 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | D     | 308 | VAL  | CA-C  | -5.74 | 1.45        | 1.52     |
| 1   | C     | 506 | TYR  | CA-C  | -5.73 | 1.45        | 1.52     |
| 8   | N     | 264 | LYS  | CA-C  | -5.71 | 1.45        | 1.52     |
| 8   | N     | 254 | THR  | CA-C  | -5.71 | 1.45        | 1.52     |
| 2   | E     | 156 | SER  | CA-C  | -5.70 | 1.45        | 1.52     |
| 2   | F     | 287 | MET  | CA-C  | -5.70 | 1.45        | 1.52     |
| 2   | E     | 283 | TYR  | CA-C  | -5.69 | 1.45        | 1.52     |
| 1   | C     | 393 | GLU  | CA-C  | -5.69 | 1.47        | 1.53     |
| 1   | A     | 164 | GLY  | CA-C  | -5.68 | 1.45        | 1.51     |
| 2   | E     | 35  | ILE  | CA-C  | -5.68 | 1.45        | 1.52     |
| 1   | C     | 30  | VAL  | N-CA  | -5.67 | 1.39        | 1.46     |
| 2   | F     | 243 | GLU  | CA-C  | -5.67 | 1.45        | 1.52     |
| 1   | C     | 483 | VAL  | CA-C  | -5.67 | 1.45        | 1.52     |
| 1   | B     | 357 | ARG  | CA-C  | -5.67 | 1.45        | 1.52     |
| 1   | C     | 101 | TYR  | CA-C  | -5.66 | 1.45        | 1.52     |
| 1   | A     | 511 | LYS  | CA-C  | -5.66 | 1.46        | 1.53     |
| 1   | A     | 257 | GLU  | CA-C  | -5.65 | 1.45        | 1.52     |
| 2   | E     | 98  | LYS  | CA-C  | -5.65 | 1.47        | 1.52     |
| 1   | C     | 468 | VAL  | CA-C  | -5.65 | 1.46        | 1.52     |
| 2   | F     | 8   | TYR  | CA-C  | -5.65 | 1.46        | 1.52     |
| 8   | N     | 54  | ARG  | CA-C  | -5.65 | 1.45        | 1.52     |
| 2   | D     | 171 | ALA  | CA-C  | -5.64 | 1.46        | 1.52     |
| 1   | A     | 89  | ARG  | CA-C  | -5.64 | 1.45        | 1.52     |
| 1   | C     | 46  | THR  | CA-C  | -5.64 | 1.45        | 1.52     |
| 1   | A     | 429 | SER  | CA-C  | -5.62 | 1.46        | 1.52     |
| 1   | B     | 252 | TYR  | CA-C  | -5.62 | 1.46        | 1.52     |
| 4   | H     | 85  | ASP  | CA-C  | -5.62 | 1.47        | 1.53     |
| 3   | G     | 184 | GLU  | CA-C  | -5.62 | 1.45        | 1.52     |
| 1   | B     | 480 | GLU  | CA-C  | -5.62 | 1.45        | 1.52     |
| 1   | B     | 50  | GLN  | CA-C  | -5.61 | 1.46        | 1.52     |
| 2   | E     | 318 | ASP  | CA-C  | -5.61 | 1.47        | 1.53     |
| 2   | E     | 304 | LYS  | CA-C  | -5.61 | 1.45        | 1.52     |
| 1   | A     | 16  | ALA  | CA-C  | -5.60 | 1.45        | 1.52     |
| 1   | C     | 553 | TYR  | N-CA  | -5.60 | 1.41        | 1.46     |
| 1   | A     | 24  | MET  | CA-C  | -5.60 | 1.45        | 1.52     |
| 1   | A     | 29  | LYS  | CA-C  | -5.60 | 1.46        | 1.52     |
| 2   | F     | 152 | ILE  | CA-C  | -5.60 | 1.45        | 1.52     |
| 1   | A     | 536 | ILE  | CA-C  | -5.59 | 1.45        | 1.52     |
| 2   | F     | 245 | LEU  | N-CA  | -5.58 | 1.40        | 1.46     |
| 1   | B     | 299 | ARG  | CA-C  | -5.58 | 1.45        | 1.52     |
| 1   | C     | 519 | ILE  | N-CA  | -5.58 | 1.39        | 1.46     |
| 2   | D     | 42  | VAL  | CA-C  | -5.58 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | D     | 450 | GLU  | CA-C  | -5.57 | 1.47        | 1.53     |
| 2   | E     | 27  | LEU  | CA-C  | -5.57 | 1.46        | 1.52     |
| 1   | A     | 273 | THR  | N-CA  | -5.56 | 1.40        | 1.46     |
| 2   | E     | 93  | PHE  | CA-C  | -5.56 | 1.45        | 1.52     |
| 2   | F     | 142 | ASN  | CA-C  | -5.56 | 1.45        | 1.52     |
| 1   | B     | 332 | GLU  | CA-C  | -5.55 | 1.45        | 1.52     |
| 1   | B     | 378 | VAL  | CA-C  | -5.55 | 1.46        | 1.52     |
| 2   | F     | 77  | GLU  | CA-C  | -5.55 | 1.45        | 1.52     |
| 2   | D     | 247 | PHE  | CA-C  | -5.55 | 1.45        | 1.52     |
| 1   | B     | 19  | MET  | CA-C  | -5.53 | 1.46        | 1.52     |
| 2   | D     | 152 | ILE  | CA-C  | -5.53 | 1.45        | 1.52     |
| 1   | B     | 466 | GLU  | CA-C  | -5.52 | 1.45        | 1.52     |
| 2   | E     | 349 | TYR  | N-CA  | -5.52 | 1.40        | 1.46     |
| 1   | B     | 10  | ALA  | CA-C  | -5.52 | 1.46        | 1.53     |
| 2   | D     | 278 | PRO  | CA-C  | -5.52 | 1.46        | 1.52     |
| 1   | A     | 3   | GLN  | CA-C  | -5.52 | 1.46        | 1.52     |
| 1   | A     | 116 | LYS  | CA-C  | -5.52 | 1.45        | 1.52     |
| 1   | B     | 330 | TRP  | CA-C  | -5.51 | 1.45        | 1.52     |
| 3   | G     | 184 | GLU  | N-CA  | -5.51 | 1.39        | 1.46     |
| 1   | B     | 305 | VAL  | CA-C  | -5.51 | 1.45        | 1.52     |
| 2   | D     | 325 | ILE  | N-CA  | -5.51 | 1.39        | 1.46     |
| 2   | D     | 34  | ASP  | CA-C  | -5.50 | 1.45        | 1.52     |
| 1   | A     | 237 | THR  | CA-C  | -5.50 | 1.45        | 1.52     |
| 1   | B     | 257 | GLU  | CA-C  | -5.50 | 1.46        | 1.52     |
| 1   | B     | 215 | LEU  | CA-C  | -5.50 | 1.45        | 1.53     |
| 2   | E     | 56  | VAL  | CA-C  | -5.50 | 1.46        | 1.52     |
| 2   | F     | 291 | LEU  | CA-C  | -5.49 | 1.45        | 1.52     |
| 2   | E     | 364 | ASN  | CA-C  | -5.49 | 1.45        | 1.53     |
| 8   | N     | 402 | VAL  | CA-C  | -5.49 | 1.46        | 1.52     |
| 1   | C     | 457 | LEU  | CA-C  | -5.48 | 1.45        | 1.52     |
| 2   | E     | 169 | ARG  | CA-C  | -5.48 | 1.45        | 1.52     |
| 1   | A     | 289 | ALA  | CA-C  | -5.46 | 1.46        | 1.52     |
| 2   | E     | 294 | ILE  | CA-C  | -5.46 | 1.46        | 1.52     |
| 1   | C     | 241 | LEU  | CA-C  | -5.45 | 1.45        | 1.52     |
| 1   | C     | 395 | VAL  | N-CA  | -5.45 | 1.39        | 1.46     |
| 1   | B     | 206 | LEU  | CA-C  | -5.44 | 1.46        | 1.52     |
| 3   | G     | 180 | GLN  | CA-C  | -5.43 | 1.45        | 1.52     |
| 1   | A     | 352 | PRO  | CA-C  | -5.43 | 1.44        | 1.52     |
| 7   | M     | 163 | ARG  | CA-C  | -5.43 | 1.45        | 1.52     |
| 1   | B     | 346 | ALA  | CA-C  | -5.42 | 1.45        | 1.52     |
| 8   | N     | 491 | HIS  | CA-C  | -5.41 | 1.45        | 1.52     |
| 1   | C     | 106 | VAL  | CA-C  | -5.41 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 24  | MET  | CA-C  | -5.41 | 1.45        | 1.52     |
| 1   | A     | 6   | ILE  | CA-C  | -5.40 | 1.46        | 1.52     |
| 2   | F     | 84  | VAL  | CA-C  | -5.40 | 1.45        | 1.52     |
| 2   | F     | 81  | ARG  | N-CA  | -5.39 | 1.39        | 1.46     |
| 1   | A     | 15  | ILE  | N-CA  | -5.39 | 1.40        | 1.46     |
| 1   | C     | 338 | SER  | CA-C  | -5.38 | 1.46        | 1.52     |
| 1   | C     | 444 | ALA  | CA-C  | -5.38 | 1.46        | 1.52     |
| 2   | F     | 219 | LEU  | N-CA  | -5.38 | 1.39        | 1.45     |
| 1   | C     | 478 | ASP  | CA-C  | -5.38 | 1.46        | 1.52     |
| 1   | C     | 10  | ALA  | CA-C  | -5.38 | 1.46        | 1.52     |
| 1   | C     | 477 | GLN  | CA-C  | -5.38 | 1.46        | 1.52     |
| 1   | B     | 320 | VAL  | CA-C  | -5.37 | 1.46        | 1.52     |
| 1   | B     | 287 | LEU  | CA-C  | -5.37 | 1.46        | 1.52     |
| 2   | E     | 253 | VAL  | CA-C  | -5.37 | 1.45        | 1.52     |
| 1   | B     | 447 | TYR  | CA-C  | -5.37 | 1.46        | 1.52     |
| 1   | A     | 90  | PRO  | CA-C  | -5.36 | 1.45        | 1.52     |
| 1   | A     | 384 | VAL  | CA-C  | -5.36 | 1.46        | 1.52     |
| 1   | B     | 362 | TYR  | CA-C  | -5.36 | 1.45        | 1.52     |
| 1   | C     | 20  | LEU  | CA-C  | -5.36 | 1.46        | 1.52     |
| 5   | K     | 88  | TYR  | CA-C  | -5.35 | 1.45        | 1.52     |
| 1   | A     | 496 | GLN  | CA-C  | -5.35 | 1.46        | 1.52     |
| 6   | L     | 70  | THR  | CA-C  | -5.35 | 1.46        | 1.52     |
| 1   | A     | 117 | TRP  | CA-C  | -5.35 | 1.46        | 1.52     |
| 2   | E     | 242 | ALA  | CA-C  | -5.34 | 1.46        | 1.52     |
| 2   | F     | 283 | TYR  | CA-C  | -5.34 | 1.46        | 1.52     |
| 2   | D     | 331 | TYR  | CA-C  | -5.34 | 1.46        | 1.52     |
| 1   | B     | 141 | PHE  | CA-C  | -5.34 | 1.47        | 1.53     |
| 1   | A     | 538 | GLU  | N-CA  | -5.33 | 1.40        | 1.46     |
| 2   | F     | 7   | GLU  | CA-C  | -5.33 | 1.46        | 1.52     |
| 1   | B     | 101 | TYR  | CA-C  | -5.33 | 1.46        | 1.53     |
| 2   | E     | 256 | ILE  | N-CA  | -5.32 | 1.39        | 1.46     |
| 2   | F     | 158 | LEU  | CA-C  | -5.32 | 1.47        | 1.52     |
| 2   | F     | 316 | MET  | CA-C  | -5.32 | 1.48        | 1.52     |
| 1   | A     | 304 | TYR  | CA-C  | -5.31 | 1.45        | 1.52     |
| 8   | N     | 544 | ILE  | CA-C  | -5.31 | 1.46        | 1.52     |
| 2   | E     | 6   | LYS  | CA-C  | -5.31 | 1.46        | 1.52     |
| 1   | B     | 159 | GLU  | CA-C  | -5.30 | 1.46        | 1.52     |
| 1   | C     | 214 | VAL  | CA-C  | -5.30 | 1.46        | 1.52     |
| 1   | B     | 336 | GLU  | CA-C  | -5.30 | 1.46        | 1.52     |
| 2   | E     | 208 | PHE  | CA-C  | -5.30 | 1.45        | 1.52     |
| 1   | C     | 407 | TRP  | CA-C  | -5.29 | 1.46        | 1.52     |
| 2   | D     | 35  | ILE  | CA-C  | -5.29 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | E     | 103 | LEU  | CA-C  | -5.29 | 1.47        | 1.52     |
| 1   | C     | 550 | ARG  | CA-C  | -5.29 | 1.46        | 1.53     |
| 3   | G     | 188 | ARG  | N-CA  | -5.29 | 1.40        | 1.46     |
| 1   | B     | 206 | LEU  | N-CA  | -5.28 | 1.39        | 1.45     |
| 1   | A     | 398 | SER  | CA-C  | -5.28 | 1.46        | 1.53     |
| 1   | C     | 492 | GLU  | CA-C  | -5.28 | 1.45        | 1.52     |
| 1   | C     | 328 | SER  | CA-C  | -5.28 | 1.45        | 1.52     |
| 2   | E     | 431 | SER  | CA-C  | -5.28 | 1.46        | 1.52     |
| 1   | B     | 519 | ILE  | N-CA  | -5.27 | 1.39        | 1.46     |
| 2   | F     | 394 | LYS  | CA-C  | -5.27 | 1.46        | 1.52     |
| 1   | A     | 14  | VAL  | CA-C  | -5.26 | 1.46        | 1.52     |
| 2   | F     | 131 | ILE  | N-CA  | -5.26 | 1.40        | 1.46     |
| 2   | F     | 254 | LEU  | N-CA  | -5.26 | 1.40        | 1.46     |
| 1   | A     | 240 | SER  | CA-C  | -5.26 | 1.45        | 1.52     |
| 1   | B     | 72  | ALA  | CA-C  | -5.26 | 1.46        | 1.52     |
| 1   | B     | 165 | GLU  | CA-C  | -5.26 | 1.46        | 1.52     |
| 1   | C     | 30  | VAL  | CA-C  | -5.26 | 1.46        | 1.52     |
| 2   | F     | 259 | ASP  | CA-C  | -5.26 | 1.45        | 1.52     |
| 1   | C     | 66  | SER  | CA-C  | -5.25 | 1.46        | 1.52     |
| 2   | D     | 132 | GLN  | CA-C  | -5.25 | 1.46        | 1.52     |
| 2   | E     | 242 | ALA  | N-CA  | -5.25 | 1.39        | 1.46     |
| 1   | B     | 254 | GLY  | CA-C  | -5.25 | 1.48        | 1.52     |
| 1   | B     | 458 | LEU  | CA-C  | -5.25 | 1.45        | 1.52     |
| 1   | B     | 491 | ARG  | N-CA  | -5.25 | 1.39        | 1.46     |
| 2   | D     | 198 | GLN  | CA-C  | -5.24 | 1.45        | 1.52     |
| 1   | B     | 158 | LYS  | CA-C  | -5.24 | 1.46        | 1.53     |
| 1   | A     | 244 | TRP  | CA-C  | -5.24 | 1.46        | 1.52     |
| 1   | C     | 120 | THR  | CA-C  | -5.24 | 1.48        | 1.52     |
| 2   | E     | 232 | ILE  | N-CA  | -5.24 | 1.40        | 1.46     |
| 2   | E     | 136 | SER  | CA-C  | -5.23 | 1.46        | 1.52     |
| 4   | H     | 34  | GLU  | CA-C  | -5.23 | 1.46        | 1.52     |
| 7   | M     | 168 | LEU  | CA-C  | -5.23 | 1.46        | 1.52     |
| 1   | B     | 17  | LYS  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | B     | 20  | LEU  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | B     | 518 | MET  | CA-C  | -5.22 | 1.46        | 1.52     |
| 2   | E     | 219 | LEU  | N-CA  | -5.22 | 1.40        | 1.46     |
| 1   | C     | 273 | THR  | CA-C  | -5.22 | 1.46        | 1.52     |
| 2   | E     | 257 | LEU  | CA-C  | -5.22 | 1.46        | 1.52     |
| 2   | F     | 258 | THR  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | B     | 209 | MET  | CA-C  | -5.21 | 1.45        | 1.52     |
| 2   | E     | 190 | VAL  | CA-C  | -5.21 | 1.46        | 1.52     |
| 1   | C     | 337 | ILE  | CA-C  | -5.21 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 212 | LEU  | CA-C  | -5.21 | 1.46        | 1.52     |
| 2   | F     | 89  | LEU  | CA-C  | -5.20 | 1.45        | 1.52     |
| 1   | B     | 282 | MET  | CA-C  | -5.19 | 1.45        | 1.52     |
| 1   | C     | 470 | LEU  | CA-C  | -5.19 | 1.45        | 1.52     |
| 1   | C     | 354 | LEU  | CA-C  | -5.18 | 1.45        | 1.52     |
| 2   | D     | 153 | PHE  | CA-C  | -5.18 | 1.46        | 1.52     |
| 1   | A     | 396 | THR  | CA-C  | -5.16 | 1.45        | 1.52     |
| 1   | B     | 166 | TYR  | CA-C  | -5.16 | 1.46        | 1.52     |
| 2   | D     | 309 | THR  | CA-C  | -5.16 | 1.46        | 1.52     |
| 2   | E     | 388 | ASN  | CA-C  | -5.15 | 1.45        | 1.52     |
| 1   | A     | 83  | ILE  | CA-C  | -5.15 | 1.46        | 1.52     |
| 2   | E     | 310 | GLN  | CA-C  | -5.15 | 1.46        | 1.52     |
| 1   | C     | 213 | ASP  | CA-C  | -5.15 | 1.47        | 1.53     |
| 1   | A     | 141 | PHE  | CA-C  | -5.15 | 1.46        | 1.52     |
| 2   | D     | 199 | ARG  | N-CA  | -5.13 | 1.40        | 1.46     |
| 2   | F     | 252 | HIS  | CA-C  | -5.13 | 1.46        | 1.52     |
| 2   | E     | 316 | MET  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | A     | 53  | GLU  | CA-C  | -5.13 | 1.46        | 1.52     |
| 2   | F     | 218 | VAL  | CA-C  | -5.13 | 1.46        | 1.52     |
| 4   | H     | 87  | GLU  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | A     | 111 | LEU  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | B     | 331 | ALA  | CA-C  | -5.13 | 1.45        | 1.52     |
| 1   | C     | 180 | GLU  | CA-C  | -5.13 | 1.46        | 1.52     |
| 2   | F     | 248 | GLU  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | C     | 143 | PHE  | CA-C  | -5.12 | 1.46        | 1.52     |
| 1   | C     | 397 | GLN  | CA-C  | -5.12 | 1.46        | 1.52     |
| 2   | D     | 131 | ILE  | N-CA  | -5.12 | 1.40        | 1.46     |
| 2   | F     | 419 | GLU  | N-CA  | -5.12 | 1.40        | 1.46     |
| 1   | A     | 265 | VAL  | CA-C  | -5.12 | 1.46        | 1.52     |
| 2   | F     | 220 | PHE  | N-CA  | -5.12 | 1.39        | 1.46     |
| 1   | B     | 80  | LEU  | CA-C  | -5.12 | 1.46        | 1.52     |
| 8   | N     | 620 | PRO  | CA-C  | -5.12 | 1.44        | 1.52     |
| 2   | F     | 18  | LEU  | N-CA  | -5.11 | 1.39        | 1.45     |
| 1   | C     | 313 | PHE  | CA-C  | -5.11 | 1.45        | 1.52     |
| 1   | A     | 323 | MET  | CA-C  | -5.11 | 1.46        | 1.53     |
| 1   | C     | 211 | ILE  | N-CA  | -5.11 | 1.40        | 1.46     |
| 1   | A     | 95  | ARG  | CA-C  | -5.11 | 1.46        | 1.52     |
| 1   | B     | 14  | VAL  | CA-C  | -5.11 | 1.46        | 1.52     |
| 2   | E     | 425 | GLN  | CA-C  | -5.11 | 1.46        | 1.52     |
| 1   | A     | 418 | HIS  | CA-C  | -5.10 | 1.46        | 1.52     |
| 2   | D     | 251 | TYR  | CA-C  | -5.10 | 1.46        | 1.52     |
| 2   | F     | 418 | PHE  | CA-C  | -5.10 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 301 | ALA  | N-CA  | -5.09 | 1.40        | 1.46     |
| 1   | A     | 47  | ALA  | CA-C  | -5.09 | 1.46        | 1.52     |
| 1   | A     | 322 | LEU  | CA-C  | -5.09 | 1.46        | 1.52     |
| 1   | A     | 520 | LEU  | CA-C  | -5.09 | 1.46        | 1.52     |
| 2   | D     | 72  | SER  | CA-C  | -5.09 | 1.46        | 1.52     |
| 8   | N     | 263 | LEU  | CA-C  | -5.08 | 1.46        | 1.52     |
| 2   | D     | 250 | ASP  | CA-C  | -5.07 | 1.46        | 1.53     |
| 2   | D     | 254 | LEU  | N-CA  | -5.07 | 1.39        | 1.46     |
| 1   | B     | 356 | ALA  | N-CA  | -5.07 | 1.40        | 1.46     |
| 1   | A     | 84  | TYR  | CA-C  | -5.07 | 1.46        | 1.52     |
| 2   | D     | 333 | THR  | CA-C  | -5.06 | 1.46        | 1.53     |
| 2   | F     | 275 | GLU  | CA-C  | -5.06 | 1.46        | 1.52     |
| 1   | B     | 418 | HIS  | CA-C  | -5.06 | 1.46        | 1.52     |
| 2   | E     | 398 | ILE  | N-CA  | -5.05 | 1.40        | 1.46     |
| 7   | M     | 294 | GLU  | CA-C  | -5.05 | 1.46        | 1.52     |
| 1   | B     | 102 | ILE  | N-CA  | -5.05 | 1.40        | 1.46     |
| 1   | C     | 47  | ALA  | CA-C  | -5.05 | 1.46        | 1.52     |
| 2   | D     | 13  | TYR  | CA-C  | -5.05 | 1.46        | 1.52     |
| 2   | E     | 43  | ARG  | CA-C  | -5.05 | 1.46        | 1.52     |
| 2   | D     | 219 | LEU  | CA-C  | -5.04 | 1.46        | 1.52     |
| 2   | D     | 310 | GLN  | CA-C  | -5.04 | 1.46        | 1.52     |
| 2   | E     | 258 | THR  | CA-C  | -5.04 | 1.46        | 1.53     |
| 2   | F     | 70  | THR  | CA-C  | -5.04 | 1.46        | 1.52     |
| 2   | D     | 229 | ILE  | N-CA  | -5.04 | 1.40        | 1.46     |
| 8   | N     | 65  | HIS  | CA-C  | -5.04 | 1.46        | 1.52     |
| 1   | A     | 22  | ALA  | CA-C  | -5.04 | 1.49        | 1.52     |
| 3   | G     | 67  | ALA  | CA-C  | -5.04 | 1.46        | 1.52     |
| 2   | F     | 78  | ASP  | N-CA  | -5.03 | 1.40        | 1.46     |
| 1   | A     | 5   | VAL  | CA-C  | -5.03 | 1.46        | 1.52     |
| 1   | C     | 318 | PHE  | CA-C  | -5.03 | 1.46        | 1.52     |
| 1   | C     | 423 | ASN  | CA-C  | -5.02 | 1.46        | 1.52     |
| 3   | G     | 4   | VAL  | N-CA  | -5.02 | 1.40        | 1.46     |
| 4   | H     | 35  | THR  | CA-C  | -5.02 | 1.46        | 1.52     |
| 6   | J     | 187 | TRP  | CA-C  | -5.02 | 1.46        | 1.53     |
| 1   | B     | 204 | PRO  | CA-C  | -5.02 | 1.46        | 1.52     |
| 2   | D     | 88  | MET  | N-CA  | -5.02 | 1.41        | 1.46     |
| 1   | B     | 292 | SER  | N-CA  | -5.01 | 1.39        | 1.46     |
| 2   | E     | 138 | ILE  | N-CA  | -5.01 | 1.40        | 1.46     |
| 3   | G     | 191 | THR  | CA-C  | -5.01 | 1.46        | 1.52     |
| 1   | C     | 273 | THR  | N-CA  | -5.01 | 1.39        | 1.46     |
| 1   | C     | 413 | LEU  | CA-C  | -5.00 | 1.46        | 1.52     |

All (1172) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 84  | TYR  | N-CA-C | -13.56 | 99.17       | 114.62   |
| 1   | B     | 185 | HIS  | CA-C-N | 12.57  | 141.27      | 121.66   |
| 1   | B     | 185 | HIS  | C-N-CA | 12.57  | 141.27      | 121.66   |
| 6   | J     | 53  | TYR  | N-CA-C | -12.37 | 95.54       | 112.12   |
| 2   | D     | 408 | ASP  | N-CA-C | -11.51 | 98.92       | 113.43   |
| 1   | C     | 517 | LYS  | N-CA-C | -11.40 | 99.86       | 113.88   |
| 2   | D     | 208 | PHE  | N-CA-C | -11.09 | 97.93       | 112.68   |
| 1   | A     | 410 | ASP  | CA-C-N | 11.00  | 135.02      | 120.28   |
| 1   | A     | 410 | ASP  | C-N-CA | 11.00  | 135.02      | 120.28   |
| 2   | E     | 292 | ALA  | N-CA-C | -10.96 | 98.10       | 112.68   |
| 9   | O     | 40  | ALA  | CA-C-N | 10.93  | 132.11      | 119.98   |
| 9   | O     | 40  | ALA  | C-N-CA | 10.93  | 132.11      | 119.98   |
| 1   | A     | 263 | THR  | N-CA-C | -10.88 | 100.54      | 114.04   |
| 6   | L     | 53  | TYR  | N-CA-C | -10.84 | 97.60       | 112.12   |
| 2   | F     | 273 | ALA  | N-CA-C | -10.67 | 98.49       | 112.68   |
| 9   | W     | 40  | ALA  | CA-C-N | 10.29  | 131.40      | 119.98   |
| 9   | W     | 40  | ALA  | C-N-CA | 10.29  | 131.40      | 119.98   |
| 2   | F     | 77  | GLU  | CA-C-N | 10.28  | 134.41      | 120.54   |
| 2   | F     | 77  | GLU  | C-N-CA | 10.28  | 134.41      | 120.54   |
| 3   | G     | 208 | GLU  | N-CA-C | -10.12 | 103.09      | 114.62   |
| 1   | B     | 553 | TYR  | N-CA-C | -10.08 | 103.13      | 114.62   |
| 1   | B     | 442 | ASN  | N-CA-C | -9.99  | 98.44       | 112.13   |
| 1   | A     | 67  | THR  | N-CA-C | -9.83  | 103.41      | 114.62   |
| 1   | A     | 461 | GLU  | N-CA-C | -9.81  | 99.88       | 112.93   |
| 2   | F     | 139 | ASP  | N-CA-C | -9.78  | 102.42      | 114.75   |
| 2   | E     | 272 | ALA  | N-CA-C | -9.65  | 101.27      | 113.43   |
| 3   | G     | 9   | MET  | CA-C-N | 9.46   | 134.69      | 120.31   |
| 3   | G     | 9   | MET  | C-N-CA | 9.46   | 134.69      | 120.31   |
| 9   | V     | 58  | PHE  | N-CA-C | 9.45   | 121.18      | 111.07   |
| 8   | N     | 326 | TRP  | N-CA-C | -9.44  | 101.32      | 113.12   |
| 1   | A     | 538 | GLU  | N-CA-C | -9.42  | 99.50       | 112.12   |
| 1   | B     | 563 | PHE  | CA-C-N | 9.40   | 133.64      | 120.29   |
| 1   | B     | 563 | PHE  | C-N-CA | 9.40   | 133.64      | 120.29   |
| 1   | C     | 483 | VAL  | N-CA-C | -9.39  | 101.70      | 110.53   |
| 2   | F     | 335 | GLY  | N-CA-C | -9.31  | 98.00       | 110.58   |
| 9   | X     | 60  | LEU  | N-CA-C | 9.16   | 121.26      | 111.28   |
| 2   | F     | 76  | VAL  | N-CA-C | -9.15  | 102.41      | 110.74   |
| 1   | A     | 430 | LEU  | CA-C-N | 9.11   | 132.84      | 120.54   |
| 1   | A     | 430 | LEU  | C-N-CA | 9.11   | 132.84      | 120.54   |
| 1   | B     | 398 | SER  | N-CA-C | -9.10  | 101.95      | 113.23   |
| 2   | F     | 412 | LEU  | N-CA-C | -8.98  | 97.82       | 111.56   |
| 3   | G     | 105 | LYS  | N-CA-C | -8.92  | 94.34       | 109.24   |
| 1   | B     | 528 | ALA  | N-CA-C | -8.90  | 102.33      | 113.55   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | Q     | 58  | PHE  | N-CA-C | 8.81  | 120.89      | 111.28   |
| 6   | J     | 132 | GLU  | N-CA-C | -8.77 | 103.00      | 114.31   |
| 1   | A     | 355 | ALA  | N-CA-C | -8.76 | 102.73      | 112.72   |
| 1   | B     | 424 | TRP  | CA-C-N | 8.74  | 131.99      | 120.28   |
| 1   | B     | 424 | TRP  | C-N-CA | 8.74  | 131.99      | 120.28   |
| 1   | B     | 210 | ARG  | CA-C-N | 8.71  | 131.53      | 120.56   |
| 1   | B     | 210 | ARG  | C-N-CA | 8.71  | 131.53      | 120.56   |
| 9   | P     | 60  | LEU  | CA-C-N | 8.70  | 130.96      | 120.09   |
| 9   | P     | 60  | LEU  | C-N-CA | 8.70  | 130.96      | 120.09   |
| 2   | E     | 161 | ASN  | N-CA-C | -8.64 | 99.60       | 112.04   |
| 2   | D     | 161 | ASN  | CA-C-N | 8.64  | 132.20      | 120.54   |
| 2   | D     | 161 | ASN  | C-N-CA | 8.64  | 132.20      | 120.54   |
| 2   | D     | 416 | ASP  | N-CA-C | -8.62 | 100.88      | 111.40   |
| 6   | J     | 175 | TRP  | CA-C-N | 8.60  | 133.38      | 120.31   |
| 6   | J     | 175 | TRP  | C-N-CA | 8.60  | 133.38      | 120.31   |
| 9   | S     | 37  | ILE  | CA-C-N | 8.56  | 129.49      | 119.98   |
| 9   | S     | 37  | ILE  | C-N-CA | 8.56  | 129.49      | 119.98   |
| 9   | P     | 59  | LEU  | CA-C-N | 8.53  | 132.06      | 120.38   |
| 9   | P     | 59  | LEU  | C-N-CA | 8.53  | 132.06      | 120.38   |
| 2   | F     | 73  | VAL  | CA-C-N | 8.48  | 133.69      | 122.42   |
| 2   | F     | 73  | VAL  | C-N-CA | 8.48  | 133.69      | 122.42   |
| 2   | E     | 255 | VAL  | N-CA-C | -8.37 | 96.42       | 108.48   |
| 8   | N     | 381 | GLY  | N-CA-C | -8.35 | 101.14      | 112.57   |
| 1   | A     | 465 | GLN  | CA-C-N | 8.34  | 137.46      | 121.54   |
| 1   | A     | 465 | GLN  | C-N-CA | 8.34  | 137.46      | 121.54   |
| 2   | F     | 142 | ASN  | N-CA-C | -8.28 | 95.99       | 108.99   |
| 1   | B     | 454 | ILE  | N-CA-C | -8.27 | 104.70      | 111.81   |
| 2   | F     | 450 | GLU  | N-CA-C | -8.25 | 103.66      | 114.31   |
| 2   | E     | 242 | ALA  | N-CA-C | -8.24 | 101.72      | 112.68   |
| 9   | P     | 58  | PHE  | N-CA-C | 8.21  | 119.86      | 111.07   |
| 9   | T     | 40  | ALA  | CA-C-N | 8.19  | 129.07      | 119.98   |
| 9   | T     | 40  | ALA  | C-N-CA | 8.19  | 129.07      | 119.98   |
| 2   | E     | 21  | VAL  | N-CA-C | -8.18 | 96.59       | 107.88   |
| 1   | C     | 237 | THR  | CA-C-N | -8.11 | 109.92      | 122.49   |
| 1   | C     | 237 | THR  | C-N-CA | -8.11 | 109.92      | 122.49   |
| 2   | E     | 292 | ALA  | CA-C-N | 8.09  | 132.19      | 120.38   |
| 2   | E     | 292 | ALA  | C-N-CA | 8.09  | 132.19      | 120.38   |
| 1   | C     | 54  | ASP  | CA-C-N | 8.08  | 132.96      | 120.75   |
| 1   | C     | 54  | ASP  | C-N-CA | 8.08  | 132.96      | 120.75   |
| 2   | E     | 232 | ILE  | N-CA-C | -8.07 | 103.98      | 113.42   |
| 2   | E     | 399 | ILE  | N-CA-C | 8.07  | 118.11      | 110.53   |
| 2   | F     | 21  | VAL  | N-CA-C | -8.05 | 97.72       | 108.35   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 2   | ILE  | N-CA-C | -8.05 | 96.85       | 108.36   |
| 2   | F     | 401 | GLU  | N-CA-C | -8.04 | 100.94      | 111.71   |
| 9   | R     | 59  | LEU  | CA-C-N | 8.03  | 131.04      | 120.28   |
| 9   | R     | 59  | LEU  | C-N-CA | 8.03  | 131.04      | 120.28   |
| 4   | H     | 7   | PRO  | CA-C-N | 8.01  | 131.81      | 120.28   |
| 4   | H     | 7   | PRO  | C-N-CA | 8.01  | 131.81      | 120.28   |
| 1   | C     | 263 | THR  | CA-C-N | 8.00  | 130.84      | 120.44   |
| 1   | C     | 263 | THR  | C-N-CA | 8.00  | 130.84      | 120.44   |
| 2   | E     | 407 | ASN  | N-CA-C | -7.97 | 101.68      | 111.40   |
| 7   | M     | 316 | VAL  | N-CA-C | -7.96 | 106.15      | 113.71   |
| 9   | Y     | 51  | ASN  | CA-C-N | 7.93  | 131.25      | 120.38   |
| 9   | Y     | 51  | ASN  | C-N-CA | 7.93  | 131.25      | 120.38   |
| 1   | C     | 449 | GLU  | N-CA-C | -7.91 | 101.96      | 111.69   |
| 9   | S     | 66  | VAL  | CA-C-N | 7.91  | 131.29      | 120.46   |
| 9   | S     | 66  | VAL  | C-N-CA | 7.91  | 131.29      | 120.46   |
| 9   | X     | 59  | LEU  | CA-C-N | 7.83  | 130.78      | 120.28   |
| 9   | X     | 59  | LEU  | C-N-CA | 7.83  | 130.78      | 120.28   |
| 9   | W     | 57  | ILE  | N-CA-C | 7.77  | 118.57      | 110.72   |
| 2   | D     | 122 | VAL  | N-CA-C | -7.77 | 105.44      | 112.90   |
| 1   | C     | 551 | ALA  | N-CA-C | -7.74 | 104.99      | 114.75   |
| 9   | P     | 52  | PHE  | N-CA-C | 7.74  | 119.72      | 111.28   |
| 7   | M     | 316 | VAL  | CA-C-N | 7.73  | 130.64      | 120.28   |
| 7   | M     | 316 | VAL  | C-N-CA | 7.73  | 130.64      | 120.28   |
| 1   | B     | 150 | PRO  | N-CA-C | -7.73 | 101.27      | 110.70   |
| 9   | O     | 48  | ASP  | N-CA-C | -7.71 | 97.56       | 109.52   |
| 9   | V     | 59  | LEU  | CA-C-N | 7.70  | 130.59      | 120.28   |
| 9   | V     | 59  | LEU  | C-N-CA | 7.70  | 130.59      | 120.28   |
| 2   | F     | 331 | TYR  | N-CA-C | -7.69 | 104.51      | 114.04   |
| 2   | F     | 202 | SER  | N-CA-C | -7.67 | 104.06      | 113.50   |
| 2   | D     | 410 | ARG  | N-CA-C | -7.65 | 103.55      | 113.12   |
| 2   | F     | 138 | ILE  | N-CA-C | -7.65 | 105.10      | 111.91   |
| 2   | D     | 451 | LEU  | N-CA-C | -7.60 | 95.64       | 108.26   |
| 2   | F     | 264 | CYS  | N-CA-C | -7.58 | 103.64      | 113.12   |
| 3   | G     | 27  | LEU  | N-CA-C | -7.54 | 103.02      | 112.90   |
| 2   | F     | 418 | PHE  | N-CA-C | -7.54 | 101.97      | 112.45   |
| 1   | B     | 239 | GLN  | N-CA-C | -7.53 | 104.24      | 113.50   |
| 9   | P     | 54  | THR  | CA-C-N | 7.53  | 130.36      | 120.28   |
| 9   | P     | 54  | THR  | C-N-CA | 7.53  | 130.36      | 120.28   |
| 6   | L     | 173 | ARG  | CA-C-N | 7.51  | 130.35      | 120.28   |
| 6   | L     | 173 | ARG  | C-N-CA | 7.51  | 130.35      | 120.28   |
| 1   | B     | 309 | ILE  | N-CA-C | -7.51 | 102.81      | 111.00   |
| 1   | A     | 576 | ALA  | N-CA-C | -7.49 | 103.45      | 112.59   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 294 | ILE  | N-CA-C | -7.48 | 103.93      | 110.74   |
| 2   | D     | 370 | LYS  | N-CA-C | -7.47 | 105.33      | 114.75   |
| 3   | G     | 189 | GLU  | CA-C-N | 7.46  | 131.15      | 120.79   |
| 3   | G     | 189 | GLU  | C-N-CA | 7.46  | 131.15      | 120.79   |
| 8   | N     | 535 | PHE  | CA-C-N | 7.45  | 130.12      | 120.44   |
| 8   | N     | 535 | PHE  | C-N-CA | 7.45  | 130.12      | 120.44   |
| 1   | C     | 319 | SER  | CA-C-N | 7.43  | 131.54      | 120.69   |
| 1   | C     | 319 | SER  | C-N-CA | 7.43  | 131.54      | 120.69   |
| 1   | B     | 351 | PRO  | N-CA-C | -7.42 | 101.64      | 110.70   |
| 2   | F     | 260 | MET  | CA-C-N | 7.42  | 135.72      | 121.54   |
| 2   | F     | 260 | MET  | C-N-CA | 7.42  | 135.72      | 121.54   |
| 9   | W     | 49  | ARG  | CA-C-N | 7.42  | 130.96      | 120.28   |
| 9   | W     | 49  | ARG  | C-N-CA | 7.42  | 130.96      | 120.28   |
| 2   | D     | 375 | HIS  | CA-C-N | 7.41  | 130.53      | 120.38   |
| 2   | D     | 375 | HIS  | C-N-CA | 7.41  | 130.53      | 120.38   |
| 1   | C     | 425 | ASN  | N-CA-C | -7.40 | 104.29      | 112.72   |
| 1   | C     | 176 | GLU  | CA-C-N | 7.39  | 130.04      | 120.44   |
| 1   | C     | 176 | GLU  | C-N-CA | 7.39  | 130.04      | 120.44   |
| 9   | X     | 10  | LEU  | CA-C-N | 7.39  | 130.18      | 120.28   |
| 9   | X     | 10  | LEU  | C-N-CA | 7.39  | 130.18      | 120.28   |
| 3   | G     | 190 | ASP  | CA-C-N | 7.38  | 130.04      | 120.44   |
| 3   | G     | 190 | ASP  | C-N-CA | 7.38  | 130.04      | 120.44   |
| 6   | L     | 173 | ARG  | N-CA-C | -7.38 | 101.73      | 111.24   |
| 8   | N     | 84  | LEU  | CA-C-N | 7.38  | 130.16      | 120.28   |
| 8   | N     | 84  | LEU  | C-N-CA | 7.38  | 130.16      | 120.28   |
| 6   | L     | 132 | GLU  | N-CA-C | -7.37 | 104.90      | 114.04   |
| 3   | G     | 161 | VAL  | CA-C-N | 7.37  | 131.03      | 120.79   |
| 3   | G     | 161 | VAL  | C-N-CA | 7.37  | 131.03      | 120.79   |
| 1   | A     | 5   | VAL  | N-CA-C | -7.37 | 97.51       | 108.12   |
| 9   | Y     | 60  | LEU  | N-CA-C | 7.36  | 119.31      | 111.28   |
| 1   | B     | 393 | GLU  | CA-C-N | 7.36  | 126.99      | 119.19   |
| 1   | B     | 393 | GLU  | C-N-CA | 7.36  | 126.99      | 119.19   |
| 1   | C     | 399 | THR  | N-CA-C | -7.36 | 104.55      | 113.97   |
| 1   | A     | 350 | TYR  | CA-C-N | -7.36 | 112.80      | 120.38   |
| 1   | A     | 350 | TYR  | C-N-CA | -7.36 | 112.80      | 120.38   |
| 9   | S     | 42  | VAL  | CA-C-N | 7.35  | 129.33      | 120.14   |
| 9   | S     | 42  | VAL  | C-N-CA | 7.35  | 129.33      | 120.14   |
| 6   | L     | 46  | GLU  | CA-C-N | 7.35  | 131.00      | 120.79   |
| 6   | L     | 46  | GLU  | C-N-CA | 7.35  | 131.00      | 120.79   |
| 2   | D     | 401 | GLU  | N-CA-C | -7.33 | 101.64      | 110.44   |
| 9   | R     | 9   | GLY  | CA-C-N | 7.33  | 130.84      | 120.28   |
| 9   | R     | 9   | GLY  | C-N-CA | 7.33  | 130.84      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 72  | ALA  | N-CA-C | -7.32 | 95.13       | 107.80   |
| 9   | U     | 68  | PHE  | CA-C-N | 7.32  | 128.10      | 119.98   |
| 9   | U     | 68  | PHE  | C-N-CA | 7.32  | 128.10      | 119.98   |
| 2   | E     | 245 | LEU  | N-CA-C | -7.31 | 104.17      | 113.23   |
| 9   | X     | 42  | VAL  | N-CA-C | 7.30  | 118.06      | 110.62   |
| 1   | C     | 122 | MET  | N-CA-C | -7.29 | 101.55      | 110.88   |
| 3   | G     | 121 | ALA  | CA-C-N | 7.28  | 130.04      | 120.28   |
| 3   | G     | 121 | ALA  | C-N-CA | 7.28  | 130.04      | 120.28   |
| 1   | B     | 76  | GLY  | CA-C-N | 7.28  | 128.94      | 119.84   |
| 1   | B     | 76  | GLY  | C-N-CA | 7.28  | 128.94      | 119.84   |
| 1   | C     | 293 | ASN  | N-CA-C | -7.28 | 103.83      | 114.39   |
| 8   | N     | 400 | PRO  | CA-C-N | 7.27  | 130.03      | 120.28   |
| 8   | N     | 400 | PRO  | C-N-CA | 7.27  | 130.03      | 120.28   |
| 3   | G     | 4   | VAL  | N-CA-C | -7.27 | 94.23       | 109.34   |
| 1   | A     | 500 | TYR  | N-CA-C | -7.26 | 103.57      | 113.30   |
| 2   | E     | 325 | ILE  | CA-C-N | 7.25  | 126.96      | 119.56   |
| 2   | E     | 325 | ILE  | C-N-CA | 7.25  | 126.96      | 119.56   |
| 2   | E     | 455 | SER  | CA-C-N | 7.25  | 130.31      | 120.38   |
| 2   | E     | 455 | SER  | C-N-CA | 7.25  | 130.31      | 120.38   |
| 9   | Q     | 18  | GLY  | CA-C-N | 7.25  | 129.99      | 120.28   |
| 9   | Q     | 18  | GLY  | C-N-CA | 7.25  | 129.99      | 120.28   |
| 2   | E     | 401 | GLU  | N-CA-C | -7.24 | 102.38      | 112.45   |
| 1   | B     | 177 | ASP  | N-CA-C | -7.24 | 104.70      | 113.97   |
| 1   | A     | 525 | GLU  | N-CA-C | -7.23 | 104.71      | 113.97   |
| 1   | B     | 441 | GLU  | N-CA-C | -7.22 | 104.09      | 113.12   |
| 9   | U     | 40  | ALA  | CA-C-N | 7.19  | 128.08      | 120.03   |
| 9   | U     | 40  | ALA  | C-N-CA | 7.19  | 128.08      | 120.03   |
| 1   | A     | 48  | PHE  | N-CA-C | -7.17 | 97.91       | 109.96   |
| 2   | F     | 166 | GLN  | N-CA-C | -7.17 | 103.15      | 110.97   |
| 1   | C     | 381 | VAL  | CA-C-N | 7.17  | 129.17      | 120.92   |
| 1   | C     | 381 | VAL  | C-N-CA | 7.17  | 129.17      | 120.92   |
| 1   | B     | 205 | PHE  | N-CA-C | -7.16 | 96.73       | 108.41   |
| 5   | K     | 107 | LEU  | CA-C-N | 7.15  | 130.19      | 120.54   |
| 5   | K     | 107 | LEU  | C-N-CA | 7.15  | 130.19      | 120.54   |
| 2   | F     | 286 | TYR  | CA-C-N | 7.15  | 130.16      | 120.44   |
| 2   | F     | 286 | TYR  | C-N-CA | 7.15  | 130.16      | 120.44   |
| 1   | C     | 341 | LEU  | N-CA-C | -7.14 | 104.18      | 113.17   |
| 1   | B     | 232 | SER  | CA-C-N | 7.13  | 135.39      | 121.41   |
| 1   | B     | 232 | SER  | C-N-CA | 7.13  | 135.39      | 121.41   |
| 5   | I     | 23  | ILE  | CA-C-N | 7.13  | 131.51      | 120.82   |
| 5   | I     | 23  | ILE  | C-N-CA | 7.13  | 131.51      | 120.82   |
| 2   | D     | 87  | GLU  | N-CA-C | -7.12 | 101.11      | 111.30   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | D     | 136 | SER  | CA-C-N | 7.12  | 135.14      | 121.54   |
| 2   | D     | 136 | SER  | C-N-CA | 7.12  | 135.14      | 121.54   |
| 9   | Q     | 37  | ILE  | CA-C-N | 7.09  | 127.86      | 119.98   |
| 9   | Q     | 37  | ILE  | C-N-CA | 7.09  | 127.86      | 119.98   |
| 1   | A     | 458 | LEU  | CA-C-N | 7.04  | 130.04      | 120.54   |
| 1   | A     | 458 | LEU  | C-N-CA | 7.04  | 130.04      | 120.54   |
| 8   | N     | 546 | LEU  | N-CA-C | -7.02 | 104.68      | 113.18   |
| 6   | L     | 79  | VAL  | N-CA-C | -7.01 | 104.02      | 110.82   |
| 2   | F     | 287 | MET  | N-CA-C | -7.00 | 103.58      | 111.14   |
| 1   | C     | 511 | LYS  | N-CA-C | -6.99 | 102.87      | 111.40   |
| 8   | N     | 248 | THR  | CA-C-N | 6.99  | 129.65      | 120.28   |
| 8   | N     | 248 | THR  | C-N-CA | 6.99  | 129.65      | 120.28   |
| 1   | C     | 446 | ASP  | N-CA-C | -6.99 | 103.08      | 112.94   |
| 9   | R     | 79  | ARG  | N-CA-C | -6.99 | 103.26      | 114.09   |
| 1   | B     | 224 | ALA  | N-CA-C | -6.98 | 97.73       | 108.76   |
| 2   | E     | 414 | PHE  | N-CA-C | -6.97 | 104.91      | 113.41   |
| 1   | B     | 486 | VAL  | CA-C-N | 6.96  | 127.82      | 120.03   |
| 1   | B     | 486 | VAL  | C-N-CA | 6.96  | 127.82      | 120.03   |
| 9   | R     | 37  | ILE  | CA-C-N | 6.96  | 127.70      | 119.98   |
| 9   | R     | 37  | ILE  | C-N-CA | 6.96  | 127.70      | 119.98   |
| 9   | U     | 59  | LEU  | CA-C-N | 6.95  | 129.59      | 120.28   |
| 9   | U     | 59  | LEU  | C-N-CA | 6.95  | 129.59      | 120.28   |
| 8   | N     | 324 | PRO  | CA-C-N | 6.94  | 127.52      | 119.47   |
| 8   | N     | 324 | PRO  | C-N-CA | 6.94  | 127.52      | 119.47   |
| 3   | G     | 10  | ASN  | N-CA-C | -6.93 | 103.78      | 111.82   |
| 2   | F     | 283 | TYR  | CA-C-N | 6.93  | 128.50      | 119.84   |
| 2   | F     | 283 | TYR  | C-N-CA | 6.93  | 128.50      | 119.84   |
| 1   | B     | 143 | PHE  | CA-C-N | 6.93  | 134.77      | 121.54   |
| 1   | B     | 143 | PHE  | C-N-CA | 6.93  | 134.77      | 121.54   |
| 8   | N     | 601 | ALA  | CA-C-N | 6.91  | 127.64      | 119.98   |
| 8   | N     | 601 | ALA  | C-N-CA | 6.91  | 127.64      | 119.98   |
| 2   | D     | 68  | LEU  | N-CA-C | -6.90 | 103.39      | 114.09   |
| 4   | H     | 98  | ILE  | CA-C-N | 6.90  | 126.66      | 120.10   |
| 4   | H     | 98  | ILE  | C-N-CA | 6.90  | 126.66      | 120.10   |
| 2   | F     | 220 | PHE  | N-CA-C | -6.89 | 96.12       | 110.80   |
| 1   | C     | 492 | GLU  | N-CA-C | -6.89 | 103.22      | 111.69   |
| 9   | T     | 59  | LEU  | N-CA-C | 6.88  | 118.78      | 111.28   |
| 9   | P     | 40  | ALA  | CA-C-N | 6.88  | 127.62      | 119.98   |
| 9   | P     | 40  | ALA  | C-N-CA | 6.88  | 127.62      | 119.98   |
| 2   | E     | 256 | ILE  | N-CA-C | -6.87 | 95.04       | 109.34   |
| 2   | E     | 369 | GLY  | CA-C-N | 6.87  | 129.80      | 120.38   |
| 2   | E     | 369 | GLY  | C-N-CA | 6.87  | 129.80      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 442 | LEU  | N-CA-C | -6.87 | 105.03      | 113.41   |
| 5   | K     | 22  | LEU  | CA-C-N | 6.86  | 134.32      | 121.97   |
| 5   | K     | 22  | LEU  | C-N-CA | 6.86  | 134.32      | 121.97   |
| 9   | T     | 74  | PHE  | N-CA-C | 6.83  | 118.38      | 111.07   |
| 1   | B     | 525 | GLU  | N-CA-C | -6.83 | 103.07      | 111.40   |
| 2   | F     | 229 | ILE  | N-CA-C | -6.83 | 104.20      | 110.82   |
| 1   | A     | 133 | MET  | N-CA-C | -6.82 | 98.65       | 108.60   |
| 2   | F     | 433 | GLU  | N-CA-C | -6.81 | 102.98      | 112.45   |
| 8   | N     | 99  | GLU  | CA-C-N | 6.81  | 127.54      | 119.98   |
| 8   | N     | 99  | GLU  | C-N-CA | 6.81  | 127.54      | 119.98   |
| 6   | L     | 119 | LYS  | N-CA-C | -6.81 | 104.00      | 112.72   |
| 1   | B     | 564 | GLU  | N-CA-C | -6.81 | 103.94      | 111.36   |
| 1   | A     | 548 | ILE  | CA-C-N | 6.80  | 128.70      | 120.13   |
| 1   | A     | 548 | ILE  | C-N-CA | 6.80  | 128.70      | 120.13   |
| 1   | B     | 203 | THR  | CA-C-N | 6.80  | 126.76      | 120.03   |
| 1   | B     | 203 | THR  | C-N-CA | 6.80  | 126.76      | 120.03   |
| 2   | E     | 208 | PHE  | N-CA-C | -6.80 | 105.14      | 113.50   |
| 2   | D     | 462 | TYR  | N-CA-C | -6.79 | 98.69       | 108.60   |
| 5   | K     | 24  | LYS  | CA-C-N | 6.79  | 130.23      | 120.79   |
| 5   | K     | 24  | LYS  | C-N-CA | 6.79  | 130.23      | 120.79   |
| 1   | B     | 497 | GLN  | N-CA-C | -6.78 | 99.93       | 109.69   |
| 1   | C     | 355 | ALA  | N-CA-C | -6.78 | 103.82      | 111.07   |
| 7   | M     | 107 | ARG  | CA-C-N | 6.77  | 128.31      | 119.84   |
| 7   | M     | 107 | ARG  | C-N-CA | 6.77  | 128.31      | 119.84   |
| 2   | D     | 286 | TYR  | N-CA-C | -6.77 | 104.77      | 113.16   |
| 8   | N     | 98  | ALA  | CA-C-N | 6.77  | 129.35      | 120.28   |
| 8   | N     | 98  | ALA  | C-N-CA | 6.77  | 129.35      | 120.28   |
| 2   | D     | 246 | ALA  | N-CA-C | -6.76 | 103.52      | 111.03   |
| 8   | N     | 254 | THR  | N-CA-C | -6.76 | 103.91      | 111.28   |
| 2   | D     | 201 | LEU  | N-CA-C | -6.75 | 102.53      | 111.24   |
| 7   | M     | 109 | PHE  | CA-C-N | 6.73  | 129.98      | 120.28   |
| 7   | M     | 109 | PHE  | C-N-CA | 6.73  | 129.98      | 120.28   |
| 3   | G     | 17  | GLN  | CA-C-N | 6.72  | 129.61      | 120.54   |
| 3   | G     | 17  | GLN  | C-N-CA | 6.72  | 129.61      | 120.54   |
| 1   | B     | 381 | VAL  | CA-C-N | 6.72  | 128.09      | 121.57   |
| 1   | B     | 381 | VAL  | C-N-CA | 6.72  | 128.09      | 121.57   |
| 2   | D     | 415 | ALA  | N-CA-C | -6.72 | 104.90      | 113.23   |
| 9   | Q     | 19  | MET  | CA-C-N | 6.72  | 127.44      | 119.98   |
| 9   | Q     | 19  | MET  | C-N-CA | 6.72  | 127.44      | 119.98   |
| 9   | W     | 62  | PRO  | CA-C-N | 6.72  | 131.35      | 120.60   |
| 9   | W     | 62  | PRO  | C-N-CA | 6.72  | 131.35      | 120.60   |
| 3   | G     | 94  | GLU  | N-CA-C | -6.72 | 97.95       | 108.90   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | G     | 124 | LEU  | N-CA-C | 6.70  | 119.44      | 111.33   |
| 8   | N     | 336 | PHE  | N-CA-C | -6.70 | 105.14      | 113.38   |
| 8   | N     | 627 | GLU  | N-CA-C | -6.69 | 103.15      | 112.45   |
| 9   | P     | 26  | ALA  | CA-C-N | 6.68  | 129.23      | 120.28   |
| 9   | P     | 26  | ALA  | C-N-CA | 6.68  | 129.23      | 120.28   |
| 9   | O     | 37  | ILE  | CA-C-N | 6.68  | 127.39      | 119.98   |
| 9   | O     | 37  | ILE  | C-N-CA | 6.68  | 127.39      | 119.98   |
| 9   | Y     | 37  | ILE  | CA-C-N | 6.67  | 127.39      | 119.98   |
| 9   | Y     | 37  | ILE  | C-N-CA | 6.67  | 127.39      | 119.98   |
| 9   | O     | 35  | ALA  | N-CA-C | 6.67  | 118.20      | 111.07   |
| 1   | B     | 346 | ALA  | N-CA-C | -6.66 | 99.19       | 109.24   |
| 2   | D     | 276 | GLU  | N-CA-C | -6.65 | 99.24       | 109.14   |
| 1   | B     | 4   | GLY  | N-CA-C | -6.64 | 101.47      | 110.43   |
| 2   | D     | 175 | PRO  | N-CA-C | -6.64 | 105.29      | 114.98   |
| 1   | A     | 64  | VAL  | N-CA-C | -6.63 | 98.16       | 108.44   |
| 1   | A     | 522 | PHE  | N-CA-C | -6.63 | 105.01      | 113.23   |
| 1   | C     | 338 | SER  | CA-C-N | 6.60  | 129.42      | 120.38   |
| 1   | C     | 338 | SER  | C-N-CA | 6.60  | 129.42      | 120.38   |
| 8   | N     | 491 | HIS  | CA-C-N | 6.60  | 129.78      | 120.28   |
| 8   | N     | 491 | HIS  | C-N-CA | 6.60  | 129.78      | 120.28   |
| 2   | E     | 175 | PRO  | N-CA-C | -6.59 | 107.07      | 114.92   |
| 2   | E     | 87  | GLU  | N-CA-C | -6.59 | 104.26      | 112.90   |
| 9   | T     | 76  | LEU  | CA-C-N | 6.59  | 134.13      | 121.54   |
| 9   | T     | 76  | LEU  | C-N-CA | 6.59  | 134.13      | 121.54   |
| 3   | G     | 25  | VAL  | CA-C-N | 6.58  | 129.43      | 120.54   |
| 3   | G     | 25  | VAL  | C-N-CA | 6.58  | 129.43      | 120.54   |
| 1   | B     | 160 | VAL  | N-CA-C | -6.58 | 95.65       | 109.34   |
| 7   | M     | 224 | PHE  | N-CA-C | -6.58 | 103.67      | 112.94   |
| 8   | N     | 397 | LYS  | N-CA-C | 6.58  | 118.20      | 108.60   |
| 9   | Q     | 79  | ARG  | N-CA-C | -6.57 | 105.57      | 112.93   |
| 9   | U     | 66  | VAL  | N-CA-C | 6.57  | 116.73      | 110.42   |
| 1   | C     | 114 | GLU  | N-CA-C | -6.56 | 105.57      | 113.97   |
| 4   | H     | 39  | ARG  | N-CA-C | -6.56 | 104.20      | 112.93   |
| 3   | G     | 156 | LYS  | CA-C-N | 6.56  | 129.31      | 120.65   |
| 3   | G     | 156 | LYS  | C-N-CA | 6.56  | 129.31      | 120.65   |
| 2   | F     | 294 | ILE  | N-CA-C | -6.56 | 105.15      | 113.22   |
| 8   | N     | 459 | THR  | CA-C-N | 6.56  | 129.07      | 120.28   |
| 8   | N     | 459 | THR  | C-N-CA | 6.56  | 129.07      | 120.28   |
| 1   | B     | 438 | TRP  | N-CA-C | -6.56 | 104.76      | 112.89   |
| 2   | E     | 402 | ASP  | N-CA-C | -6.56 | 99.34       | 109.24   |
| 1   | A     | 563 | PHE  | N-CA-C | -6.55 | 103.41      | 111.40   |
| 1   | C     | 430 | LEU  | N-CA-C | -6.55 | 103.45      | 112.03   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 369 | ILE  | N-CA-C | -6.54 | 98.92       | 108.87   |
| 1   | A     | 273 | THR  | N-CA-C | -6.54 | 96.39       | 108.02   |
| 2   | D     | 287 | MET  | CA-C-N | 6.54  | 129.33      | 120.38   |
| 2   | D     | 287 | MET  | C-N-CA | 6.54  | 129.33      | 120.38   |
| 2   | E     | 244 | TYR  | N-CA-C | -6.53 | 103.37      | 112.45   |
| 1   | A     | 534 | VAL  | CA-C-N | 6.53  | 134.01      | 121.54   |
| 1   | A     | 534 | VAL  | C-N-CA | 6.53  | 134.01      | 121.54   |
| 1   | C     | 422 | ILE  | N-CA-C | -6.53 | 99.27       | 108.80   |
| 2   | F     | 453 | ARG  | N-CA-C | -6.53 | 104.09      | 111.14   |
| 9   | Y     | 40  | ALA  | CA-C-N | 6.53  | 127.22      | 119.98   |
| 9   | Y     | 40  | ALA  | C-N-CA | 6.53  | 127.22      | 119.98   |
| 8   | N     | 649 | ARG  | CA-C-N | 6.52  | 129.32      | 120.38   |
| 8   | N     | 649 | ARG  | C-N-CA | 6.52  | 129.32      | 120.38   |
| 2   | D     | 17  | PRO  | CA-C-N | 6.51  | 133.98      | 121.54   |
| 2   | D     | 17  | PRO  | C-N-CA | 6.51  | 133.98      | 121.54   |
| 4   | H     | 88  | GLY  | CA-C-N | 6.51  | 129.01      | 120.28   |
| 4   | H     | 88  | GLY  | C-N-CA | 6.51  | 129.01      | 120.28   |
| 1   | B     | 532 | ARG  | N-CA-C | -6.50 | 105.31      | 112.72   |
| 1   | C     | 452 | ASP  | N-CA-C | -6.50 | 104.04      | 112.23   |
| 9   | O     | 49  | ARG  | CA-C-N | 6.50  | 128.99      | 120.28   |
| 9   | O     | 49  | ARG  | C-N-CA | 6.50  | 128.99      | 120.28   |
| 2   | D     | 346 | LYS  | N-CA-C | -6.49 | 105.90      | 113.88   |
| 1   | C     | 113 | ARG  | N-CA-C | -6.49 | 103.69      | 112.26   |
| 1   | C     | 414 | ALA  | CA-C-N | 6.48  | 129.61      | 120.28   |
| 1   | C     | 414 | ALA  | C-N-CA | 6.48  | 129.61      | 120.28   |
| 2   | E     | 257 | LEU  | N-CA-C | -6.47 | 99.15       | 109.76   |
| 1   | B     | 295 | PRO  | CA-C-N | 6.47  | 129.65      | 120.53   |
| 1   | B     | 295 | PRO  | C-N-CA | 6.47  | 129.65      | 120.53   |
| 2   | F     | 291 | LEU  | N-CA-C | -6.46 | 103.74      | 111.69   |
| 9   | V     | 58  | PHE  | CA-C-N | 6.45  | 129.56      | 120.28   |
| 9   | V     | 58  | PHE  | C-N-CA | 6.45  | 129.56      | 120.28   |
| 3   | G     | 157 | THR  | N-CA-C | -6.45 | 103.94      | 110.97   |
| 2   | D     | 323 | HIS  | CA-C-N | 6.44  | 126.07      | 119.56   |
| 2   | D     | 323 | HIS  | C-N-CA | 6.44  | 126.07      | 119.56   |
| 2   | E     | 198 | GLN  | N-CA-C | -6.43 | 103.51      | 112.45   |
| 1   | C     | 239 | GLN  | CA-C-N | 6.42  | 128.78      | 120.44   |
| 1   | C     | 239 | GLN  | C-N-CA | 6.42  | 128.78      | 120.44   |
| 8   | N     | 630 | THR  | N-CA-C | -6.42 | 105.74      | 112.93   |
| 1   | A     | 499 | ALA  | N-CA-C | -6.42 | 105.41      | 112.72   |
| 1   | C     | 203 | THR  | N-CA-C | -6.40 | 100.66      | 110.32   |
| 1   | C     | 495 | LEU  | N-CA-C | -6.40 | 106.06      | 114.31   |
| 1   | B     | 18  | GLY  | N-CA-C | -6.39 | 106.31      | 115.64   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 99  | GLY  | N-CA-C | -6.38 | 98.05       | 113.18   |
| 1   | C     | 185 | HIS  | CA-C-N | 6.38  | 129.93      | 120.87   |
| 1   | C     | 185 | HIS  | C-N-CA | 6.38  | 129.93      | 120.87   |
| 2   | F     | 120 | ASN  | N-CA-C | -6.37 | 99.20       | 109.40   |
| 1   | A     | 236 | VAL  | CA-C-N | 6.37  | 131.31      | 121.19   |
| 1   | A     | 236 | VAL  | C-N-CA | 6.37  | 131.31      | 121.19   |
| 3   | G     | 191 | THR  | N-CA-C | -6.36 | 104.26      | 111.07   |
| 1   | C     | 460 | ARG  | N-CA-C | -6.36 | 104.22      | 112.23   |
| 1   | A     | 357 | ARG  | CA-C-N | 6.35  | 129.08      | 120.44   |
| 1   | A     | 357 | ARG  | C-N-CA | 6.35  | 129.08      | 120.44   |
| 2   | D     | 261 | THR  | N-CA-C | -6.35 | 104.05      | 110.97   |
| 1   | B     | 370 | THR  | CA-C-N | 6.35  | 129.08      | 120.38   |
| 1   | B     | 370 | THR  | C-N-CA | 6.35  | 129.08      | 120.38   |
| 2   | D     | 413 | GLN  | N-CA-C | 6.35  | 120.59      | 112.34   |
| 2   | D     | 290 | ASP  | N-CA-C | -6.34 | 103.89      | 111.69   |
| 2   | F     | 421 | PHE  | N-CA-C | -6.34 | 104.25      | 112.68   |
| 1   | B     | 357 | ARG  | N-CA-C | -6.34 | 103.64      | 112.45   |
| 1   | C     | 536 | ILE  | CA-C-N | 6.33  | 128.76      | 120.28   |
| 1   | C     | 536 | ILE  | C-N-CA | 6.33  | 128.76      | 120.28   |
| 2   | E     | 140 | VAL  | N-CA-C | -6.32 | 96.19       | 109.34   |
| 2   | F     | 428 | GLN  | N-CA-C | -6.32 | 97.25       | 108.13   |
| 1   | B     | 373 | GLY  | N-CA-C | -6.31 | 105.97      | 115.32   |
| 2   | D     | 440 | TRP  | N-CA-C | -6.31 | 104.63      | 112.90   |
| 1   | B     | 550 | ARG  | N-CA-C | -6.31 | 105.16      | 112.92   |
| 2   | F     | 230 | GLU  | CA-C-N | 6.31  | 131.22      | 121.19   |
| 2   | F     | 230 | GLU  | C-N-CA | 6.31  | 131.22      | 121.19   |
| 1   | C     | 473 | PRO  | CA-C-N | 6.31  | 128.73      | 120.28   |
| 1   | C     | 473 | PRO  | C-N-CA | 6.31  | 128.73      | 120.28   |
| 5   | K     | 31  | LYS  | CA-C-N | 6.30  | 129.05      | 120.54   |
| 5   | K     | 31  | LYS  | C-N-CA | 6.30  | 129.05      | 120.54   |
| 3   | G     | 77  | ALA  | CA-C-N | 6.29  | 128.00      | 120.14   |
| 3   | G     | 77  | ALA  | C-N-CA | 6.29  | 128.00      | 120.14   |
| 7   | M     | 194 | LEU  | CA-C-N | 6.29  | 128.71      | 120.28   |
| 7   | M     | 194 | LEU  | C-N-CA | 6.29  | 128.71      | 120.28   |
| 8   | N     | 5   | MET  | N-CA-C | -6.29 | 98.96       | 108.96   |
| 7   | M     | 297 | ALA  | CA-C-N | 6.29  | 128.48      | 120.56   |
| 7   | M     | 297 | ALA  | C-N-CA | 6.29  | 128.48      | 120.56   |
| 2   | D     | 62  | GLU  | N-CA-C | 6.29  | 119.94      | 110.64   |
| 9   | P     | 68  | PHE  | CA-C-N | 6.29  | 126.96      | 119.98   |
| 9   | P     | 68  | PHE  | C-N-CA | 6.29  | 126.96      | 119.98   |
| 9   | Q     | 54  | THR  | CA-C-N | 6.29  | 128.70      | 120.28   |
| 9   | Q     | 54  | THR  | C-N-CA | 6.29  | 128.70      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 68  | GLY  | N-CA-C | -6.28 | 106.47      | 115.64   |
| 6   | L     | 53  | TYR  | CA-C-N | 6.28  | 128.61      | 120.44   |
| 6   | L     | 53  | TYR  | C-N-CA | 6.28  | 128.61      | 120.44   |
| 2   | E     | 77  | GLU  | N-CA-C | -6.28 | 99.75       | 109.24   |
| 8   | N     | 328 | LYS  | N-CA-C | 6.28  | 121.29      | 112.75   |
| 6   | L     | 64  | GLY  | N-CA-C | 6.27  | 120.26      | 112.73   |
| 1   | B     | 231 | GLY  | N-CA-C | -6.27 | 107.23      | 114.69   |
| 2   | D     | 198 | GLN  | CA-C-N | 6.27  | 128.59      | 120.44   |
| 2   | D     | 198 | GLN  | C-N-CA | 6.27  | 128.59      | 120.44   |
| 3   | G     | 103 | ARG  | N-CA-C | -6.26 | 97.47       | 110.80   |
| 2   | F     | 258 | THR  | CA-C-N | 6.26  | 133.49      | 121.54   |
| 2   | F     | 258 | THR  | C-N-CA | 6.26  | 133.49      | 121.54   |
| 1   | C     | 457 | LEU  | N-CA-C | -6.25 | 103.77      | 111.40   |
| 2   | D     | 100 | ILE  | N-CA-C | -6.25 | 99.04       | 108.17   |
| 2   | F     | 340 | SER  | CA-C-N | 6.25  | 128.66      | 120.28   |
| 2   | F     | 340 | SER  | C-N-CA | 6.25  | 128.66      | 120.28   |
| 1   | C     | 547 | ARG  | N-CA-C | -6.25 | 104.00      | 111.69   |
| 5   | I     | 22  | LEU  | CA-C-N | 6.25  | 133.22      | 121.97   |
| 5   | I     | 22  | LEU  | C-N-CA | 6.25  | 133.22      | 121.97   |
| 1   | C     | 482 | LEU  | CA-C-N | 6.24  | 128.55      | 120.56   |
| 1   | C     | 482 | LEU  | C-N-CA | 6.24  | 128.55      | 120.56   |
| 2   | D     | 294 | ILE  | N-CA-C | -6.24 | 105.64      | 111.45   |
| 9   | Z     | 37  | ILE  | CA-C-N | 6.24  | 126.90      | 119.98   |
| 9   | Z     | 37  | ILE  | C-N-CA | 6.24  | 126.90      | 119.98   |
| 4   | H     | 62  | LEU  | N-CA-C | -6.23 | 104.40      | 112.68   |
| 2   | F     | 160 | ALA  | CA-C-N | 6.22  | 133.42      | 121.54   |
| 2   | F     | 160 | ALA  | C-N-CA | 6.22  | 133.42      | 121.54   |
| 1   | B     | 323 | MET  | CA-C-N | 6.21  | 130.73      | 121.72   |
| 1   | B     | 323 | MET  | C-N-CA | 6.21  | 130.73      | 121.72   |
| 9   | P     | 17  | VAL  | N-CA-C | 6.21  | 116.33      | 110.30   |
| 9   | Z     | 36  | ARG  | N-CA-C | 6.21  | 117.84      | 111.14   |
| 5   | K     | 95  | GLU  | CA-C-N | 6.20  | 128.59      | 120.28   |
| 5   | K     | 95  | GLU  | C-N-CA | 6.20  | 128.59      | 120.28   |
| 9   | U     | 63  | GLU  | CA-C-N | 6.20  | 129.20      | 120.28   |
| 9   | U     | 63  | GLU  | C-N-CA | 6.20  | 129.20      | 120.28   |
| 2   | E     | 142 | ASN  | N-CA-C | -6.19 | 106.26      | 113.88   |
| 3   | G     | 64  | LEU  | N-CA-C | -6.19 | 104.44      | 111.07   |
| 1   | B     | 491 | ARG  | N-CA-C | -6.19 | 97.62       | 110.80   |
| 8   | N     | 608 | ILE  | CA-C-N | 6.18  | 128.56      | 120.28   |
| 8   | N     | 608 | ILE  | C-N-CA | 6.18  | 128.56      | 120.28   |
| 2   | F     | 100 | ILE  | CA-C-N | 6.17  | 129.17      | 120.28   |
| 2   | F     | 100 | ILE  | C-N-CA | 6.17  | 129.17      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | L     | 171 | MET  | N-CA-C | -6.16 | 104.48      | 111.07   |
| 2   | F     | 449 | GLY  | N-CA-C | -6.16 | 106.92      | 114.92   |
| 2   | E     | 283 | TYR  | CA-C-N | 6.14  | 126.17      | 119.90   |
| 2   | E     | 283 | TYR  | C-N-CA | 6.14  | 126.17      | 119.90   |
| 9   | R     | 62  | PRO  | CA-C-N | 6.14  | 130.42      | 120.60   |
| 9   | R     | 62  | PRO  | C-N-CA | 6.14  | 130.42      | 120.60   |
| 1   | C     | 512 | ALA  | CA-C-N | 6.14  | 128.82      | 120.54   |
| 1   | C     | 512 | ALA  | C-N-CA | 6.14  | 128.82      | 120.54   |
| 2   | E     | 26  | ASP  | N-CA-C | -6.13 | 104.62      | 113.21   |
| 1   | A     | 475 | ALA  | N-CA-C | -6.13 | 103.12      | 112.99   |
| 2   | D     | 288 | TYR  | CA-C-N | 6.11  | 128.79      | 120.54   |
| 2   | D     | 288 | TYR  | C-N-CA | 6.11  | 128.79      | 120.54   |
| 6   | L     | 135 | ALA  | N-CA-C | -6.10 | 104.55      | 112.23   |
| 9   | X     | 59  | LEU  | N-CA-C | 6.10  | 118.72      | 111.71   |
| 5   | I     | 37  | LEU  | CA-C-N | 6.09  | 128.76      | 120.54   |
| 5   | I     | 37  | LEU  | C-N-CA | 6.09  | 128.76      | 120.54   |
| 1   | B     | 286 | VAL  | CA-C-N | 6.09  | 130.52      | 122.30   |
| 1   | B     | 286 | VAL  | C-N-CA | 6.09  | 130.52      | 122.30   |
| 9   | Y     | 10  | LEU  | CA-C-N | 6.08  | 128.35      | 120.44   |
| 9   | Y     | 10  | LEU  | C-N-CA | 6.08  | 128.35      | 120.44   |
| 3   | G     | 143 | THR  | N-CA-C | -6.08 | 104.00      | 112.45   |
| 1   | A     | 102 | ILE  | N-CA-C | -6.08 | 99.49       | 108.85   |
| 2   | E     | 293 | THR  | CA-C-N | 6.08  | 128.29      | 120.88   |
| 2   | E     | 293 | THR  | C-N-CA | 6.08  | 128.29      | 120.88   |
| 1   | C     | 501 | HIS  | CA-C-N | 6.08  | 128.34      | 120.44   |
| 1   | C     | 501 | HIS  | C-N-CA | 6.08  | 128.34      | 120.44   |
| 1   | A     | 324 | ALA  | N-CA-C | -6.06 | 99.51       | 108.79   |
| 1   | B     | 209 | MET  | CA-C-N | 6.06  | 133.11      | 121.54   |
| 1   | B     | 209 | MET  | C-N-CA | 6.06  | 133.11      | 121.54   |
| 2   | E     | 177 | LEU  | N-CA-C | -6.06 | 103.33      | 111.87   |
| 1   | C     | 462 | ALA  | CA-C-N | 6.06  | 126.81      | 120.03   |
| 1   | C     | 462 | ALA  | C-N-CA | 6.06  | 126.81      | 120.03   |
| 2   | D     | 54  | TYR  | CA-C-N | 6.05  | 131.43      | 121.39   |
| 2   | D     | 54  | TYR  | C-N-CA | 6.05  | 131.43      | 121.39   |
| 2   | D     | 405 | THR  | N-CA-C | -6.05 | 100.33      | 108.86   |
| 9   | X     | 58  | PHE  | N-CA-C | 6.05  | 117.54      | 111.07   |
| 2   | D     | 93  | PHE  | CA-C-N | 6.05  | 129.71      | 120.82   |
| 2   | D     | 93  | PHE  | C-N-CA | 6.05  | 129.71      | 120.82   |
| 4   | H     | 42  | TYR  | N-CA-C | -6.05 | 100.39      | 108.74   |
| 9   | Q     | 59  | LEU  | CA-C-N | 6.05  | 128.38      | 120.28   |
| 9   | Q     | 59  | LEU  | C-N-CA | 6.05  | 128.38      | 120.28   |
| 2   | E     | 158 | LEU  | N-CA-C | -6.04 | 101.19      | 110.32   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | N     | 399 | LYS  | CA-C-N | 6.04  | 127.40      | 119.84   |
| 8   | N     | 399 | LYS  | C-N-CA | 6.04  | 127.40      | 119.84   |
| 9   | W     | 26  | ALA  | CA-C-N | 6.04  | 128.37      | 120.28   |
| 9   | W     | 26  | ALA  | C-N-CA | 6.04  | 128.37      | 120.28   |
| 2   | F     | 406 | GLU  | CA-C-N | 6.03  | 128.68      | 120.54   |
| 2   | F     | 406 | GLU  | C-N-CA | 6.03  | 128.68      | 120.54   |
| 1   | A     | 209 | MET  | CA-C-N | 6.03  | 133.05      | 121.54   |
| 1   | A     | 209 | MET  | C-N-CA | 6.03  | 133.05      | 121.54   |
| 3   | G     | 71  | ASP  | N-CA-C | -6.02 | 105.11      | 112.88   |
| 1   | C     | 174 | VAL  | N-CA-C | -6.02 | 99.60       | 108.99   |
| 8   | N     | 354 | PHE  | N-CA-C | 6.02  | 117.84      | 111.28   |
| 9   | U     | 7   | SER  | N-CA-C | -6.02 | 105.52      | 112.92   |
| 9   | U     | 58  | PHE  | CA-C-N | 6.02  | 128.94      | 120.28   |
| 9   | U     | 58  | PHE  | C-N-CA | 6.02  | 128.94      | 120.28   |
| 3   | G     | 69  | ALA  | CA-C-N | 6.02  | 131.67      | 121.14   |
| 3   | G     | 69  | ALA  | C-N-CA | 6.02  | 131.67      | 121.14   |
| 1   | B     | 447 | TYR  | N-CA-C | -6.01 | 96.52       | 109.81   |
| 8   | N     | 503 | GLY  | CA-C-N | 6.01  | 126.65      | 119.98   |
| 8   | N     | 503 | GLY  | C-N-CA | 6.01  | 126.65      | 119.98   |
| 1   | B     | 436 | ASP  | CA-C-N | 6.01  | 125.49      | 119.24   |
| 1   | B     | 436 | ASP  | C-N-CA | 6.01  | 125.49      | 119.24   |
| 6   | J     | 99  | GLU  | N-CA-C | -6.01 | 105.71      | 113.16   |
| 8   | N     | 1   | MET  | CA-C-N | 6.01  | 128.71      | 120.35   |
| 8   | N     | 1   | MET  | C-N-CA | 6.01  | 128.71      | 120.35   |
| 8   | N     | 152 | LEU  | N-CA-C | 6.01  | 117.91      | 111.36   |
| 1   | C     | 272 | LEU  | N-CA-C | -6.00 | 100.62      | 109.81   |
| 2   | D     | 260 | MET  | CA-C-N | 6.00  | 128.58      | 120.65   |
| 2   | D     | 260 | MET  | C-N-CA | 6.00  | 128.58      | 120.65   |
| 5   | K     | 31  | LYS  | N-CA-C | -6.00 | 104.69      | 112.68   |
| 2   | F     | 364 | ASN  | N-CA-C | -5.98 | 105.90      | 112.72   |
| 8   | N     | 220 | LEU  | CA-C-N | 5.98  | 128.29      | 120.28   |
| 8   | N     | 220 | LEU  | C-N-CA | 5.98  | 128.29      | 120.28   |
| 8   | N     | 402 | VAL  | CA-C-N | 5.98  | 128.65      | 120.46   |
| 8   | N     | 402 | VAL  | C-N-CA | 5.98  | 128.65      | 120.46   |
| 2   | D     | 421 | PHE  | N-CA-C | -5.98 | 104.69      | 111.14   |
| 2   | E     | 54  | TYR  | N-CA-C | -5.97 | 100.93      | 108.45   |
| 8   | N     | 613 | THR  | N-CA-C | -5.97 | 106.00      | 113.28   |
| 5   | K     | 23  | ILE  | CA-C-N | 5.97  | 129.77      | 120.82   |
| 5   | K     | 23  | ILE  | C-N-CA | 5.97  | 129.77      | 120.82   |
| 2   | E     | 456 | LYS  | CA-C-N | 5.96  | 132.92      | 121.54   |
| 2   | E     | 456 | LYS  | C-N-CA | 5.96  | 132.92      | 121.54   |
| 3   | G     | 15  | ARG  | N-CA-C | -5.96 | 104.36      | 111.69   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | F     | 213 | ALA  | N-CA-C | -5.95 | 105.88      | 113.02   |
| 9   | W     | 59  | LEU  | CA-C-N | 5.95  | 128.25      | 120.28   |
| 9   | W     | 59  | LEU  | C-N-CA | 5.95  | 128.25      | 120.28   |
| 9   | Z     | 64  | THR  | CA-C-N | 5.95  | 128.25      | 120.28   |
| 9   | Z     | 64  | THR  | C-N-CA | 5.95  | 128.25      | 120.28   |
| 1   | B     | 576 | ALA  | N-CA-C | -5.95 | 107.26      | 114.75   |
| 9   | V     | 40  | ALA  | CA-C-N | 5.94  | 126.58      | 119.98   |
| 9   | V     | 40  | ALA  | C-N-CA | 5.94  | 126.58      | 119.98   |
| 2   | E     | 86  | LYS  | N-CA-C | -5.94 | 104.69      | 112.41   |
| 7   | M     | 115 | LEU  | CA-C-N | 5.94  | 125.95      | 119.89   |
| 7   | M     | 115 | LEU  | C-N-CA | 5.94  | 125.95      | 119.89   |
| 1   | B     | 430 | LEU  | N-CA-C | -5.94 | 106.00      | 113.72   |
| 9   | U     | 19  | MET  | CA-C-N | 5.93  | 126.53      | 120.00   |
| 9   | U     | 19  | MET  | C-N-CA | 5.93  | 126.53      | 120.00   |
| 9   | T     | 56  | LEU  | N-CA-C | -5.93 | 104.90      | 111.36   |
| 2   | F     | 326 | PRO  | N-CA-C | -5.92 | 100.28      | 112.47   |
| 9   | U     | 10  | LEU  | CA-C-N | 5.91  | 128.19      | 120.28   |
| 9   | U     | 10  | LEU  | C-N-CA | 5.91  | 128.19      | 120.28   |
| 9   | Z     | 11  | ASP  | N-CA-C | 5.91  | 117.39      | 111.07   |
| 1   | A     | 484 | ILE  | N-CA-C | -5.90 | 104.98      | 113.07   |
| 8   | N     | 191 | LYS  | CA-C-N | 5.90  | 128.19      | 120.28   |
| 8   | N     | 191 | LYS  | C-N-CA | 5.90  | 128.19      | 120.28   |
| 2   | D     | 420 | ARG  | CA-C-N | 5.90  | 128.47      | 120.44   |
| 2   | D     | 420 | ARG  | C-N-CA | 5.90  | 128.47      | 120.44   |
| 2   | E     | 263 | TYR  | CA-C-N | 5.90  | 128.99      | 120.38   |
| 2   | E     | 263 | TYR  | C-N-CA | 5.90  | 128.99      | 120.38   |
| 2   | D     | 342 | GLU  | N-CA-C | -5.90 | 104.70      | 112.72   |
| 8   | N     | 20  | LEU  | CA-C-N | 5.89  | 128.17      | 120.28   |
| 8   | N     | 20  | LEU  | C-N-CA | 5.89  | 128.17      | 120.28   |
| 2   | F     | 147 | GLY  | CA-C-N | 5.89  | 132.79      | 121.54   |
| 2   | F     | 147 | GLY  | C-N-CA | 5.89  | 132.79      | 121.54   |
| 1   | B     | 271 | GLU  | N-CA-C | -5.88 | 106.44      | 113.97   |
| 9   | W     | 61  | LEU  | CA-C-N | 5.88  | 125.75      | 119.28   |
| 9   | W     | 61  | LEU  | C-N-CA | 5.88  | 125.75      | 119.28   |
| 9   | O     | 66  | VAL  | CA-C-N | 5.88  | 128.51      | 120.46   |
| 9   | O     | 66  | VAL  | C-N-CA | 5.88  | 128.51      | 120.46   |
| 2   | E     | 323 | HIS  | CA-C-N | 5.88  | 127.19      | 119.84   |
| 2   | E     | 323 | HIS  | C-N-CA | 5.88  | 127.19      | 119.84   |
| 9   | W     | 43  | GLY  | CA-C-N | 5.87  | 128.15      | 120.28   |
| 9   | W     | 43  | GLY  | C-N-CA | 5.87  | 128.15      | 120.28   |
| 7   | M     | 26  | GLN  | CA-C-N | 5.87  | 128.14      | 120.28   |
| 7   | M     | 26  | GLN  | C-N-CA | 5.87  | 128.14      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | Q     | 60  | LEU  | CA-C-N | 5.87  | 127.43      | 120.09   |
| 9   | Q     | 60  | LEU  | C-N-CA | 5.87  | 127.43      | 120.09   |
| 3   | G     | 191 | THR  | CA-C-N | 5.87  | 128.14      | 120.28   |
| 3   | G     | 191 | THR  | C-N-CA | 5.87  | 128.14      | 120.28   |
| 4   | H     | 13  | PHE  | CA-C-N | 5.86  | 128.93      | 120.38   |
| 4   | H     | 13  | PHE  | C-N-CA | 5.86  | 128.93      | 120.38   |
| 2   | F     | 265 | GLU  | CA-C-N | 5.86  | 128.40      | 120.38   |
| 2   | F     | 265 | GLU  | C-N-CA | 5.86  | 128.40      | 120.38   |
| 5   | I     | 31  | LYS  | CA-C-N | 5.85  | 128.39      | 120.38   |
| 5   | I     | 31  | LYS  | C-N-CA | 5.85  | 128.39      | 120.38   |
| 2   | E     | 138 | ILE  | N-CA-C | -5.85 | 105.42      | 110.74   |
| 2   | F     | 121 | PRO  | CA-C-N | 5.84  | 128.47      | 120.46   |
| 2   | F     | 121 | PRO  | C-N-CA | 5.84  | 128.47      | 120.46   |
| 1   | B     | 14  | VAL  | N-CA-C | -5.84 | 100.07      | 108.42   |
| 1   | B     | 410 | ASP  | CA-C-N | 5.84  | 128.03      | 120.44   |
| 1   | B     | 410 | ASP  | C-N-CA | 5.84  | 128.03      | 120.44   |
| 8   | N     | 365 | ASP  | CA-C-N | 5.84  | 128.77      | 120.53   |
| 8   | N     | 365 | ASP  | C-N-CA | 5.84  | 128.77      | 120.53   |
| 9   | Y     | 56  | LEU  | CA-C-N | 5.84  | 128.46      | 120.46   |
| 9   | Y     | 56  | LEU  | C-N-CA | 5.84  | 128.46      | 120.46   |
| 1   | B     | 570 | ILE  | N-CA-C | -5.84 | 105.16      | 110.82   |
| 9   | U     | 39  | ALA  | CA-C-N | 5.84  | 128.69      | 120.28   |
| 9   | U     | 39  | ALA  | C-N-CA | 5.84  | 128.69      | 120.28   |
| 9   | V     | 26  | ALA  | CA-C-N | 5.84  | 128.10      | 120.28   |
| 9   | V     | 26  | ALA  | C-N-CA | 5.84  | 128.10      | 120.28   |
| 1   | A     | 529 | ALA  | N-CA-C | -5.83 | 104.28      | 111.40   |
| 9   | U     | 67  | ILE  | N-CA-C | 5.83  | 116.57      | 110.62   |
| 1   | A     | 142 | GLY  | N-CA-C | -5.83 | 105.44      | 112.49   |
| 1   | A     | 196 | GLN  | CA-C-N | 5.83  | 132.67      | 121.54   |
| 1   | A     | 196 | GLN  | C-N-CA | 5.83  | 132.67      | 121.54   |
| 1   | B     | 202 | ASN  | N-CA-C | -5.82 | 107.98      | 114.62   |
| 9   | W     | 54  | THR  | CA-C-N | 5.82  | 128.08      | 120.28   |
| 9   | W     | 54  | THR  | C-N-CA | 5.82  | 128.08      | 120.28   |
| 9   | X     | 45  | ILE  | CA-C-N | 5.82  | 128.01      | 120.44   |
| 9   | X     | 45  | ILE  | C-N-CA | 5.82  | 128.01      | 120.44   |
| 9   | W     | 53  | GLY  | CA-C-N | 5.82  | 128.01      | 120.44   |
| 9   | W     | 53  | GLY  | C-N-CA | 5.82  | 128.01      | 120.44   |
| 1   | B     | 352 | PRO  | N-CA-C | -5.82 | 107.08      | 114.35   |
| 2   | E     | 246 | ALA  | N-CA-C | -5.82 | 104.31      | 111.40   |
| 9   | U     | 74  | PHE  | N-CA-C | 5.81  | 117.29      | 111.07   |
| 1   | B     | 246 | ASN  | N-CA-C | -5.81 | 103.77      | 112.54   |
| 1   | C     | 213 | ASP  | N-CA-C | -5.81 | 102.67      | 111.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 227 | PRO  | CA-C-N | 5.81  | 128.65      | 120.28   |
| 2   | E     | 227 | PRO  | C-N-CA | 5.81  | 128.65      | 120.28   |
| 9   | T     | 39  | ALA  | CA-C-N | 5.81  | 128.06      | 120.28   |
| 9   | T     | 39  | ALA  | C-N-CA | 5.81  | 128.06      | 120.28   |
| 3   | G     | 67  | ALA  | N-CA-C | -5.81 | 104.86      | 112.41   |
| 1   | A     | 200 | ASP  | CA-C-N | 5.80  | 125.81      | 119.89   |
| 1   | A     | 200 | ASP  | C-N-CA | 5.80  | 125.81      | 119.89   |
| 2   | F     | 98  | LYS  | CA-C-N | 5.80  | 127.09      | 119.84   |
| 2   | F     | 98  | LYS  | C-N-CA | 5.80  | 127.09      | 119.84   |
| 5   | I     | 31  | LYS  | N-CA-C | -5.79 | 104.97      | 112.68   |
| 1   | B     | 30  | VAL  | N-CA-C | -5.79 | 100.14      | 108.42   |
| 1   | B     | 277 | THR  | N-CA-C | -5.79 | 98.47       | 110.80   |
| 4   | H     | 6   | ASP  | CA-C-N | 5.78  | 124.98      | 118.97   |
| 4   | H     | 6   | ASP  | C-N-CA | 5.78  | 124.98      | 118.97   |
| 1   | B     | 186 | THR  | N-CA-C | 5.78  | 117.47      | 109.15   |
| 3   | G     | 127 | SER  | CA-C-N | 5.77  | 128.01      | 120.28   |
| 3   | G     | 127 | SER  | C-N-CA | 5.77  | 128.01      | 120.28   |
| 1   | B     | 338 | SER  | CA-C-N | 5.77  | 127.94      | 120.44   |
| 1   | B     | 338 | SER  | C-N-CA | 5.77  | 127.94      | 120.44   |
| 2   | D     | 286 | TYR  | CA-C-N | 5.77  | 130.36      | 121.19   |
| 2   | D     | 286 | TYR  | C-N-CA | 5.77  | 130.36      | 121.19   |
| 1   | B     | 147 | ILE  | CA-C-N | 5.76  | 129.02      | 120.95   |
| 1   | B     | 147 | ILE  | C-N-CA | 5.76  | 129.02      | 120.95   |
| 2   | D     | 46  | GLN  | N-CA-C | 5.76  | 119.07      | 110.14   |
| 8   | N     | 156 | ALA  | CA-C-N | 5.76  | 128.00      | 120.28   |
| 8   | N     | 156 | ALA  | C-N-CA | 5.76  | 128.00      | 120.28   |
| 9   | P     | 44  | ALA  | N-CA-C | 5.76  | 117.56      | 111.28   |
| 2   | D     | 369 | GLY  | N-CA-C | -5.75 | 107.38      | 115.32   |
| 1   | B     | 274 | ASP  | N-CA-C | -5.75 | 102.18      | 110.40   |
| 9   | O     | 15  | ILE  | CA-C-N | 5.75  | 127.98      | 120.28   |
| 9   | O     | 15  | ILE  | C-N-CA | 5.75  | 127.98      | 120.28   |
| 1   | A     | 110 | ALA  | N-CA-C | -5.74 | 106.82      | 113.88   |
| 1   | A     | 291 | THR  | CA-C-N | 5.74  | 127.97      | 120.28   |
| 1   | A     | 291 | THR  | C-N-CA | 5.74  | 127.97      | 120.28   |
| 2   | F     | 90  | GLY  | N-CA-C | -5.74 | 105.26      | 113.86   |
| 5   | I     | 102 | LYS  | CA-C-N | 5.73  | 128.43      | 120.63   |
| 5   | I     | 102 | LYS  | C-N-CA | 5.73  | 128.43      | 120.63   |
| 2   | F     | 358 | LEU  | CA-C-N | 5.73  | 130.52      | 121.99   |
| 2   | F     | 358 | LEU  | C-N-CA | 5.73  | 130.52      | 121.99   |
| 3   | G     | 160 | ARG  | N-CA-C | 5.73  | 117.60      | 111.36   |
| 1   | C     | 435 | LEU  | N-CA-C | -5.73 | 106.06      | 113.16   |
| 1   | A     | 511 | LYS  | N-CA-C | -5.72 | 102.80      | 111.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 311 | GLU  | N-CA-C | -5.72 | 104.42      | 111.40   |
| 6   | L     | 125 | PRO  | N-CA-C | -5.72 | 106.55      | 114.27   |
| 1   | B     | 571 | GLN  | N-CA-C | -5.71 | 106.27      | 113.18   |
| 1   | C     | 62  | GLU  | CA-C-N | 5.71  | 125.72      | 119.89   |
| 1   | C     | 62  | GLU  | C-N-CA | 5.71  | 125.72      | 119.89   |
| 9   | X     | 53  | GLY  | N-CA-C | 5.71  | 119.58      | 112.73   |
| 1   | C     | 412 | SER  | CA-C-N | 5.71  | 128.19      | 120.65   |
| 1   | C     | 412 | SER  | C-N-CA | 5.71  | 128.19      | 120.65   |
| 1   | A     | 98  | THR  | N-CA-C | -5.71 | 103.80      | 112.99   |
| 1   | B     | 190 | ARG  | N-CA-C | -5.71 | 106.30      | 113.72   |
| 3   | G     | 142 | ASN  | N-CA-C | -5.70 | 106.95      | 114.31   |
| 7   | M     | 27  | GLU  | CA-C-N | 5.70  | 128.49      | 120.28   |
| 7   | M     | 27  | GLU  | C-N-CA | 5.70  | 128.49      | 120.28   |
| 2   | F     | 286 | TYR  | N-CA-C | -5.70 | 106.09      | 113.16   |
| 6   | L     | 141 | GLU  | N-CA-C | -5.70 | 100.28      | 108.60   |
| 9   | Q     | 56  | LEU  | N-CA-C | -5.70 | 104.99      | 111.14   |
| 2   | D     | 364 | ASN  | N-CA-C | -5.69 | 100.51      | 109.50   |
| 8   | N     | 330 | PHE  | CA-C-N | 5.69  | 128.48      | 120.28   |
| 8   | N     | 330 | PHE  | C-N-CA | 5.69  | 128.48      | 120.28   |
| 1   | A     | 548 | ILE  | N-CA-C | -5.69 | 104.80      | 111.00   |
| 1   | A     | 406 | PHE  | CA-C-N | 5.69  | 131.76      | 123.12   |
| 1   | A     | 406 | PHE  | C-N-CA | 5.69  | 131.76      | 123.12   |
| 9   | S     | 53  | GLY  | CA-C-N | 5.69  | 127.90      | 120.28   |
| 9   | S     | 53  | GLY  | C-N-CA | 5.69  | 127.90      | 120.28   |
| 2   | D     | 131 | ILE  | CA-C-N | 5.69  | 129.98      | 122.30   |
| 2   | D     | 131 | ILE  | C-N-CA | 5.69  | 129.98      | 122.30   |
| 9   | Z     | 16  | ALA  | N-CA-C | 5.68  | 117.55      | 111.36   |
| 9   | Y     | 28  | LEU  | CA-C-N | 5.67  | 126.27      | 119.98   |
| 9   | Y     | 28  | LEU  | C-N-CA | 5.67  | 126.27      | 119.98   |
| 3   | G     | 8   | ARG  | CA-C-N | 5.67  | 132.36      | 121.54   |
| 3   | G     | 8   | ARG  | C-N-CA | 5.67  | 132.36      | 121.54   |
| 6   | L     | 116 | PRO  | N-CA-C | -5.66 | 106.76      | 114.80   |
| 1   | B     | 350 | TYR  | N-CA-C | -5.66 | 102.64      | 109.72   |
| 8   | N     | 324 | PRO  | CA-C-O | -5.66 | 112.35      | 120.56   |
| 9   | X     | 63  | GLU  | CA-C-N | 5.65  | 128.42      | 120.28   |
| 9   | X     | 63  | GLU  | C-N-CA | 5.65  | 128.42      | 120.28   |
| 2   | E     | 242 | ALA  | CA-C-N | 5.65  | 132.34      | 121.54   |
| 2   | E     | 242 | ALA  | C-N-CA | 5.65  | 132.34      | 121.54   |
| 2   | F     | 381 | GLN  | N-CA-C | -5.65 | 98.76       | 110.80   |
| 2   | E     | 450 | GLU  | N-CA-C | -5.65 | 104.96      | 113.89   |
| 1   | C     | 248 | ASP  | N-CA-C | -5.65 | 106.52      | 113.41   |
| 9   | W     | 12  | ARG  | CA-C-N | 5.65  | 126.25      | 119.98   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | W     | 12  | ARG  | C-N-CA | 5.65  | 126.25      | 119.98   |
| 9   | Q     | 53  | GLY  | N-CA-C | 5.64  | 119.49      | 112.73   |
| 3   | G     | 193 | ARG  | N-CA-C | -5.63 | 105.05      | 111.14   |
| 9   | W     | 37  | ILE  | CA-C-N | 5.63  | 126.23      | 119.98   |
| 9   | W     | 37  | ILE  | C-N-CA | 5.63  | 126.23      | 119.98   |
| 2   | F     | 383 | TYR  | N-CA-C | -5.63 | 104.78      | 111.03   |
| 1   | A     | 543 | PRO  | CA-C-N | 5.63  | 128.17      | 120.46   |
| 1   | A     | 543 | PRO  | C-N-CA | 5.63  | 128.17      | 120.46   |
| 7   | M     | 28  | ALA  | CA-C-N | 5.63  | 128.38      | 120.28   |
| 7   | M     | 28  | ALA  | C-N-CA | 5.63  | 128.38      | 120.28   |
| 2   | E     | 135 | ILE  | CA-C-N | 5.62  | 127.81      | 120.28   |
| 2   | E     | 135 | ILE  | C-N-CA | 5.62  | 127.81      | 120.28   |
| 2   | F     | 423 | ILE  | N-CA-C | -5.61 | 105.38      | 110.82   |
| 2   | D     | 226 | ASP  | CA-C-O | -5.61 | 115.08      | 120.97   |
| 9   | Z     | 52  | PHE  | N-CA-C | 5.61  | 117.40      | 111.28   |
| 1   | A     | 325 | ASP  | CA-C-N | 5.61  | 130.09      | 122.07   |
| 1   | A     | 325 | ASP  | C-N-CA | 5.61  | 130.09      | 122.07   |
| 3   | G     | 205 | GLU  | N-CA-C | -5.61 | 106.20      | 113.16   |
| 8   | N     | 387 | GLU  | CA-C-O | -5.61 | 112.48      | 120.16   |
| 6   | J     | 174 | ALA  | N-CA-C | 5.60  | 117.47      | 111.36   |
| 2   | D     | 220 | PHE  | N-CA-C | -5.60 | 101.35      | 110.20   |
| 6   | L     | 27  | ALA  | N-CA-C | -5.60 | 104.80      | 111.69   |
| 9   | S     | 52  | PHE  | N-CA-C | 5.60  | 117.38      | 111.28   |
| 3   | G     | 200 | LYS  | CA-C-N | 5.60  | 128.42      | 120.53   |
| 3   | G     | 200 | LYS  | C-N-CA | 5.60  | 128.42      | 120.53   |
| 2   | F     | 239 | LEU  | N-CA-C | -5.60 | 104.87      | 110.97   |
| 2   | F     | 453 | ARG  | CA-C-N | 5.59  | 128.91      | 120.75   |
| 2   | F     | 453 | ARG  | C-N-CA | 5.59  | 128.91      | 120.75   |
| 8   | N     | 216 | ALA  | CA-C-N | 5.59  | 127.77      | 120.28   |
| 8   | N     | 216 | ALA  | C-N-CA | 5.59  | 127.77      | 120.28   |
| 5   | K     | 32  | GLN  | CA-C-N | 5.59  | 127.70      | 120.44   |
| 5   | K     | 32  | GLN  | C-N-CA | 5.59  | 127.70      | 120.44   |
| 2   | E     | 363 | ASN  | N-CA-C | -5.58 | 107.11      | 114.31   |
| 1   | A     | 461 | GLU  | CA-C-N | 5.58  | 130.06      | 121.19   |
| 1   | A     | 461 | GLU  | C-N-CA | 5.58  | 130.06      | 121.19   |
| 1   | B     | 299 | ARG  | N-CA-C | -5.58 | 104.83      | 111.69   |
| 4   | H     | 3   | VAL  | N-CA-C | 5.58  | 118.46      | 110.09   |
| 1   | A     | 130 | ARG  | N-CA-C | -5.58 | 100.83      | 109.14   |
| 2   | D     | 309 | THR  | N-CA-C | -5.57 | 99.01       | 108.26   |
| 2   | E     | 196 | ILE  | N-CA-C | 5.57  | 120.93      | 109.34   |
| 1   | B     | 220 | MET  | N-CA-C | -5.57 | 105.26      | 113.61   |
| 8   | N     | 324 | PRO  | N-CA-C | 5.57  | 117.49      | 110.70   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | R     | 58  | PHE  | N-CA-C | 5.56  | 117.02      | 111.07   |
| 2   | F     | 370 | LYS  | N-CA-C | -5.56 | 98.95       | 110.80   |
| 4   | H     | 58  | ALA  | N-CA-C | -5.56 | 105.12      | 111.07   |
| 1   | A     | 11  | GLY  | CA-C-N | 5.55  | 126.78      | 119.84   |
| 1   | A     | 11  | GLY  | C-N-CA | 5.55  | 126.78      | 119.84   |
| 2   | D     | 169 | ARG  | N-CA-C | -5.55 | 106.18      | 113.12   |
| 2   | E     | 435 | SER  | CA-C-N | 5.55  | 132.15      | 121.54   |
| 2   | E     | 435 | SER  | C-N-CA | 5.55  | 132.15      | 121.54   |
| 7   | M     | 23  | SER  | CA-C-N | 5.55  | 127.65      | 120.44   |
| 7   | M     | 23  | SER  | C-N-CA | 5.55  | 127.65      | 120.44   |
| 1   | C     | 241 | LEU  | N-CA-C | -5.54 | 105.32      | 111.36   |
| 9   | V     | 55  | ALA  | CA-C-N | 5.54  | 128.16      | 120.29   |
| 9   | V     | 55  | ALA  | C-N-CA | 5.54  | 128.16      | 120.29   |
| 8   | N     | 203 | ARG  | N-CA-C | -5.53 | 102.29      | 110.48   |
| 2   | E     | 456 | LYS  | CA-C-O | 5.53  | 126.60      | 120.63   |
| 8   | N     | 505 | LEU  | N-CA-C | 5.53  | 117.31      | 111.28   |
| 8   | N     | 537 | LEU  | N-CA-C | -5.53 | 106.20      | 113.17   |
| 1   | A     | 350 | TYR  | O-C-N  | -5.53 | 114.96      | 121.32   |
| 2   | D     | 148 | GLN  | N-CA-C | 5.53  | 115.84      | 108.38   |
| 2   | E     | 321 | ARG  | N-CA-C | -5.53 | 106.54      | 113.28   |
| 1   | C     | 109 | HIS  | N-CA-C | -5.52 | 101.28      | 110.17   |
| 2   | E     | 112 | LEU  | CA-C-N | 5.52  | 125.53      | 119.89   |
| 2   | E     | 112 | LEU  | C-N-CA | 5.52  | 125.53      | 119.89   |
| 1   | C     | 30  | VAL  | N-CA-C | -5.52 | 99.86       | 108.81   |
| 7   | M     | 5   | PHE  | CA-C-N | 5.52  | 127.99      | 120.54   |
| 7   | M     | 5   | PHE  | C-N-CA | 5.52  | 127.99      | 120.54   |
| 9   | X     | 56  | LEU  | N-CA-C | -5.52 | 105.18      | 111.14   |
| 2   | E     | 254 | LEU  | N-CA-C | -5.51 | 99.74       | 108.73   |
| 6   | J     | 100 | TRP  | CA-C-O | -5.51 | 112.61      | 120.16   |
| 1   | C     | 529 | ALA  | N-CA-C | -5.51 | 104.92      | 111.03   |
| 1   | B     | 292 | SER  | N-CA-C | -5.50 | 106.24      | 113.17   |
| 2   | F     | 48  | ILE  | N-CA-C | -5.50 | 101.16      | 108.96   |
| 1   | B     | 122 | MET  | N-CA-C | -5.49 | 105.19      | 112.94   |
| 2   | D     | 197 | THR  | CA-C-N | 5.49  | 132.02      | 121.54   |
| 2   | D     | 197 | THR  | C-N-CA | 5.49  | 132.02      | 121.54   |
| 1   | A     | 33  | GLU  | N-CA-C | -5.49 | 106.63      | 113.38   |
| 9   | P     | 57  | ILE  | N-CA-C | 5.49  | 116.26      | 110.72   |
| 1   | C     | 500 | TYR  | N-CA-C | -5.48 | 106.36      | 113.16   |
| 9   | P     | 79  | ARG  | N-CA-C | -5.48 | 106.75      | 113.50   |
| 1   | C     | 553 | TYR  | N-CA-C | -5.47 | 104.47      | 113.50   |
| 2   | D     | 88  | MET  | N-CA-C | -5.47 | 104.18      | 112.99   |
| 1   | A     | 298 | ALA  | CA-C-N | 5.46  | 128.15      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 298 | ALA  | C-N-CA | 5.46  | 128.15      | 120.28   |
| 2   | D     | 114 | ILE  | CA-C-N | 5.46  | 127.60      | 120.28   |
| 2   | D     | 114 | ILE  | C-N-CA | 5.46  | 127.60      | 120.28   |
| 1   | B     | 149 | VAL  | N-CA-C | -5.46 | 103.94      | 109.02   |
| 1   | C     | 528 | ALA  | N-CA-C | -5.46 | 106.66      | 113.38   |
| 9   | V     | 56  | LEU  | N-CA-C | -5.46 | 105.41      | 111.36   |
| 2   | E     | 167 | ILE  | N-CA-C | -5.45 | 105.06      | 111.00   |
| 6   | J     | 23  | ALA  | CA-C-N | 5.45  | 127.52      | 120.44   |
| 6   | J     | 23  | ALA  | C-N-CA | 5.45  | 127.52      | 120.44   |
| 9   | U     | 35  | ALA  | N-CA-C | 5.45  | 116.90      | 111.07   |
| 1   | B     | 78  | GLY  | CA-C-N | 5.44  | 127.83      | 120.65   |
| 1   | B     | 78  | GLY  | C-N-CA | 5.44  | 127.83      | 120.65   |
| 2   | E     | 395 | LEU  | CA-C-N | 5.44  | 127.53      | 120.56   |
| 2   | E     | 395 | LEU  | C-N-CA | 5.44  | 127.53      | 120.56   |
| 8   | N     | 499 | VAL  | CA-C-N | 5.44  | 126.02      | 119.98   |
| 8   | N     | 499 | VAL  | C-N-CA | 5.44  | 126.02      | 119.98   |
| 9   | T     | 77  | ASN  | N-CA-C | 5.44  | 122.38      | 110.80   |
| 9   | Q     | 11  | ASP  | N-CA-C | 5.43  | 116.89      | 111.07   |
| 9   | P     | 76  | LEU  | N-CA-C | 5.43  | 116.88      | 111.07   |
| 2   | E     | 40  | GLY  | N-CA-C | -5.43 | 107.62      | 115.27   |
| 1   | C     | 423 | ASN  | CA-C-N | 5.42  | 127.99      | 120.29   |
| 1   | C     | 423 | ASN  | C-N-CA | 5.42  | 127.99      | 120.29   |
| 5   | K     | 111 | VAL  | CA-C-N | 5.42  | 127.81      | 120.38   |
| 5   | K     | 111 | VAL  | C-N-CA | 5.42  | 127.81      | 120.38   |
| 1   | B     | 389 | GLY  | N-CA-C | -5.42 | 107.79      | 115.43   |
| 3   | G     | 155 | LYS  | CA-C-N | 5.42  | 127.80      | 120.38   |
| 3   | G     | 155 | LYS  | C-N-CA | 5.42  | 127.80      | 120.38   |
| 2   | D     | 433 | GLU  | CA-C-N | 5.42  | 127.80      | 120.38   |
| 2   | D     | 433 | GLU  | C-N-CA | 5.42  | 127.80      | 120.38   |
| 2   | F     | 72  | SER  | N-CA-C | -5.42 | 101.27      | 108.74   |
| 1   | B     | 102 | ILE  | N-CA-C | -5.41 | 100.52      | 108.85   |
| 1   | A     | 2   | ILE  | N-CA-C | -5.41 | 100.90      | 108.80   |
| 9   | X     | 48  | ASP  | CA-C-N | 5.41  | 128.53      | 120.31   |
| 9   | X     | 48  | ASP  | C-N-CA | 5.41  | 128.53      | 120.31   |
| 2   | E     | 211 | THR  | N-CA-C | -5.41 | 105.32      | 112.94   |
| 5   | I     | 107 | LEU  | CA-C-N | 5.41  | 127.84      | 120.54   |
| 5   | I     | 107 | LEU  | C-N-CA | 5.41  | 127.84      | 120.54   |
| 7   | M     | 6   | ALA  | CA-C-N | 5.41  | 127.47      | 120.44   |
| 7   | M     | 6   | ALA  | C-N-CA | 5.41  | 127.47      | 120.44   |
| 2   | E     | 315 | SER  | N-CA-C | -5.40 | 102.75      | 110.59   |
| 1   | B     | 425 | ASN  | N-CA-C | -5.40 | 105.39      | 111.28   |
| 2   | D     | 62  | GLU  | CA-C-N | 5.40  | 129.74      | 120.72   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | D     | 62  | GLU  | C-N-CA | 5.40  | 129.74      | 120.72   |
| 1   | B     | 26  | ASP  | CA-C-N | 5.40  | 129.28      | 121.18   |
| 1   | B     | 26  | ASP  | C-N-CA | 5.40  | 129.28      | 121.18   |
| 1   | C     | 411 | ALA  | N-CA-C | 5.40  | 119.87      | 113.12   |
| 1   | C     | 358 | LEU  | N-CA-C | -5.39 | 104.35      | 111.96   |
| 1   | B     | 426 | GLY  | CA-C-N | 5.39  | 131.84      | 121.54   |
| 1   | B     | 426 | GLY  | C-N-CA | 5.39  | 131.84      | 121.54   |
| 1   | C     | 331 | ALA  | CA-C-N | 5.39  | 128.04      | 120.28   |
| 1   | C     | 331 | ALA  | C-N-CA | 5.39  | 128.04      | 120.28   |
| 4   | H     | 30  | GLN  | CA-C-N | 5.39  | 131.83      | 121.54   |
| 4   | H     | 30  | GLN  | C-N-CA | 5.39  | 131.83      | 121.54   |
| 8   | N     | 273 | ARG  | CA-C-N | 5.39  | 127.77      | 120.44   |
| 8   | N     | 273 | ARG  | C-N-CA | 5.39  | 127.77      | 120.44   |
| 2   | F     | 198 | GLN  | CA-C-N | 5.38  | 127.76      | 120.65   |
| 2   | F     | 198 | GLN  | C-N-CA | 5.38  | 127.76      | 120.65   |
| 1   | B     | 475 | ALA  | CA-C-N | 5.38  | 131.82      | 121.54   |
| 1   | B     | 475 | ALA  | C-N-CA | 5.38  | 131.82      | 121.54   |
| 6   | J     | 41  | LEU  | N-CA-C | -5.38 | 104.98      | 112.45   |
| 9   | Q     | 26  | ALA  | CA-C-N | 5.37  | 127.48      | 120.28   |
| 9   | Q     | 26  | ALA  | C-N-CA | 5.37  | 127.48      | 120.28   |
| 9   | X     | 46  | ALA  | CA-C-N | 5.37  | 127.75      | 120.44   |
| 9   | X     | 46  | ALA  | C-N-CA | 5.37  | 127.75      | 120.44   |
| 2   | E     | 410 | ARG  | CA-C-N | 5.37  | 128.25      | 120.79   |
| 2   | E     | 410 | ARG  | C-N-CA | 5.37  | 128.25      | 120.79   |
| 2   | F     | 40  | GLY  | N-CA-C | -5.37 | 108.22      | 115.36   |
| 9   | T     | 55  | ALA  | CA-C-N | 5.37  | 127.92      | 120.29   |
| 9   | T     | 55  | ALA  | C-N-CA | 5.37  | 127.92      | 120.29   |
| 1   | C     | 187 | TRP  | CA-C-N | 5.37  | 125.13      | 119.76   |
| 1   | C     | 187 | TRP  | C-N-CA | 5.37  | 125.13      | 119.76   |
| 5   | I     | 35  | GLU  | N-CA-C | -5.37 | 106.58      | 113.23   |
| 3   | G     | 20  | LEU  | N-CA-C | -5.37 | 105.07      | 111.03   |
| 2   | D     | 292 | ALA  | CA-C-N | 5.36  | 129.18      | 120.60   |
| 2   | D     | 292 | ALA  | C-N-CA | 5.36  | 129.18      | 120.60   |
| 2   | E     | 445 | MET  | N-CA-C | -5.36 | 106.24      | 112.89   |
| 2   | E     | 436 | LEU  | CA-C-N | 5.36  | 131.78      | 121.54   |
| 2   | E     | 436 | LEU  | C-N-CA | 5.36  | 131.78      | 121.54   |
| 2   | E     | 183 | LYS  | CA-C-N | 5.35  | 127.45      | 120.28   |
| 2   | E     | 183 | LYS  | C-N-CA | 5.35  | 127.45      | 120.28   |
| 8   | N     | 277 | ALA  | N-CA-C | -5.35 | 99.40       | 110.80   |
| 2   | D     | 453 | ARG  | N-CA-C | -5.35 | 104.03      | 110.88   |
| 1   | C     | 211 | ILE  | N-CA-C | -5.35 | 98.22       | 109.34   |
| 1   | A     | 341 | LEU  | N-CA-C | -5.34 | 102.29      | 110.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | N     | 554 | GLN  | N-CA-C | -5.34 | 105.62      | 111.82   |
| 4   | H     | 6   | ASP  | N-CA-C | -5.34 | 101.65      | 109.50   |
| 8   | N     | 549 | PRO  | CA-C-N | 5.34  | 129.63      | 120.72   |
| 8   | N     | 549 | PRO  | C-N-CA | 5.34  | 129.63      | 120.72   |
| 6   | J     | 29  | ALA  | CA-C-N | 5.33  | 127.28      | 120.56   |
| 6   | J     | 29  | ALA  | C-N-CA | 5.33  | 127.28      | 120.56   |
| 8   | N     | 512 | ALA  | CA-C-N | 5.33  | 127.95      | 120.28   |
| 8   | N     | 512 | ALA  | C-N-CA | 5.33  | 127.95      | 120.28   |
| 8   | N     | 603 | VAL  | CA-C-N | 5.33  | 127.42      | 120.28   |
| 8   | N     | 603 | VAL  | C-N-CA | 5.33  | 127.42      | 120.28   |
| 1   | C     | 351 | PRO  | N-CA-C | -5.33 | 104.20      | 110.70   |
| 8   | N     | 28  | GLY  | CA-C-N | 5.32  | 127.75      | 120.35   |
| 8   | N     | 28  | GLY  | C-N-CA | 5.32  | 127.75      | 120.35   |
| 9   | O     | 39  | ALA  | CA-C-N | 5.32  | 127.41      | 120.28   |
| 9   | O     | 39  | ALA  | C-N-CA | 5.32  | 127.41      | 120.28   |
| 2   | E     | 441 | ALA  | N-CA-C | -5.32 | 106.30      | 112.89   |
| 9   | W     | 53  | GLY  | N-CA-C | 5.32  | 119.11      | 112.73   |
| 1   | A     | 479 | ALA  | CA-C-N | 5.31  | 127.66      | 120.65   |
| 1   | A     | 479 | ALA  | C-N-CA | 5.31  | 127.66      | 120.65   |
| 8   | N     | 515 | TYR  | N-CA-C | -5.31 | 107.45      | 114.04   |
| 8   | N     | 630 | THR  | CA-C-N | 5.31  | 130.10      | 122.35   |
| 8   | N     | 630 | THR  | C-N-CA | 5.31  | 130.10      | 122.35   |
| 3   | G     | 151 | GLY  | CA-C-N | 5.31  | 128.17      | 120.79   |
| 3   | G     | 151 | GLY  | C-N-CA | 5.31  | 128.17      | 120.79   |
| 2   | F     | 455 | SER  | CA-C-N | 5.31  | 127.92      | 120.28   |
| 2   | F     | 455 | SER  | C-N-CA | 5.31  | 127.92      | 120.28   |
| 9   | W     | 58  | PHE  | N-CA-C | 5.31  | 116.75      | 111.07   |
| 9   | Y     | 26  | ALA  | CA-C-N | 5.30  | 127.39      | 120.28   |
| 9   | Y     | 26  | ALA  | C-N-CA | 5.30  | 127.39      | 120.28   |
| 1   | B     | 388 | GLY  | N-CA-C | -5.30 | 107.30      | 115.73   |
| 5   | I     | 43  | GLU  | CA-C-N | 5.30  | 127.65      | 120.65   |
| 5   | I     | 43  | GLU  | C-N-CA | 5.30  | 127.65      | 120.65   |
| 1   | B     | 248 | ASP  | N-CA-C | -5.30 | 99.51       | 110.80   |
| 8   | N     | 454 | ILE  | CA-C-N | 5.30  | 127.91      | 120.28   |
| 8   | N     | 454 | ILE  | C-N-CA | 5.30  | 127.91      | 120.28   |
| 2   | D     | 19  | LEU  | CA-C-N | 5.30  | 128.62      | 121.05   |
| 2   | D     | 19  | LEU  | C-N-CA | 5.30  | 128.62      | 121.05   |
| 3   | G     | 171 | GLY  | N-CA-C | -5.30 | 106.08      | 112.49   |
| 7   | M     | 108 | PRO  | CA-C-N | 5.30  | 127.38      | 120.28   |
| 7   | M     | 108 | PRO  | C-N-CA | 5.30  | 127.38      | 120.28   |
| 2   | F     | 84  | VAL  | N-CA-C | -5.29 | 101.36      | 108.35   |
| 1   | C     | 261 | GLU  | N-CA-C | -5.29 | 106.77      | 113.18   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | M     | 76  | VAL  | N-CA-C | -5.29 | 98.33       | 109.34   |
| 1   | C     | 14  | VAL  | CA-C-N | 5.29  | 130.14      | 123.10   |
| 1   | C     | 14  | VAL  | C-N-CA | 5.29  | 130.14      | 123.10   |
| 9   | Y     | 22  | ALA  | CA-C-N | 5.29  | 127.33      | 120.56   |
| 9   | Y     | 22  | ALA  | C-N-CA | 5.29  | 127.33      | 120.56   |
| 4   | H     | 9   | THR  | N-CA-C | -5.29 | 107.00      | 113.50   |
| 2   | F     | 170 | GLN  | N-CA-C | 5.28  | 117.04      | 111.28   |
| 1   | C     | 21  | GLY  | N-CA-C | -5.28 | 108.34      | 115.36   |
| 2   | D     | 237 | MET  | N-CA-C | -5.27 | 104.44      | 111.24   |
| 6   | L     | 54  | ARG  | N-CA-C | -5.27 | 105.43      | 111.07   |
| 1   | A     | 326 | SER  | CA-C-N | 5.27  | 127.77      | 120.29   |
| 1   | A     | 326 | SER  | C-N-CA | 5.27  | 127.77      | 120.29   |
| 8   | N     | 645 | PHE  | CA-C-N | 5.27  | 127.65      | 120.54   |
| 8   | N     | 645 | PHE  | C-N-CA | 5.27  | 127.65      | 120.54   |
| 7   | M     | 229 | ARG  | CA-C-N | 5.27  | 127.29      | 120.44   |
| 7   | M     | 229 | ARG  | C-N-CA | 5.27  | 127.29      | 120.44   |
| 1   | C     | 424 | TRP  | N-CA-C | -5.26 | 105.62      | 111.36   |
| 9   | V     | 68  | PHE  | CA-C-N | 5.26  | 125.82      | 119.98   |
| 9   | V     | 68  | PHE  | C-N-CA | 5.26  | 125.82      | 119.98   |
| 3   | G     | 122 | TYR  | N-CA-C | -5.26 | 105.55      | 111.28   |
| 8   | N     | 350 | VAL  | N-CA-C | 5.26  | 115.99      | 110.62   |
| 8   | N     | 495 | PHE  | CA-C-N | 5.26  | 127.85      | 120.28   |
| 8   | N     | 495 | PHE  | C-N-CA | 5.26  | 127.85      | 120.28   |
| 9   | P     | 75  | ILE  | N-CA-C | 5.25  | 115.98      | 110.62   |
| 2   | D     | 53  | GLU  | N-CA-C | -5.25 | 107.42      | 113.88   |
| 1   | A     | 26  | ASP  | CA-C-N | 5.25  | 131.42      | 121.97   |
| 1   | A     | 26  | ASP  | C-N-CA | 5.25  | 131.42      | 121.97   |
| 1   | A     | 245 | SER  | CA-C-N | 5.25  | 131.56      | 121.54   |
| 1   | A     | 245 | SER  | C-N-CA | 5.25  | 131.56      | 121.54   |
| 1   | A     | 288 | ILE  | N-CA-C | -5.25 | 101.42      | 108.35   |
| 2   | E     | 209 | GLU  | N-CA-C | -5.25 | 106.72      | 113.23   |
| 9   | X     | 18  | GLY  | CA-C-N | 5.25  | 127.31      | 120.28   |
| 9   | X     | 18  | GLY  | C-N-CA | 5.25  | 127.31      | 120.28   |
| 9   | Y     | 68  | PHE  | CA-C-N | 5.25  | 125.81      | 119.98   |
| 9   | Y     | 68  | PHE  | C-N-CA | 5.25  | 125.81      | 119.98   |
| 3   | G     | 60  | ALA  | CA-C-N | 5.25  | 129.53      | 121.19   |
| 3   | G     | 60  | ALA  | C-N-CA | 5.25  | 129.53      | 121.19   |
| 2   | D     | 143 | THR  | N-CA-C | -5.24 | 100.85      | 109.40   |
| 2   | F     | 461 | LYS  | N-CA-C | -5.24 | 107.26      | 113.97   |
| 1   | A     | 277 | THR  | N-CA-C | -5.24 | 107.43      | 113.88   |
| 9   | T     | 76  | LEU  | N-CA-C | 5.24  | 116.68      | 111.07   |
| 9   | U     | 37  | ILE  | CA-C-N | 5.24  | 125.80      | 119.98   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | U     | 37  | ILE  | C-N-CA | 5.24  | 125.80      | 119.98   |
| 9   | Z     | 19  | MET  | CA-C-N | 5.24  | 125.80      | 119.98   |
| 9   | Z     | 19  | MET  | C-N-CA | 5.24  | 125.80      | 119.98   |
| 7   | M     | 210 | SER  | N-CA-C | -5.24 | 105.65      | 111.36   |
| 5   | K     | 35  | GLU  | N-CA-C | -5.24 | 106.89      | 113.28   |
| 8   | N     | 12  | GLY  | CA-C-N | 5.24  | 126.39      | 119.84   |
| 8   | N     | 12  | GLY  | C-N-CA | 5.24  | 126.39      | 119.84   |
| 2   | E     | 421 | PHE  | CA-C-N | 5.23  | 128.66      | 120.82   |
| 2   | E     | 421 | PHE  | C-N-CA | 5.23  | 128.66      | 120.82   |
| 2   | F     | 187 | PHE  | N-CA-C | -5.23 | 98.73       | 107.99   |
| 8   | N     | 164 | ARG  | N-CA-C | -5.22 | 106.68      | 113.16   |
| 1   | C     | 12  | PRO  | N-CA-C | -5.22 | 107.93      | 114.20   |
| 9   | O     | 28  | LEU  | CA-C-N | 5.22  | 125.78      | 119.98   |
| 9   | O     | 28  | LEU  | C-N-CA | 5.22  | 125.78      | 119.98   |
| 8   | N     | 153 | VAL  | CA-C-N | 5.22  | 127.27      | 120.28   |
| 8   | N     | 153 | VAL  | C-N-CA | 5.22  | 127.27      | 120.28   |
| 1   | B     | 89  | ARG  | CA-C-N | 5.22  | 126.03      | 119.98   |
| 1   | B     | 89  | ARG  | C-N-CA | 5.22  | 126.03      | 119.98   |
| 7   | M     | 84  | VAL  | N-CA-C | -5.22 | 105.45      | 110.72   |
| 2   | E     | 377 | GLN  | N-CA-C | -5.22 | 106.42      | 112.89   |
| 8   | N     | 75  | GLU  | CA-C-N | 5.22  | 126.03      | 119.98   |
| 8   | N     | 75  | GLU  | C-N-CA | 5.22  | 126.03      | 119.98   |
| 1   | C     | 254 | GLY  | N-CA-C | -5.21 | 102.33      | 111.46   |
| 2   | E     | 110 | LYS  | N-CA-C | -5.21 | 100.39      | 108.42   |
| 1   | B     | 187 | TRP  | CA-C-N | 5.21  | 126.35      | 119.84   |
| 1   | B     | 187 | TRP  | C-N-CA | 5.21  | 126.35      | 119.84   |
| 9   | W     | 42  | VAL  | CA-C-N | 5.21  | 126.65      | 120.14   |
| 9   | W     | 42  | VAL  | C-N-CA | 5.21  | 126.65      | 120.14   |
| 2   | E     | 287 | MET  | CA-C-N | 5.21  | 127.57      | 120.54   |
| 2   | E     | 287 | MET  | C-N-CA | 5.21  | 127.57      | 120.54   |
| 8   | N     | 43  | TYR  | N-CA-C | -5.21 | 104.67      | 112.54   |
| 9   | W     | 35  | ALA  | N-CA-C | 5.21  | 116.64      | 111.07   |
| 8   | N     | 547 | MET  | N-CA-C | -5.21 | 105.64      | 112.72   |
| 9   | T     | 79  | ARG  | N-CA-C | -5.20 | 106.19      | 112.54   |
| 2   | F     | 157 | GLY  | N-CA-C | -5.20 | 107.46      | 115.73   |
| 3   | G     | 179 | ILE  | CA-C-N | 5.20  | 131.47      | 121.54   |
| 3   | G     | 179 | ILE  | C-N-CA | 5.20  | 131.47      | 121.54   |
| 9   | V     | 19  | MET  | CA-C-N | 5.20  | 125.72      | 120.00   |
| 9   | V     | 19  | MET  | C-N-CA | 5.20  | 125.72      | 120.00   |
| 9   | T     | 26  | ALA  | CA-C-N | 5.20  | 127.25      | 120.28   |
| 9   | T     | 26  | ALA  | C-N-CA | 5.20  | 127.25      | 120.28   |
| 2   | D     | 416 | ASP  | CA-C-N | 5.20  | 127.50      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | D     | 416 | ASP  | C-N-CA | 5.20  | 127.50      | 120.38   |
| 6   | J     | 135 | ALA  | N-CA-C | -5.19 | 106.09      | 112.90   |
| 8   | N     | 650 | GLU  | N-CA-C | 5.19  | 117.61      | 111.33   |
| 1   | C     | 473 | PRO  | N-CA-C | -5.19 | 101.78      | 112.47   |
| 9   | R     | 68  | PHE  | CA-C-N | 5.19  | 125.74      | 119.98   |
| 9   | R     | 68  | PHE  | C-N-CA | 5.19  | 125.74      | 119.98   |
| 8   | N     | 14  | LYS  | CA-C-N | 5.18  | 126.61      | 120.14   |
| 8   | N     | 14  | LYS  | C-N-CA | 5.18  | 126.61      | 120.14   |
| 9   | R     | 42  | VAL  | N-CA-C | 5.18  | 115.90      | 110.62   |
| 9   | S     | 10  | LEU  | CA-C-N | 5.18  | 127.17      | 120.44   |
| 9   | S     | 10  | LEU  | C-N-CA | 5.18  | 127.17      | 120.44   |
| 1   | C     | 33  | GLU  | N-CA-C | -5.17 | 104.78      | 111.71   |
| 8   | N     | 211 | LEU  | CA-C-N | 5.17  | 125.41      | 119.83   |
| 8   | N     | 211 | LEU  | C-N-CA | 5.17  | 125.41      | 119.83   |
| 1   | B     | 555 | SER  | N-CA-C | -5.17 | 101.56      | 109.41   |
| 4   | H     | 28  | GLU  | N-CA-C | -5.17 | 105.86      | 113.61   |
| 1   | A     | 414 | ALA  | N-CA-C | -5.17 | 104.60      | 112.04   |
| 1   | C     | 36  | VAL  | CA-C-N | -5.17 | 117.11      | 122.69   |
| 1   | C     | 36  | VAL  | C-N-CA | -5.17 | 117.11      | 122.69   |
| 8   | N     | 584 | ALA  | N-CA-C | -5.16 | 106.94      | 114.12   |
| 8   | N     | 640 | ARG  | CA-C-N | 5.16  | 125.16      | 119.89   |
| 8   | N     | 640 | ARG  | C-N-CA | 5.16  | 125.16      | 119.89   |
| 1   | C     | 262 | MET  | CA-C-N | 5.16  | 127.20      | 120.28   |
| 1   | C     | 262 | MET  | C-N-CA | 5.16  | 127.20      | 120.28   |
| 8   | N     | 89  | LYS  | CA-C-N | 5.16  | 127.19      | 120.28   |
| 8   | N     | 89  | LYS  | C-N-CA | 5.16  | 127.19      | 120.28   |
| 9   | W     | 15  | ILE  | CA-C-N | 5.16  | 127.19      | 120.28   |
| 9   | W     | 15  | ILE  | C-N-CA | 5.16  | 127.19      | 120.28   |
| 5   | I     | 91  | ARG  | N-CA-C | -5.15 | 106.15      | 112.90   |
| 2   | F     | 56  | VAL  | N-CA-C | -5.15 | 100.70      | 108.12   |
| 9   | Z     | 79  | ARG  | N-CA-C | -5.15 | 107.03      | 113.72   |
| 1   | C     | 431 | PHE  | N-CA-C | -5.15 | 104.70      | 112.99   |
| 9   | Q     | 60  | LEU  | N-CA-C | 5.14  | 116.89      | 111.28   |
| 2   | D     | 316 | MET  | N-CA-C | -5.14 | 104.22      | 110.13   |
| 4   | H     | 40  | GLY  | N-CA-C | -5.14 | 107.97      | 115.63   |
| 6   | L     | 41  | LEU  | N-CA-C | -5.14 | 104.64      | 112.04   |
| 8   | N     | 460 | ALA  | CA-C-N | 5.14  | 127.17      | 120.28   |
| 8   | N     | 460 | ALA  | C-N-CA | 5.14  | 127.17      | 120.28   |
| 3   | G     | 193 | ARG  | CA-C-N | 5.14  | 127.16      | 120.28   |
| 3   | G     | 193 | ARG  | C-N-CA | 5.14  | 127.16      | 120.28   |
| 2   | F     | 336 | GLN  | N-CA-C | -5.13 | 99.87       | 110.80   |
| 9   | W     | 16  | ALA  | CA-C-N | 5.13  | 127.12      | 120.70   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | W     | 16  | ALA  | C-N-CA | 5.13  | 127.12      | 120.70   |
| 1   | C     | 511 | LYS  | CA-C-N | 5.13  | 127.11      | 120.44   |
| 1   | C     | 511 | LYS  | C-N-CA | 5.13  | 127.11      | 120.44   |
| 8   | N     | 489 | HIS  | N-CA-C | -5.13 | 107.07      | 113.38   |
| 1   | A     | 7   | GLN  | N-CA-C | -5.13 | 106.16      | 112.72   |
| 7   | M     | 311 | LEU  | CA-C-N | 5.12  | 126.25      | 119.84   |
| 7   | M     | 311 | LEU  | C-N-CA | 5.12  | 126.25      | 119.84   |
| 2   | E     | 319 | ASP  | N-CA-C | -5.12 | 106.72      | 113.17   |
| 2   | D     | 30  | GLY  | N-CA-C | -5.12 | 108.64      | 115.40   |
| 2   | F     | 380 | ASP  | N-CA-C | -5.12 | 106.72      | 113.17   |
| 8   | N     | 209 | GLY  | CA-C-N | 5.12  | 127.56      | 120.29   |
| 8   | N     | 209 | GLY  | C-N-CA | 5.12  | 127.56      | 120.29   |
| 1   | A     | 556 | GLU  | N-CA-C | -5.12 | 106.99      | 113.18   |
| 6   | L     | 132 | GLU  | CA-C-N | 5.12  | 127.40      | 120.65   |
| 6   | L     | 132 | GLU  | C-N-CA | 5.12  | 127.40      | 120.65   |
| 1   | A     | 215 | LEU  | N-CA-C | -5.11 | 104.67      | 112.04   |
| 1   | A     | 466 | GLU  | N-CA-C | 5.11  | 121.69      | 110.80   |
| 6   | J     | 22  | GLU  | CA-C-N | 5.11  | 127.13      | 120.28   |
| 6   | J     | 22  | GLU  | C-N-CA | 5.11  | 127.13      | 120.28   |
| 8   | N     | 543 | ARG  | CA-C-N | 5.11  | 131.17      | 121.97   |
| 8   | N     | 543 | ARG  | C-N-CA | 5.11  | 131.17      | 121.97   |
| 2   | F     | 355 | LEU  | CA-C-O | -5.11 | 113.63      | 118.33   |
| 5   | K     | 108 | ASP  | CA-C-N | 5.11  | 127.54      | 120.29   |
| 5   | K     | 108 | ASP  | C-N-CA | 5.11  | 127.54      | 120.29   |
| 7   | M     | 291 | LYS  | CA-C-N | 5.11  | 127.12      | 120.28   |
| 7   | M     | 291 | LYS  | C-N-CA | 5.11  | 127.12      | 120.28   |
| 8   | N     | 401 | GLN  | CA-C-N | 5.11  | 127.00      | 120.56   |
| 8   | N     | 401 | GLN  | C-N-CA | 5.11  | 127.00      | 120.56   |
| 9   | O     | 10  | LEU  | CA-C-N | 5.11  | 127.08      | 120.44   |
| 9   | O     | 10  | LEU  | C-N-CA | 5.11  | 127.08      | 120.44   |
| 2   | D     | 193 | ALA  | N-CA-C | 5.10  | 116.63      | 108.41   |
| 1   | C     | 340 | ARG  | N-CA-C | -5.10 | 106.57      | 112.89   |
| 6   | J     | 79  | VAL  | N-CA-C | -5.10 | 106.10      | 110.74   |
| 8   | N     | 558 | ILE  | CA-C-N | 5.09  | 127.53      | 120.29   |
| 8   | N     | 558 | ILE  | C-N-CA | 5.09  | 127.53      | 120.29   |
| 8   | N     | 180 | VAL  | N-CA-C | -5.09 | 100.98      | 108.11   |
| 2   | D     | 34  | ASP  | N-CA-C | -5.08 | 101.01      | 108.79   |
| 2   | F     | 265 | GLU  | N-CA-C | -5.08 | 104.82      | 111.02   |
| 1   | A     | 531 | LYS  | N-CA-C | -5.08 | 106.93      | 113.23   |
| 1   | C     | 153 | VAL  | N-CA-C | -5.08 | 98.77       | 109.34   |
| 2   | F     | 172 | THR  | CA-C-N | 5.08  | 127.89      | 120.98   |
| 2   | F     | 172 | THR  | C-N-CA | 5.08  | 127.89      | 120.98   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | Q     | 45  | ILE  | CA-C-N | 5.08  | 127.05      | 120.44   |
| 9   | Q     | 45  | ILE  | C-N-CA | 5.08  | 127.05      | 120.44   |
| 2   | F     | 87  | GLU  | N-CA-C | -5.08 | 105.83      | 112.23   |
| 6   | L     | 21  | GLN  | CA-C-N | 5.08  | 127.04      | 120.44   |
| 6   | L     | 21  | GLN  | C-N-CA | 5.08  | 127.04      | 120.44   |
| 9   | O     | 26  | ALA  | CA-C-N | 5.08  | 127.04      | 120.44   |
| 9   | O     | 26  | ALA  | C-N-CA | 5.08  | 127.04      | 120.44   |
| 9   | X     | 14  | LEU  | CA-C-N | 5.08  | 127.63      | 120.42   |
| 9   | X     | 14  | LEU  | C-N-CA | 5.08  | 127.63      | 120.42   |
| 2   | E     | 431 | SER  | CA-C-N | 5.07  | 127.68      | 120.53   |
| 2   | E     | 431 | SER  | C-N-CA | 5.07  | 127.68      | 120.53   |
| 9   | R     | 10  | LEU  | CA-C-N | 5.07  | 127.03      | 120.44   |
| 9   | R     | 10  | LEU  | C-N-CA | 5.07  | 127.03      | 120.44   |
| 1   | C     | 172 | VAL  | N-CA-C | -5.07 | 107.49      | 113.42   |
| 2   | E     | 279 | GLY  | N-CA-C | -5.07 | 108.62      | 115.36   |
| 2   | F     | 80  | ALA  | N-CA-C | -5.07 | 100.00      | 110.80   |
| 2   | D     | 458 | HIS  | CA-C-N | 5.07  | 128.61      | 120.30   |
| 2   | D     | 458 | HIS  | C-N-CA | 5.07  | 128.61      | 120.30   |
| 6   | J     | 53  | TYR  | CA-C-N | 5.07  | 127.03      | 120.44   |
| 6   | J     | 53  | TYR  | C-N-CA | 5.07  | 127.03      | 120.44   |
| 8   | N     | 234 | VAL  | CA-C-N | 5.07  | 127.07      | 120.28   |
| 8   | N     | 234 | VAL  | C-N-CA | 5.07  | 127.07      | 120.28   |
| 8   | N     | 421 | GLY  | CA-C-N | 5.07  | 127.62      | 120.42   |
| 8   | N     | 421 | GLY  | C-N-CA | 5.07  | 127.62      | 120.42   |
| 9   | Z     | 18  | GLY  | CA-C-N | 5.07  | 127.07      | 120.28   |
| 9   | Z     | 18  | GLY  | C-N-CA | 5.07  | 127.07      | 120.28   |
| 1   | C     | 271 | GLU  | N-CA-C | -5.06 | 105.83      | 112.72   |
| 1   | C     | 67  | THR  | N-CA-C | -5.06 | 107.14      | 113.72   |
| 7   | M     | 170 | LYS  | CA-C-N | 5.06  | 127.06      | 120.28   |
| 7   | M     | 170 | LYS  | C-N-CA | 5.06  | 127.06      | 120.28   |
| 9   | T     | 45  | ILE  | CA-C-N | 5.06  | 127.02      | 120.44   |
| 9   | T     | 45  | ILE  | C-N-CA | 5.06  | 127.02      | 120.44   |
| 1   | B     | 537 | ASP  | CA-C-N | 5.06  | 127.56      | 120.28   |
| 1   | B     | 537 | ASP  | C-N-CA | 5.06  | 127.56      | 120.28   |
| 7   | M     | 161 | LEU  | N-CA-C | 5.06  | 117.19      | 111.02   |
| 2   | E     | 109 | GLU  | N-CA-C | -5.05 | 106.03      | 113.61   |
| 5   | I     | 33  | LEU  | CA-C-N | 5.05  | 127.56      | 120.28   |
| 5   | I     | 33  | LEU  | C-N-CA | 5.05  | 127.56      | 120.28   |
| 1   | C     | 460 | ARG  | CA-C-N | 5.05  | 127.75      | 120.38   |
| 1   | C     | 460 | ARG  | C-N-CA | 5.05  | 127.75      | 120.38   |
| 1   | A     | 386 | PRO  | N-CA-C | -5.04 | 104.55      | 110.70   |
| 5   | I     | 113 | LEU  | N-CA-C | -5.04 | 105.70      | 111.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | P     | 49  | ARG  | CA-C-N | 5.04  | 127.03      | 120.28   |
| 9   | P     | 49  | ARG  | C-N-CA | 5.04  | 127.03      | 120.28   |
| 1   | A     | 368 | VAL  | N-CA-C | 5.04  | 117.74      | 109.78   |
| 1   | C     | 102 | ILE  | N-CA-C | -5.04 | 101.23      | 108.48   |
| 1   | B     | 150 | PRO  | CA-C-N | 5.04  | 126.13      | 119.84   |
| 1   | B     | 150 | PRO  | C-N-CA | 5.04  | 126.13      | 119.84   |
| 4   | H     | 72  | LEU  | N-CA-C | -5.03 | 97.59       | 107.91   |
| 8   | N     | 17  | ALA  | N-CA-C | 5.03  | 117.42      | 111.33   |
| 9   | P     | 39  | ALA  | CA-C-N | 5.03  | 127.02      | 120.28   |
| 9   | P     | 39  | ALA  | C-N-CA | 5.03  | 127.02      | 120.28   |
| 9   | Y     | 66  | VAL  | CA-C-N | 5.03  | 127.34      | 120.46   |
| 9   | Y     | 66  | VAL  | C-N-CA | 5.03  | 127.34      | 120.46   |
| 1   | A     | 421 | ALA  | CA-C-N | 5.02  | 128.10      | 120.77   |
| 1   | A     | 421 | ALA  | C-N-CA | 5.02  | 128.10      | 120.77   |
| 9   | U     | 26  | ALA  | CA-C-N | 5.02  | 127.01      | 120.28   |
| 9   | U     | 26  | ALA  | C-N-CA | 5.02  | 127.01      | 120.28   |
| 1   | C     | 519 | ILE  | CA-C-N | 5.02  | 128.35      | 120.82   |
| 1   | C     | 519 | ILE  | C-N-CA | 5.02  | 128.35      | 120.82   |
| 1   | B     | 519 | ILE  | CA-C-N | 5.02  | 129.17      | 121.19   |
| 1   | B     | 519 | ILE  | C-N-CA | 5.02  | 129.17      | 121.19   |
| 6   | L     | 108 | ALA  | CA-C-N | 5.02  | 127.41      | 120.29   |
| 6   | L     | 108 | ALA  | C-N-CA | 5.02  | 127.41      | 120.29   |
| 6   | J     | 9   | SER  | CA-C-N | 5.01  | 127.25      | 120.38   |
| 6   | J     | 9   | SER  | C-N-CA | 5.01  | 127.25      | 120.38   |
| 1   | C     | 108 | VAL  | N-CA-C | -5.01 | 100.69      | 108.95   |
| 8   | N     | 548 | ILE  | CA-C-N | 5.01  | 126.10      | 119.84   |
| 8   | N     | 548 | ILE  | C-N-CA | 5.01  | 126.10      | 119.84   |
| 2   | F     | 162 | GLU  | N-CA-C | -5.00 | 103.28      | 111.04   |
| 5   | I     | 49  | LYS  | CA-C-N | 5.00  | 127.25      | 120.44   |
| 5   | I     | 49  | LYS  | C-N-CA | 5.00  | 127.25      | 120.44   |
| 9   | T     | 66  | VAL  | CA-C-N | 5.00  | 127.32      | 120.46   |
| 9   | T     | 66  | VAL  | C-N-CA | 5.00  | 127.32      | 120.46   |
| 1   | A     | 170 | GLU  | N-CA-C | -5.00 | 103.89      | 110.39   |
| 1   | A     | 486 | VAL  | CA-C-N | 5.00  | 125.63      | 120.03   |
| 1   | A     | 486 | VAL  | C-N-CA | 5.00  | 125.63      | 120.03   |
| 9   | P     | 61  | LEU  | CA-C-N | 5.00  | 124.78      | 119.28   |
| 9   | P     | 61  | LEU  | C-N-CA | 5.00  | 124.78      | 119.28   |

There are no chirality outliers.

All (144) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 112 | ASP  | Peptide |
| 1   | A     | 200 | ASP  | Peptide |
| 1   | A     | 258 | ARG  | Peptide |
| 1   | A     | 262 | MET  | Peptide |
| 1   | A     | 323 | MET  | Peptide |
| 1   | A     | 326 | SER  | Peptide |
| 1   | A     | 350 | TYR  | Peptide |
| 1   | A     | 366 | GLY  | Peptide |
| 1   | A     | 368 | VAL  | Peptide |
| 1   | A     | 384 | VAL  | Peptide |
| 1   | A     | 392 | SER  | Peptide |
| 1   | A     | 40  | ILE  | Peptide |
| 1   | A     | 575 | LYS  | Peptide |
| 1   | A     | 94  | ILE  | Peptide |
| 1   | B     | 142 | GLY  | Peptide |
| 1   | B     | 199 | LEU  | Peptide |
| 1   | B     | 206 | LEU  | Peptide |
| 1   | B     | 220 | MET  | Peptide |
| 1   | B     | 223 | THR  | Peptide |
| 1   | B     | 254 | GLY  | Peptide |
| 1   | B     | 290 | ASN  | Peptide |
| 1   | B     | 31  | GLY  | Peptide |
| 1   | B     | 325 | ASP  | Peptide |
| 1   | B     | 34  | GLY  | Peptide |
| 1   | B     | 345 | PRO  | Peptide |
| 1   | B     | 352 | PRO  | Peptide |
| 1   | B     | 392 | SER  | Peptide |
| 1   | B     | 45  | ASP  | Peptide |
| 1   | B     | 55  | THR  | Peptide |
| 1   | C     | 108 | VAL  | Peptide |
| 1   | C     | 18  | GLY  | Peptide |
| 1   | C     | 209 | MET  | Peptide |
| 1   | C     | 213 | ASP  | Peptide |
| 1   | C     | 237 | THR  | Peptide |
| 1   | C     | 238 | GLN  | Peptide |
| 1   | C     | 254 | GLY  | Peptide |
| 1   | C     | 272 | LEU  | Peptide |
| 1   | C     | 291 | THR  | Peptide |
| 1   | C     | 318 | PHE  | Peptide |
| 1   | C     | 320 | VAL  | Peptide |
| 1   | C     | 34  | GLY  | Peptide |
| 1   | C     | 351 | PRO  | Peptide |
| 1   | C     | 391 | MET  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | C     | 415 | PHE  | Peptide |
| 1   | C     | 417 | ARG  | Peptide |
| 1   | C     | 436 | ASP  | Peptide |
| 1   | C     | 441 | GLU  | Peptide |
| 1   | C     | 477 | GLN  | Peptide |
| 1   | C     | 50  | GLN  | Peptide |
| 1   | C     | 506 | TYR  | Peptide |
| 2   | D     | 129 | GLN  | Peptide |
| 2   | D     | 145 | VAL  | Peptide |
| 2   | D     | 153 | PHE  | Peptide |
| 2   | D     | 160 | ALA  | Peptide |
| 2   | D     | 25  | LYS  | Peptide |
| 2   | D     | 286 | TYR  | Peptide |
| 2   | D     | 319 | ASP  | Peptide |
| 2   | D     | 404 | LEU  | Peptide |
| 2   | D     | 59  | VAL  | Peptide |
| 2   | D     | 8   | TYR  | Peptide |
| 2   | E     | 158 | LEU  | Peptide |
| 2   | E     | 160 | ALA  | Peptide |
| 2   | E     | 175 | PRO  | Peptide |
| 2   | E     | 214 | LEU  | Peptide |
| 2   | E     | 228 | THR  | Peptide |
| 2   | E     | 241 | VAL  | Peptide |
| 2   | E     | 25  | LYS  | Peptide |
| 2   | E     | 257 | LEU  | Peptide |
| 2   | E     | 271 | GLY  | Peptide |
| 2   | E     | 272 | ALA  | Peptide |
| 2   | E     | 319 | ASP  | Peptide |
| 2   | E     | 335 | GLY  | Peptide |
| 2   | E     | 346 | LYS  | Peptide |
| 2   | E     | 400 | GLY  | Peptide |
| 2   | E     | 401 | GLU  | Peptide |
| 2   | E     | 63  | THR  | Peptide |
| 2   | E     | 70  | THR  | Peptide |
| 2   | F     | 135 | ILE  | Peptide |
| 2   | F     | 14  | ILE  | Peptide |
| 2   | F     | 186 | PRO  | Peptide |
| 2   | F     | 192 | ALA  | Peptide |
| 2   | F     | 213 | ALA  | Peptide |
| 2   | F     | 214 | LEU  | Peptide |
| 2   | F     | 216 | ARG  | Peptide |
| 2   | F     | 225 | ASP  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | F     | 283 | TYR  | Peptide |
| 2   | F     | 316 | MET  | Peptide |
| 2   | F     | 318 | ASP  | Peptide |
| 2   | F     | 369 | GLY  | Peptide |
| 2   | F     | 426 | GLY  | Peptide |
| 2   | F     | 6   | LYS  | Peptide |
| 2   | F     | 81  | ARG  | Peptide |
| 2   | F     | 94  | ASN  | Peptide |
| 3   | G     | 106 | ALA  | Peptide |
| 3   | G     | 119 | THR  | Peptide |
| 3   | G     | 120 | PRO  | Peptide |
| 3   | G     | 24  | GLY  | Peptide |
| 3   | G     | 26  | ASP  | Peptide |
| 3   | G     | 5   | SER  | Peptide |
| 3   | G     | 76  | VAL  | Peptide |
| 4   | H     | 5   | ALA  | Peptide |
| 4   | H     | 54  | ASP  | Peptide |
| 4   | H     | 71  | LEU  | Peptide |
| 4   | H     | 96  | LYS  | Peptide |
| 4   | H     | 99  | GLY  | Peptide |
| 6   | J     | 162 | GLN  | Peptide |
| 6   | L     | 141 | GLU  | Peptide |
| 6   | L     | 144 | ALA  | Peptide |
| 6   | L     | 157 | ALA  | Peptide |
| 6   | L     | 159 | GLY  | Peptide |
| 6   | L     | 178 | MET  | Peptide |
| 6   | L     | 94  | LEU  | Peptide |
| 7   | M     | 120 | ARG  | Peptide |
| 7   | M     | 183 | LEU  | Peptide |
| 7   | M     | 74  | ARG  | Peptide |
| 7   | M     | 75  | LEU  | Peptide |
| 8   | N     | 271 | SER  | Peptide |
| 8   | N     | 289 | LYS  | Peptide |
| 8   | N     | 297 | HIS  | Peptide |
| 8   | N     | 340 | PRO  | Peptide |
| 8   | N     | 354 | PHE  | Peptide |
| 8   | N     | 384 | LYS  | Peptide |
| 8   | N     | 387 | GLU  | Peptide |
| 8   | N     | 44  | GLN  | Peptide |
| 8   | N     | 449 | ILE  | Peptide |
| 8   | N     | 5   | MET  | Peptide |
| 8   | N     | 587 | GLU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 8   | N     | 635 | TYR  | Peptide |
| 8   | N     | 641 | PRO  | Peptide |
| 8   | N     | 82  | GLU  | Peptide |
| 9   | O     | 46  | ALA  | Peptide |
| 9   | O     | 47  | GLU  | Peptide |
| 9   | P     | 59  | LEU  | Peptide |
| 9   | P     | 60  | LEU  | Peptide |
| 9   | Q     | 60  | LEU  | Peptide |
| 9   | R     | 41  | GLY  | Peptide |
| 9   | R     | 48  | ASP  | Peptide |
| 9   | T     | 60  | LEU  | Peptide |
| 9   | T     | 76  | LEU  | Peptide |
| 9   | V     | 48  | ASP  | Peptide |
| 9   | V     | 59  | LEU  | Peptide |
| 9   | V     | 60  | LEU  | Peptide |
| 9   | X     | 41  | GLY  | Peptide |
| 9   | X     | 59  | LEU  | Peptide |

## 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     | 2307  | 0        | 654      | 4       | 0            |
| 1   | B     | 2307  | 0        | 654      | 6       | 0            |
| 1   | C     | 2307  | 0        | 654      | 8       | 0            |
| 2   | D     | 1835  | 0        | 512      | 5       | 0            |
| 2   | E     | 1835  | 0        | 512      | 2       | 0            |
| 2   | F     | 1835  | 0        | 512      | 6       | 0            |
| 3   | G     | 839   | 0        | 230      | 1       | 0            |
| 4   | H     | 399   | 0        | 119      | 1       | 0            |
| 5   | I     | 399   | 0        | 100      | 0       | 0            |
| 5   | K     | 399   | 0        | 100      | 0       | 0            |
| 6   | J     | 738   | 0        | 192      | 2       | 0            |
| 6   | L     | 738   | 0        | 192      | 0       | 0            |
| 7   | M     | 1279  | 0        | 357      | 0       | 0            |
| 8   | N     | 2526  | 0        | 709      | 1       | 0            |
| 9   | O     | 303   | 0        | 102      | 0       | 0            |
| 9   | P     | 303   | 0        | 102      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | Q     | 303   | 0        | 102      | 0       | 0            |
| 9   | R     | 303   | 0        | 102      | 1       | 0            |
| 9   | S     | 303   | 0        | 102      | 1       | 0            |
| 9   | T     | 303   | 0        | 102      | 0       | 0            |
| 9   | U     | 303   | 0        | 102      | 0       | 0            |
| 9   | V     | 303   | 0        | 102      | 0       | 0            |
| 9   | W     | 303   | 0        | 102      | 0       | 0            |
| 9   | X     | 303   | 0        | 102      | 0       | 0            |
| 9   | Y     | 303   | 0        | 102      | 0       | 0            |
| 9   | Z     | 303   | 0        | 102      | 0       | 0            |
| 10  | B     | 27    | 0        | 12       | 0       | 0            |
| 10  | C     | 27    | 0        | 12       | 0       | 0            |
| All | All   | 23433 | 0        | 6745     | 34      | 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 1.

All (34) 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:D:95:GLY:H    | 2:D:221:LEU:H   | 1.38                     | 0.69              |
| 1:A:26:ASP:H    | 1:A:39:ILE:H    | 1.44                     | 0.65              |
| 1:C:30:VAL:H    | 1:C:35:LEU:H    | 1.49                     | 0.59              |
| 6:J:151:GLY:HA2 | 6:J:167:LEU:H   | 1.67                     | 0.58              |
| 1:B:30:VAL:H    | 1:B:35:LEU:H    | 1.52                     | 0.58              |
| 3:G:8:ARG:C     | 3:G:10:ASN:H    | 2.15                     | 0.54              |
| 6:J:151:GLY:CA  | 6:J:167:LEU:H   | 2.23                     | 0.52              |
| 2:D:90:GLY:H    | 2:D:217:SER:H   | 1.61                     | 0.49              |
| 9:R:11:ASP:H    | 9:S:8:GLY:HA2   | 1.78                     | 0.49              |
| 1:C:21:GLY:HA2  | 2:F:68:LEU:H    | 1.77                     | 0.48              |
| 1:C:151:PRO:C   | 1:C:153:VAL:H   | 2.21                     | 0.48              |
| 2:F:329:THR:C   | 2:F:331:TYR:H   | 2.23                     | 0.47              |
| 1:C:24:MET:H    | 2:F:66:LEU:N    | 2.12                     | 0.47              |
| 1:C:30:VAL:H    | 1:C:35:LEU:N    | 2.11                     | 0.47              |
| 8:N:363:VAL:C   | 8:N:425:GLY:HA2 | 2.40                     | 0.47              |
| 1:C:58:LEU:H    | 2:E:29:TYR:H    | 1.63                     | 0.46              |
| 1:A:348:GLU:C   | 1:A:350:TYR:H   | 2.24                     | 0.46              |
| 2:D:341:ARG:C   | 2:D:343:LEU:H   | 2.24                     | 0.45              |
| 1:B:542:LEU:C   | 1:B:544:VAL:H   | 2.24                     | 0.45              |
| 2:F:8:TYR:H     | 2:F:73:VAL:H    | 1.65                     | 0.45              |
| 4:H:50:ALA:C    | 4:H:52:LEU:H    | 2.23                     | 0.45              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 2:F:285:GLY:C | 2:F:287:MET:H   | 2.23                     | 0.44              |
| 1:A:370:THR:H | 1:A:374:GLU:H   | 1.65                     | 0.43              |
| 1:B:260:ASN:C | 1:B:262:MET:H   | 2.27                     | 0.43              |
| 1:B:489:ILE:C | 1:B:491:ARG:H   | 2.26                     | 0.43              |
| 1:C:551:ALA:C | 1:C:553:TYR:H   | 2.26                     | 0.43              |
| 2:D:299:GLY:H | 2:D:308:VAL:H   | 1.66                     | 0.43              |
| 2:E:240:THR:C | 2:E:242:ALA:H   | 2.27                     | 0.42              |
| 1:C:28:CYS:H  | 1:C:37:GLY:H    | 1.65                     | 0.42              |
| 1:A:536:ILE:C | 1:A:538:GLU:H   | 2.27                     | 0.42              |
| 1:B:117:TRP:H | 1:B:166:TYR:H   | 1.68                     | 0.41              |
| 2:F:246:ALA:O | 2:F:306:GLY:HA3 | 2.20                     | 0.41              |
| 2:D:85:SER:C  | 2:D:87:GLU:H    | 2.29                     | 0.41              |
| 1:B:340:ARG:C | 1:B:342:GLU:H   | 2.29                     | 0.41              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 1   | A     | 575/578 (100%) | 443 (77%) | 90 (16%) | 42 (7%)  | 1           | 10 |
| 1   | B     | 575/578 (100%) | 456 (79%) | 84 (15%) | 35 (6%)  | 1           | 13 |
| 1   | C     | 575/578 (100%) | 453 (79%) | 86 (15%) | 36 (6%)  | 1           | 12 |
| 2   | D     | 457/478 (96%)  | 323 (71%) | 96 (21%) | 38 (8%)  | 0           | 9  |
| 2   | E     | 457/478 (96%)  | 357 (78%) | 56 (12%) | 44 (10%) | 0           | 7  |
| 2   | F     | 457/478 (96%)  | 336 (74%) | 77 (17%) | 44 (10%) | 0           | 7  |
| 3   | G     | 208/223 (93%)  | 149 (72%) | 35 (17%) | 24 (12%) | 0           | 5  |
| 4   | H     | 98/104 (94%)   | 74 (76%)  | 13 (13%) | 11 (11%) | 0           | 5  |
| 5   | I     | 98/120 (82%)   | 93 (95%)  | 3 (3%)   | 2 (2%)   | 6           | 31 |
| 5   | K     | 98/120 (82%)   | 95 (97%)  | 1 (1%)   | 2 (2%)   | 6           | 31 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 6   | J     | 181/188 (96%)   | 159 (88%)  | 17 (9%)   | 5 (3%)   | 4           | 24  |
| 6   | L     | 181/188 (96%)   | 155 (86%)  | 18 (10%)  | 8 (4%)   | 2           | 17  |
| 7   | M     | 318/323 (98%)   | 299 (94%)  | 11 (4%)   | 8 (2%)   | 4           | 26  |
| 8   | N     | 628/652 (96%)   | 550 (88%)  | 44 (7%)   | 34 (5%)  | 1           | 14  |
| 9   | O     | 74/99 (75%)     | 71 (96%)   | 3 (4%)    | 0        | 100         | 100 |
| 9   | P     | 74/99 (75%)     | 72 (97%)   | 1 (1%)    | 1 (1%)   | 9           | 40  |
| 9   | Q     | 74/99 (75%)     | 73 (99%)   | 1 (1%)    | 0        | 100         | 100 |
| 9   | R     | 74/99 (75%)     | 71 (96%)   | 2 (3%)    | 1 (1%)   | 9           | 40  |
| 9   | S     | 74/99 (75%)     | 70 (95%)   | 4 (5%)    | 0        | 100         | 100 |
| 9   | T     | 74/99 (75%)     | 72 (97%)   | 1 (1%)    | 1 (1%)   | 9           | 40  |
| 9   | U     | 74/99 (75%)     | 70 (95%)   | 3 (4%)    | 1 (1%)   | 9           | 40  |
| 9   | V     | 74/99 (75%)     | 71 (96%)   | 3 (4%)    | 0        | 100         | 100 |
| 9   | W     | 74/99 (75%)     | 71 (96%)   | 1 (1%)    | 2 (3%)   | 4           | 25  |
| 9   | X     | 74/99 (75%)     | 73 (99%)   | 1 (1%)    | 0        | 100         | 100 |
| 9   | Y     | 74/99 (75%)     | 72 (97%)   | 2 (3%)    | 0        | 100         | 100 |
| 9   | Z     | 74/99 (75%)     | 73 (99%)   | 1 (1%)    | 0        | 100         | 100 |
| All | All   | 5794/6274 (92%) | 4801 (83%) | 654 (11%) | 339 (6%) | 2           | 13  |

All (339) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | GLU  |
| 1   | A     | 134 | VAL  |
| 1   | A     | 159 | GLU  |
| 1   | A     | 197 | ARG  |
| 1   | A     | 202 | ASN  |
| 1   | A     | 210 | ARG  |
| 1   | A     | 247 | ALA  |
| 1   | A     | 303 | ILE  |
| 1   | A     | 304 | TYR  |
| 1   | A     | 305 | VAL  |
| 1   | A     | 351 | PRO  |
| 1   | A     | 466 | GLU  |
| 1   | A     | 535 | SER  |
| 1   | B     | 45  | ASP  |
| 1   | B     | 77  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 207 | THR  |
| 1   | B     | 223 | THR  |
| 1   | B     | 233 | GLY  |
| 1   | B     | 342 | GLU  |
| 1   | B     | 427 | SER  |
| 1   | B     | 432 | THR  |
| 1   | B     | 444 | ALA  |
| 1   | B     | 476 | LEU  |
| 1   | C     | 163 | ALA  |
| 1   | C     | 405 | ALA  |
| 1   | C     | 416 | ARG  |
| 1   | C     | 471 | VAL  |
| 1   | C     | 480 | GLU  |
| 2   | D     | 7   | GLU  |
| 2   | D     | 18  | LEU  |
| 2   | D     | 26  | ASP  |
| 2   | D     | 101 | ASP  |
| 2   | D     | 137 | THR  |
| 2   | D     | 216 | ARG  |
| 2   | D     | 307 | SER  |
| 2   | D     | 355 | LEU  |
| 2   | D     | 357 | SER  |
| 2   | D     | 419 | GLU  |
| 2   | E     | 15  | SER  |
| 2   | E     | 25  | LYS  |
| 2   | E     | 128 | GLU  |
| 2   | E     | 139 | ASP  |
| 2   | E     | 145 | VAL  |
| 2   | E     | 151 | PRO  |
| 2   | E     | 159 | PRO  |
| 2   | E     | 196 | ILE  |
| 2   | E     | 327 | ASP  |
| 2   | E     | 428 | GLN  |
| 2   | F     | 49  | GLU  |
| 2   | F     | 67  | ASP  |
| 2   | F     | 113 | PRO  |
| 2   | F     | 151 | PRO  |
| 2   | F     | 210 | ARG  |
| 2   | F     | 284 | PRO  |
| 2   | F     | 298 | ALA  |
| 2   | F     | 318 | ASP  |
| 2   | F     | 354 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 362 | MET  |
| 2   | F     | 395 | LEU  |
| 3   | G     | 7   | THR  |
| 3   | G     | 80  | ALA  |
| 3   | G     | 81  | LEU  |
| 3   | G     | 117 | VAL  |
| 3   | G     | 167 | VAL  |
| 4   | H     | 53  | PRO  |
| 4   | H     | 79  | GLU  |
| 5   | I     | 23  | ILE  |
| 6   | J     | 163 | VAL  |
| 5   | K     | 23  | ILE  |
| 6   | L     | 180 | SER  |
| 7   | M     | 4   | ASP  |
| 7   | M     | 108 | PRO  |
| 8   | N     | 37  | PRO  |
| 8   | N     | 39  | ALA  |
| 8   | N     | 72  | LEU  |
| 8   | N     | 294 | LEU  |
| 8   | N     | 348 | THR  |
| 8   | N     | 388 | PRO  |
| 8   | N     | 523 | TRP  |
| 8   | N     | 544 | ILE  |
| 9   | T     | 77  | ASN  |
| 1   | A     | 132 | GLY  |
| 1   | A     | 195 | VAL  |
| 1   | A     | 196 | GLN  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 227 | PRO  |
| 1   | A     | 229 | PRO  |
| 1   | A     | 340 | ARG  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 413 | LEU  |
| 1   | A     | 443 | VAL  |
| 1   | A     | 471 | VAL  |
| 1   | A     | 510 | LYS  |
| 1   | B     | 85  | ASP  |
| 1   | B     | 163 | ALA  |
| 1   | B     | 210 | ARG  |
| 1   | B     | 275 | PRO  |
| 1   | B     | 392 | SER  |
| 1   | B     | 463 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 512 | ALA  |
| 1   | C     | 25  | TYR  |
| 1   | C     | 64  | VAL  |
| 1   | C     | 194 | PRO  |
| 1   | C     | 202 | ASN  |
| 1   | C     | 227 | PRO  |
| 1   | C     | 245 | SER  |
| 1   | C     | 326 | SER  |
| 2   | D     | 128 | GLU  |
| 2   | D     | 215 | SER  |
| 2   | D     | 239 | LEU  |
| 2   | D     | 256 | ILE  |
| 2   | D     | 298 | ALA  |
| 2   | D     | 332 | ILE  |
| 2   | D     | 336 | GLN  |
| 2   | D     | 399 | ILE  |
| 2   | E     | 30  | GLY  |
| 2   | E     | 53  | GLU  |
| 2   | E     | 71  | THR  |
| 2   | E     | 101 | ASP  |
| 2   | E     | 140 | VAL  |
| 2   | E     | 178 | SER  |
| 2   | E     | 194 | MET  |
| 2   | E     | 354 | PRO  |
| 2   | E     | 360 | ARG  |
| 2   | E     | 375 | HIS  |
| 2   | E     | 389 | GLY  |
| 2   | E     | 436 | LEU  |
| 2   | F     | 79  | VAL  |
| 2   | F     | 114 | ILE  |
| 2   | F     | 148 | GLN  |
| 2   | F     | 237 | MET  |
| 2   | F     | 293 | THR  |
| 2   | F     | 330 | GLY  |
| 2   | F     | 351 | PRO  |
| 2   | F     | 370 | LYS  |
| 3   | G     | 4   | VAL  |
| 3   | G     | 66  | LEU  |
| 3   | G     | 87  | GLU  |
| 3   | G     | 89  | VAL  |
| 3   | G     | 99  | SER  |
| 3   | G     | 112 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 114 | LEU  |
| 3   | G     | 119 | THR  |
| 3   | G     | 134 | ALA  |
| 3   | G     | 168 | VAL  |
| 3   | G     | 174 | ALA  |
| 4   | H     | 15  | LEU  |
| 4   | H     | 21  | TYR  |
| 6   | J     | 121 | LEU  |
| 6   | J     | 154 | ALA  |
| 6   | L     | 140 | VAL  |
| 8   | N     | 77  | ALA  |
| 8   | N     | 185 | LYS  |
| 8   | N     | 277 | ALA  |
| 8   | N     | 395 | ALA  |
| 8   | N     | 520 | GLN  |
| 8   | N     | 586 | ALA  |
| 8   | N     | 593 | GLY  |
| 8   | N     | 637 | GLU  |
| 9   | W     | 6   | ALA  |
| 1   | A     | 246 | ASN  |
| 1   | A     | 302 | SER  |
| 1   | A     | 397 | GLN  |
| 1   | A     | 474 | ASP  |
| 1   | B     | 23  | ARG  |
| 1   | B     | 88  | GLN  |
| 1   | B     | 278 | GLY  |
| 1   | B     | 354 | LEU  |
| 1   | B     | 375 | GLU  |
| 1   | B     | 387 | PRO  |
| 1   | B     | 443 | VAL  |
| 1   | C     | 45  | ASP  |
| 1   | C     | 57  | GLY  |
| 1   | C     | 207 | THR  |
| 1   | C     | 234 | LYS  |
| 1   | C     | 243 | LYS  |
| 1   | C     | 282 | MET  |
| 1   | C     | 302 | SER  |
| 1   | C     | 352 | PRO  |
| 1   | C     | 392 | SER  |
| 1   | C     | 510 | LYS  |
| 2   | D     | 10  | GLY  |
| 2   | D     | 64  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 67  | ASP  |
| 2   | D     | 159 | PRO  |
| 2   | D     | 166 | GLN  |
| 2   | D     | 240 | THR  |
| 2   | E     | 215 | SER  |
| 2   | E     | 276 | GLU  |
| 2   | E     | 336 | GLN  |
| 2   | E     | 356 | PRO  |
| 2   | E     | 390 | VAL  |
| 2   | F     | 24  | ALA  |
| 2   | F     | 62  | GLU  |
| 2   | F     | 77  | GLU  |
| 2   | F     | 80  | ALA  |
| 2   | F     | 119 | LEU  |
| 2   | F     | 128 | GLU  |
| 2   | F     | 164 | ALA  |
| 2   | F     | 168 | ALA  |
| 3   | G     | 116 | PRO  |
| 3   | G     | 180 | GLN  |
| 4   | H     | 25  | SER  |
| 4   | H     | 77  | LEU  |
| 6   | J     | 138 | ARG  |
| 6   | L     | 96  | GLN  |
| 6   | L     | 160 | LYS  |
| 7   | M     | 245 | SER  |
| 8   | N     | 35  | LEU  |
| 8   | N     | 42  | ALA  |
| 8   | N     | 74  | ALA  |
| 8   | N     | 271 | SER  |
| 8   | N     | 387 | GLU  |
| 8   | N     | 400 | PRO  |
| 8   | N     | 519 | LEU  |
| 9   | U     | 77  | ASN  |
| 1   | A     | 25  | TYR  |
| 1   | A     | 390 | ASP  |
| 1   | B     | 25  | TYR  |
| 1   | B     | 408 | ARG  |
| 1   | C     | 36  | VAL  |
| 1   | C     | 304 | TYR  |
| 1   | C     | 473 | PRO  |
| 1   | C     | 484 | ILE  |
| 2   | D     | 96  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 343 | LEU  |
| 2   | D     | 351 | PRO  |
| 2   | D     | 354 | PRO  |
| 2   | D     | 435 | SER  |
| 2   | E     | 17  | PRO  |
| 2   | E     | 275 | GLU  |
| 2   | E     | 278 | PRO  |
| 2   | E     | 383 | TYR  |
| 2   | E     | 415 | ALA  |
| 2   | E     | 429 | ASN  |
| 2   | E     | 434 | GLU  |
| 2   | F     | 88  | MET  |
| 2   | F     | 133 | THR  |
| 2   | F     | 227 | PRO  |
| 2   | F     | 275 | GLU  |
| 2   | F     | 326 | PRO  |
| 2   | F     | 336 | GLN  |
| 2   | F     | 452 | LYS  |
| 4   | H     | 52  | LEU  |
| 4   | H     | 71  | LEU  |
| 4   | H     | 96  | LYS  |
| 5   | I     | 104 | MET  |
| 6   | L     | 95  | PRO  |
| 6   | L     | 157 | ALA  |
| 6   | L     | 179 | SER  |
| 7   | M     | 144 | GLY  |
| 8   | N     | 36  | ARG  |
| 8   | N     | 136 | PRO  |
| 8   | N     | 162 | GLU  |
| 8   | N     | 270 | ALA  |
| 8   | N     | 590 | GLY  |
| 8   | N     | 640 | ARG  |
| 9   | R     | 7   | SER  |
| 1   | A     | 66  | SER  |
| 1   | A     | 219 | ALA  |
| 1   | A     | 359 | ALA  |
| 1   | A     | 395 | VAL  |
| 1   | B     | 36  | VAL  |
| 1   | B     | 284 | ARG  |
| 1   | B     | 331 | ALA  |
| 1   | B     | 417 | ARG  |
| 1   | B     | 563 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 70  | PRO  |
| 1   | C     | 71  | LEU  |
| 1   | C     | 100 | ILE  |
| 1   | C     | 247 | ALA  |
| 2   | D     | 17  | PRO  |
| 2   | D     | 23  | ASN  |
| 2   | D     | 190 | VAL  |
| 2   | D     | 191 | PHE  |
| 2   | D     | 270 | ILE  |
| 2   | D     | 457 | ASP  |
| 2   | E     | 243 | GLU  |
| 2   | E     | 362 | MET  |
| 2   | E     | 437 | GLN  |
| 2   | F     | 99  | PRO  |
| 2   | F     | 175 | PRO  |
| 2   | F     | 259 | ASP  |
| 2   | F     | 372 | ARG  |
| 3   | G     | 6   | PRO  |
| 3   | G     | 123 | THR  |
| 3   | G     | 153 | GLU  |
| 4   | H     | 5   | ALA  |
| 4   | H     | 54  | ASP  |
| 6   | J     | 144 | ALA  |
| 7   | M     | 76  | VAL  |
| 7   | M     | 217 | PHE  |
| 8   | N     | 295 | ALA  |
| 9   | W     | 48  | ASP  |
| 1   | A     | 54  | ASP  |
| 1   | A     | 432 | THR  |
| 1   | B     | 326 | SER  |
| 1   | C     | 486 | VAL  |
| 2   | D     | 340 | SER  |
| 2   | E     | 106 | ILE  |
| 2   | E     | 222 | ASN  |
| 2   | E     | 263 | TYR  |
| 2   | E     | 355 | LEU  |
| 2   | E     | 430 | ARG  |
| 2   | E     | 435 | SER  |
| 2   | F     | 23  | ASN  |
| 2   | F     | 69  | ALA  |
| 3   | G     | 86  | LEU  |
| 5   | K     | 104 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | M     | 277 | VAL  |
| 8   | N     | 297 | HIS  |
| 8   | N     | 545 | TRP  |
| 8   | N     | 585 | LEU  |
| 9   | P     | 6   | ALA  |
| 1   | A     | 296 | VAL  |
| 2   | D     | 235 | PRO  |
| 2   | F     | 96  | ILE  |
| 1   | A     | 394 | PRO  |
| 1   | B     | 51  | VAL  |
| 2   | F     | 205 | ILE  |
| 3   | G     | 154 | ILE  |
| 3   | G     | 179 | ILE  |
| 1   | A     | 27  | ILE  |
| 1   | B     | 5   | VAL  |
| 1   | C     | 211 | ILE  |
| 1   | C     | 443 | VAL  |
| 2   | F     | 117 | LEU  |
| 6   | L     | 163 | VAL  |
| 1   | A     | 40  | ILE  |
| 1   | C     | 345 | PRO  |
| 1   | C     | 402 | ILE  |
| 1   | C     | 560 | PRO  |
| 2   | D     | 356 | PRO  |
| 2   | F     | 10  | GLY  |
| 8   | N     | 444 | PRO  |
| 1   | A     | 515 | ILE  |
| 1   | B     | 514 | GLY  |
| 2   | E     | 324 | PRO  |
| 7   | M     | 78  | GLY  |

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 10  | ADP  | B     | 600 | -    | 28,29,29     | 1.21 | 1 (3%)      | 43,45,45    | 0.99 | 1 (2%)      |
| 10  | ADP  | C     | 600 | -    | 28,29,29     | 0.90 | 1 (3%)      | 43,45,45    | 1.02 | 2 (4%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 10  | ADP  | B     | 600 | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 10  | ADP  | C     | 600 | -    | -       | 8/16/32/32 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 10  | B     | 600 | ADP  | PA-O3A | 5.21 | 1.65        | 1.59     |
| 10  | C     | 600 | ADP  | PA-O3A | 2.02 | 1.61        | 1.59     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 10  | C     | 600 | ADP  | N6-C6-N1 | 3.79  | 126.81      | 118.38   |
| 10  | B     | 600 | ADP  | N6-C6-N1 | 3.12  | 125.33      | 118.38   |
| 10  | C     | 600 | ADP  | C5-C6-N6 | -2.35 | 117.48      | 123.29   |

There are no chirality outliers.

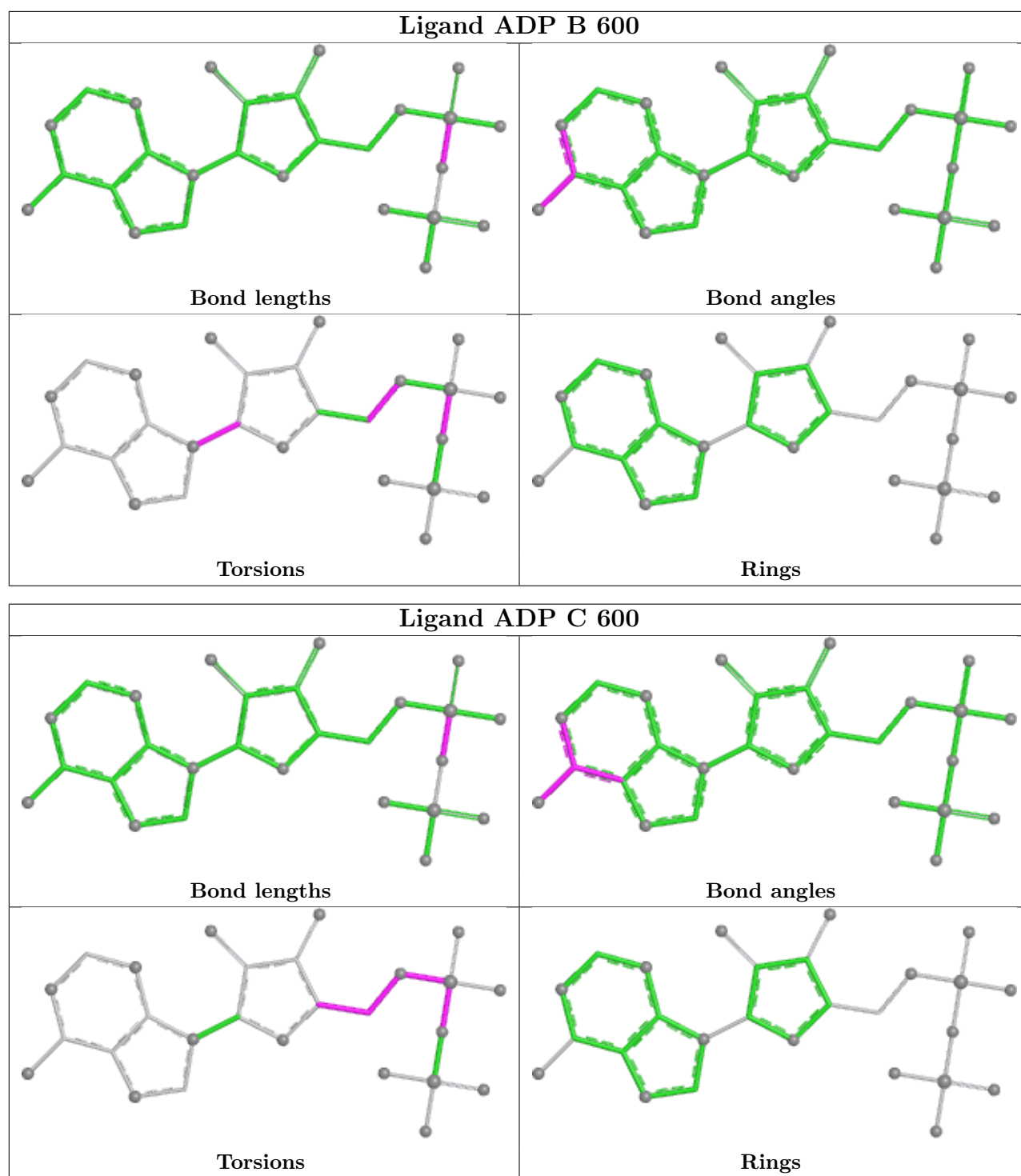
All (14) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | B     | 600 | ADP  | PB-O3A-PA-O5'   |
| 10  | C     | 600 | ADP  | C5'-O5'-PA-O1A  |
| 10  | C     | 600 | ADP  | C5'-O5'-PA-O2A  |
| 10  | C     | 600 | ADP  | C5'-O5'-PA-O3A  |
| 10  | C     | 600 | ADP  | O4'-C4'-C5'-O5' |
| 10  | C     | 600 | ADP  | C3'-C4'-C5'-O5' |
| 10  | B     | 600 | ADP  | C2'-C1'-N9-C8   |
| 10  | C     | 600 | ADP  | PB-O3A-PA-O2A   |
| 10  | C     | 600 | ADP  | C4'-C5'-O5'-PA  |
| 10  | B     | 600 | ADP  | C2'-C1'-N9-C4   |
| 10  | B     | 600 | ADP  | C4'-C5'-O5'-PA  |
| 10  | B     | 600 | ADP  | O4'-C1'-N9-C8   |
| 10  | B     | 600 | ADP  | PB-O3A-PA-O1A   |
| 10  | C     | 600 | ADP  | PB-O3A-PA-O1A   |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

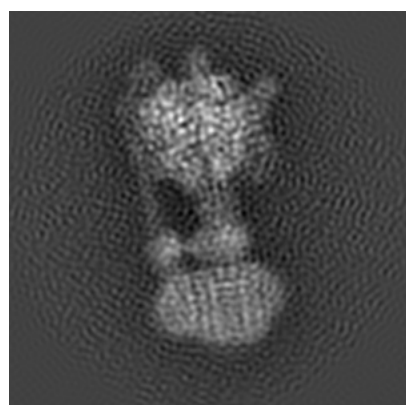
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6812. These allow visual inspection of the internal detail of the map and identification of artifacts.

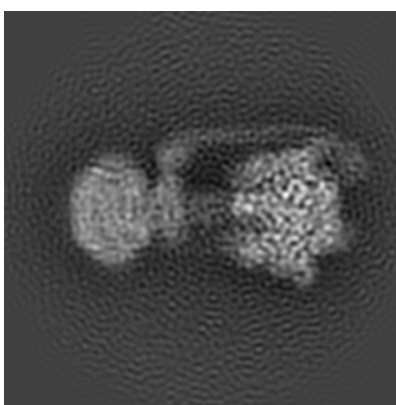
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

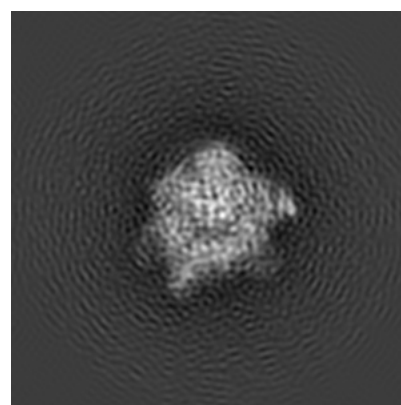
#### 6.1.1 Primary map



X



Y



Z

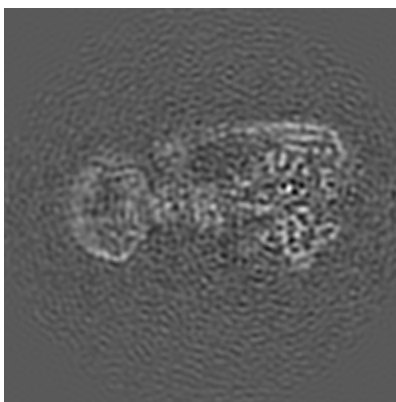
The images above show the map projected in three orthogonal directions.

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

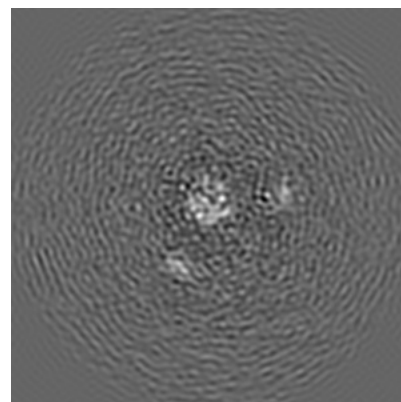
#### 6.2.1 Primary map



X Index: 118



Y Index: 118



Z Index: 118

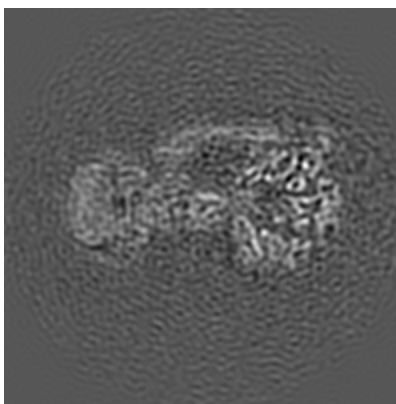
The images above show central slices of the map in three orthogonal directions.

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

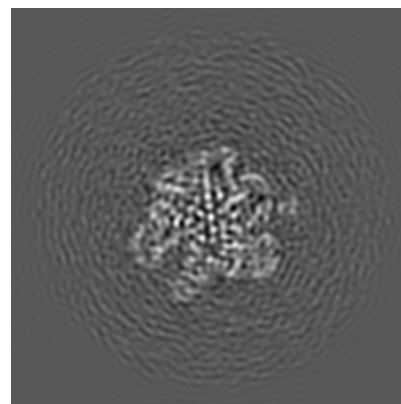
### 6.3.1 Primary map



X Index: 118



Y Index: 123

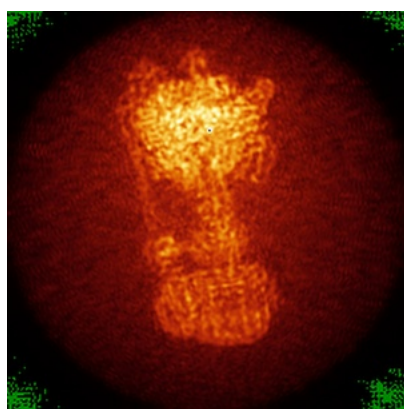


Z Index: 175

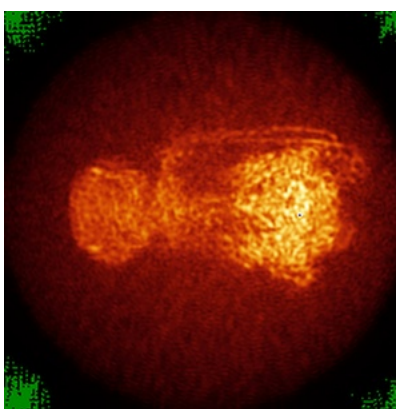
The images above show the largest variance slices of the map in three orthogonal directions.

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

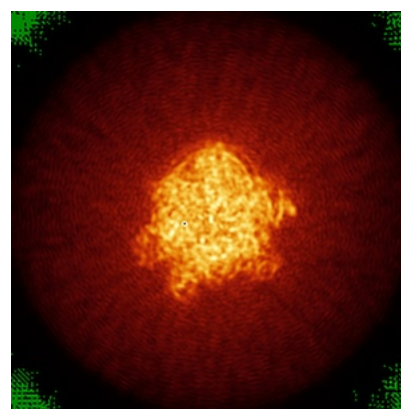
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

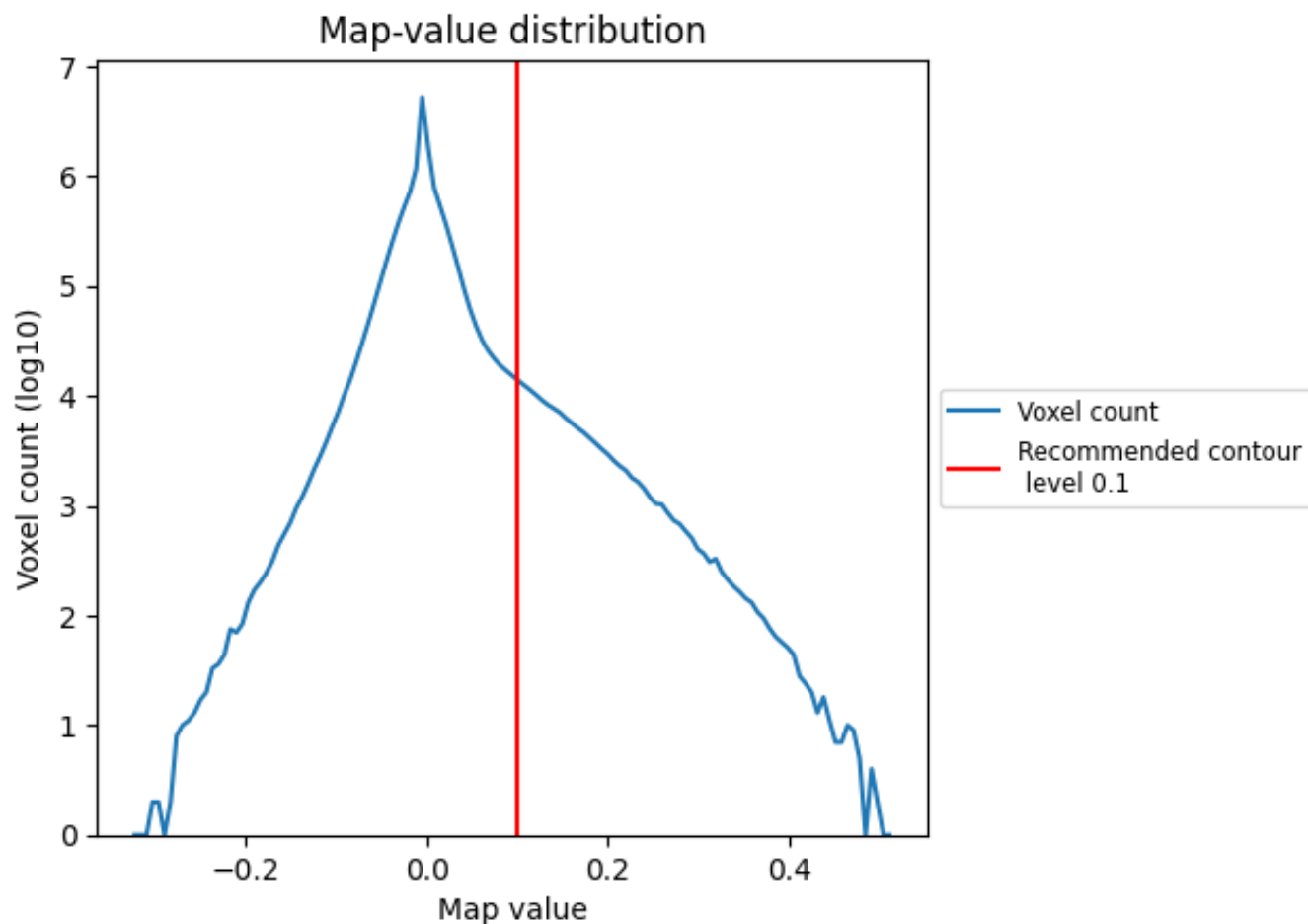
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

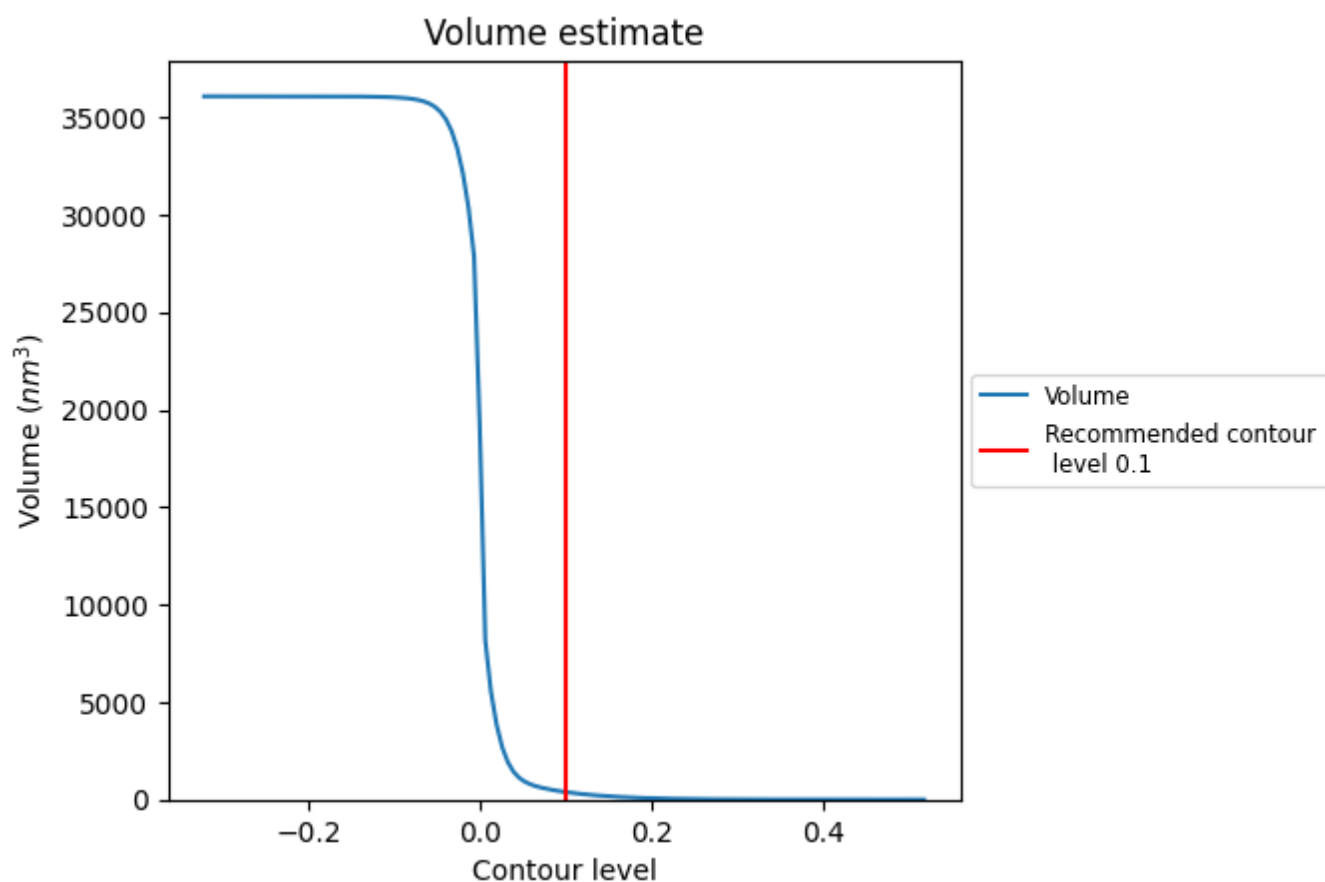
This section contains the results of statistical analysis of the map.

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



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

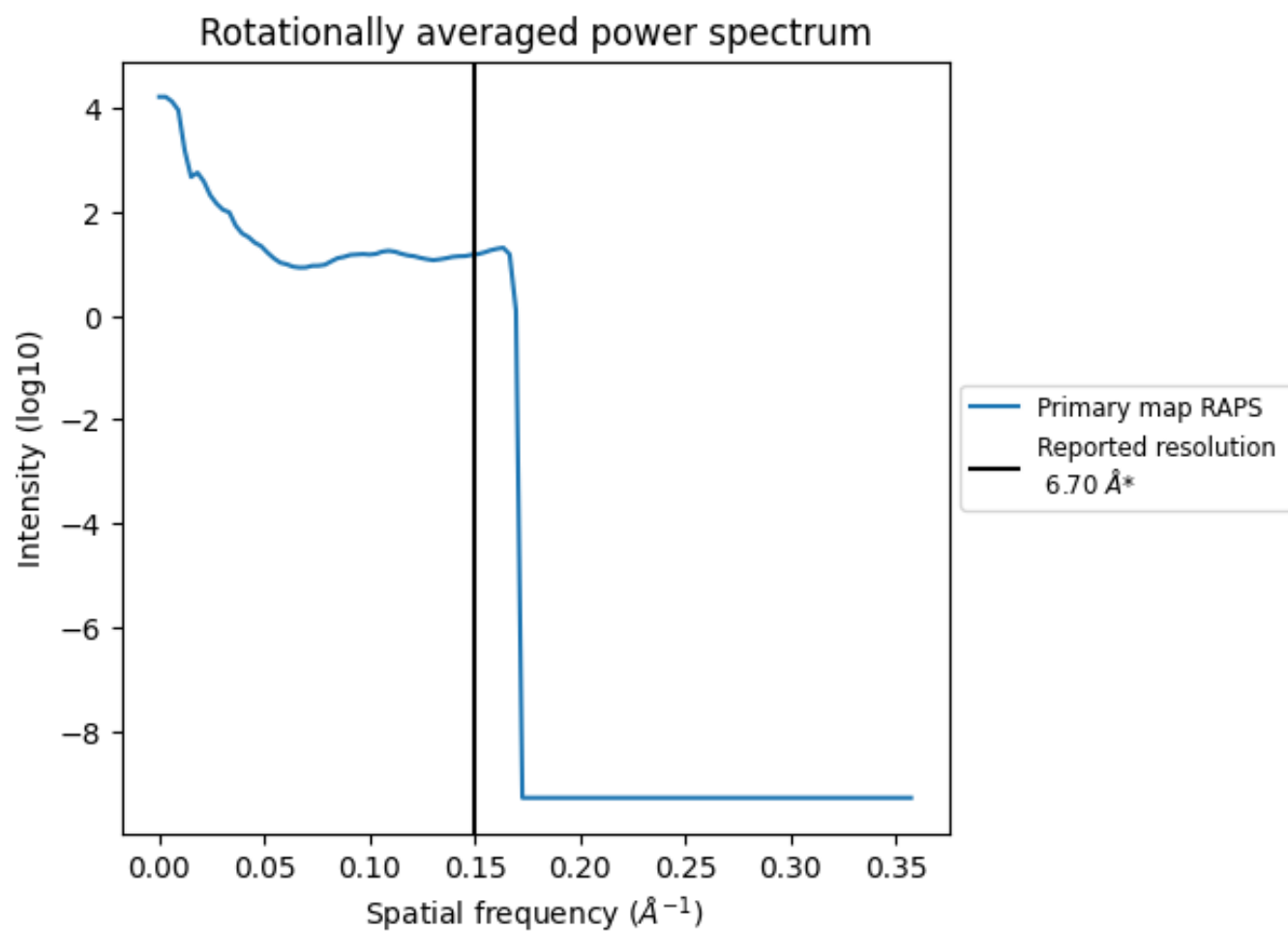
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 382 nm<sup>3</sup>; this corresponds to an approximate mass of 345 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 ⓘ

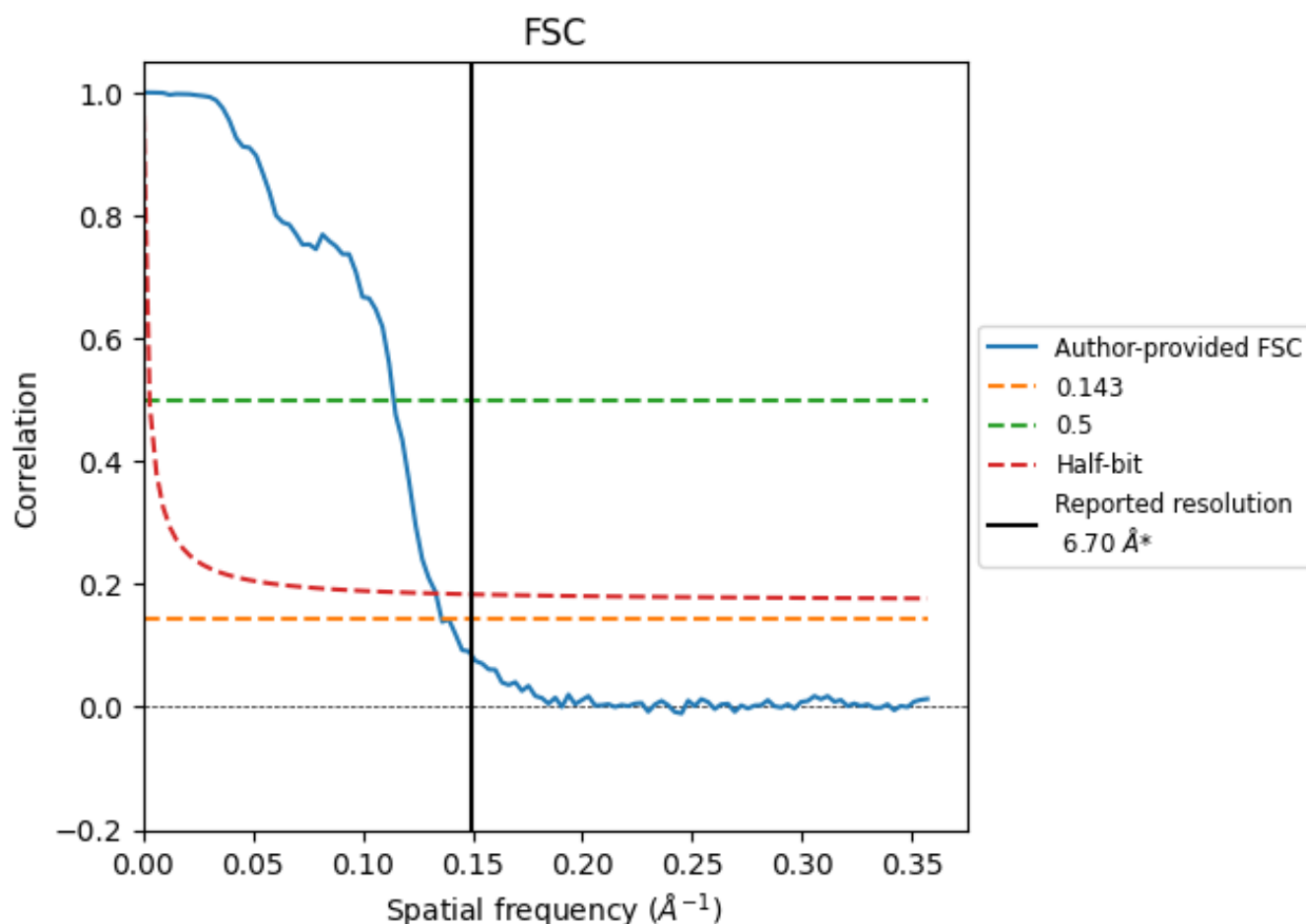


\*Reported resolution corresponds to spatial frequency of 0.149 Å<sup>-1</sup>

## 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 0.149 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

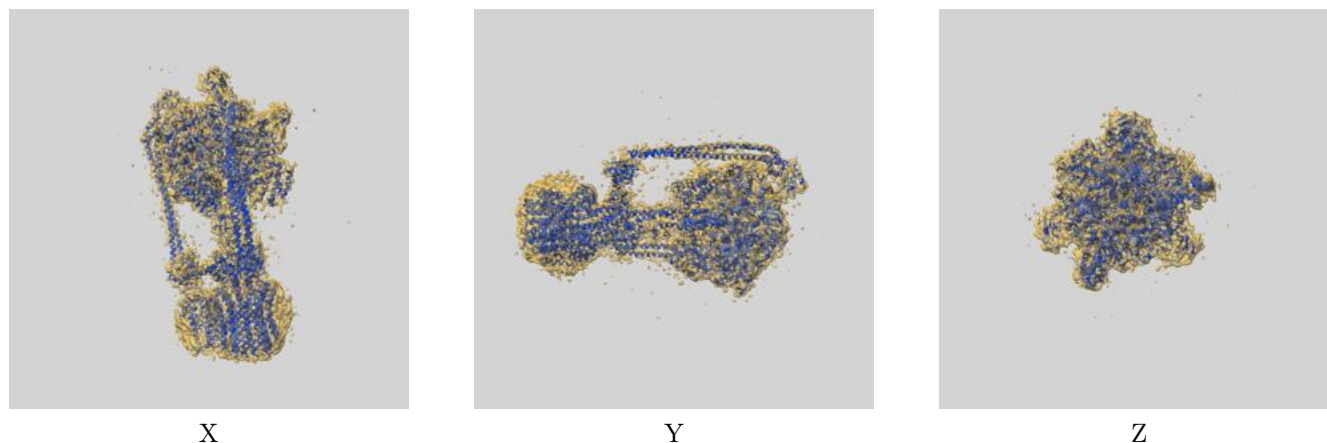
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 6.70                               | -    | -        |
| Author-provided FSC curve | 7.36                               | 8.76 | 7.50     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

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

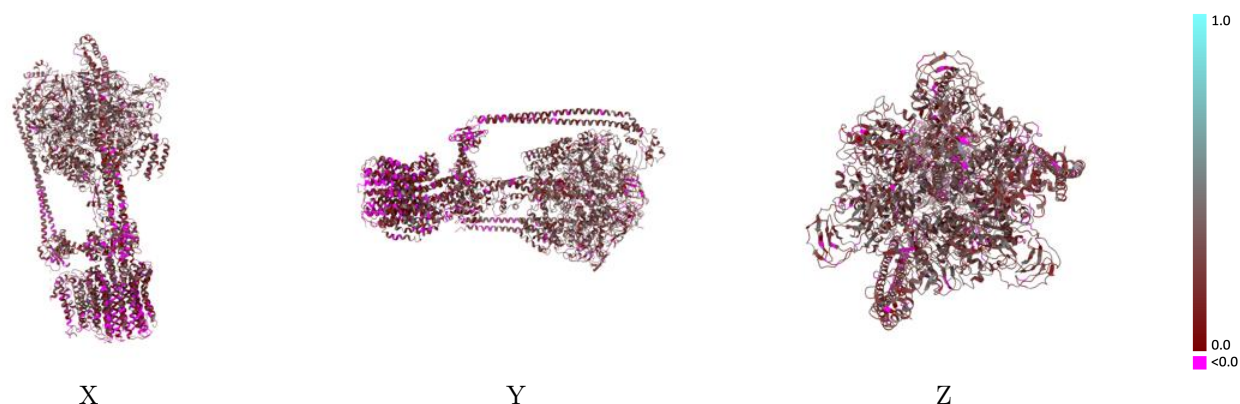
This section contains information regarding the fit between EMDB map EMD-6812 and PDB model 5Y5Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



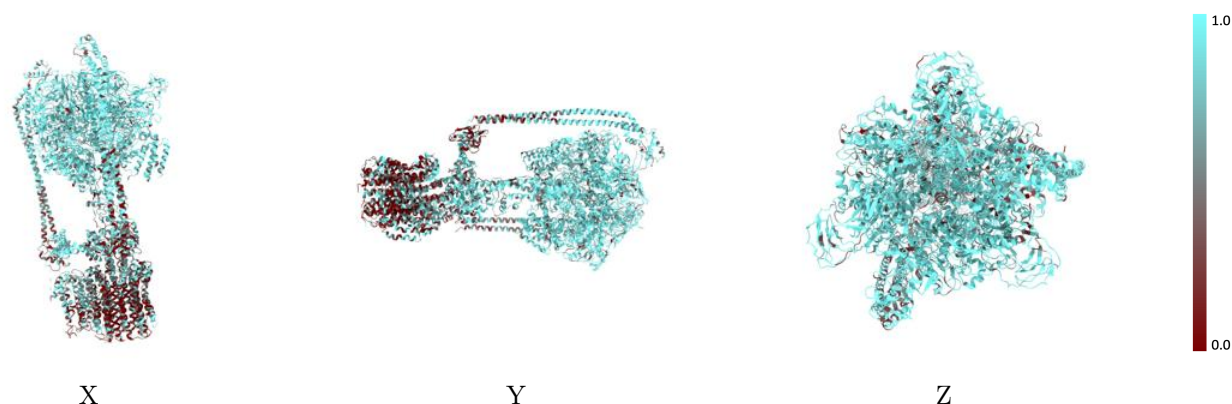
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



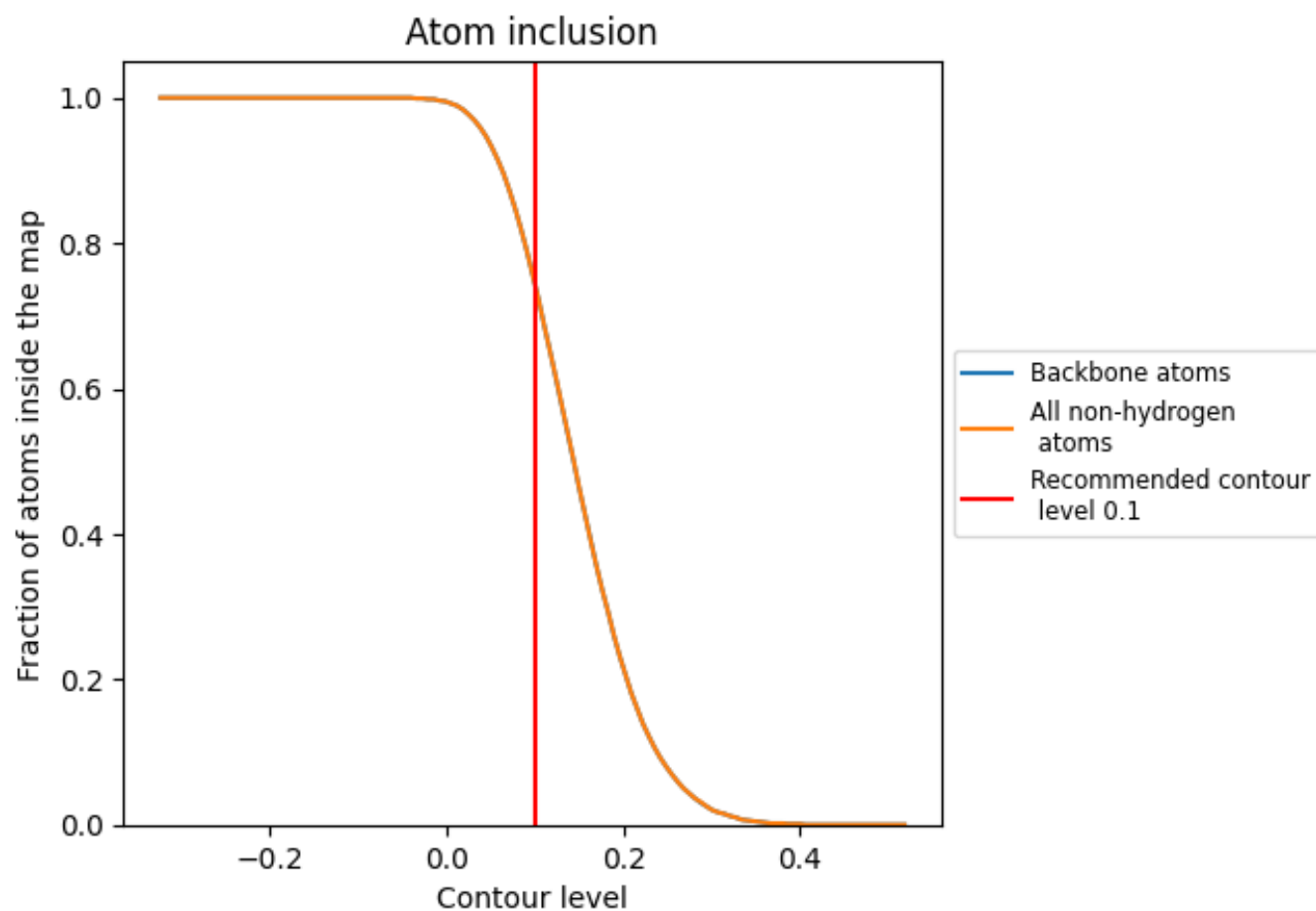
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7460   |  0.2370   |
| A     |  0.8670   |  0.2730   |
| B     |  0.9040   |  0.2900   |
| C     |  0.8770   |  0.2870   |
| D     |  0.8550   |  0.2730   |
| E     |  0.8920   |  0.2970   |
| F     |  0.8890   |  0.2930   |
| G     |  0.8000   |  0.2580   |
| H     |  0.7720   |  0.2460   |
| I     |  0.6320   |  0.2000   |
| J     |  0.7610   |  0.2210   |
| K     |  0.7590   |  0.2140   |
| L     |  0.7520   |  0.2230   |
| M     |  0.6710   |  0.2040   |
| N     |  0.5810  |  0.1750  |
| O     |  0.4190 |  0.1400 |
| P     |  0.4220 |  0.1550 |
| Q     |  0.3270 |  0.1020 |
| R     |  0.4090 |  0.1420 |
| S     |  0.4490 |  0.1150 |
| T     |  0.4220 |  0.1040 |
| U     |  0.4720 |  0.1320 |
| V     |  0.3760 |  0.1220 |
| W     |  0.2570 |  0.0640 |
| X     |  0.4460 |  0.1430 |
| Y     |  0.5150 |  0.1720 |
| Z     |  0.4780 |  0.1810 |

