



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:37 AM UTC

PDB ID : 5REQ / pdb_00005req
Title : Methylmalonyl-COA MUTASE, Y89F Mutant, substrate complex
Authors : Evans, P.R.; Thomae, N.H.
Deposited on : 1998-08-03
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

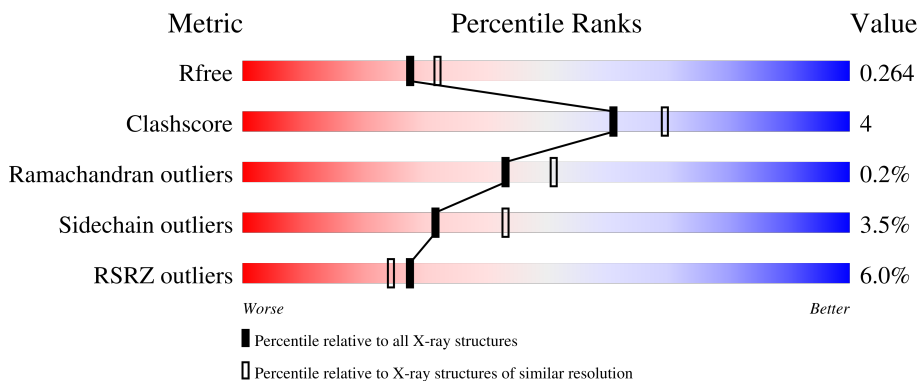
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 180053 | 6164 (2.20-2.20) |
| Clashscore | 190562 | 6851 (2.20-2.20) |
| Ramachandran outliers | 187476 | 6768 (2.20-2.20) |
| Sidechain outliers | 187428 | 6769 (2.20-2.20) |
| RSRZ outliers | 180081 | 6166 (2.20-2.20) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 727 | |
| 1 | C | 727 | |
| 2 | B | 637 | |
| 2 | D | 637 | |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22112 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 725 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5574 | 3526 | 966 | 1058 | 24 | | | |
| 1 | C | 725 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5574 | 3526 | 966 | 1058 | 24 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 89 | PHE | TYR | engineered mutation | UNP P11653 |
| C | 89 | PHE | TYR | engineered mutation | UNP P11653 |

- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT).

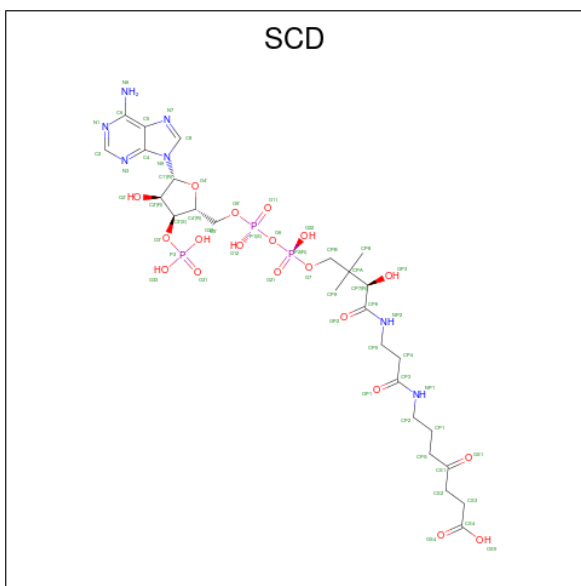
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | B | 619 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4722 | 2976 | 821 | 912 | 13 | | | |
| 2 | D | 619 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4722 | 2976 | 821 | 912 | 13 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 203 | GLY | ALA | SEE REMARK 999 | UNP P11652 |
| D | 203 | GLY | ALA | SEE REMARK 999 | UNP P11652 |
| B | 330 | GLU | ASP | SEE REMARK 999 | UNP P11652 |
| D | 330 | GLU | ASP | SEE REMARK 999 | UNP P11652 |
| B | 331 | LEU | VAL | SEE REMARK 999 | UNP P11652 |
| D | 331 | LEU | VAL | SEE REMARK 999 | UNP P11652 |

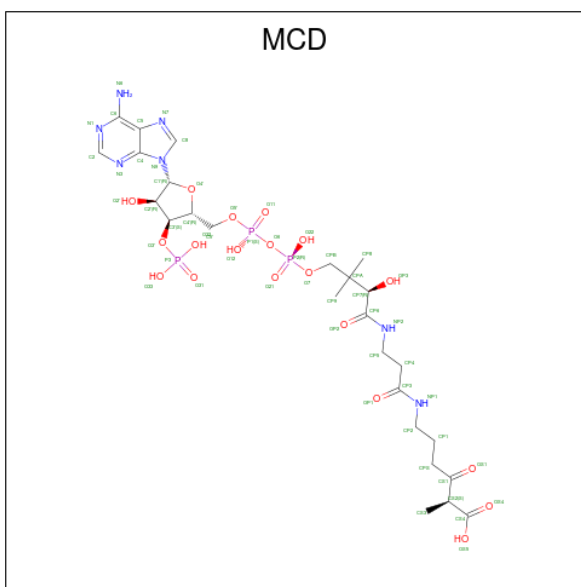
- Molecule 3 is SUCCINYL(CARBADETHIA)-COENZYME A (CCD ID: SCD) (formula:

$C_{26}H_{42}N_7O_{19}P_3$).



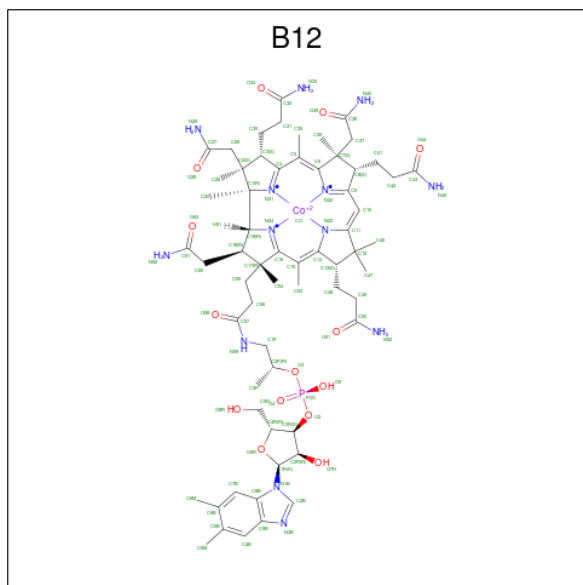
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|---|----|---------|---------|---|
| | | | Total | C | N | O | | | P |
| 3 | A | 1 | Total | C | N | O | P | 0 | 1 |
| | | | 55 | 26 | 7 | 19 | 3 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 1 |
| | | | 55 | 26 | 7 | 19 | 3 | | |

- Molecule 4 is METHYLMALONYL(CARBADETHIA)-COENZYME A (CCD ID: MCD) (formula: $C_{26}H_{42}N_7O_{19}P_3$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| | | | Total | C | N | O | P | | |
| 4 | A | 1 | 55 | 26 | 7 | 19 | 3 | 0 | 1 |
| 4 | C | 1 | 55 | 26 | 7 | 19 | 3 | 0 | 1 |

- Molecule 5 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|----|----|----|---------|---------|---|
| | | | Total | C | Co | N | O | | | P |
| 5 | A | 1 | 91 | 62 | 1 | 13 | 14 | 1 | 0 | 0 |
| 5 | C | 1 | 91 | 62 | 1 | 13 | 14 | 1 | 0 | 0 |

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6 | B | 1 | Total C O 6 3 3 | 0 | 0 |
| 6 | B | 1 | Total C O 6 3 3 | 0 | 0 |
| 6 | D | 1 | Total C O 6 3 3 | 0 | 0 |
| 6 | D | 1 | Total C O 6 3 3 | 0 | 0 |

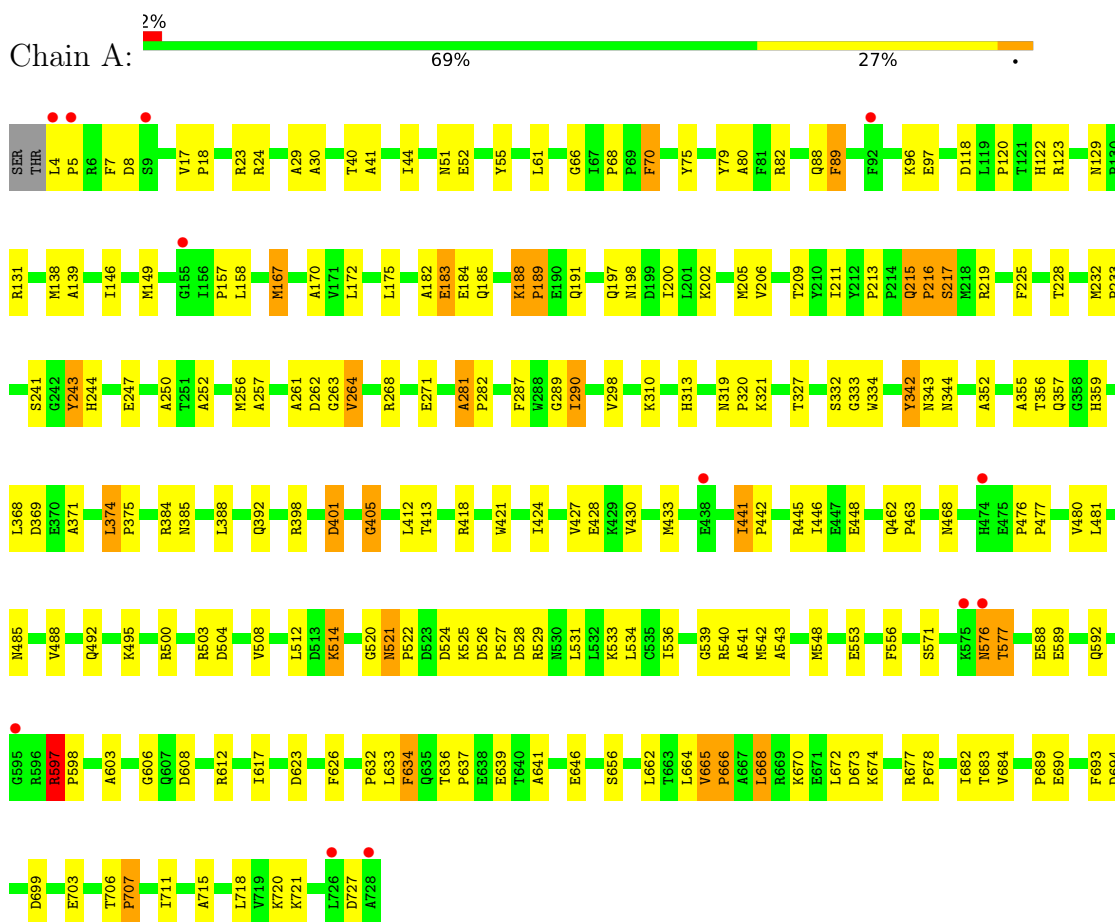
- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 7 | A | 356 | Total O 356 356 | 0 | 0 |
| 7 | B | 192 | Total O 192 192 | 0 | 0 |
| 7 | C | 353 | Total O 353 353 | 0 | 0 |
| 7 | D | 193 | Total O 193 193 | 0 | 0 |

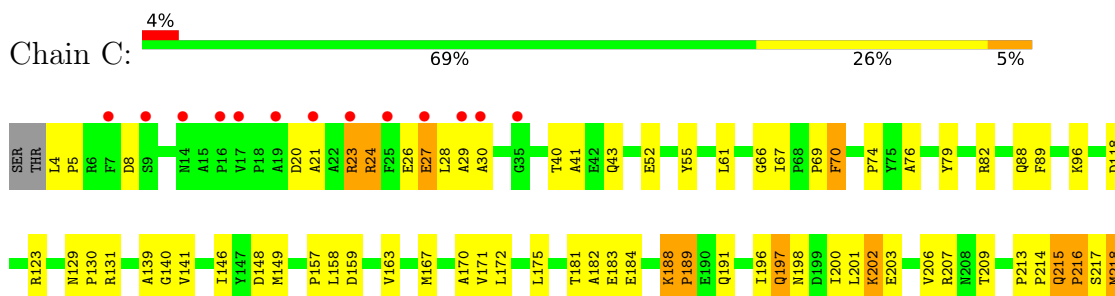
3 Residue-property plots

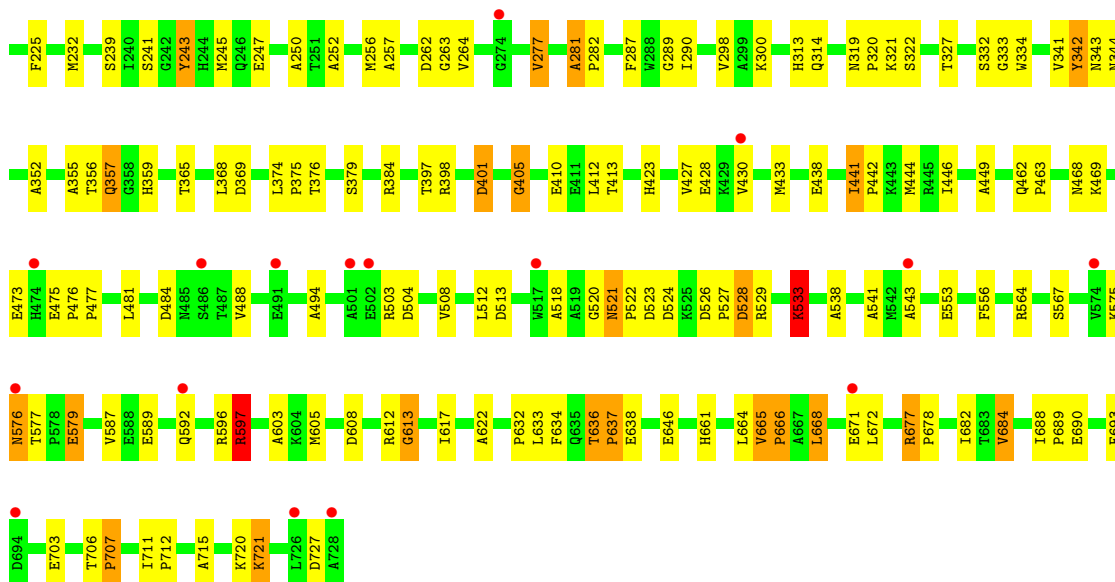
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT)

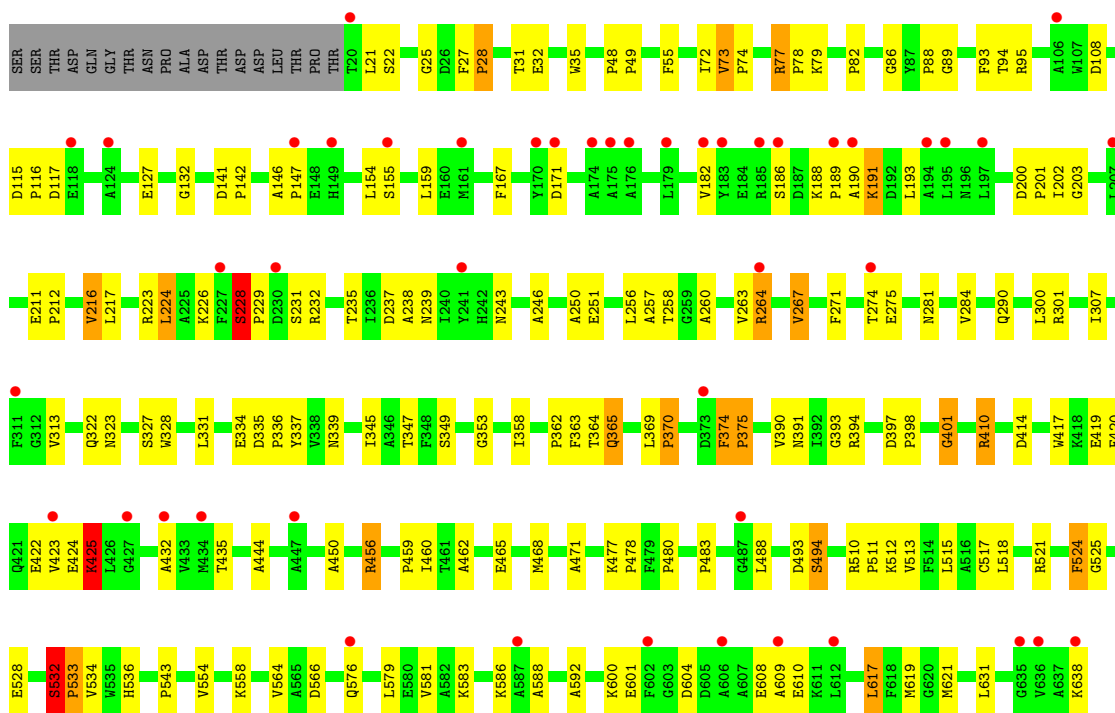


- Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT)

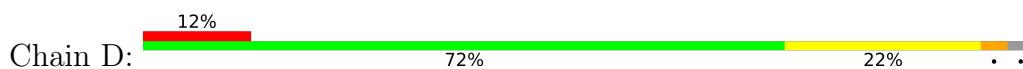


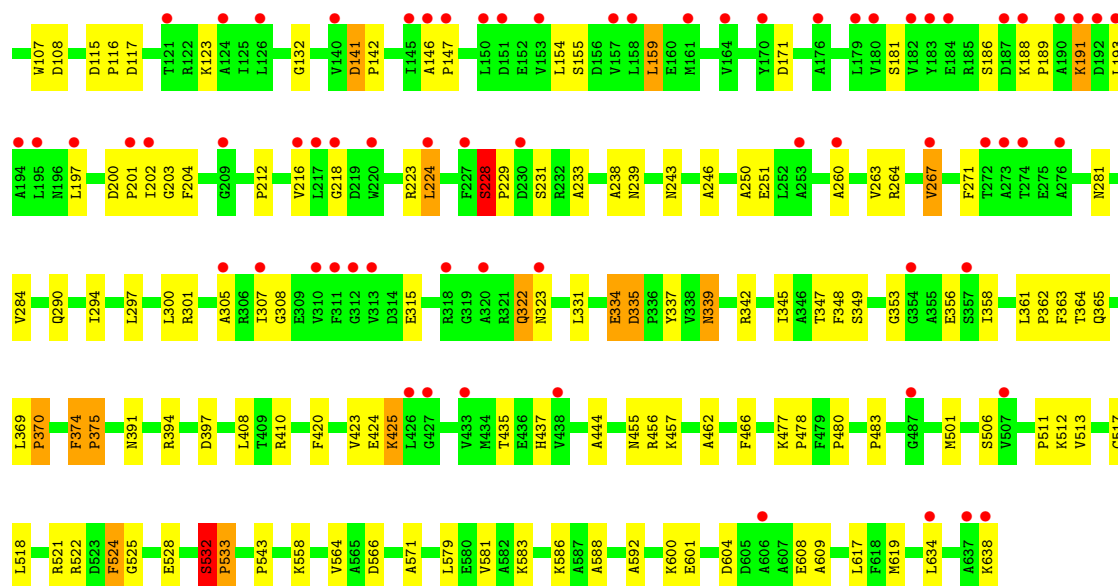


• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT)



• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT)





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 120.20Å 161.89Å 88.70Å 90.00° 104.88° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.20 20.00 – 2.20 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (20.00-2.20) 99.8 (20.00-2.20) | Depositor EDS |
| R_{merge} | 0.05 | Depositor |
| R_{sym} | 0.05 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.88 (at 2.20Å) | Xtrriage |
| Refinement program | REFMAC | Depositor |
| R, R_{free} | 0.246 , 0.292 0.230 , 0.264 | Depositor DCC |
| R_{free} test set | 8387 reflections (5.07%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 34.4 | Xtrriage |
| Anisotropy | 0.333 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 42.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 22112 | wwPDB-VP |
| Average B, all atoms (Å ²) | 43.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MCD, SCD, B12, GOL

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.63 | 0/5691 | 2.19 | 293/7728 (3.8%) |
| 1 | C | 0.64 | 0/5691 | 2.19 | 290/7728 (3.8%) |
| 2 | B | 0.56 | 0/4812 | 2.04 | 224/6533 (3.4%) |
| 2 | D | 0.55 | 0/4812 | 2.03 | 196/6533 (3.0%) |
| All | All | 0.60 | 0/21006 | 2.12 | 1003/28522 (3.5%) |

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 | 9 |
| 1 | C | 0 | 12 |
| 2 | B | 0 | 2 |
| 2 | D | 0 | 4 |
| All | All | 0 | 27 |

There are no bond length outliers.

All (1003) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 23 | ARG | CD-NE-CZ | 18.37 | 150.12 | 124.40 |
| 1 | C | 384 | ARG | CD-NE-CZ | 12.37 | 141.72 | 124.40 |
| 2 | B | 77 | ARG | CD-NE-CZ | 12.03 | 141.24 | 124.40 |
| 1 | A | 576 | ASN | CA-CB-CG | 11.68 | 124.28 | 112.60 |
| 1 | C | 41 | ALA | CA-C-N | 11.67 | 140.21 | 120.72 |
| 1 | C | 41 | ALA | C-N-CA | 11.67 | 140.21 | 120.72 |
| 2 | D | 77 | ARG | CD-NE-CZ | 11.32 | 140.24 | 124.40 |
| 1 | C | 597 | ARG | CD-NE-CZ | 11.30 | 140.22 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1 | A | 597 | ARG | CD-NE-CZ | 11.18 | 140.05 | 124.40 |
| 1 | C | 462 | GLN | CA-C-O | 10.68 | 126.23 | 119.29 |
| 1 | C | 333 | GLY | O-C-N | -10.51 | 112.09 | 122.18 |
| 1 | A | 70 | PHE | CA-CB-CG | 10.39 | 124.19 | 113.80 |
| 1 | C | 690 | GLU | CA-C-N | 9.96 | 133.63 | 120.28 |
| 1 | C | 690 | GLU | C-N-CA | 9.96 | 133.63 | 120.28 |
| 1 | C | 596 | ARG | CD-NE-CZ | 9.92 | 138.29 | 124.40 |
| 1 | C | 476 | PRO | N-CA-CB | 9.67 | 108.60 | 103.19 |
| 1 | A | 690 | GLU | CA-C-N | 9.59 | 135.94 | 120.60 |
| 1 | A | 690 | GLU | C-N-CA | 9.59 | 135.94 | 120.60 |
| 2 | D | 335 | ASP | CA-CB-CG | 9.55 | 122.15 | 112.60 |
| 1 | A | 319 | ASN | CA-C-O | 9.44 | 126.31 | 119.32 |
| 1 | A | 693 | PHE | CA-CB-CG | 9.41 | 123.21 | 113.80 |
| 1 | C | 576 | ASN | CA-CB-CG | 9.33 | 121.93 | 112.60 |
| 1 | C | 225 | PHE | CA-CB-CG | 9.28 | 123.08 | 113.80 |
| 1 | A | 41 | ALA | CA-C-N | 9.00 | 139.12 | 121.58 |
| 1 | A | 41 | ALA | C-N-CA | 9.00 | 139.12 | 121.58 |
| 2 | B | 524 | PHE | CA-CB-CG | 8.94 | 122.74 | 113.80 |
| 1 | A | 333 | GLY | O-C-N | -8.93 | 113.61 | 122.18 |
| 2 | D | 238 | ALA | CA-C-N | 8.84 | 133.74 | 120.31 |
| 2 | D | 238 | ALA | C-N-CA | 8.84 | 133.74 | 120.31 |
| 1 | C | 693 | PHE | CA-CB-CG | 8.75 | 122.55 | 113.80 |
| 1 | C | 89 | PHE | CA-CB-CG | 8.73 | 122.53 | 113.80 |
| 1 | A | 287 | PHE | CA-CB-CG | 8.72 | 122.52 | 113.80 |
| 2 | B | 601 | GLU | CA-C-N | 8.67 | 138.49 | 121.58 |
| 2 | B | 601 | GLU | C-N-CA | 8.67 | 138.49 | 121.58 |
| 1 | C | 423 | HIS | CA-CB-CG | 8.66 | 122.46 | 113.80 |
| 1 | C | 287 | PHE | CA-CB-CG | 8.63 | 122.44 | 113.80 |
| 2 | B | 238 | ALA | CA-C-N | 8.63 | 132.71 | 120.28 |
| 2 | B | 238 | ALA | C-N-CA | 8.63 | 132.71 | 120.28 |
| 2 | D | 524 | PHE | CA-CB-CG | 8.53 | 122.33 | 113.80 |
| 1 | C | 727 | ASP | CA-CB-CG | 8.42 | 121.02 | 112.60 |
| 2 | B | 93 | PHE | CA-C-N | 8.30 | 131.74 | 120.54 |
| 2 | B | 93 | PHE | C-N-CA | 8.30 | 131.74 | 120.54 |
| 1 | A | 384 | ARG | CD-NE-CZ | 8.27 | 135.98 | 124.40 |
| 2 | D | 93 | PHE | CA-C-N | 8.21 | 131.12 | 120.44 |
| 2 | D | 93 | PHE | C-N-CA | 8.21 | 131.12 | 120.44 |
| 2 | B | 339 | ASN | CA-C-N | 8.20 | 130.89 | 120.56 |
| 2 | B | 339 | ASN | C-N-CA | 8.20 | 130.89 | 120.56 |
| 2 | D | 337 | TYR | CA-C-N | 8.16 | 133.36 | 120.47 |
| 2 | D | 337 | TYR | C-N-CA | 8.16 | 133.36 | 120.47 |
| 1 | A | 313 | HIS | CA-C-N | 8.11 | 131.49 | 120.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 313 | HIS | C-N-CA | 8.11 | 131.49 | 120.38 |
| 2 | D | 339 | ASN | CA-C-N | 8.10 | 131.05 | 120.60 |
| 2 | D | 339 | ASN | C-N-CA | 8.10 | 131.05 | 120.60 |
| 2 | D | 528 | GLU | CA-C-N | 8.05 | 128.92 | 119.98 |
| 2 | D | 528 | GLU | C-N-CA | 8.05 | 128.92 | 119.98 |
| 2 | B | 117 | ASP | CA-CB-CG | 8.04 | 120.64 | 112.60 |
| 2 | B | 78 | PRO | CA-C-N | 8.00 | 133.40 | 120.60 |
| 2 | B | 78 | PRO | C-N-CA | 8.00 | 133.40 | 120.60 |
| 2 | B | 600 | LYS | CA-C-N | 7.98 | 134.05 | 120.72 |
| 2 | B | 600 | LYS | C-N-CA | 7.98 | 134.05 | 120.72 |
| 2 | D | 521 | ARG | CA-C-N | 7.94 | 131.25 | 120.38 |
| 2 | D | 521 | ARG | C-N-CA | 7.94 | 131.25 | 120.38 |
| 2 | B | 32 | GLU | CA-C-N | 7.87 | 131.16 | 120.54 |
| 2 | B | 32 | GLU | C-N-CA | 7.87 | 131.16 | 120.54 |
| 1 | C | 313 | HIS | CA-C-N | 7.84 | 131.83 | 120.38 |
| 1 | C | 313 | HIS | C-N-CA | 7.84 | 131.83 | 120.38 |
| 2 | B | 369 | LEU | CA-C-O | 7.82 | 126.76 | 120.19 |
| 2 | B | 86 | GLY | O-C-N | -7.82 | 114.39 | 122.60 |
| 2 | B | 335 | ASP | CA-CB-CG | 7.81 | 120.41 | 112.60 |
| 2 | B | 154 | LEU | CA-C-N | 7.80 | 130.73 | 120.28 |
| 2 | B | 154 | LEU | C-N-CA | 7.80 | 130.73 | 120.28 |
| 1 | A | 333 | GLY | CA-C-N | 7.79 | 131.05 | 120.38 |
| 1 | A | 333 | GLY | C-N-CA | 7.79 | 131.05 | 120.38 |
| 2 | D | 307 | ILE | CA-C-N | 7.79 | 128.75 | 120.03 |
| 2 | D | 307 | ILE | C-N-CA | 7.79 | 128.75 | 120.03 |
| 1 | C | 52 | GLU | N-CA-C | 7.78 | 122.45 | 113.19 |
| 1 | C | 149 | MET | CA-C-N | 7.77 | 130.54 | 120.44 |
| 1 | C | 149 | MET | C-N-CA | 7.77 | 130.54 | 120.44 |
| 1 | C | 183 | GLU | O-C-N | -7.72 | 114.06 | 122.09 |
| 2 | D | 601 | GLU | CA-C-N | 7.71 | 136.62 | 121.58 |
| 2 | D | 601 | GLU | C-N-CA | 7.71 | 136.62 | 121.58 |
| 1 | A | 369 | ASP | CA-C-N | 7.65 | 130.87 | 120.38 |
| 1 | A | 369 | ASP | C-N-CA | 7.65 | 130.87 | 120.38 |
| 1 | A | 699 | ASP | CA-CB-CG | 7.65 | 120.25 | 112.60 |
| 1 | C | 213 | PRO | CA-C-N | 7.65 | 127.20 | 119.24 |
| 1 | C | 213 | PRO | C-N-CA | 7.65 | 127.20 | 119.24 |
| 1 | A | 149 | MET | CA-C-N | 7.63 | 130.36 | 120.44 |
| 1 | A | 149 | MET | C-N-CA | 7.63 | 130.36 | 120.44 |
| 1 | C | 41 | ALA | O-C-N | -7.62 | 113.31 | 122.22 |
| 1 | A | 327 | THR | N-CA-C | 7.61 | 121.52 | 109.50 |
| 1 | A | 334 | TRP | CA-C-N | 7.60 | 131.23 | 120.28 |
| 1 | A | 334 | TRP | C-N-CA | 7.60 | 131.23 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 633 | LEU | CA-C-N | 7.59 | 134.96 | 123.05 |
| 1 | C | 633 | LEU | C-N-CA | 7.59 | 134.96 | 123.05 |
| 1 | A | 526 | ASP | CA-CB-CG | 7.51 | 120.11 | 112.60 |
| 2 | D | 466 | PHE | CA-C-O | 7.51 | 126.27 | 120.26 |
| 2 | B | 239 | ASN | CA-C-N | 7.49 | 129.99 | 120.56 |
| 2 | B | 239 | ASN | C-N-CA | 7.49 | 129.99 | 120.56 |
| 1 | C | 184 | GLU | CA-C-N | 7.49 | 134.84 | 121.66 |
| 1 | C | 184 | GLU | C-N-CA | 7.49 | 134.84 | 121.66 |
| 2 | B | 202 | ILE | CA-C-N | 7.47 | 128.27 | 119.98 |
| 2 | B | 202 | ILE | C-N-CA | 7.47 | 128.27 | 119.98 |
| 1 | A | 79 | TYR | CA-C-N | 7.46 | 130.28 | 120.28 |
| 1 | A | 79 | TYR | C-N-CA | 7.46 | 130.28 | 120.28 |
| 1 | A | 633 | LEU | O-C-N | -7.46 | 113.55 | 122.65 |
| 1 | C | 55 | TYR | N-CA-C | 7.44 | 121.46 | 112.38 |
| 2 | D | 89 | GLY | CA-C-N | 7.44 | 133.42 | 122.71 |
| 2 | D | 89 | GLY | C-N-CA | 7.44 | 133.42 | 122.71 |
| 2 | D | 600 | LYS | CA-C-N | 7.43 | 134.15 | 121.14 |
| 2 | D | 600 | LYS | C-N-CA | 7.43 | 134.15 | 121.14 |
| 1 | A | 146 | ILE | CA-C-N | 7.42 | 130.55 | 120.54 |
| 1 | A | 146 | ILE | C-N-CA | 7.42 | 130.55 | 120.54 |
| 1 | C | 319 | ASN | CA-C-O | 7.39 | 125.72 | 119.66 |
| 1 | C | 521 | ASN | CA-CB-CG | 7.38 | 119.98 | 112.60 |
| 1 | A | 727 | ASP | CA-CB-CG | 7.37 | 119.97 | 112.60 |
| 1 | C | 333 | GLY | CA-C-N | 7.36 | 130.47 | 120.38 |
| 1 | C | 333 | GLY | C-N-CA | 7.36 | 130.47 | 120.38 |
| 1 | C | 677 | ARG | O-C-N | -7.35 | 114.92 | 121.17 |
| 2 | D | 78 | PRO | CA-C-N | 7.34 | 132.34 | 120.60 |
| 2 | D | 78 | PRO | C-N-CA | 7.34 | 132.34 | 120.60 |
| 1 | C | 320 | PRO | CA-C-N | 7.33 | 130.83 | 120.28 |
| 1 | C | 320 | PRO | C-N-CA | 7.33 | 130.83 | 120.28 |
| 1 | C | 216 | PRO | CA-C-N | 7.30 | 130.07 | 120.28 |
| 1 | C | 216 | PRO | C-N-CA | 7.30 | 130.07 | 120.28 |
| 1 | A | 424 | ILE | CA-C-N | 7.28 | 129.91 | 120.44 |
| 1 | A | 424 | ILE | C-N-CA | 7.28 | 129.91 | 120.44 |
| 1 | A | 526 | ASP | CA-C-O | 7.26 | 126.44 | 119.62 |
| 2 | B | 424 | GLU | CA-C-N | 7.24 | 130.71 | 120.28 |
| 2 | B | 424 | GLU | C-N-CA | 7.24 | 130.71 | 120.28 |
| 1 | A | 89 | PHE | CA-CB-CG | 7.23 | 121.03 | 113.80 |
| 1 | A | 678 | PRO | CA-C-N | 7.22 | 132.96 | 120.68 |
| 1 | A | 678 | PRO | C-N-CA | 7.22 | 132.96 | 120.68 |
| 1 | A | 398 | ARG | N-CA-C | 7.21 | 120.00 | 111.71 |
| 1 | C | 209 | THR | N-CA-CB | 7.21 | 121.99 | 111.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 320 | PRO | CA-C-N | 7.20 | 130.65 | 120.28 |
| 1 | A | 320 | PRO | C-N-CA | 7.20 | 130.65 | 120.28 |
| 1 | C | 369 | ASP | CA-C-N | 7.20 | 130.24 | 120.38 |
| 1 | C | 369 | ASP | C-N-CA | 7.20 | 130.24 | 120.38 |
| 2 | D | 132 | GLY | N-CA-C | 7.19 | 124.89 | 115.40 |
| 1 | C | 319 | ASN | CA-C-N | 7.19 | 126.81 | 119.19 |
| 1 | C | 319 | ASN | C-N-CA | 7.19 | 126.81 | 119.19 |
| 1 | A | 343 | ASN | CA-C-N | 7.17 | 129.90 | 120.28 |
| 1 | A | 343 | ASN | C-N-CA | 7.17 | 129.90 | 120.28 |
| 1 | C | 61 | LEU | N-CA-C | 7.17 | 121.47 | 112.87 |
| 1 | A | 633 | LEU | CA-C-N | 7.14 | 132.75 | 122.40 |
| 1 | A | 633 | LEU | C-N-CA | 7.14 | 132.75 | 122.40 |
| 2 | D | 154 | LEU | CA-C-N | 7.14 | 129.84 | 120.28 |
| 2 | D | 154 | LEU | C-N-CA | 7.14 | 129.84 | 120.28 |
| 2 | B | 95 | ARG | N-CA-C | 7.13 | 119.91 | 111.71 |
| 1 | A | 225 | PHE | CA-CB-CG | 7.10 | 120.90 | 113.80 |
| 1 | A | 342 | TYR | CA-C-N | 7.08 | 131.08 | 120.31 |
| 1 | A | 342 | TYR | C-N-CA | 7.08 | 131.08 | 120.31 |
| 1 | C | 375 | PRO | N-CA-CB | 7.08 | 109.51 | 103.35 |
| 1 | C | 82 | ARG | CD-NE-CZ | 7.07 | 134.30 | 124.40 |
| 2 | B | 228 | SER | CA-C-N | 7.07 | 126.70 | 119.56 |
| 2 | B | 228 | SER | C-N-CA | 7.07 | 126.70 | 119.56 |
| 1 | C | 327 | THR | N-CA-C | 7.07 | 121.05 | 109.24 |
| 2 | D | 363 | PHE | CA-CB-CG | 7.06 | 120.86 | 113.80 |
| 2 | B | 401 | GLY | O-C-N | -7.01 | 115.36 | 122.65 |
| 1 | A | 662 | LEU | N-CA-C | 6.98 | 120.69 | 111.75 |
| 1 | C | 334 | TRP | CA-C-N | 6.98 | 131.77 | 120.60 |
| 1 | C | 334 | TRP | C-N-CA | 6.98 | 131.77 | 120.60 |
| 2 | B | 89 | GLY | CA-C-N | 6.98 | 132.76 | 122.71 |
| 2 | B | 89 | GLY | C-N-CA | 6.98 | 132.76 | 122.71 |
| 1 | A | 206 | VAL | CB-CA-C | -6.96 | 99.87 | 111.29 |
| 1 | A | 526 | ASP | CA-C-N | 6.95 | 126.93 | 119.28 |
| 1 | A | 526 | ASP | C-N-CA | 6.95 | 126.93 | 119.28 |
| 1 | A | 577 | THR | CA-C-N | 6.94 | 126.46 | 119.24 |
| 1 | A | 577 | THR | C-N-CA | 6.94 | 126.46 | 119.24 |
| 1 | C | 130 | PRO | CA-C-N | 6.93 | 130.26 | 120.28 |
| 1 | C | 130 | PRO | C-N-CA | 6.93 | 130.26 | 120.28 |
| 1 | C | 298 | VAL | O-C-N | -6.93 | 115.12 | 121.91 |
| 1 | C | 633 | LEU | O-C-N | -6.89 | 114.25 | 122.65 |
| 2 | B | 511 | PRO | N-CA-CB | 6.88 | 109.44 | 103.31 |
| 1 | C | 24 | ARG | CD-NE-CZ | 6.88 | 134.03 | 124.40 |
| 2 | B | 28 | PRO | N-CA-CB | 6.88 | 109.33 | 103.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 241 | SER | N-CA-C | 6.87 | 121.03 | 109.76 |
| 2 | D | 146 | ALA | CA-C-N | 6.84 | 126.81 | 119.28 |
| 2 | D | 146 | ALA | C-N-CA | 6.84 | 126.81 | 119.28 |
| 1 | C | 677 | ARG | CA-CB-CG | 6.84 | 127.79 | 114.10 |
| 2 | B | 301 | ARG | CA-C-O | -6.83 | 113.31 | 120.55 |
| 2 | D | 322 | GLN | CA-C-O | 6.83 | 127.87 | 120.43 |
| 1 | A | 52 | GLU | CA-C-N | 6.83 | 132.12 | 120.72 |
| 1 | A | 52 | GLU | C-N-CA | 6.83 | 132.12 | 120.72 |
| 1 | A | 209 | THR | N-CA-CB | 6.82 | 121.43 | 111.54 |
| 2 | D | 117 | ASP | CA-CB-CG | 6.82 | 119.42 | 112.60 |
| 1 | A | 673 | ASP | CA-C-N | 6.82 | 130.34 | 120.38 |
| 1 | A | 673 | ASP | C-N-CA | 6.82 | 130.34 | 120.38 |
| 1 | C | 678 | PRO | CA-C-N | 6.80 | 132.24 | 120.68 |
| 1 | C | 678 | PRO | C-N-CA | 6.80 | 132.24 | 120.68 |
| 2 | D | 267 | VAL | CA-C-N | 6.79 | 129.94 | 120.29 |
| 2 | D | 267 | VAL | C-N-CA | 6.79 | 129.94 | 120.29 |
| 2 | D | 543 | PRO | N-CA-CB | 6.79 | 109.25 | 103.35 |
| 1 | A | 334 | TRP | O-C-N | -6.77 | 114.94 | 122.12 |
| 2 | D | 24 | ALA | CA-C-N | 6.75 | 132.35 | 120.74 |
| 2 | D | 24 | ALA | C-N-CA | 6.75 | 132.35 | 120.74 |
| 2 | B | 528 | GLU | CA-C-N | 6.74 | 127.46 | 119.98 |
| 2 | B | 528 | GLU | C-N-CA | 6.74 | 127.46 | 119.98 |
| 1 | C | 526 | ASP | CA-C-N | 6.72 | 126.34 | 119.56 |
| 1 | C | 526 | ASP | C-N-CA | 6.72 | 126.34 | 119.56 |
| 2 | D | 423 | VAL | CA-C-N | 6.71 | 129.28 | 120.28 |
| 2 | D | 423 | VAL | C-N-CA | 6.71 | 129.28 | 120.28 |
| 2 | D | 239 | ASN | CA-C-N | 6.71 | 129.25 | 120.60 |
| 2 | D | 239 | ASN | C-N-CA | 6.71 | 129.25 | 120.60 |
| 1 | C | 707 | PRO | N-CA-CB | 6.71 | 109.15 | 103.25 |
| 2 | D | 525 | GLY | CA-C-N | 6.70 | 127.56 | 119.99 |
| 2 | D | 525 | GLY | C-N-CA | 6.70 | 127.56 | 119.99 |
| 2 | B | 423 | VAL | CA-C-N | 6.69 | 129.25 | 120.28 |
| 2 | B | 423 | VAL | C-N-CA | 6.69 | 129.25 | 120.28 |
| 1 | A | 183 | GLU | O-C-N | -6.69 | 115.13 | 122.09 |
| 2 | D | 32 | GLU | CA-C-N | 6.66 | 129.54 | 120.54 |
| 2 | D | 32 | GLU | C-N-CA | 6.66 | 129.54 | 120.54 |
| 2 | D | 48 | PRO | CA-C-N | 6.66 | 126.61 | 119.28 |
| 2 | D | 48 | PRO | C-N-CA | 6.66 | 126.61 | 119.28 |
| 1 | A | 216 | PRO | CA-C-N | 6.66 | 129.20 | 120.28 |
| 1 | A | 216 | PRO | C-N-CA | 6.66 | 129.20 | 120.28 |
| 2 | D | 353 | GLY | CA-C-N | 6.65 | 131.69 | 120.91 |
| 2 | D | 353 | GLY | C-N-CA | 6.65 | 131.69 | 120.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 243 | TYR | CA-C-N | 6.64 | 129.18 | 120.28 |
| 1 | C | 243 | TYR | C-N-CA | 6.64 | 129.18 | 120.28 |
| 1 | A | 243 | TYR | CA-C-N | 6.63 | 129.46 | 120.38 |
| 1 | A | 243 | TYR | C-N-CA | 6.63 | 129.46 | 120.38 |
| 1 | C | 5 | PRO | N-CA-CB | 6.62 | 109.21 | 103.31 |
| 1 | A | 641 | ALA | CA-C-N | 6.61 | 129.04 | 120.44 |
| 1 | A | 641 | ALA | C-N-CA | 6.61 | 129.04 | 120.44 |
| 2 | B | 146 | ALA | CA-C-N | 6.60 | 126.54 | 119.28 |
| 2 | B | 146 | ALA | C-N-CA | 6.60 | 126.54 | 119.28 |
| 1 | A | 241 | SER | N-CA-C | 6.60 | 120.59 | 109.76 |
| 2 | D | 462 | ALA | CA-C-N | 6.59 | 133.83 | 121.97 |
| 2 | D | 462 | ALA | C-N-CA | 6.59 | 133.83 | 121.97 |
| 1 | A | 612 | ARG | CA-C-N | 6.58 | 127.24 | 119.94 |
| 1 | A | 612 | ARG | C-N-CA | 6.58 | 127.24 | 119.94 |
| 1 | A | 626 | PHE | CA-CB-CG | 6.58 | 120.38 | 113.80 |
| 2 | B | 77 | ARG | CA-C-N | 6.58 | 126.82 | 119.32 |
| 2 | B | 77 | ARG | C-N-CA | 6.58 | 126.82 | 119.32 |
| 2 | B | 48 | PRO | CA-C-N | 6.55 | 126.49 | 119.28 |
| 2 | B | 48 | PRO | C-N-CA | 6.55 | 126.49 | 119.28 |
| 1 | A | 52 | GLU | N-CA-C | 6.55 | 120.73 | 112.87 |
| 2 | D | 420 | PHE | CA-CB-CG | 6.55 | 120.35 | 113.80 |
| 1 | C | 334 | TRP | O-C-N | -6.54 | 115.19 | 122.12 |
| 1 | A | 388 | LEU | CA-C-N | 6.54 | 128.94 | 120.44 |
| 1 | A | 388 | LEU | C-N-CA | 6.54 | 128.94 | 120.44 |
| 2 | D | 370 | PRO | N-CA-CB | 6.53 | 108.99 | 103.25 |
| 1 | C | 504 | ASP | CA-C-N | 6.52 | 126.29 | 119.05 |
| 1 | C | 504 | ASP | C-N-CA | 6.52 | 126.29 | 119.05 |
| 2 | D | 533 | PRO | N-CA-CB | 6.52 | 110.50 | 103.33 |
| 2 | D | 202 | ILE | CA-C-N | 6.51 | 127.20 | 119.98 |
| 2 | D | 202 | ILE | C-N-CA | 6.51 | 127.20 | 119.98 |
| 1 | A | 646 | GLU | N-CA-C | 6.50 | 120.31 | 112.38 |
| 2 | D | 455 | ASN | CA-C-N | 6.50 | 131.82 | 122.40 |
| 2 | D | 455 | ASN | C-N-CA | 6.50 | 131.82 | 122.40 |
| 1 | C | 131 | ARG | N-CA-C | 6.49 | 119.17 | 111.71 |
| 1 | A | 711 | ILE | CA-C-N | 6.49 | 126.41 | 119.28 |
| 1 | A | 711 | ILE | C-N-CA | 6.49 | 126.41 | 119.28 |
| 2 | D | 82 | PRO | N-CA-CB | 6.49 | 108.99 | 103.35 |
| 2 | D | 95 | ARG | N-CA-C | 6.48 | 119.16 | 111.71 |
| 1 | A | 677 | ARG | O-C-N | -6.47 | 115.43 | 121.32 |
| 1 | C | 413 | THR | CA-C-N | 6.47 | 129.24 | 120.44 |
| 1 | C | 413 | THR | C-N-CA | 6.47 | 129.24 | 120.44 |
| 1 | A | 244 | HIS | CA-C-N | 6.46 | 128.94 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 244 | HIS | C-N-CA | 6.46 | 128.94 | 120.28 |
| 1 | A | 368 | LEU | N-CA-C | 6.46 | 119.13 | 111.71 |
| 2 | B | 212 | PRO | N-CA-CB | 6.45 | 108.91 | 103.17 |
| 1 | C | 198 | ASN | CA-CB-CG | 6.45 | 119.05 | 112.60 |
| 1 | C | 313 | HIS | O-C-N | -6.45 | 115.28 | 122.12 |
| 2 | B | 132 | GLY | N-CA-C | 6.44 | 123.91 | 115.40 |
| 1 | A | 344 | ASN | CA-C-N | 6.43 | 128.67 | 120.56 |
| 1 | A | 344 | ASN | C-N-CA | 6.43 | 128.67 | 120.56 |
| 2 | B | 257 | ALA | CA-C-N | 6.43 | 128.90 | 120.28 |
| 2 | B | 257 | ALA | C-N-CA | 6.43 | 128.90 | 120.28 |
| 1 | A | 369 | ASP | O-C-N | -6.43 | 114.14 | 122.37 |
| 1 | C | 88 | GLN | CA-C-N | 6.42 | 129.94 | 120.95 |
| 1 | C | 88 | GLN | C-N-CA | 6.42 | 129.94 | 120.95 |
| 2 | D | 424 | GLU | CA-C-N | 6.41 | 129.51 | 120.28 |
| 2 | D | 424 | GLU | C-N-CA | 6.41 | 129.51 | 120.28 |
| 1 | A | 17 | VAL | CA-C-O | 6.41 | 122.93 | 119.15 |
| 1 | A | 188 | LYS | CA-C-N | 6.40 | 126.32 | 119.28 |
| 1 | A | 188 | LYS | C-N-CA | 6.40 | 126.32 | 119.28 |
| 2 | B | 95 | ARG | CG-CD-NE | 6.40 | 126.08 | 112.00 |
| 1 | C | 70 | PHE | O-C-N | -6.40 | 114.58 | 122.57 |
| 2 | D | 67 | VAL | CA-C-N | 6.39 | 133.08 | 122.66 |
| 2 | D | 67 | VAL | C-N-CA | 6.39 | 133.08 | 122.66 |
| 1 | A | 504 | ASP | CA-C-N | 6.39 | 126.14 | 119.05 |
| 1 | A | 504 | ASP | C-N-CA | 6.39 | 126.14 | 119.05 |
| 1 | C | 410 | GLU | CA-C-O | -6.38 | 113.78 | 120.55 |
| 2 | B | 73 | VAL | CA-C-N | 6.37 | 125.95 | 119.19 |
| 2 | B | 73 | VAL | C-N-CA | 6.37 | 125.95 | 119.19 |
| 2 | B | 397 | ASP | CA-C-N | 6.37 | 126.28 | 119.28 |
| 2 | B | 397 | ASP | C-N-CA | 6.37 | 126.28 | 119.28 |
| 2 | D | 363 | PHE | CA-C-N | 6.36 | 134.65 | 121.94 |
| 2 | D | 363 | PHE | C-N-CA | 6.36 | 134.65 | 121.94 |
| 2 | B | 480 | PRO | N-CA-CB | 6.35 | 108.84 | 103.25 |
| 1 | A | 184 | GLU | CA-C-N | 6.34 | 133.85 | 122.06 |
| 1 | A | 184 | GLU | C-N-CA | 6.34 | 133.85 | 122.06 |
| 1 | C | 427 | VAL | CA-C-N | 6.34 | 129.41 | 120.28 |
| 1 | C | 427 | VAL | C-N-CA | 6.34 | 129.41 | 120.28 |
| 1 | C | 527 | PRO | N-CA-CB | 6.34 | 109.59 | 103.51 |
| 1 | A | 694 | ASP | CA-C-N | 6.32 | 128.75 | 120.28 |
| 1 | A | 694 | ASP | C-N-CA | 6.32 | 128.75 | 120.28 |
| 1 | C | 477 | PRO | N-CA-CB | 6.32 | 108.94 | 103.31 |
| 1 | C | 183 | GLU | CA-C-N | 6.31 | 130.70 | 120.60 |
| 1 | C | 183 | GLU | C-N-CA | 6.31 | 130.70 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 343 | ASN | CA-C-N | 6.31 | 129.37 | 120.28 |
| 1 | C | 343 | ASN | C-N-CA | 6.31 | 129.37 | 120.28 |
| 1 | C | 352 | ALA | CA-C-O | 6.31 | 127.11 | 120.42 |
| 1 | A | 170 | ALA | CA-C-N | 6.31 | 129.38 | 120.42 |
| 1 | A | 170 | ALA | C-N-CA | 6.31 | 129.38 | 120.42 |
| 1 | A | 129 | ASN | CA-C-N | 6.30 | 126.04 | 119.05 |
| 1 | A | 129 | ASN | C-N-CA | 6.30 | 126.04 | 119.05 |
| 1 | A | 556 | PHE | N-CA-C | 6.30 | 120.17 | 112.23 |
| 1 | C | 215 | GLN | CA-C-N | 6.30 | 126.04 | 119.05 |
| 1 | C | 215 | GLN | C-N-CA | 6.30 | 126.04 | 119.05 |
| 1 | A | 707 | PRO | N-CA-CB | 6.29 | 108.78 | 103.25 |
| 1 | C | 262 | ASP | CA-C-N | 6.29 | 126.96 | 119.98 |
| 1 | C | 262 | ASP | C-N-CA | 6.29 | 126.96 | 119.98 |
| 2 | D | 511 | PRO | N-CA-CB | 6.28 | 108.82 | 103.35 |
| 1 | A | 129 | ASN | CA-C-O | 6.28 | 125.66 | 119.51 |
| 1 | C | 430 | VAL | O-C-N | -6.28 | 114.72 | 122.57 |
| 2 | B | 536 | HIS | CA-C-N | 6.26 | 128.68 | 120.60 |
| 2 | B | 536 | HIS | C-N-CA | 6.26 | 128.68 | 120.60 |
| 2 | D | 28 | PRO | N-CA-CB | 6.25 | 108.75 | 103.25 |
| 1 | C | 170 | ALA | CA-C-N | 6.25 | 129.02 | 120.46 |
| 1 | C | 170 | ALA | C-N-CA | 6.25 | 129.02 | 120.46 |
| 2 | D | 263 | VAL | N-CA-C | -6.24 | 104.66 | 110.53 |
| 1 | A | 588 | GLU | CA-C-N | 6.23 | 129.25 | 120.28 |
| 1 | A | 588 | GLU | C-N-CA | 6.23 | 129.25 | 120.28 |
| 1 | A | 321 | LYS | CA-C-N | 6.22 | 128.62 | 120.28 |
| 1 | A | 321 | LYS | C-N-CA | 6.22 | 128.62 | 120.28 |
| 1 | A | 319 | ASN | CA-C-N | 6.22 | 126.12 | 119.28 |
| 1 | A | 319 | ASN | C-N-CA | 6.22 | 126.12 | 119.28 |
| 2 | B | 25 | GLY | O-C-N | -6.22 | 115.62 | 122.84 |
| 1 | A | 633 | LEU | CA-C-O | 6.21 | 129.07 | 121.99 |
| 1 | C | 206 | VAL | CB-CA-C | -6.21 | 101.10 | 111.29 |
| 2 | B | 337 | TYR | CA-C-N | 6.21 | 130.95 | 120.64 |
| 2 | B | 337 | TYR | C-N-CA | 6.21 | 130.95 | 120.64 |
| 1 | A | 182 | ALA | CA-C-N | 6.21 | 128.92 | 120.54 |
| 1 | A | 182 | ALA | C-N-CA | 6.21 | 128.92 | 120.54 |
| 1 | A | 462 | GLN | CA-C-O | 6.20 | 123.32 | 119.29 |
| 1 | A | 715 | ALA | CA-C-N | 6.20 | 128.59 | 120.60 |
| 1 | A | 715 | ALA | C-N-CA | 6.20 | 128.59 | 120.60 |
| 2 | D | 308 | GLY | CA-C-N | 6.20 | 128.59 | 120.28 |
| 2 | D | 308 | GLY | C-N-CA | 6.20 | 128.59 | 120.28 |
| 1 | C | 314 | GLN | O-C-N | -6.20 | 115.14 | 122.20 |
| 1 | A | 477 | PRO | N-CA-CB | 6.19 | 108.82 | 103.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 5 | PRO | N-CA-CB | 6.19 | 108.82 | 103.31 |
| 2 | B | 374 | PHE | CA-C-N | 6.19 | 126.09 | 119.28 |
| 2 | B | 374 | PHE | C-N-CA | 6.19 | 126.09 | 119.28 |
| 1 | C | 79 | TYR | CA-C-N | 6.19 | 128.89 | 120.54 |
| 1 | C | 79 | TYR | C-N-CA | 6.19 | 128.89 | 120.54 |
| 1 | A | 157 | PRO | N-CA-CB | 6.18 | 108.67 | 103.17 |
| 1 | A | 413 | THR | CA-C-N | 6.18 | 128.48 | 120.44 |
| 1 | A | 413 | THR | C-N-CA | 6.18 | 128.48 | 120.44 |
| 1 | C | 412 | LEU | CA-C-N | 6.18 | 128.48 | 120.44 |
| 1 | C | 412 | LEU | C-N-CA | 6.18 | 128.48 | 120.44 |
| 1 | A | 548 | MET | CA-C-N | 6.18 | 129.06 | 120.29 |
| 1 | A | 548 | MET | C-N-CA | 6.18 | 129.06 | 120.29 |
| 1 | A | 213 | PRO | CA-C-N | 6.18 | 125.67 | 119.24 |
| 1 | A | 213 | PRO | C-N-CA | 6.18 | 125.67 | 119.24 |
| 2 | B | 94 | THR | CA-C-N | 6.18 | 129.17 | 120.28 |
| 2 | B | 94 | THR | C-N-CA | 6.18 | 129.17 | 120.28 |
| 1 | A | 401 | ASP | CA-C-N | 6.17 | 125.90 | 119.05 |
| 1 | A | 401 | ASP | C-N-CA | 6.17 | 125.90 | 119.05 |
| 1 | A | 82 | ARG | CD-NE-CZ | 6.16 | 133.03 | 124.40 |
| 2 | B | 483 | PRO | N-CA-CB | 6.16 | 108.80 | 103.31 |
| 2 | D | 189 | PRO | N-CA-CB | 6.16 | 108.65 | 103.17 |
| 2 | B | 190 | ALA | N-CA-C | 6.16 | 118.78 | 111.33 |
| 2 | D | 397 | ASP | CA-C-N | 6.15 | 126.33 | 119.32 |
| 2 | D | 397 | ASP | C-N-CA | 6.15 | 126.33 | 119.32 |
| 2 | D | 115 | ASP | CA-CB-CG | 6.15 | 118.75 | 112.60 |
| 1 | C | 633 | LEU | CA-C-O | 6.15 | 129.00 | 121.99 |
| 1 | A | 520 | GLY | O-C-N | -6.14 | 115.74 | 122.68 |
| 2 | D | 228 | SER | CA-C-N | 6.14 | 126.67 | 120.04 |
| 2 | D | 228 | SER | C-N-CA | 6.14 | 126.67 | 120.04 |
| 1 | A | 232 | MET | CA-C-N | 6.13 | 125.75 | 119.56 |
| 1 | A | 232 | MET | C-N-CA | 6.13 | 125.75 | 119.56 |
| 1 | C | 612 | ARG | CA-C-N | 6.13 | 126.74 | 119.94 |
| 1 | C | 612 | ARG | C-N-CA | 6.13 | 126.74 | 119.94 |
| 1 | A | 521 | ASN | CA-CB-CG | 6.13 | 118.73 | 112.60 |
| 1 | C | 522 | PRO | N-CA-CB | 6.12 | 108.20 | 103.30 |
| 1 | A | 41 | ALA | O-C-N | -6.12 | 114.23 | 122.43 |
| 1 | C | 410 | GLU | CB-CG-CD | 6.12 | 123.00 | 112.60 |
| 1 | A | 197 | GLN | O-C-N | -6.12 | 115.67 | 122.03 |
| 2 | B | 363 | PHE | CA-C-N | 6.11 | 135.82 | 121.52 |
| 2 | B | 363 | PHE | C-N-CA | 6.11 | 135.82 | 121.52 |
| 2 | D | 586 | LYS | CA-C-N | 6.11 | 128.97 | 120.29 |
| 2 | D | 586 | LYS | C-N-CA | 6.11 | 128.97 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 463 | PRO | N-CA-CB | 6.11 | 108.66 | 103.35 |
| 2 | D | 212 | PRO | N-CA-CB | 6.10 | 108.60 | 103.17 |
| 2 | B | 534 | VAL | CA-C-N | 6.10 | 128.45 | 120.28 |
| 2 | B | 534 | VAL | C-N-CA | 6.10 | 128.45 | 120.28 |
| 1 | C | 398 | ARG | N-CA-C | 6.10 | 117.93 | 111.28 |
| 1 | C | 504 | ASP | CA-CB-CG | 6.09 | 118.69 | 112.60 |
| 1 | A | 371 | ALA | CA-C-N | 6.08 | 129.22 | 123.08 |
| 1 | A | 371 | ALA | C-N-CA | 6.08 | 129.22 | 123.08 |
| 2 | B | 82 | PRO | N-CA-CB | 6.08 | 108.64 | 103.35 |
| 1 | C | 188 | LYS | CA-C-N | 6.07 | 125.96 | 119.28 |
| 1 | C | 188 | LYS | C-N-CA | 6.07 | 125.96 | 119.28 |
| 2 | D | 77 | ARG | CA-C-N | 6.07 | 126.51 | 119.47 |
| 2 | D | 77 | ARG | C-N-CA | 6.07 | 126.51 | 119.47 |
| 1 | C | 637 | PRO | CA-C-N | 6.07 | 128.90 | 120.29 |
| 1 | C | 637 | PRO | C-N-CA | 6.07 | 128.90 | 120.29 |
| 2 | D | 571 | ALA | CA-C-N | 6.07 | 128.41 | 120.28 |
| 2 | D | 571 | ALA | C-N-CA | 6.07 | 128.41 | 120.28 |
| 2 | B | 363 | PHE | CA-CB-CG | 6.06 | 119.86 | 113.80 |
| 2 | D | 243 | ASN | N-CA-C | 6.06 | 119.78 | 112.38 |
| 1 | C | 463 | PRO | N-CA-CB | 6.06 | 108.62 | 103.35 |
| 2 | B | 420 | PHE | CA-CB-CG | 6.03 | 119.83 | 113.80 |
| 1 | A | 262 | ASP | CA-C-N | 6.03 | 126.78 | 120.03 |
| 1 | A | 262 | ASP | C-N-CA | 6.03 | 126.78 | 120.03 |
| 1 | C | 52 | GLU | CA-C-N | 6.03 | 133.34 | 121.58 |
| 1 | C | 52 | GLU | C-N-CA | 6.03 | 133.34 | 121.58 |
| 2 | B | 532 | SER | CA-C-N | 6.03 | 126.19 | 119.32 |
| 2 | B | 532 | SER | C-N-CA | 6.03 | 126.19 | 119.32 |
| 2 | B | 229 | PRO | CA-C-N | 6.03 | 129.47 | 120.31 |
| 2 | B | 229 | PRO | C-N-CA | 6.03 | 129.47 | 120.31 |
| 1 | C | 197 | GLN | O-C-N | -6.02 | 115.77 | 122.03 |
| 1 | C | 298 | VAL | CA-C-N | 6.02 | 128.34 | 120.28 |
| 1 | C | 298 | VAL | C-N-CA | 6.02 | 128.34 | 120.28 |
| 1 | C | 577 | THR | CA-C-N | 6.01 | 126.17 | 119.32 |
| 1 | C | 577 | THR | C-N-CA | 6.01 | 126.17 | 119.32 |
| 2 | D | 115 | ASP | CA-C-N | 6.01 | 125.22 | 118.97 |
| 2 | D | 115 | ASP | C-N-CA | 6.01 | 125.22 | 118.97 |
| 1 | C | 401 | ASP | CA-C-N | 6.00 | 125.72 | 119.05 |
| 1 | C | 401 | ASP | C-N-CA | 6.00 | 125.72 | 119.05 |
| 2 | B | 159 | LEU | N-CA-C | 6.00 | 119.86 | 112.54 |
| 1 | C | 397 | THR | O-C-N | -6.00 | 114.45 | 122.49 |
| 1 | C | 181 | THR | CA-C-N | 6.00 | 128.63 | 120.54 |
| 1 | C | 181 | THR | C-N-CA | 6.00 | 128.63 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 375 | PRO | N-CA-CB | 6.00 | 108.64 | 103.31 |
| 1 | A | 608 | ASP | CA-CB-CG | 5.99 | 118.59 | 112.60 |
| 2 | B | 267 | VAL | CA-C-N | 5.99 | 128.31 | 120.28 |
| 2 | B | 267 | VAL | C-N-CA | 5.99 | 128.31 | 120.28 |
| 1 | A | 636 | THR | CA-C-N | 5.98 | 125.60 | 119.56 |
| 1 | A | 636 | THR | C-N-CA | 5.98 | 125.60 | 119.56 |
| 2 | B | 370 | PRO | N-CA-CB | 5.97 | 108.51 | 103.25 |
| 1 | C | 182 | ALA | CA-C-N | 5.97 | 128.60 | 120.54 |
| 1 | C | 182 | ALA | C-N-CA | 5.97 | 128.60 | 120.54 |
| 2 | D | 480 | PRO | N-CA-CB | 5.97 | 108.50 | 103.25 |
| 2 | D | 301 | ARG | CA-C-O | -5.97 | 114.51 | 120.90 |
| 2 | B | 232 | ARG | CD-NE-CZ | 5.96 | 132.75 | 124.40 |
| 1 | C | 129 | ASN | CA-C-N | 5.96 | 125.67 | 119.05 |
| 1 | C | 129 | ASN | C-N-CA | 5.96 | 125.67 | 119.05 |
| 2 | D | 483 | PRO | N-CA-CB | 5.96 | 108.63 | 103.27 |
| 1 | C | 636 | THR | CA-C-N | 5.95 | 125.66 | 119.05 |
| 1 | C | 636 | THR | C-N-CA | 5.95 | 125.66 | 119.05 |
| 2 | D | 260 | ALA | CA-C-N | 5.94 | 128.24 | 120.28 |
| 2 | D | 260 | ALA | C-N-CA | 5.94 | 128.24 | 120.28 |
| 2 | B | 189 | PRO | CA-C-N | 5.93 | 128.51 | 120.38 |
| 2 | B | 189 | PRO | C-N-CA | 5.93 | 128.51 | 120.38 |
| 1 | C | 342 | TYR | CA-C-N | 5.93 | 128.82 | 120.28 |
| 1 | C | 342 | TYR | C-N-CA | 5.93 | 128.82 | 120.28 |
| 1 | A | 428 | GLU | CA-C-N | 5.93 | 129.32 | 120.31 |
| 1 | A | 428 | GLU | C-N-CA | 5.93 | 129.32 | 120.31 |
| 1 | C | 526 | ASP | CA-C-O | 5.93 | 125.05 | 119.59 |
| 2 | B | 258 | THR | CA-C-N | 5.93 | 126.52 | 119.94 |
| 2 | B | 258 | THR | C-N-CA | 5.93 | 126.52 | 119.94 |
| 1 | C | 521 | ASN | O-C-N | -5.92 | 116.04 | 121.37 |
| 2 | B | 543 | PRO | N-CA-CB | 5.92 | 108.83 | 103.33 |
| 1 | A | 52 | GLU | O-C-N | -5.91 | 114.57 | 122.43 |
| 1 | C | 263 | GLY | O-C-N | -5.91 | 116.52 | 122.19 |
| 2 | D | 294 | ILE | CA-C-N | 5.91 | 128.20 | 120.28 |
| 2 | D | 294 | ILE | C-N-CA | 5.91 | 128.20 | 120.28 |
| 2 | D | 374 | PHE | CA-C-N | 5.91 | 125.45 | 119.19 |
| 2 | D | 374 | PHE | C-N-CA | 5.91 | 125.45 | 119.19 |
| 2 | D | 141 | ASP | CA-C-N | 5.90 | 125.60 | 119.05 |
| 2 | D | 141 | ASP | C-N-CA | 5.90 | 125.60 | 119.05 |
| 1 | C | 711 | ILE | CA-C-N | 5.89 | 125.59 | 119.05 |
| 1 | C | 711 | ILE | C-N-CA | 5.89 | 125.59 | 119.05 |
| 2 | D | 609 | ALA | CA-C-N | 5.89 | 128.17 | 120.28 |
| 2 | D | 609 | ALA | C-N-CA | 5.89 | 128.17 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 69 | PRO | CA-C-N | 5.89 | 130.76 | 122.46 |
| 1 | C | 69 | PRO | C-N-CA | 5.89 | 130.76 | 122.46 |
| 2 | D | 147 | PRO | CA-C-N | 5.89 | 133.06 | 121.58 |
| 2 | D | 147 | PRO | C-N-CA | 5.89 | 133.06 | 121.58 |
| 2 | D | 455 | ASN | CA-C-O | 5.88 | 126.23 | 119.35 |
| 1 | C | 589 | GLU | CA-C-N | 5.88 | 128.09 | 120.44 |
| 1 | C | 589 | GLU | C-N-CA | 5.88 | 128.09 | 120.44 |
| 1 | A | 405 | GLY | O-C-N | -5.88 | 116.54 | 122.65 |
| 2 | B | 521 | ARG | CA-C-N | 5.88 | 128.48 | 120.54 |
| 2 | B | 521 | ARG | C-N-CA | 5.88 | 128.48 | 120.54 |
| 2 | B | 307 | ILE | CA-C-N | 5.88 | 126.50 | 119.98 |
| 2 | B | 307 | ILE | C-N-CA | 5.88 | 126.50 | 119.98 |
| 1 | C | 613 | GLY | CA-C-N | 5.87 | 128.07 | 120.44 |
| 1 | C | 613 | GLY | C-N-CA | 5.87 | 128.07 | 120.44 |
| 2 | D | 532 | SER | CA-C-N | 5.87 | 125.56 | 119.05 |
| 2 | D | 532 | SER | C-N-CA | 5.87 | 125.56 | 119.05 |
| 2 | B | 141 | ASP | CA-C-N | 5.87 | 125.56 | 119.05 |
| 2 | B | 141 | ASP | C-N-CA | 5.87 | 125.56 | 119.05 |
| 1 | A | 55 | TYR | N-CA-C | 5.87 | 118.62 | 111.82 |
| 2 | B | 115 | ASP | CA-C-N | 5.87 | 125.07 | 118.97 |
| 2 | B | 115 | ASP | C-N-CA | 5.87 | 125.07 | 118.97 |
| 1 | C | 494 | ALA | CA-C-N | 5.86 | 128.13 | 120.28 |
| 1 | C | 494 | ALA | C-N-CA | 5.86 | 128.13 | 120.28 |
| 1 | A | 412 | LEU | CA-C-N | 5.86 | 128.06 | 120.44 |
| 1 | A | 412 | LEU | C-N-CA | 5.86 | 128.06 | 120.44 |
| 1 | C | 428 | GLU | CA-C-N | 5.86 | 128.13 | 120.28 |
| 1 | C | 428 | GLU | C-N-CA | 5.86 | 128.13 | 120.28 |
| 2 | D | 200 | ASP | CA-C-N | 5.86 | 125.56 | 119.05 |
| 2 | D | 200 | ASP | C-N-CA | 5.86 | 125.56 | 119.05 |
| 1 | C | 468 | ASN | CA-CB-CG | 5.86 | 118.45 | 112.60 |
| 1 | C | 438 | GLU | CA-C-N | 5.85 | 128.12 | 120.28 |
| 1 | C | 438 | GLU | C-N-CA | 5.85 | 128.12 | 120.28 |
| 1 | C | 556 | PHE | N-CA-C | 5.84 | 119.59 | 112.23 |
| 2 | D | 444 | ALA | CA-C-N | 5.83 | 128.03 | 120.44 |
| 2 | D | 444 | ALA | C-N-CA | 5.83 | 128.03 | 120.44 |
| 1 | C | 146 | ILE | O-C-N | -5.82 | 116.22 | 121.87 |
| 1 | C | 216 | PRO | N-CA-CB | 5.82 | 109.73 | 103.33 |
| 1 | A | 80 | ALA | CA-C-O | -5.82 | 114.38 | 120.55 |
| 1 | A | 205 | MET | CA-C-O | -5.82 | 114.71 | 120.82 |
| 1 | A | 527 | PRO | N-CA-CB | 5.81 | 109.67 | 103.39 |
| 1 | C | 608 | ASP | CA-CB-CG | 5.81 | 118.41 | 112.60 |
| 1 | C | 527 | PRO | CA-C-N | 5.80 | 130.41 | 120.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 527 | PRO | C-N-CA | 5.80 | 130.41 | 120.72 |
| 1 | C | 518 | ALA | CA-C-O | -5.80 | 114.41 | 120.55 |
| 1 | C | 140 | GLY | O-C-N | -5.79 | 118.36 | 123.92 |
| 2 | D | 84 | LYS | CA-C-O | -5.79 | 113.99 | 120.54 |
| 1 | A | 146 | ILE | O-C-N | -5.79 | 116.25 | 121.87 |
| 2 | B | 264 | ARG | CD-NE-CZ | 5.79 | 132.50 | 124.40 |
| 1 | A | 215 | GLN | CA-C-N | 5.78 | 125.47 | 119.05 |
| 1 | A | 215 | GLN | C-N-CA | 5.78 | 125.47 | 119.05 |
| 1 | A | 589 | GLU | CA-C-N | 5.78 | 128.50 | 120.29 |
| 1 | A | 589 | GLU | C-N-CA | 5.78 | 128.50 | 120.29 |
| 2 | D | 478 | PRO | N-CA-CB | 5.78 | 108.34 | 103.25 |
| 1 | A | 703 | GLU | CA-CB-CG | 5.77 | 125.64 | 114.10 |
| 2 | B | 417 | TRP | CA-C-N | 5.77 | 128.02 | 120.28 |
| 2 | B | 417 | TRP | C-N-CA | 5.77 | 128.02 | 120.28 |
| 1 | A | 684 | VAL | N-CA-CB | 5.77 | 119.37 | 111.41 |
| 1 | A | 7 | PHE | N-CA-C | 5.77 | 119.94 | 113.02 |
| 2 | D | 25 | GLY | CA-C-N | 5.77 | 131.23 | 121.14 |
| 2 | D | 25 | GLY | C-N-CA | 5.77 | 131.23 | 121.14 |
| 1 | A | 504 | ASP | CA-CB-CG | 5.76 | 118.36 | 112.60 |
| 1 | A | 66 | GLY | O-C-N | -5.76 | 115.22 | 122.41 |
| 1 | C | 43 | GLN | CA-C-O | 5.76 | 128.12 | 120.98 |
| 1 | A | 636 | THR | N-CA-C | -5.75 | 101.67 | 110.07 |
| 1 | C | 703 | GLU | CA-CB-CG | 5.75 | 125.61 | 114.10 |
| 2 | D | 466 | PHE | O-C-N | -5.75 | 118.88 | 121.53 |
| 1 | A | 639 | GLU | CA-C-N | 5.75 | 128.45 | 120.29 |
| 1 | A | 639 | GLU | C-N-CA | 5.75 | 128.45 | 120.29 |
| 2 | B | 450 | ALA | CA-C-N | 5.74 | 127.90 | 120.44 |
| 2 | B | 450 | ALA | C-N-CA | 5.74 | 127.90 | 120.44 |
| 2 | B | 576 | GLN | N-CA-C | 5.74 | 118.02 | 111.02 |
| 1 | C | 333 | GLY | CA-C-O | 5.73 | 127.19 | 121.00 |
| 1 | C | 672 | LEU | CA-C-N | 5.73 | 127.95 | 120.28 |
| 1 | C | 672 | LEU | C-N-CA | 5.73 | 127.95 | 120.28 |
| 1 | C | 711 | ILE | CA-C-O | 5.72 | 123.06 | 118.71 |
| 2 | D | 203 | GLY | CA-C-N | 5.72 | 127.88 | 120.44 |
| 2 | D | 203 | GLY | C-N-CA | 5.72 | 127.88 | 120.44 |
| 2 | B | 200 | ASP | CA-C-N | 5.71 | 125.39 | 119.05 |
| 2 | B | 200 | ASP | C-N-CA | 5.71 | 125.39 | 119.05 |
| 1 | A | 445 | ARG | CA-C-N | 5.71 | 128.28 | 120.46 |
| 1 | A | 445 | ARG | C-N-CA | 5.71 | 128.28 | 120.46 |
| 1 | A | 677 | ARG | CA-CB-CG | 5.71 | 125.52 | 114.10 |
| 1 | C | 148 | ASP | CA-C-N | 5.71 | 127.93 | 120.28 |
| 1 | C | 148 | ASP | C-N-CA | 5.71 | 127.93 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 412 | LEU | O-C-N | -5.71 | 116.07 | 122.12 |
| 1 | A | 219 | ARG | CA-C-N | 5.71 | 127.75 | 120.56 |
| 1 | A | 219 | ARG | C-N-CA | 5.71 | 127.75 | 120.56 |
| 2 | B | 462 | ALA | CA-C-N | 5.70 | 132.24 | 121.97 |
| 2 | B | 462 | ALA | C-N-CA | 5.70 | 132.24 | 121.97 |
| 1 | A | 313 | HIS | O-C-N | -5.70 | 116.08 | 122.12 |
| 1 | C | 587 | VAL | CA-C-N | 5.70 | 127.92 | 120.28 |
| 1 | C | 587 | VAL | C-N-CA | 5.70 | 127.92 | 120.28 |
| 1 | A | 522 | PRO | N-CA-CB | 5.70 | 108.37 | 103.36 |
| 1 | C | 332 | SER | CA-C-O | 5.69 | 127.39 | 120.62 |
| 1 | A | 66 | GLY | CA-C-N | 5.69 | 132.66 | 122.13 |
| 1 | A | 66 | GLY | C-N-CA | 5.69 | 132.66 | 122.13 |
| 1 | C | 343 | ASN | O-C-N | -5.69 | 115.56 | 122.22 |
| 2 | D | 339 | ASN | O-C-N | -5.69 | 114.99 | 122.39 |
| 2 | B | 72 | ILE | CB-CG1-CD1 | 5.69 | 125.75 | 113.80 |
| 1 | A | 198 | ASN | CA-CB-CG | 5.68 | 118.28 | 112.60 |
| 1 | C | 523 | ASP | CA-C-N | 5.68 | 128.16 | 120.38 |
| 1 | C | 523 | ASP | C-N-CA | 5.68 | 128.16 | 120.38 |
| 1 | A | 97 | GLU | CA-C-N | 5.67 | 127.82 | 120.44 |
| 1 | A | 97 | GLU | C-N-CA | 5.67 | 127.82 | 120.44 |
| 2 | B | 127 | GLU | CA-C-N | 5.67 | 126.23 | 119.94 |
| 2 | B | 127 | GLU | C-N-CA | 5.67 | 126.23 | 119.94 |
| 2 | D | 116 | PRO | N-CA-CB | 5.67 | 109.30 | 103.23 |
| 1 | A | 666 | PRO | N-CA-CB | 5.67 | 109.29 | 103.23 |
| 2 | D | 455 | ASN | O-C-N | -5.65 | 115.28 | 122.34 |
| 2 | B | 390 | VAL | O-C-N | -5.64 | 115.52 | 122.18 |
| 1 | A | 427 | VAL | CA-C-N | 5.64 | 128.89 | 120.31 |
| 1 | A | 427 | VAL | C-N-CA | 5.64 | 128.89 | 120.31 |
| 2 | B | 78 | PRO | O-C-N | -5.64 | 115.75 | 122.24 |
| 2 | B | 494 | SER | CA-C-N | 5.64 | 127.84 | 120.28 |
| 2 | B | 494 | SER | C-N-CA | 5.64 | 127.84 | 120.28 |
| 1 | C | 123 | ARG | CA-C-N | 5.64 | 131.32 | 120.66 |
| 1 | C | 123 | ARG | C-N-CA | 5.64 | 131.32 | 120.66 |
| 1 | C | 488 | VAL | N-CA-CB | 5.64 | 117.15 | 110.55 |
| 1 | C | 677 | ARG | CA-C-N | 5.64 | 126.13 | 120.04 |
| 1 | C | 677 | ARG | C-N-CA | 5.64 | 126.13 | 120.04 |
| 1 | C | 157 | PRO | N-CA-CB | 5.64 | 108.19 | 103.17 |
| 1 | C | 30 | ALA | CA-C-N | 5.63 | 128.87 | 120.31 |
| 1 | C | 30 | ALA | C-N-CA | 5.63 | 128.87 | 120.31 |
| 2 | D | 141 | ASP | CA-CB-CG | 5.63 | 118.23 | 112.60 |
| 1 | A | 368 | LEU | CA-C-N | 5.63 | 132.00 | 122.65 |
| 1 | A | 368 | LEU | C-N-CA | 5.63 | 132.00 | 122.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 88 | PRO | N-CA-CB | 5.63 | 108.58 | 103.34 |
| 1 | C | 520 | GLY | O-C-N | -5.63 | 116.32 | 122.68 |
| 2 | B | 419 | GLU | CA-C-N | 5.62 | 127.75 | 120.44 |
| 2 | B | 419 | GLU | C-N-CA | 5.62 | 127.75 | 120.44 |
| 2 | B | 586 | LYS | CA-C-N | 5.62 | 127.82 | 120.28 |
| 2 | B | 586 | LYS | C-N-CA | 5.62 | 127.82 | 120.28 |
| 2 | B | 362 | PRO | N-CA-CB | 5.62 | 108.24 | 103.35 |
| 2 | B | 328 | TRP | CA-C-N | 5.62 | 128.37 | 120.28 |
| 2 | B | 328 | TRP | C-N-CA | 5.62 | 128.37 | 120.28 |
| 1 | A | 531 | LEU | N-CA-C | 5.61 | 118.33 | 111.82 |
| 1 | C | 118 | ASP | CA-CB-CG | 5.61 | 118.21 | 112.60 |
| 1 | C | 720 | LYS | CA-C-N | 5.61 | 127.80 | 120.28 |
| 1 | C | 720 | LYS | C-N-CA | 5.61 | 127.80 | 120.28 |
| 1 | C | 665 | VAL | CA-C-N | 5.61 | 125.27 | 119.05 |
| 1 | C | 665 | VAL | C-N-CA | 5.61 | 125.27 | 119.05 |
| 1 | C | 715 | ALA | CA-C-N | 5.60 | 128.11 | 120.77 |
| 1 | C | 715 | ALA | C-N-CA | 5.60 | 128.11 | 120.77 |
| 1 | A | 528 | ASP | CA-C-N | 5.60 | 132.48 | 122.06 |
| 1 | A | 528 | ASP | C-N-CA | 5.60 | 132.48 | 122.06 |
| 2 | D | 361 | LEU | CA-C-O | 5.60 | 126.00 | 120.17 |
| 2 | B | 35 | TRP | CA-C-N | 5.60 | 128.10 | 120.54 |
| 2 | B | 35 | TRP | C-N-CA | 5.60 | 128.10 | 120.54 |
| 2 | B | 211 | GLU | CA-C-O | 5.60 | 124.89 | 120.19 |
| 1 | C | 449 | ALA | CA-C-N | 5.60 | 128.82 | 120.31 |
| 1 | C | 449 | ALA | C-N-CA | 5.60 | 128.82 | 120.31 |
| 1 | A | 637 | PRO | CA-C-N | 5.58 | 130.13 | 120.58 |
| 1 | A | 637 | PRO | C-N-CA | 5.58 | 130.13 | 120.58 |
| 1 | C | 528 | ASP | CA-C-N | 5.58 | 132.44 | 122.06 |
| 1 | C | 528 | ASP | C-N-CA | 5.58 | 132.44 | 122.06 |
| 2 | B | 345 | ILE | CA-C-N | 5.56 | 128.19 | 120.29 |
| 2 | B | 345 | ILE | C-N-CA | 5.56 | 128.19 | 120.29 |
| 1 | A | 539 | GLY | CA-C-N | 5.56 | 128.76 | 120.31 |
| 1 | A | 539 | GLY | C-N-CA | 5.56 | 128.76 | 120.31 |
| 1 | C | 282 | PRO | N-CA-CB | 5.56 | 109.04 | 103.48 |
| 2 | B | 375 | PRO | N-CA-CB | 5.56 | 109.39 | 103.39 |
| 2 | B | 116 | PRO | N-CA-CB | 5.55 | 109.17 | 103.23 |
| 2 | B | 55 | PHE | N-CA-CB | 5.55 | 118.26 | 109.82 |
| 1 | A | 18 | PRO | N-CA-CB | 5.55 | 109.08 | 103.25 |
| 2 | D | 86 | GLY | O-C-N | -5.55 | 116.77 | 122.60 |
| 2 | D | 457 | LYS | CA-C-N | 5.55 | 131.29 | 123.30 |
| 2 | D | 457 | LYS | C-N-CA | 5.55 | 131.29 | 123.30 |
| 2 | D | 369 | LEU | CA-C-O | 5.54 | 125.58 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | D | 251 | GLU | CB-CG-CD | 5.53 | 122.01 | 112.60 |
| 1 | A | 632 | PRO | N-CA-CB | 5.53 | 109.19 | 103.38 |
| 1 | C | 721 | LYS | CA-C-N | 5.53 | 127.63 | 120.44 |
| 1 | C | 721 | LYS | C-N-CA | 5.53 | 127.63 | 120.44 |
| 2 | D | 362 | PRO | N-CA-CB | 5.53 | 108.59 | 103.39 |
| 2 | B | 608 | GLU | CA-C-N | 5.53 | 127.95 | 120.38 |
| 2 | B | 608 | GLU | C-N-CA | 5.53 | 127.95 | 120.38 |
| 2 | D | 24 | ALA | O-C-N | -5.52 | 114.37 | 122.43 |
| 1 | A | 441 | ILE | CA-C-N | 5.52 | 124.98 | 119.24 |
| 1 | A | 441 | ILE | C-N-CA | 5.52 | 124.98 | 119.24 |
| 1 | A | 158 | LEU | N-CA-C | 5.52 | 119.88 | 113.20 |
| 1 | C | 579 | GLU | CA-C-N | 5.52 | 127.51 | 120.56 |
| 1 | C | 579 | GLU | C-N-CA | 5.52 | 127.51 | 120.56 |
| 1 | C | 202 | LYS | CA-C-N | 5.51 | 127.94 | 120.44 |
| 1 | C | 202 | LYS | C-N-CA | 5.51 | 127.94 | 120.44 |
| 2 | B | 263 | VAL | N-CA-C | -5.51 | 105.48 | 110.82 |
| 2 | D | 229 | PRO | CA-C-N | 5.50 | 130.04 | 120.68 |
| 2 | D | 229 | PRO | C-N-CA | 5.50 | 130.04 | 120.68 |
| 1 | A | 281 | ALA | CA-C-N | 5.50 | 125.17 | 119.56 |
| 1 | A | 281 | ALA | C-N-CA | 5.50 | 125.17 | 119.56 |
| 2 | D | 223 | ARG | CA-C-N | 5.50 | 132.02 | 122.56 |
| 2 | D | 223 | ARG | C-N-CA | 5.50 | 132.02 | 122.56 |
| 2 | B | 25 | GLY | CA-C-N | 5.50 | 130.76 | 121.14 |
| 2 | B | 25 | GLY | C-N-CA | 5.50 | 130.76 | 121.14 |
| 1 | C | 622 | ALA | CA-C-N | 5.50 | 129.90 | 120.72 |
| 1 | C | 622 | ALA | C-N-CA | 5.50 | 129.90 | 120.72 |
| 1 | A | 216 | PRO | N-CA-CB | 5.49 | 109.37 | 103.33 |
| 2 | B | 478 | PRO | N-CA-CB | 5.48 | 108.07 | 103.25 |
| 2 | B | 339 | ASN | O-C-N | -5.48 | 115.09 | 122.43 |
| 1 | A | 448 | GLU | CA-C-N | 5.47 | 127.62 | 120.28 |
| 1 | A | 448 | GLU | C-N-CA | 5.47 | 127.62 | 120.28 |
| 2 | B | 190 | ALA | O-C-N | -5.47 | 116.32 | 122.12 |
| 1 | C | 189 | PRO | N-CA-CB | 5.47 | 109.30 | 103.39 |
| 2 | D | 345 | ILE | CA-C-N | 5.46 | 127.54 | 120.44 |
| 2 | D | 345 | ILE | C-N-CA | 5.46 | 127.54 | 120.44 |
| 2 | B | 465 | GLU | O-C-N | -5.46 | 116.88 | 123.27 |
| 2 | D | 78 | PRO | O-C-N | -5.46 | 115.57 | 122.17 |
| 1 | A | 233 | PRO | N-CA-CB | 5.46 | 108.75 | 103.51 |
| 2 | B | 191 | LYS | CA-C-N | 5.45 | 131.26 | 121.66 |
| 2 | B | 191 | LYS | C-N-CA | 5.45 | 131.26 | 121.66 |
| 1 | C | 661 | HIS | N-CA-C | 5.45 | 117.98 | 111.71 |
| 1 | C | 232 | MET | CA-C-N | 5.45 | 125.54 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 232 | MET | C-N-CA | 5.45 | 125.54 | 119.87 |
| 1 | C | 488 | VAL | CB-CA-C | -5.45 | 104.99 | 111.97 |
| 1 | A | 524 | ASP | N-CA-C | 5.45 | 117.22 | 111.28 |
| 2 | B | 533 | PRO | N-CA-CB | 5.44 | 109.47 | 103.26 |
| 2 | B | 108 | ASP | CA-CB-CG | 5.43 | 118.03 | 112.60 |
| 2 | D | 48 | PRO | N-CA-CB | 5.43 | 108.35 | 103.08 |
| 1 | A | 333 | GLY | CA-C-O | 5.43 | 126.86 | 121.00 |
| 1 | C | 281 | ALA | O-C-N | -5.43 | 115.61 | 120.71 |
| 2 | D | 204 | PHE | CA-C-N | 5.43 | 127.87 | 120.54 |
| 2 | D | 204 | PHE | C-N-CA | 5.43 | 127.87 | 120.54 |
| 2 | B | 229 | PRO | N-CA-CB | 5.43 | 108.72 | 103.51 |
| 1 | C | 344 | ASN | CA-C-N | 5.43 | 127.40 | 120.56 |
| 1 | C | 344 | ASN | C-N-CA | 5.43 | 127.40 | 120.56 |
| 1 | A | 44 | ILE | N-CA-C | -5.42 | 101.80 | 107.60 |
| 2 | B | 48 | PRO | N-CA-CB | 5.42 | 108.34 | 103.08 |
| 1 | A | 476 | PRO | N-CA-CB | 5.42 | 108.33 | 103.08 |
| 2 | D | 159 | LEU | N-CA-C | 5.42 | 119.15 | 112.54 |
| 2 | D | 364 | THR | CA-C-N | 5.42 | 129.26 | 120.60 |
| 2 | D | 364 | THR | C-N-CA | 5.42 | 129.26 | 120.60 |
| 2 | D | 466 | PHE | CB-CA-C | -5.42 | 107.36 | 111.20 |
| 1 | C | 524 | ASP | N-CA-C | 5.41 | 117.88 | 111.33 |
| 1 | A | 61 | LEU | N-CA-C | 5.40 | 118.97 | 112.38 |
| 1 | A | 257 | ALA | N-CA-C | 5.40 | 117.17 | 111.28 |
| 1 | A | 189 | PRO | N-CA-CB | 5.40 | 109.22 | 103.39 |
| 1 | A | 332 | SER | CA-C-O | 5.40 | 127.04 | 120.62 |
| 1 | C | 28 | LEU | CA-C-N | 5.40 | 127.45 | 120.44 |
| 1 | C | 28 | LEU | C-N-CA | 5.40 | 127.45 | 120.44 |
| 1 | A | 118 | ASP | CA-CB-CG | 5.39 | 118.00 | 112.60 |
| 2 | D | 191 | LYS | N-CA-C | 5.39 | 119.48 | 113.01 |
| 2 | D | 462 | ALA | O-C-N | -5.39 | 115.26 | 122.00 |
| 2 | B | 251 | GLU | CB-CG-CD | 5.39 | 121.77 | 112.60 |
| 2 | B | 155 | SER | N-CA-C | 5.39 | 117.16 | 111.28 |
| 2 | D | 68 | ASP | CA-CB-CG | 5.39 | 117.99 | 112.60 |
| 1 | A | 263 | GLY | O-C-N | -5.39 | 116.95 | 122.17 |
| 1 | A | 282 | PRO | N-CA-CB | 5.39 | 108.87 | 103.48 |
| 1 | C | 678 | PRO | N-CA-CB | 5.38 | 108.31 | 103.20 |
| 2 | D | 315 | GLU | N-CA-C | 5.38 | 117.15 | 111.28 |
| 2 | B | 422 | GLU | CA-C-N | 5.38 | 128.06 | 120.42 |
| 2 | B | 422 | GLU | C-N-CA | 5.38 | 128.06 | 120.42 |
| 1 | C | 262 | ASP | O-C-N | -5.38 | 116.49 | 122.09 |
| 2 | B | 525 | GLY | CA-C-N | 5.38 | 126.06 | 119.99 |
| 2 | B | 525 | GLY | C-N-CA | 5.38 | 126.06 | 119.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 214 | PRO | N-CA-CB | 5.38 | 109.01 | 103.15 |
| 1 | C | 541 | ALA | CA-C-N | 5.38 | 131.81 | 121.54 |
| 1 | C | 541 | ALA | C-N-CA | 5.38 | 131.81 | 121.54 |
| 2 | B | 617 | LEU | N-CA-CB | 5.37 | 118.99 | 110.55 |
| 2 | B | 536 | HIS | O-C-N | -5.37 | 115.23 | 122.43 |
| 1 | C | 441 | ILE | CA-C-N | 5.37 | 124.83 | 119.24 |
| 1 | C | 441 | ILE | C-N-CA | 5.37 | 124.83 | 119.24 |
| 1 | A | 421 | TRP | CA-C-N | 5.37 | 125.94 | 119.98 |
| 1 | A | 421 | TRP | C-N-CA | 5.37 | 125.94 | 119.98 |
| 2 | B | 335 | ASP | CA-C-N | 5.37 | 124.98 | 119.56 |
| 2 | B | 335 | ASP | C-N-CA | 5.37 | 124.98 | 119.56 |
| 1 | A | 290 | ILE | N-CA-CB | 5.36 | 118.73 | 112.35 |
| 2 | B | 349 | SER | CA-C-N | 5.36 | 127.46 | 120.28 |
| 2 | B | 349 | SER | C-N-CA | 5.36 | 127.46 | 120.28 |
| 1 | C | 322 | SER | O-C-N | -5.36 | 116.44 | 122.12 |
| 2 | B | 609 | ALA | N-CA-C | 5.35 | 117.81 | 111.33 |
| 1 | A | 261 | ALA | O-C-N | -5.35 | 116.05 | 122.15 |
| 2 | B | 365 | GLN | N-CA-C | 5.35 | 119.06 | 112.54 |
| 2 | D | 123 | LYS | CA-C-N | 5.35 | 127.76 | 120.54 |
| 2 | D | 123 | LYS | C-N-CA | 5.35 | 127.76 | 120.54 |
| 2 | B | 327 | SER | N-CA-C | 5.35 | 117.93 | 109.96 |
| 1 | A | 598 | PRO | N-CA-CB | 5.35 | 108.08 | 103.27 |
| 2 | D | 229 | PRO | N-CA-CB | 5.34 | 108.28 | 103.20 |
| 2 | B | 142 | PRO | N-CA-CB | 5.34 | 109.21 | 103.33 |
| 2 | B | 147 | PRO | CA-C-N | 5.34 | 132.00 | 121.58 |
| 2 | B | 147 | PRO | C-N-CA | 5.34 | 132.00 | 121.58 |
| 1 | C | 556 | PHE | CA-CB-CG | 5.34 | 119.14 | 113.80 |
| 1 | C | 484 | ASP | CA-CB-CG | 5.34 | 117.94 | 112.60 |
| 2 | B | 456 | ARG | O-C-N | -5.34 | 113.29 | 122.20 |
| 2 | D | 349 | SER | CA-C-N | 5.34 | 127.43 | 120.28 |
| 2 | D | 349 | SER | C-N-CA | 5.34 | 127.43 | 120.28 |
| 1 | C | 159 | ASP | CA-CB-CG | 5.33 | 117.93 | 112.60 |
| 2 | D | 558 | LYS | O-C-N | -5.33 | 116.47 | 122.12 |
| 2 | D | 604 | ASP | CA-C-N | 5.33 | 131.18 | 122.65 |
| 2 | D | 604 | ASP | C-N-CA | 5.33 | 131.18 | 122.65 |
| 1 | C | 52 | GLU | O-C-N | -5.32 | 113.89 | 122.41 |
| 1 | C | 66 | GLY | N-CA-C | 5.32 | 122.69 | 115.30 |
| 1 | C | 469 | LYS | CA-C-N | 5.32 | 130.50 | 122.68 |
| 1 | C | 469 | LYS | C-N-CA | 5.32 | 130.50 | 122.68 |
| 1 | A | 281 | ALA | O-C-N | -5.32 | 115.21 | 121.32 |
| 1 | A | 665 | VAL | CA-C-N | 5.31 | 124.50 | 118.97 |
| 1 | A | 665 | VAL | C-N-CA | 5.31 | 124.50 | 118.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 182 | VAL | CA-C-N | 5.31 | 128.39 | 120.31 |
| 2 | B | 182 | VAL | C-N-CA | 5.31 | 128.39 | 120.31 |
| 1 | A | 500 | ARG | CA-C-N | 5.31 | 127.83 | 120.29 |
| 1 | A | 500 | ARG | C-N-CA | 5.31 | 127.83 | 120.29 |
| 2 | D | 566 | ASP | CA-CB-CG | 5.31 | 117.91 | 112.60 |
| 2 | B | 398 | PRO | N-CA-CB | 5.31 | 109.12 | 103.39 |
| 1 | C | 368 | LEU | N-CA-C | 5.31 | 118.86 | 112.38 |
| 1 | C | 632 | PRO | N-CA-CB | 5.30 | 108.29 | 103.15 |
| 2 | D | 425 | LYS | CA-C-N | 5.30 | 131.92 | 121.58 |
| 2 | D | 425 | LYS | C-N-CA | 5.30 | 131.92 | 121.58 |
| 1 | C | 597 | ARG | NE-CZ-NH1 | 5.30 | 126.80 | 121.50 |
| 1 | A | 82 | ARG | CA-C-O | 5.30 | 124.62 | 119.22 |
| 2 | B | 510 | ARG | CA-C-O | 5.30 | 124.16 | 119.71 |
| 1 | C | 603 | ALA | CA-C-O | 5.30 | 126.33 | 120.71 |
| 2 | B | 444 | ALA | CA-C-N | 5.29 | 127.64 | 120.44 |
| 2 | B | 444 | ALA | C-N-CA | 5.29 | 127.64 | 120.44 |
| 1 | A | 184 | GLU | O-C-N | -5.29 | 115.34 | 122.43 |
| 2 | B | 235 | THR | N-CA-CB | 5.29 | 119.50 | 110.87 |
| 1 | C | 646 | GLU | N-CA-C | 5.29 | 117.80 | 111.71 |
| 1 | A | 689 | PRO | N-CA-CB | 5.29 | 107.95 | 103.35 |
| 1 | C | 538 | ALA | CA-C-N | 5.29 | 125.85 | 119.98 |
| 1 | C | 538 | ALA | C-N-CA | 5.29 | 125.85 | 119.98 |
| 1 | A | 720 | LYS | CA-C-N | 5.28 | 127.36 | 120.28 |
| 1 | A | 720 | LYS | C-N-CA | 5.28 | 127.36 | 120.28 |
| 2 | B | 631 | LEU | CA-C-N | 5.28 | 127.30 | 120.44 |
| 2 | B | 631 | LEU | C-N-CA | 5.28 | 127.30 | 120.44 |
| 1 | A | 244 | HIS | CA-CB-CG | -5.28 | 108.52 | 113.80 |
| 2 | B | 167 | PHE | CA-CB-CG | 5.28 | 119.08 | 113.80 |
| 2 | D | 78 | PRO | N-CA-CB | 5.28 | 109.21 | 103.30 |
| 2 | B | 201 | PRO | N-CA-CB | 5.28 | 109.13 | 103.33 |
| 2 | B | 604 | ASP | CA-C-N | 5.28 | 131.09 | 122.65 |
| 2 | B | 604 | ASP | C-N-CA | 5.28 | 131.09 | 122.65 |
| 2 | D | 335 | ASP | CA-C-N | 5.28 | 124.89 | 119.56 |
| 2 | D | 335 | ASP | C-N-CA | 5.28 | 124.89 | 119.56 |
| 2 | B | 217 | LEU | CA-C-N | 5.27 | 125.95 | 119.99 |
| 2 | B | 217 | LEU | C-N-CA | 5.27 | 125.95 | 119.99 |
| 1 | A | 298 | VAL | CA-C-N | 5.27 | 127.34 | 120.28 |
| 1 | A | 298 | VAL | C-N-CA | 5.27 | 127.34 | 120.28 |
| 2 | B | 260 | ALA | CA-C-N | 5.27 | 127.34 | 120.28 |
| 2 | B | 260 | ALA | C-N-CA | 5.27 | 127.34 | 120.28 |
| 1 | C | 158 | LEU | CA-C-N | 5.27 | 129.64 | 120.68 |
| 1 | C | 158 | LEU | C-N-CA | 5.27 | 129.64 | 120.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 184 | GLU | N-CA-C | 5.27 | 118.81 | 112.38 |
| 1 | C | 433 | MET | N-CA-C | 5.27 | 117.10 | 111.36 |
| 2 | B | 588 | ALA | N-CA-C | 5.27 | 119.57 | 113.20 |
| 1 | C | 8 | ASP | CA-CB-CG | 5.27 | 117.87 | 112.60 |
| 1 | A | 175 | LEU | CA-C-N | 5.26 | 127.33 | 120.28 |
| 1 | A | 175 | LEU | C-N-CA | 5.26 | 127.33 | 120.28 |
| 1 | C | 198 | ASN | N-CA-CB | -5.26 | 103.91 | 111.70 |
| 2 | D | 437 | HIS | CA-CB-CG | -5.26 | 108.54 | 113.80 |
| 1 | A | 634 | PHE | CA-CB-CG | 5.26 | 119.06 | 113.80 |
| 1 | A | 211 | ILE | N-CA-CB | 5.25 | 119.89 | 111.23 |
| 1 | A | 433 | MET | N-CA-C | 5.25 | 117.91 | 111.82 |
| 2 | D | 108 | ASP | CA-CB-CG | 5.25 | 117.85 | 112.60 |
| 1 | A | 88 | GLN | CA-C-N | 5.25 | 128.80 | 121.24 |
| 1 | A | 88 | GLN | C-N-CA | 5.25 | 128.80 | 121.24 |
| 1 | C | 26 | GLU | CA-C-O | -5.25 | 114.96 | 120.63 |
| 2 | D | 88 | PRO | N-CA-CB | 5.25 | 108.17 | 103.19 |
| 2 | D | 218 | GLY | CA-C-N | 5.25 | 127.31 | 120.28 |
| 2 | D | 218 | GLY | C-N-CA | 5.25 | 127.31 | 120.28 |
| 1 | A | 217 | SER | CA-C-N | 5.24 | 128.27 | 120.31 |
| 1 | A | 217 | SER | C-N-CA | 5.24 | 128.27 | 120.31 |
| 2 | B | 189 | PRO | N-CA-CB | 5.23 | 108.74 | 103.25 |
| 2 | D | 142 | PRO | N-CA-CB | 5.23 | 109.08 | 103.33 |
| 2 | B | 610 | GLU | N-CA-C | 5.22 | 117.72 | 111.71 |
| 1 | A | 668 | LEU | CA-C-N | 5.22 | 127.59 | 120.54 |
| 1 | A | 668 | LEU | C-N-CA | 5.22 | 127.59 | 120.54 |
| 1 | C | 20 | ASP | CA-C-N | 5.22 | 128.04 | 120.79 |
| 1 | C | 20 | ASP | C-N-CA | 5.22 | 128.04 | 120.79 |
| 1 | C | 172 | LEU | O-C-N | -5.22 | 116.26 | 120.38 |
| 2 | B | 31 | THR | CA-C-N | 5.21 | 127.21 | 120.44 |
| 2 | B | 31 | THR | C-N-CA | 5.21 | 127.21 | 120.44 |
| 1 | A | 673 | ASP | O-C-N | -5.21 | 116.68 | 122.09 |
| 1 | A | 646 | GLU | CA-C-N | 5.20 | 130.53 | 122.26 |
| 1 | A | 646 | GLU | C-N-CA | 5.20 | 130.53 | 122.26 |
| 2 | D | 56 | ALA | CA-C-N | 5.20 | 127.25 | 120.28 |
| 2 | D | 56 | ALA | C-N-CA | 5.20 | 127.25 | 120.28 |
| 1 | C | 553 | GLU | CA-C-N | 5.19 | 127.55 | 120.54 |
| 1 | C | 553 | GLU | C-N-CA | 5.19 | 127.55 | 120.54 |
| 2 | B | 364 | THR | CA-C-N | 5.19 | 129.39 | 120.72 |
| 2 | B | 364 | THR | C-N-CA | 5.19 | 129.39 | 120.72 |
| 1 | C | 158 | LEU | N-CA-C | 5.19 | 119.60 | 113.16 |
| 1 | A | 29 | ALA | CA-C-N | 5.19 | 127.23 | 120.28 |
| 1 | A | 29 | ALA | C-N-CA | 5.19 | 127.23 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 243 | ASN | CA-C-N | 5.18 | 131.69 | 122.06 |
| 2 | B | 243 | ASN | C-N-CA | 5.18 | 131.69 | 122.06 |
| 1 | C | 379 | SER | CA-C-N | 5.18 | 127.74 | 120.28 |
| 1 | C | 379 | SER | C-N-CA | 5.18 | 127.74 | 120.28 |
| 1 | A | 488 | VAL | N-CA-CB | 5.17 | 117.19 | 110.57 |
| 1 | C | 341 | VAL | N-CA-C | 5.17 | 119.28 | 112.04 |
| 1 | C | 368 | LEU | CA-C-N | 5.17 | 131.23 | 122.65 |
| 1 | C | 368 | LEU | C-N-CA | 5.17 | 131.23 | 122.65 |
| 1 | C | 666 | PRO | N-CA-CB | 5.17 | 109.02 | 103.33 |
| 2 | D | 601 | GLU | O-C-N | -5.17 | 115.33 | 122.46 |
| 2 | B | 510 | ARG | CA-C-N | 5.17 | 125.08 | 119.76 |
| 2 | B | 510 | ARG | C-N-CA | 5.17 | 125.08 | 119.76 |
| 2 | B | 203 | GLY | CA-C-N | 5.16 | 127.15 | 120.44 |
| 2 | B | 203 | GLY | C-N-CA | 5.16 | 127.15 | 120.44 |
| 1 | A | 213 | PRO | N-CA-CB | 5.16 | 108.09 | 103.08 |
| 1 | A | 674 | LYS | CA-C-N | 5.16 | 132.26 | 121.94 |
| 1 | A | 674 | LYS | C-N-CA | 5.16 | 132.26 | 121.94 |
| 2 | D | 455 | ASN | CA-CB-CG | 5.16 | 117.76 | 112.60 |
| 1 | A | 603 | ALA | N-CA-C | 5.15 | 117.89 | 109.59 |
| 1 | A | 468 | ASN | CA-CB-CG | 5.15 | 117.75 | 112.60 |
| 1 | C | 29 | ALA | CA-C-N | 5.15 | 127.19 | 120.28 |
| 1 | C | 29 | ALA | C-N-CA | 5.15 | 127.19 | 120.28 |
| 1 | C | 401 | ASP | CA-C-O | 5.15 | 127.22 | 120.16 |
| 2 | B | 275 | GLU | CA-C-N | 5.15 | 127.14 | 120.44 |
| 2 | B | 275 | GLU | C-N-CA | 5.15 | 127.14 | 120.44 |
| 1 | C | 76 | ALA | N-CA-C | 5.15 | 116.89 | 111.28 |
| 2 | D | 375 | PRO | N-CA-CB | 5.15 | 108.98 | 103.52 |
| 2 | B | 425 | LYS | CA-C-N | 5.15 | 132.24 | 121.94 |
| 2 | B | 425 | LYS | C-N-CA | 5.15 | 132.24 | 121.94 |
| 2 | B | 336 | PRO | N-CA-CB | 5.14 | 108.45 | 103.51 |
| 2 | B | 353 | GLY | CA-C-N | 5.14 | 128.56 | 121.26 |
| 2 | B | 353 | GLY | C-N-CA | 5.14 | 128.56 | 121.26 |
| 1 | A | 30 | ALA | CA-C-N | 5.14 | 128.13 | 120.31 |
| 1 | A | 30 | ALA | C-N-CA | 5.14 | 128.13 | 120.31 |
| 2 | B | 79 | LYS | CA-C-N | 5.14 | 131.61 | 121.58 |
| 2 | B | 79 | LYS | C-N-CA | 5.14 | 131.61 | 121.58 |
| 2 | D | 305 | ALA | CA-C-N | 5.14 | 128.13 | 120.31 |
| 2 | D | 305 | ALA | C-N-CA | 5.14 | 128.13 | 120.31 |
| 1 | C | 636 | THR | N-CA-C | -5.14 | 102.56 | 110.07 |
| 1 | C | 300 | LYS | O-C-N | -5.14 | 116.75 | 122.09 |
| 1 | A | 385 | ASN | CA-CB-CG | 5.13 | 117.73 | 112.60 |
| 1 | A | 228 | THR | O-C-N | -5.13 | 116.68 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 617 | ILE | CA-C-O | -5.13 | 115.73 | 121.17 |
| 1 | C | 264 | VAL | O-C-N | -5.13 | 116.81 | 121.94 |
| 2 | D | 181 | SER | CA-C-N | 5.13 | 127.48 | 120.46 |
| 2 | D | 181 | SER | C-N-CA | 5.13 | 127.48 | 120.46 |
| 1 | A | 198 | ASN | N-CA-CB | -5.12 | 104.39 | 112.13 |
| 1 | A | 690 | GLU | O-C-N | -5.12 | 116.22 | 122.22 |
| 2 | B | 390 | VAL | CA-C-O | 5.12 | 125.16 | 119.42 |
| 2 | D | 588 | ALA | N-CA-C | 5.12 | 119.25 | 113.15 |
| 2 | D | 634 | LEU | N-CA-C | 5.12 | 119.29 | 113.19 |
| 1 | A | 553 | GLU | CA-C-N | 5.12 | 127.45 | 120.54 |
| 1 | A | 553 | GLU | C-N-CA | 5.12 | 127.45 | 120.54 |
| 2 | D | 608 | GLU | CA-C-N | 5.12 | 127.40 | 120.38 |
| 2 | D | 608 | GLU | C-N-CA | 5.12 | 127.40 | 120.38 |
| 1 | A | 252 | ALA | CA-C-N | 5.12 | 128.09 | 120.31 |
| 1 | A | 252 | ALA | C-N-CA | 5.12 | 128.09 | 120.31 |
| 1 | C | 321 | LYS | O-C-N | -5.12 | 116.23 | 122.22 |
| 1 | A | 261 | ALA | N-CA-C | -5.12 | 105.78 | 111.36 |
| 1 | C | 141 | VAL | N-CA-C | 5.12 | 116.18 | 109.58 |
| 2 | B | 393 | GLY | CA-C-N | 5.11 | 127.64 | 120.28 |
| 2 | B | 393 | GLY | C-N-CA | 5.11 | 127.64 | 120.28 |
| 1 | C | 264 | VAL | CA-C-N | 5.11 | 127.13 | 120.28 |
| 1 | C | 264 | VAL | C-N-CA | 5.11 | 127.13 | 120.28 |
| 2 | D | 115 | ASP | CA-C-O | 5.11 | 124.31 | 119.76 |
| 1 | C | 475 | GLU | CA-C-N | 5.11 | 123.39 | 119.66 |
| 1 | C | 475 | GLU | C-N-CA | 5.11 | 123.39 | 119.66 |
| 1 | A | 68 | PRO | N-CA-CB | 5.11 | 108.03 | 103.08 |
| 1 | A | 131 | ARG | N-CA-C | 5.11 | 118.61 | 112.38 |
| 1 | A | 352 | ALA | CA-C-N | 5.11 | 127.08 | 120.44 |
| 1 | A | 352 | ALA | C-N-CA | 5.11 | 127.08 | 120.44 |
| 1 | A | 664 | LEU | N-CA-C | 5.11 | 116.93 | 111.36 |
| 2 | D | 94 | THR | CA-C-N | 5.11 | 127.63 | 120.28 |
| 2 | D | 94 | THR | C-N-CA | 5.11 | 127.63 | 120.28 |
| 2 | D | 408 | LEU | N-CA-C | 5.11 | 116.84 | 111.28 |
| 2 | B | 488 | LEU | N-CA-C | 5.10 | 117.74 | 110.24 |
| 1 | C | 175 | LEU | CA-C-N | 5.10 | 127.12 | 120.28 |
| 1 | C | 175 | LEU | C-N-CA | 5.10 | 127.12 | 120.28 |
| 1 | C | 475 | GLU | CA-C-O | 5.10 | 124.30 | 119.76 |
| 1 | C | 314 | GLN | CA-C-N | 5.10 | 132.14 | 121.94 |
| 1 | C | 314 | GLN | C-N-CA | 5.10 | 132.14 | 121.94 |
| 1 | A | 172 | LEU | CA-C-N | 5.10 | 124.71 | 119.05 |
| 1 | A | 172 | LEU | C-N-CA | 5.10 | 124.71 | 119.05 |
| 1 | C | 27 | GLU | CA-C-N | 5.09 | 127.06 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 27 | GLU | C-N-CA | 5.09 | 127.06 | 120.44 |
| 1 | C | 689 | PRO | N-CA-CB | 5.09 | 107.78 | 103.35 |
| 1 | A | 75 | TYR | O-C-N | -5.09 | 116.74 | 123.21 |
| 2 | B | 223 | ARG | CA-C-N | 5.09 | 131.31 | 122.56 |
| 2 | B | 223 | ARG | C-N-CA | 5.09 | 131.31 | 122.56 |
| 2 | D | 23 | LEU | O-C-N | -5.09 | 116.80 | 121.79 |
| 2 | D | 506 | SER | N-CA-C | 5.09 | 117.72 | 111.82 |
| 1 | A | 672 | LEU | CA-C-N | 5.08 | 127.40 | 120.54 |
| 1 | A | 672 | LEU | C-N-CA | 5.08 | 127.40 | 120.54 |
| 1 | A | 51 | ASN | CA-C-N | 5.08 | 130.44 | 120.99 |
| 1 | A | 51 | ASN | C-N-CA | 5.08 | 130.44 | 120.99 |
| 1 | C | 163 | VAL | CA-C-O | 5.08 | 125.67 | 120.39 |
| 1 | C | 541 | ALA | O-C-N | -5.08 | 114.87 | 122.39 |
| 1 | A | 374 | LEU | CA-C-O | 5.08 | 126.43 | 120.69 |
| 1 | A | 343 | ASN | O-C-N | -5.07 | 116.03 | 122.27 |
| 1 | C | 533 | LYS | O-C-N | -5.07 | 116.82 | 122.09 |
| 2 | B | 49 | PRO | N-CA-CB | 5.07 | 108.86 | 103.39 |
| 2 | B | 191 | LYS | N-CA-C | 5.06 | 119.09 | 113.01 |
| 1 | A | 448 | GLU | O-C-N | -5.06 | 116.86 | 122.07 |
| 1 | A | 264 | VAL | CA-C-N | 5.06 | 127.06 | 120.28 |
| 1 | A | 264 | VAL | C-N-CA | 5.06 | 127.06 | 120.28 |
| 1 | A | 504 | ASP | CA-C-O | 5.05 | 124.24 | 119.59 |
| 2 | B | 432 | ALA | CA-C-N | 5.05 | 127.38 | 120.46 |
| 2 | B | 432 | ALA | C-N-CA | 5.05 | 127.38 | 120.46 |
| 2 | B | 77 | ARG | CA-C-O | 5.05 | 126.04 | 120.94 |
| 1 | A | 8 | ASP | CA-CB-CG | 5.05 | 117.65 | 112.60 |
| 1 | A | 120 | PRO | N-CA-CB | 5.05 | 108.65 | 103.15 |
| 1 | C | 684 | VAL | N-CA-CB | 5.05 | 118.89 | 111.52 |
| 2 | D | 40 | GLU | N-CA-C | 5.05 | 116.47 | 111.07 |
| 2 | B | 190 | ALA | CA-C-N | 5.04 | 131.16 | 121.18 |
| 2 | B | 190 | ALA | C-N-CA | 5.04 | 131.16 | 121.18 |
| 2 | D | 408 | LEU | CA-C-N | 5.04 | 126.99 | 120.44 |
| 2 | D | 408 | LEU | C-N-CA | 5.04 | 126.99 | 120.44 |
| 2 | D | 501 | MET | CA-C-N | 5.04 | 127.03 | 120.28 |
| 2 | D | 501 | MET | C-N-CA | 5.04 | 127.03 | 120.28 |
| 1 | A | 385 | ASN | CA-C-N | 5.04 | 127.34 | 120.54 |
| 1 | A | 385 | ASN | C-N-CA | 5.04 | 127.34 | 120.54 |
| 2 | B | 78 | PRO | N-CA-CB | 5.04 | 109.00 | 103.26 |
| 2 | B | 237 | ASP | CA-CB-CG | 5.04 | 117.64 | 112.60 |
| 2 | B | 337 | TYR | O-C-N | -5.03 | 115.85 | 122.39 |
| 2 | B | 256 | LEU | CA-C-N | 5.03 | 126.98 | 120.44 |
| 2 | B | 256 | LEU | C-N-CA | 5.03 | 126.98 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 410 | ARG | CA-CB-CG | 5.03 | 124.16 | 114.10 |
| 1 | C | 184 | GLU | O-C-N | -5.03 | 115.85 | 122.39 |
| 1 | C | 634 | PHE | CA-CB-CG | 5.03 | 118.83 | 113.80 |
| 1 | C | 513 | ASP | O-C-N | -5.03 | 116.08 | 122.27 |
| 1 | A | 536 | ILE | CA-C-N | 5.03 | 126.97 | 120.44 |
| 1 | A | 536 | ILE | C-N-CA | 5.03 | 126.97 | 120.44 |
| 1 | C | 245 | MET | CA-C-O | -5.03 | 115.54 | 120.82 |
| 1 | A | 185 | GLN | CA-C-N | 5.03 | 130.69 | 121.85 |
| 1 | A | 185 | GLN | C-N-CA | 5.03 | 130.69 | 121.85 |
| 1 | C | 175 | LEU | O-C-N | -5.02 | 116.80 | 122.12 |
| 1 | A | 70 | PHE | O-C-N | -5.02 | 115.82 | 122.40 |
| 2 | B | 493 | ASP | CA-CB-CG | 5.02 | 117.62 | 112.60 |
| 1 | C | 257 | ALA | N-CA-C | 5.02 | 116.44 | 111.07 |
| 1 | C | 575 | LYS | CA-C-N | 5.02 | 131.12 | 121.54 |
| 1 | C | 575 | LYS | C-N-CA | 5.02 | 131.12 | 121.54 |
| 1 | C | 405 | GLY | O-C-N | -5.02 | 117.43 | 122.65 |
| 1 | A | 271 | GLU | O-C-N | -5.01 | 116.80 | 122.12 |
| 1 | A | 189 | PRO | CA-C-N | 5.01 | 129.09 | 120.72 |
| 1 | A | 189 | PRO | C-N-CA | 5.01 | 129.09 | 120.72 |
| 1 | C | 277 | VAL | O-C-N | -5.01 | 117.01 | 121.87 |
| 2 | D | 201 | PRO | N-CA-CB | 5.01 | 108.84 | 103.33 |
| 2 | B | 414 | ASP | N-CA-C | 5.01 | 116.74 | 111.28 |
| 1 | A | 418 | ARG | CA-C-N | 5.00 | 126.99 | 120.28 |
| 1 | A | 418 | ARG | C-N-CA | 5.00 | 126.99 | 120.28 |
| 2 | D | 155 | SER | N-CA-C | 5.00 | 116.73 | 111.28 |
| 1 | A | 682 | ILE | N-CA-CB | 5.00 | 118.82 | 111.52 |
| 2 | D | 243 | ASN | CA-C-N | 5.00 | 131.44 | 122.38 |
| 2 | D | 243 | ASN | C-N-CA | 5.00 | 131.44 | 122.38 |
| 1 | C | 617 | ILE | CA-C-O | -5.00 | 115.87 | 121.17 |

There are no chirality outliers.

All (27) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 167 | MET | Mainchain |
| 1 | A | 183 | GLU | Mainchain |
| 1 | A | 281 | ALA | Mainchain |
| 1 | A | 342 | TYR | Mainchain |
| 1 | A | 356 | THR | Mainchain |
| 1 | A | 40 | THR | Mainchain |
| 1 | A | 405 | GLY | Mainchain |
| 1 | A | 540 | ARG | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 70 | PHE | Mainchain |
| 2 | B | 401 | GLY | Mainchain |
| 2 | B | 456 | ARG | Mainchain |
| 1 | C | 167 | MET | Mainchain |
| 1 | C | 277 | VAL | Mainchain |
| 1 | C | 281 | ALA | Mainchain |
| 1 | C | 342 | TYR | Mainchain |
| 1 | C | 356 | THR | Mainchain |
| 1 | C | 357 | GLN | Mainchain |
| 1 | C | 376 | THR | Mainchain |
| 1 | C | 40 | THR | Mainchain |
| 1 | C | 405 | GLY | Mainchain |
| 1 | C | 677 | ARG | Mainchain |
| 1 | C | 70 | PHE | Mainchain |
| 1 | C | 74 | PRO | Mainchain |
| 2 | D | 228 | SER | Mainchain |
| 2 | D | 24 | ALA | Mainchain |
| 2 | D | 348 | PHE | Mainchain |
| 2 | D | 456 | ARG | Mainchain |

5.2 Too-close contacts [i](#)

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 | 5574 | 0 | 5486 | 37 | 2 |
| 1 | C | 5574 | 0 | 5486 | 42 | 0 |
| 2 | B | 4722 | 0 | 4642 | 34 | 0 |
| 2 | D | 4722 | 0 | 4642 | 33 | 2 |
| 3 | A | 55 | 0 | 37 | 2 | 0 |
| 3 | C | 55 | 0 | 37 | 1 | 0 |
| 4 | A | 55 | 0 | 37 | 3 | 0 |
| 4 | C | 55 | 0 | 37 | 2 | 0 |
| 5 | A | 91 | 0 | 88 | 17 | 0 |
| 5 | C | 91 | 0 | 88 | 16 | 0 |
| 6 | B | 12 | 0 | 16 | 1 | 0 |
| 6 | D | 12 | 0 | 16 | 2 | 0 |
| 7 | A | 356 | 0 | 0 | 0 | 0 |
| 7 | B | 192 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | C | 353 | 0 | 0 | 4 | 0 |
| 7 | D | 193 | 0 | 0 | 0 | 0 |
| All | All | 22112 | 0 | 20612 | 173 | 2 |

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 4.

All (173) 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) |
|---------------------|----------------------|--------------------------|-------------------|
| 5:A:1800:B12:H531 | 5:A:1800:B12:H552 | 1.46 | 0.96 |
| 5:A:1800:B12:H421 | 5:A:1800:B12:H363 | 1.46 | 0.95 |
| 1:C:21:ALA:HB3 | 7:C:4310:HOH:O | 1.72 | 0.89 |
| 1:A:357:GLN:HE22 | 2:B:290:GLN:HE22 | 1.24 | 0.85 |
| 5:C:2800:B12:H552 | 5:C:2800:B12:H531 | 1.64 | 0.80 |
| 1:C:357:GLN:HE22 | 2:D:290:GLN:HE22 | 1.32 | 0.77 |
| 5:C:2800:B12:H353 | 5:C:2800:B12:H302 | 1.67 | 0.77 |
| 1:A:290:ILE:HG13 | 1:A:355:ALA:HB2 | 1.65 | 0.76 |
| 1:C:27:GLU:HB2 | 7:C:4284:HOH:O | 1.84 | 0.75 |
| 2:B:370:PRO:HB3 | 2:B:375:PRO:HG2 | 1.69 | 0.74 |
| 1:C:290:ILE:HG13 | 1:C:355:ALA:HB2 | 1.69 | 0.74 |
| 1:A:247:GLU:HB3 | 5:A:1800:B12:H532 | 1.71 | 0.73 |
| 1:C:706:THR:HB | 1:C:707:PRO:HD2 | 1.71 | 0.72 |
| 2:D:281:ASN:HD22 | 2:D:323:ASN:HD21 | 1.36 | 0.72 |
| 2:B:468:MET:HE2 | 2:B:471:ALA:HA | 1.73 | 0.71 |
| 1:A:706:THR:HB | 1:A:707:PRO:HD2 | 1.73 | 0.71 |
| 5:A:1800:B12:H363 | 5:A:1800:B12:C42 | 2.11 | 0.70 |
| 1:C:4:LEU:HB3 | 2:D:264:ARG:HG2 | 1.76 | 0.68 |
| 2:B:73:VAL:HB | 2:B:74:PRO:HD2 | 1.77 | 0.67 |
| 2:B:617:LEU:HD22 | 2:B:621:MET:HE1 | 1.76 | 0.67 |
| 2:B:281:ASN:HD22 | 2:B:323:ASN:HD21 | 1.43 | 0.66 |
| 1:C:188:LYS:H | 1:C:191:GLN:NE2 | 1.93 | 0.66 |
| 1:C:215:GLN:HB3 | 1:C:216:PRO:HD3 | 1.76 | 0.66 |
| 1:C:247:GLU:HB3 | 5:C:2800:B12:H532 | 1.77 | 0.66 |
| 5:A:1800:B12:H353 | 5:A:1800:B12:H302 | 1.76 | 0.65 |
| 2:D:370:PRO:HB3 | 2:D:375:PRO:HG2 | 1.79 | 0.65 |
| 1:A:200:ILE:HG21 | 1:A:217:SER:HB3 | 1.79 | 0.64 |
| 2:D:564:VAL:HG22 | 2:D:592:ALA:HB3 | 1.78 | 0.64 |
| 3:A:1801[A]:SCD:OP2 | 3:A:1801[A]:SCD:HPB1 | 1.97 | 0.64 |
| 2:B:564:VAL:HG22 | 2:B:592:ALA:HB3 | 1.78 | 0.64 |
| 2:B:224:LEU:HD21 | 2:B:231:SER:HB3 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:C:23:ARG:HD2 | 7:C:4304:HOH:O | 1.99 | 0.62 |
| 2:D:374:PHE:HB3 | 2:D:375:PRO:HD3 | 1.81 | 0.62 |
| 1:A:441:ILE:HB | 1:A:442:PRO:HD3 | 1.81 | 0.62 |
| 2:D:197:LEU:HB2 | 2:D:233:ALA:HA | 1.81 | 0.62 |
| 1:A:188:LYS:H | 1:A:191:GLN:NE2 | 1.99 | 0.61 |
| 5:C:2800:B12:H531 | 5:C:2800:B12:C55 | 2.30 | 0.61 |
| 3:C:2801[A]:SCD:HPB1 | 3:C:2801[A]:SCD:OP2 | 1.99 | 0.60 |
| 5:A:1800:B12:H531 | 5:A:1800:B12:C55 | 2.28 | 0.59 |
| 2:D:73:VAL:HB | 2:D:74:PRO:HD2 | 1.85 | 0.59 |
| 2:B:532:SER:HB3 | 2:B:533:PRO:HD3 | 1.85 | 0.58 |
| 2:D:197:LEU:HD12 | 2:D:233:ALA:CB | 2.34 | 0.58 |
| 6:B:3002:GOL:O3 | 6:B:3002:GOL:O1 | 1.99 | 0.58 |
| 2:D:532:SER:HB3 | 2:D:533:PRO:HD3 | 1.85 | 0.58 |
| 2:B:284:VAL:HG11 | 2:B:322:GLN:HE21 | 1.68 | 0.57 |
| 2:D:284:VAL:HG11 | 2:D:322:GLN:HE21 | 1.69 | 0.57 |
| 2:B:374:PHE:HB3 | 2:B:375:PRO:HD3 | 1.87 | 0.57 |
| 2:B:391:ASN:HD22 | 2:B:394:ARG:HE | 1.52 | 0.57 |
| 1:A:4:LEU:HB3 | 2:B:264:ARG:HG2 | 1.85 | 0.57 |
| 5:A:1800:B12:H312 | 5:A:1800:B12:H251 | 1.88 | 0.56 |
| 1:C:441:ILE:HB | 1:C:442:PRO:HD3 | 1.87 | 0.56 |
| 4:C:2802[B]:MCD:HPB1 | 4:C:2802[B]:MCD:OP2 | 2.05 | 0.56 |
| 5:A:1800:B12:H2B | 5:A:1800:B12:O7R | 2.06 | 0.56 |
| 1:C:374:LEU:HB2 | 1:C:481:LEU:HD23 | 1.87 | 0.56 |
| 2:D:356:GLU:HA | 6:D:3004:GOL:H2 | 1.89 | 0.55 |
| 5:C:2800:B12:H301 | 5:C:2800:B12:H203 | 1.87 | 0.55 |
| 5:A:1800:B12:H203 | 5:A:1800:B12:H301 | 1.89 | 0.55 |
| 5:A:1800:B12:H312 | 5:A:1800:B12:C25 | 2.37 | 0.54 |
| 1:C:638:GLU:HA | 1:C:671:GLU:HG3 | 1.89 | 0.54 |
| 2:B:347:THR:HG23 | 2:B:358:ILE:HG21 | 1.89 | 0.54 |
| 2:B:391:ASN:ND2 | 2:B:394:ARG:HE | 2.05 | 0.54 |
| 2:D:281:ASN:ND2 | 2:D:323:ASN:HD21 | 2.05 | 0.53 |
| 1:A:215:GLN:HB3 | 1:A:216:PRO:HD3 | 1.89 | 0.53 |
| 2:B:216:VAL:HG23 | 7:B:5409:HOH:O | 2.07 | 0.53 |
| 1:C:706:THR:HB | 1:C:707:PRO:CD | 2.37 | 0.53 |
| 2:D:224:LEU:HD21 | 2:D:231:SER:HB3 | 1.89 | 0.53 |
| 2:D:513:VAL:HG13 | 2:D:564:VAL:HG12 | 1.92 | 0.52 |
| 4:A:1802[B]:MCD:NP2 | 4:A:1802[B]:MCD:HP92 | 2.21 | 0.52 |
| 1:A:512:LEU:HD21 | 1:A:543:ALA:HB1 | 1.92 | 0.52 |
| 1:C:512:LEU:HD21 | 1:C:543:ALA:HB1 | 1.92 | 0.52 |
| 6:D:3004:GOL:O1 | 6:D:3004:GOL:O3 | 2.22 | 0.52 |
| 1:C:357:GLN:HE22 | 2:D:290:GLN:NE2 | 2.05 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:C:528:ASP:HA | 1:C:533:LYS:HE3 | 1.92 | 0.51 |
| 4:A:1802[B]:MCD:HPB1 | 4:A:1802[B]:MCD:OP2 | 2.11 | 0.51 |
| 1:C:200:ILE:HG21 | 1:C:217:SER:HB3 | 1.93 | 0.51 |
| 2:B:513:VAL:HG13 | 2:B:564:VAL:HG12 | 1.93 | 0.51 |
| 1:A:250:ALA:HB2 | 1:A:446:ILE:HG12 | 1.92 | 0.50 |
| 5:C:2800:B12:H372 | 5:C:2800:B12:H351 | 1.94 | 0.50 |
| 1:C:684:VAL:HG12 | 1:C:688:ILE:HD11 | 1.94 | 0.50 |
| 2:D:77:ARG:HB3 | 2:D:78:PRO:HD2 | 1.93 | 0.50 |
| 2:B:554:VAL:HG12 | 2:B:558:LYS:HD2 | 1.93 | 0.49 |
| 1:C:250:ALA:HB2 | 1:C:446:ILE:HG12 | 1.95 | 0.49 |
| 5:C:2800:B12:C25 | 5:C:2800:B12:H312 | 2.43 | 0.49 |
| 1:C:665:VAL:N | 1:C:666:PRO:HD2 | 2.27 | 0.49 |
| 5:C:2800:B12:H312 | 5:C:2800:B12:H251 | 1.95 | 0.49 |
| 1:A:706:THR:HB | 1:A:707:PRO:CD | 2.41 | 0.48 |
| 1:A:359:HIS:CE1 | 1:A:401:ASP:H | 2.32 | 0.48 |
| 2:D:391:ASN:ND2 | 2:D:394:ARG:HE | 2.10 | 0.48 |
| 1:A:122:HIS:HA | 1:A:167:MET:HE1 | 1.96 | 0.48 |
| 1:C:359:HIS:CE1 | 1:C:401:ASP:H | 2.31 | 0.48 |
| 2:D:391:ASN:HD22 | 2:D:394:ARG:HE | 1.62 | 0.48 |
| 1:C:139:ALA:HB1 | 5:C:2800:B12:H362 | 1.96 | 0.48 |
| 1:A:243:TYR:HD1 | 1:A:289:GLY:HA2 | 1.79 | 0.48 |
| 1:A:503:ARG:HD2 | 1:A:508:VAL:HG21 | 1.95 | 0.48 |
| 1:C:188:LYS:HB3 | 1:C:189:PRO:HD2 | 1.95 | 0.48 |
| 5:C:2800:B12:H353 | 5:C:2800:B12:C30 | 2.40 | 0.47 |
| 5:A:1800:B12:H372 | 5:A:1800:B12:H351 | 1.97 | 0.47 |
| 2:B:27:PHE:HB3 | 2:B:28:PRO:HD2 | 1.97 | 0.47 |
| 2:B:331:LEU:HD13 | 2:B:365:GLN:HB3 | 1.97 | 0.47 |
| 1:C:597:ARG:HG2 | 1:C:597:ARG:HH11 | 1.80 | 0.47 |
| 5:A:1800:B12:O7R | 5:A:1800:B12:C2B | 2.63 | 0.46 |
| 4:C:2802[B]:MCD:NP2 | 4:C:2802[B]:MCD:HP92 | 2.28 | 0.46 |
| 2:D:347:THR:HG23 | 2:D:358:ILE:HG21 | 1.97 | 0.46 |
| 1:A:597:ARG:HH11 | 1:A:597:ARG:HG2 | 1.81 | 0.46 |
| 1:A:514:LYS:HD3 | 1:A:534:LEU:HD22 | 1.98 | 0.46 |
| 1:A:665:VAL:N | 1:A:666:PRO:CD | 2.79 | 0.46 |
| 2:D:339:ASN:HA | 2:D:342:ARG:HB2 | 1.97 | 0.46 |
| 5:C:2800:B12:C42 | 5:C:2800:B12:H363 | 2.47 | 0.45 |
| 2:B:518:LEU:HD21 | 2:B:581:VAL:HG11 | 1.98 | 0.45 |
| 2:D:246:ALA:HB1 | 2:D:250:ALA:HB3 | 1.98 | 0.45 |
| 1:C:21:ALA:HA | 2:D:90:VAL:HG11 | 1.98 | 0.45 |
| 2:B:274:THR:HA | 2:B:313:VAL:HG13 | 1.97 | 0.45 |
| 5:C:2800:B12:H2B | 5:C:2800:B12:O2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:92:PRO:O | 2:D:93:PHE:HB2 | 2.17 | 0.45 |
| 2:B:281:ASN:ND2 | 2:B:323:ASN:HD21 | 2.14 | 0.44 |
| 1:C:668:LEU:HD13 | 1:C:682:ILE:HG12 | 1.99 | 0.44 |
| 1:A:264:VAL:HG12 | 1:A:268:ARG:HH21 | 1.81 | 0.44 |
| 1:A:357:GLN:HE22 | 2:B:290:GLN:NE2 | 2.03 | 0.44 |
| 1:A:310:LYS:HE2 | 2:B:21:LEU:HD11 | 2.00 | 0.44 |
| 2:B:532:SER:CB | 2:B:533:PRO:HD3 | 2.47 | 0.44 |
| 1:A:188:LYS:HB3 | 1:A:189:PRO:HD2 | 1.98 | 0.44 |
| 1:A:665:VAL:N | 1:A:666:PRO:HD2 | 2.34 | 0.43 |
| 2:D:579:LEU:HG | 2:D:583:LYS:HE3 | 2.01 | 0.43 |
| 1:C:444:MET:HE2 | 1:C:564:ARG:HD3 | 1.99 | 0.43 |
| 5:C:2800:B12:HM51 | 5:C:2800:B12:HM63 | 1.85 | 0.43 |
| 1:A:139:ALA:HB1 | 5:A:1800:B12:H362 | 2.01 | 0.43 |
| 1:C:203:GLU:OE2 | 1:C:207:ARG:HD3 | 2.19 | 0.43 |
| 2:B:517:CYS:HB3 | 2:B:524:PHE:CG | 2.54 | 0.43 |
| 2:B:515:LEU:HD23 | 2:B:566:ASP:HB3 | 2.01 | 0.42 |
| 2:B:579:LEU:HG | 2:B:583:LYS:HE3 | 2.00 | 0.42 |
| 2:B:425:LYS:HZ3 | 2:B:425:LYS:HB2 | 1.83 | 0.42 |
| 1:A:492:GLN:HE22 | 1:A:495:LYS:NZ | 2.17 | 0.42 |
| 2:B:246:ALA:HB1 | 2:B:250:ALA:HB3 | 2.00 | 0.42 |
| 1:C:197:GLN:HA | 1:C:239:SER:HB3 | 2.02 | 0.42 |
| 1:A:138:MET:SD | 1:A:485:ASN:HB2 | 2.59 | 0.42 |
| 1:C:215:GLN:HB3 | 1:C:216:PRO:CD | 2.46 | 0.42 |
| 1:C:636:THR:HB | 1:C:637:PRO:HD2 | 2.01 | 0.42 |
| 2:D:334:GLU:O | 2:D:335:ASP:C | 2.63 | 0.42 |
| 1:A:541:ALA:O | 1:A:542:MET:HB2 | 2.19 | 0.42 |
| 1:C:605:MET:HE3 | 1:C:664:LEU:HB3 | 2.01 | 0.42 |
| 5:A:1800:B12:H2B | 5:A:1800:B12:O2 | 2.19 | 0.42 |
| 1:C:23:ARG:CD | 7:C:4304:HOH:O | 2.62 | 0.42 |
| 2:D:517:CYS:HB3 | 2:D:524:PHE:CG | 2.55 | 0.42 |
| 1:C:252:ALA:O | 1:C:256:MET:HG3 | 2.20 | 0.42 |
| 5:C:2800:B12:H363 | 5:C:2800:B12:H421 | 2.02 | 0.42 |
| 2:D:267:VAL:HA | 2:D:271:PHE:O | 2.20 | 0.42 |
| 1:A:571:SER:HB3 | 1:A:623:ASP:HB3 | 2.02 | 0.42 |
| 1:C:171:VAL:HG23 | 1:C:196:ILE:HG12 | 2.01 | 0.42 |
| 1:C:521:ASN:O | 1:C:529:ARG:HD3 | 2.19 | 0.42 |
| 1:C:243:TYR:HD1 | 1:C:289:GLY:HA2 | 1.85 | 0.41 |
| 1:A:521:ASN:O | 1:A:529:ARG:HD3 | 2.21 | 0.41 |
| 1:C:579:GLU:HB3 | 1:C:712:PRO:HB2 | 2.01 | 0.41 |
| 5:A:1800:B12:HM63 | 5:A:1800:B12:HM51 | 1.74 | 0.41 |
| 2:D:107:TRP:CD1 | 2:D:358:ILE:HD12 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 1:A:392:GLN:HB3 | 2:B:459:PRO:HG2 | 2.02 | 0.41 |
| 5:A:1800:B12:H262 | 5:A:1800:B12:H91 | 1.97 | 0.41 |
| 2:D:331:LEU:HD13 | 2:D:365:GLN:HB3 | 2.03 | 0.41 |
| 2:D:518:LEU:HD21 | 2:D:581:VAL:HG11 | 2.02 | 0.41 |
| 1:A:256:MET:HE2 | 1:A:256:MET:HB3 | 1.92 | 0.41 |
| 1:A:89:PHE:CE2 | 3:A:1801[A]:SCD:HS21 | 2.55 | 0.41 |
| 1:A:683:THR:HG21 | 1:A:718:LEU:HD13 | 2.02 | 0.41 |
| 2:B:267:VAL:HA | 2:B:271:PHE:O | 2.21 | 0.41 |
| 5:C:2800:B12:C61 | 5:C:2800:B12:H551 | 2.50 | 0.41 |
| 2:D:374:PHE:CB | 2:D:375:PRO:HD3 | 2.50 | 0.41 |
| 1:A:374:LEU:HB2 | 1:A:481:LEU:HD23 | 2.03 | 0.41 |
| 1:C:503:ARG:HD2 | 1:C:508:VAL:HG21 | 2.03 | 0.41 |
| 1:A:606:GLY:O | 1:A:634:PHE:HA | 2.20 | 0.40 |
| 5:A:1800:B12:H601 | 5:A:1800:B12:H252 | 2.03 | 0.40 |
| 1:C:201:LEU:HG | 1:C:218:MET:HE1 | 2.03 | 0.40 |
| 1:A:89:PHE:CE2 | 4:A:1802[B]:MCD:HS2 | 2.57 | 0.40 |
| 1:C:613:GLY:HA2 | 5:C:2800:B12:H3P1 | 2.03 | 0.40 |
| 2:D:197:LEU:HD12 | 2:D:233:ALA:HB1 | 2.03 | 0.40 |
| 2:B:460:ILE:HD13 | 2:B:494:SER:HB3 | 2.02 | 0.40 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:A:670:LYS:NZ | 2:D:20:THR:OG1[2_646] | 1.69 | 0.51 |
| 1:A:670:LYS:CD | 2:D:20:THR:O[2_646] | 2.02 | 0.18 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | 723/727 (99%) | 695 (96%) | 27 (4%) | 1 (0%) | 48 57 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|---------|----------|-------------|
| 1 | C | 723/727 (99%) | 693 (96%) | 29 (4%) | 1 (0%) | 48 57 |
| 2 | B | 617/637 (97%) | 594 (96%) | 21 (3%) | 2 (0%) | 36 42 |
| 2 | D | 617/637 (97%) | 596 (97%) | 19 (3%) | 2 (0%) | 36 42 |
| All | All | 2680/2728 (98%) | 2578 (96%) | 96 (4%) | 6 (0%) | 43 51 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 576 | ASN |
| 2 | D | 171 | ASP |
| 1 | A | 576 | ASN |
| 2 | B | 171 | ASP |
| 2 | D | 228 | SER |
| 2 | B | 228 | SER |

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1 | A | 573/590 (97%) | 558 (97%) | 15 (3%) | 40 55 |
| 1 | C | 573/590 (97%) | 559 (98%) | 14 (2%) | 43 58 |
| 2 | B | 481/509 (94%) | 461 (96%) | 20 (4%) | 26 36 |
| 2 | D | 481/509 (94%) | 457 (95%) | 24 (5%) | 22 28 |
| All | All | 2108/2198 (96%) | 2035 (96%) | 73 (4%) | 32 43 |

All (73) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 24 | ARG |
| 1 | A | 96 | LYS |
| 1 | A | 123 | ARG |
| 1 | A | 202 | LYS |
| 1 | A | 430 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 480 | VAL |
| 1 | A | 514 | LYS |
| 1 | A | 525 | LYS |
| 1 | A | 533 | LYS |
| 1 | A | 577 | THR |
| 1 | A | 592 | GLN |
| 1 | A | 597 | ARG |
| 1 | A | 656 | SER |
| 1 | A | 668 | LEU |
| 1 | A | 721 | LYS |
| 2 | B | 22 | SER |
| 2 | B | 77 | ARG |
| 2 | B | 186 | SER |
| 2 | B | 188 | LYS |
| 2 | B | 191 | LYS |
| 2 | B | 193 | LEU |
| 2 | B | 216 | VAL |
| 2 | B | 224 | LEU |
| 2 | B | 226 | LYS |
| 2 | B | 228 | SER |
| 2 | B | 300 | LEU |
| 2 | B | 334 | GLU |
| 2 | B | 410 | ARG |
| 2 | B | 425 | LYS |
| 2 | B | 435 | THR |
| 2 | B | 477 | LYS |
| 2 | B | 512 | LYS |
| 2 | B | 532 | SER |
| 2 | B | 619 | MET |
| 2 | B | 638 | LYS |
| 1 | C | 23 | ARG |
| 1 | C | 24 | ARG |
| 1 | C | 67 | ILE |
| 1 | C | 96 | LYS |
| 1 | C | 202 | LYS |
| 1 | C | 218 | MET |
| 1 | C | 365 | THR |
| 1 | C | 473 | GLU |
| 1 | C | 533 | LYS |
| 1 | C | 567 | SER |
| 1 | C | 592 | GLN |
| 1 | C | 597 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 668 | LEU |
| 1 | C | 721 | LYS |
| 2 | D | 60 | LYS |
| 2 | D | 77 | ARG |
| 2 | D | 141 | ASP |
| 2 | D | 159 | LEU |
| 2 | D | 186 | SER |
| 2 | D | 188 | LYS |
| 2 | D | 191 | LYS |
| 2 | D | 193 | LEU |
| 2 | D | 216 | VAL |
| 2 | D | 224 | LEU |
| 2 | D | 228 | SER |
| 2 | D | 297 | LEU |
| 2 | D | 300 | LEU |
| 2 | D | 334 | GLU |
| 2 | D | 410 | ARG |
| 2 | D | 425 | LYS |
| 2 | D | 435 | THR |
| 2 | D | 477 | LYS |
| 2 | D | 512 | LYS |
| 2 | D | 522 | ARG |
| 2 | D | 532 | SER |
| 2 | D | 617 | LEU |
| 2 | D | 619 | MET |
| 2 | D | 638 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 51 | ASN |
| 1 | A | 191 | GLN |
| 1 | A | 198 | ASN |
| 1 | A | 246 | GLN |
| 1 | A | 385 | ASN |
| 1 | A | 492 | GLN |
| 1 | A | 521 | ASN |
| 1 | A | 562 | GLN |
| 1 | A | 635 | GLN |
| 1 | A | 643 | GLN |
| 2 | B | 290 | GLN |
| 2 | B | 322 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 323 | ASN |
| 2 | B | 391 | ASN |
| 2 | B | 421 | GLN |
| 2 | B | 577 | GLN |
| 1 | C | 191 | GLN |
| 1 | C | 198 | ASN |
| 1 | C | 246 | GLN |
| 1 | C | 359 | HIS |
| 1 | C | 385 | ASN |
| 1 | C | 492 | GLN |
| 1 | C | 521 | ASN |
| 1 | C | 643 | GLN |
| 2 | D | 290 | GLN |
| 2 | D | 322 | GLN |
| 2 | D | 323 | ASN |
| 2 | D | 391 | ASN |

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](#)

10 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 |
| 5 | B12 | C | 2800 | 1 | 94,101,101 | 0.99 | 5 (5%) | 149,166,166 | 1.56 | 26 (17%) |
| 6 | GOL | D | 3003 | - | 5,5,5 | 0.22 | 0 | 5,5,5 | 0.41 | 0 |
| 3 | SCD | A | 1801[A] | - | 55,57,57 | 1.17 | 6 (10%) | 79,84,84 | 1.36 | 9 (11%) |
| 4 | MCD | A | 1802[B] | - | 54,57,57 | 1.20 | 5 (9%) | 78,85,85 | 1.26 | 8 (10%) |
| 6 | GOL | B | 3001 | - | 5,5,5 | 0.23 | 0 | 5,5,5 | 0.33 | 0 |
| 5 | B12 | A | 1800 | 1 | 94,101,101 | 0.96 | 3 (3%) | 149,166,166 | 1.62 | 30 (20%) |
| 6 | GOL | B | 3002 | - | 5,5,5 | 0.29 | 0 | 5,5,5 | 0.97 | 0 |
| 6 | GOL | D | 3004 | - | 5,5,5 | 0.29 | 0 | 5,5,5 | 0.67 | 0 |
| 3 | SCD | C | 2801[A] | - | 55,57,57 | 1.13 | 4 (7%) | 79,84,84 | 1.31 | 10 (12%) |
| 4 | MCD | C | 2802[B] | - | 54,57,57 | 1.18 | 5 (9%) | 78,85,85 | 1.25 | 10 (12%) |

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 |
|-----|------|-------|---------|------|---------|---------------|-----------|
| 5 | B12 | C | 2800 | 1 | - | 10/56/223/223 | 0/3/11/11 |
| 6 | GOL | D | 3003 | - | - | 4/4/4/4 | - |
| 3 | SCD | A | 1801[A] | - | - | 4/56/72/72 | 0/3/3/3 |
| 4 | MCD | A | 1802[B] | - | - | 3/59/75/75 | 0/3/3/3 |
| 6 | GOL | B | 3001 | - | - | 4/4/4/4 | - |
| 5 | B12 | A | 1800 | 1 | - | 9/56/223/223 | 0/3/11/11 |
| 6 | GOL | B | 3002 | - | - | 2/4/4/4 | - |
| 6 | GOL | D | 3004 | - | - | 2/4/4/4 | - |
| 3 | SCD | C | 2801[A] | - | - | 5/56/72/72 | 0/3/3/3 |
| 4 | MCD | C | 2802[B] | - | - | 2/59/75/75 | 0/3/3/3 |

All (28) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 4 | A | 1802[B] | MCD | CP2-NP1 | 3.67 | 1.54 | 1.46 |
| 3 | A | 1801[A] | SCD | CP2-NP1 | 3.63 | 1.54 | 1.46 |
| 4 | A | 1802[B] | MCD | CP5-NP2 | 3.51 | 1.54 | 1.46 |
| 4 | C | 2802[B] | MCD | CP5-NP2 | 3.44 | 1.53 | 1.46 |
| 4 | C | 2802[B] | MCD | CP2-NP1 | 3.31 | 1.53 | 1.46 |
| 3 | A | 1801[A] | SCD | CP5-NP2 | 3.29 | 1.53 | 1.46 |
| 3 | C | 2801[A] | SCD | CP2-NP1 | 3.14 | 1.53 | 1.46 |
| 3 | A | 1801[A] | SCD | P2-O7 | -3.12 | 1.47 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 3 | C | 2801[A] | SCD | CP5-NP2 | 3.10 | 1.53 | 1.46 |
| 4 | A | 1802[B] | MCD | P2-O7 | -2.97 | 1.47 | 1.59 |
| 3 | C | 2801[A] | SCD | P2-O7 | -2.92 | 1.48 | 1.59 |
| 5 | A | 1800 | B12 | C14-N23 | 2.89 | 1.39 | 1.35 |
| 4 | C | 2802[B] | MCD | P2-O7 | -2.82 | 1.48 | 1.59 |
| 5 | A | 1800 | B12 | C2B-N1B | -2.48 | 1.33 | 1.37 |
| 5 | C | 2800 | B12 | C14-N23 | 2.45 | 1.38 | 1.35 |
| 4 | A | 1802[B] | MCD | P2-O6 | 2.43 | 1.62 | 1.59 |
| 5 | C | 2800 | B12 | P-O2 | 2.37 | 1.66 | 1.59 |
| 5 | C | 2800 | B12 | C19-N24 | -2.33 | 1.46 | 1.49 |
| 4 | A | 1802[B] | MCD | OS4-CS4 | 2.25 | 1.28 | 1.22 |
| 5 | C | 2800 | B12 | C30-C3 | 2.21 | 1.59 | 1.54 |
| 3 | A | 1801[A] | SCD | P2-O6 | 2.20 | 1.61 | 1.59 |
| 5 | C | 2800 | B12 | C35-C5 | 2.18 | 1.55 | 1.50 |
| 3 | A | 1801[A] | SCD | OS4-CS4 | 2.15 | 1.29 | 1.22 |
| 5 | A | 1800 | B12 | P-O2 | 2.15 | 1.65 | 1.59 |
| 4 | C | 2802[B] | MCD | OS4-CS4 | 2.15 | 1.28 | 1.22 |
| 3 | C | 2801[A] | SCD | C2-N1 | 2.14 | 1.37 | 1.33 |
| 3 | A | 1801[A] | SCD | C2-N1 | 2.03 | 1.37 | 1.33 |
| 4 | C | 2802[B] | MCD | P2-O6 | 2.01 | 1.61 | 1.59 |

All (93) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 5 | A | 1800 | B12 | C16-C15-C14 | -4.85 | 113.86 | 121.26 |
| 5 | C | 2800 | B12 | C19-N24-C16 | 4.82 | 112.56 | 107.29 |
| 3 | C | 2801[A] | SCD | CP8-CPA-CPB | 4.68 | 115.95 | 108.22 |
| 4 | A | 1802[B] | MCD | CP5-NP2-CP6 | -4.66 | 114.17 | 122.55 |
| 3 | A | 1801[A] | SCD | CP8-CPA-CPB | 4.39 | 115.47 | 108.22 |
| 4 | C | 2802[B] | MCD | CP5-NP2-CP6 | -4.36 | 114.70 | 122.55 |
| 3 | C | 2801[A] | SCD | CP5-NP2-CP6 | -4.23 | 114.95 | 122.55 |
| 3 | A | 1801[A] | SCD | CP5-NP2-CP6 | -4.20 | 115.01 | 122.55 |
| 5 | C | 2800 | B12 | C20-C1-C19 | 4.17 | 113.36 | 109.35 |
| 5 | C | 2800 | B12 | C16-C15-C14 | -4.00 | 115.16 | 121.26 |
| 4 | C | 2802[B] | MCD | CP8-CPA-CPB | 3.93 | 114.71 | 108.22 |
| 5 | A | 1800 | B12 | C54-C17-C16 | -3.89 | 92.26 | 112.41 |
| 5 | C | 2800 | B12 | C54-C17-C16 | -3.81 | 92.66 | 112.41 |
| 5 | C | 2800 | B12 | C9B-C8B-N1B | 3.78 | 106.98 | 105.30 |
| 3 | A | 1801[A] | SCD | O7-CPB-CPA | -3.67 | 104.65 | 110.55 |
| 4 | A | 1802[B] | MCD | CP8-CPA-CPB | 3.65 | 114.25 | 108.22 |
| 5 | A | 1800 | B12 | C19-N24-C16 | 3.65 | 111.28 | 107.29 |
| 5 | A | 1800 | B12 | C55-C17-C18 | 3.63 | 118.05 | 111.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 4 | C | 2802[B] | MCD | O7-CPB-CPA | -3.60 | 104.75 | 110.55 |
| 5 | A | 1800 | B12 | C13-C14-C15 | -3.56 | 118.90 | 124.32 |
| 5 | C | 2800 | B12 | C55-C17-C16 | 3.55 | 123.54 | 116.59 |
| 4 | A | 1802[B] | MCD | O7-CPB-CPA | -3.54 | 104.85 | 110.55 |
| 5 | C | 2800 | B12 | C9-N22-C6 | 3.54 | 109.54 | 105.28 |
| 5 | A | 1800 | B12 | C12-C11-C10 | -3.41 | 119.01 | 123.40 |
| 5 | A | 1800 | B12 | C9B-C8B-N1B | 3.36 | 106.79 | 105.30 |
| 3 | C | 2801[A] | SCD | O7-CPB-CPA | -3.35 | 105.16 | 110.55 |
| 5 | C | 2800 | B12 | C55-C17-C18 | 3.06 | 116.95 | 111.12 |
| 3 | A | 1801[A] | SCD | CP2-NP1-CP3 | -3.06 | 117.13 | 122.82 |
| 3 | C | 2801[A] | SCD | CP9-CPA-CPB | 3.06 | 113.27 | 108.22 |
| 5 | A | 1800 | B12 | C7B-C8B-C9B | 3.05 | 126.13 | 122.47 |
| 3 | C | 2801[A] | SCD | CS3-CS2-CS1 | -3.02 | 109.22 | 113.49 |
| 3 | A | 1801[A] | SCD | OS5-CS4-CS3 | 3.02 | 123.54 | 114.00 |
| 4 | C | 2802[B] | MCD | CP9-CPA-CPB | 3.01 | 113.19 | 108.22 |
| 5 | A | 1800 | B12 | C55-C56-C57 | -2.93 | 104.72 | 111.25 |
| 4 | A | 1802[B] | MCD | CP1-CP2-NP1 | -2.91 | 104.03 | 112.20 |
| 5 | A | 1800 | B12 | C13-C14-N23 | 2.88 | 113.00 | 109.09 |
| 5 | C | 2800 | B12 | O51-C50-C49 | -2.88 | 112.36 | 121.04 |
| 4 | C | 2802[B] | MCD | CP9-CPA-CP7 | -2.87 | 103.87 | 108.77 |
| 5 | A | 1800 | B12 | C5-C6-N22 | -2.75 | 119.72 | 123.88 |
| 5 | A | 1800 | B12 | C5M-C5B-C6B | -2.73 | 115.18 | 120.76 |
| 5 | A | 1800 | B12 | C9-N22-C6 | 2.71 | 108.54 | 105.28 |
| 5 | A | 1800 | B12 | C10-C11-N23 | 2.69 | 128.97 | 124.42 |
| 5 | A | 1800 | B12 | O5-P-O4 | 2.67 | 124.89 | 112.44 |
| 3 | C | 2801[A] | SCD | OS5-CS4-CS3 | 2.63 | 122.31 | 114.00 |
| 5 | A | 1800 | B12 | O51-C50-C49 | -2.62 | 113.12 | 121.04 |
| 5 | A | 1800 | B12 | C20-C1-C2 | -2.62 | 108.96 | 113.28 |
| 5 | C | 2800 | B12 | C18-C19-N24 | 2.62 | 106.27 | 102.33 |
| 5 | C | 2800 | B12 | C2P-C1P-N59 | -2.59 | 109.11 | 112.92 |
| 5 | A | 1800 | B12 | C4B-C5B-C6B | 2.57 | 123.46 | 119.69 |
| 3 | C | 2801[A] | SCD | CP1-CP2-NP1 | -2.55 | 105.04 | 112.20 |
| 5 | A | 1800 | B12 | C55-C17-C16 | 2.52 | 121.53 | 116.59 |
| 4 | C | 2802[B] | MCD | CP1-CP2-NP1 | -2.52 | 105.13 | 112.20 |
| 5 | C | 2800 | B12 | C7B-C8B-C9B | 2.51 | 125.48 | 122.47 |
| 3 | A | 1801[A] | SCD | CP1-CP2-NP1 | -2.48 | 105.23 | 112.20 |
| 4 | C | 2802[B] | MCD | OS1-CS1-CPS | 2.48 | 125.88 | 121.68 |
| 5 | C | 2800 | B12 | C3-C4-C5 | -2.47 | 119.68 | 123.82 |
| 5 | A | 1800 | B12 | C18-C19-N24 | 2.47 | 106.04 | 102.33 |
| 3 | A | 1801[A] | SCD | OP2-CP6-NP2 | 2.41 | 128.08 | 122.98 |
| 5 | C | 2800 | B12 | C35-C5-C4 | -2.40 | 111.93 | 116.79 |
| 5 | C | 2800 | B12 | C54-C17-C55 | -2.40 | 105.28 | 109.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 5 | A | 1800 | B12 | C1P-N59-C57 | -2.39 | 117.56 | 122.69 |
| 5 | C | 2800 | B12 | C1P-N59-C57 | -2.38 | 117.59 | 122.69 |
| 5 | A | 1800 | B12 | C53-C15-C16 | 2.37 | 124.39 | 120.36 |
| 4 | A | 1802[B] | MCD | CP2-NP1-CP3 | -2.37 | 118.41 | 122.82 |
| 5 | C | 2800 | B12 | C1-C2-C3 | -2.37 | 98.62 | 101.60 |
| 5 | C | 2800 | B12 | C2-C1-C19 | -2.35 | 114.96 | 118.61 |
| 5 | A | 1800 | B12 | C3-C4-C5 | -2.35 | 119.89 | 123.82 |
| 5 | C | 2800 | B12 | C15-C16-N24 | 2.32 | 125.73 | 122.42 |
| 3 | C | 2801[A] | SCD | OS5-CS4-OS4 | -2.32 | 117.38 | 123.33 |
| 3 | C | 2801[A] | SCD | OP2-CP6-NP2 | 2.29 | 127.82 | 122.98 |
| 5 | A | 1800 | B12 | C2-C1-N21 | 2.28 | 104.95 | 101.78 |
| 4 | A | 1802[B] | MCD | OP2-CP6-CP7 | -2.28 | 114.53 | 120.89 |
| 4 | A | 1802[B] | MCD | C2'-C3'-C4' | -2.28 | 99.25 | 103.24 |
| 5 | C | 2800 | B12 | C2-C1-N21 | 2.27 | 104.94 | 101.78 |
| 5 | C | 2800 | B12 | O5-P-O4 | 2.27 | 123.01 | 112.44 |
| 5 | A | 1800 | B12 | C1-C2-C3 | -2.27 | 98.75 | 101.60 |
| 5 | A | 1800 | B12 | C42-C43-N45 | 2.27 | 123.76 | 116.49 |
| 4 | C | 2802[B] | MCD | C2'-C3'-C4' | -2.24 | 99.33 | 103.24 |
| 5 | A | 1800 | B12 | C54-C17-C18 | -2.21 | 109.81 | 112.99 |
| 5 | A | 1800 | B12 | C41-C8-C9 | -2.21 | 107.33 | 111.19 |
| 4 | A | 1802[B] | MCD | CP9-CPA-CP7 | -2.20 | 105.01 | 108.77 |
| 3 | C | 2801[A] | SCD | C2'-C3'-C4' | -2.20 | 99.38 | 103.24 |
| 5 | C | 2800 | B12 | C55-C56-C57 | -2.20 | 106.35 | 111.25 |
| 5 | C | 2800 | B12 | C13-C14-C15 | -2.19 | 120.98 | 124.32 |
| 5 | A | 1800 | B12 | C7B-C8B-N1B | -2.18 | 127.08 | 131.39 |
| 5 | C | 2800 | B12 | C8B-C9B-N3B | -2.17 | 107.65 | 110.00 |
| 5 | C | 2800 | B12 | C4B-C5B-C6B | 2.16 | 122.85 | 119.69 |
| 5 | A | 1800 | B12 | C2P-C1P-N59 | -2.15 | 109.76 | 112.92 |
| 3 | A | 1801[A] | SCD | C2'-C3'-C4' | -2.15 | 99.48 | 103.24 |
| 4 | C | 2802[B] | MCD | OP2-CP6-CP7 | -2.12 | 114.97 | 120.89 |
| 4 | C | 2802[B] | MCD | CPS-CS1-CS2 | -2.09 | 114.28 | 117.36 |
| 3 | A | 1801[A] | SCD | CP9-CPA-CPB | 2.08 | 111.66 | 108.22 |
| 5 | C | 2800 | B12 | C30-C31-C32 | 2.06 | 119.56 | 112.55 |

There are no chirality outliers.

All (45) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|---------|------|-----------------|
| 3 | C | 2801[A] | SCD | P1-O6-P2-O7 |
| 4 | A | 1802[B] | MCD | P1-O6-P2-O7 |
| 4 | C | 2802[B] | MCD | P1-O6-P2-O7 |
| 5 | A | 1800 | B12 | C2R-C1R-N1B-C2B |

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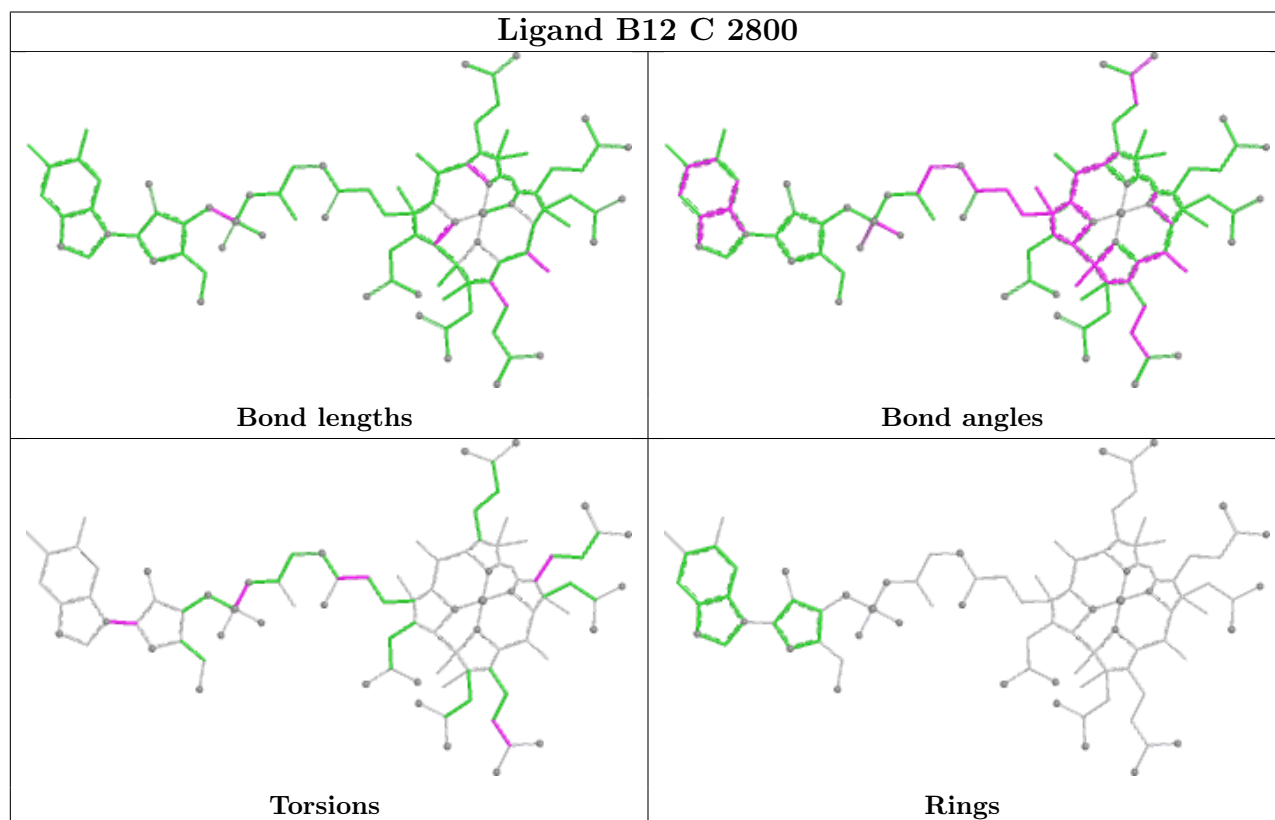
| Mol | Chain | Res | Type | Atoms |
|-----|-------|---------|------|-----------------|
| 5 | C | 2800 | B12 | C2R-C1R-N1B-C2B |
| 6 | B | 3001 | GOL | O1-C1-C2-C3 |
| 6 | B | 3001 | GOL | C1-C2-C3-O3 |
| 6 | B | 3002 | GOL | C1-C2-C3-O3 |
| 6 | D | 3003 | GOL | O1-C1-C2-C3 |
| 6 | D | 3003 | GOL | C1-C2-C3-O3 |
| 6 | D | 3004 | GOL | C1-C2-C3-O3 |
| 5 | C | 2800 | B12 | C42-C41-C8-C9 |
| 6 | B | 3001 | GOL | O1-C1-C2-O2 |
| 6 | B | 3002 | GOL | O2-C2-C3-O3 |
| 5 | A | 1800 | B12 | C16-C17-C55-C56 |
| 5 | A | 1800 | B12 | C2R-C1R-N1B-C8B |
| 5 | C | 2800 | B12 | C2R-C1R-N1B-C8B |
| 6 | B | 3001 | GOL | O2-C2-C3-O3 |
| 6 | D | 3003 | GOL | O1-C1-C2-O2 |
| 6 | D | 3004 | GOL | O2-C2-C3-O3 |
| 6 | D | 3003 | GOL | O2-C2-C3-O3 |
| 5 | A | 1800 | B12 | C41-C42-C43-O44 |
| 5 | A | 1800 | B12 | C41-C42-C43-N45 |
| 3 | A | 1801[A] | SCD | P1-O6-P2-O7 |
| 5 | A | 1800 | B12 | O6R-C1R-N1B-C8B |
| 5 | C | 2800 | B12 | O6R-C1R-N1B-C8B |
| 3 | A | 1801[A] | SCD | P2-O6-P1-O12 |
| 3 | C | 2801[A] | SCD | P2-O6-P1-O12 |
| 4 | C | 2802[B] | MCD | P2-O6-P1-O12 |
| 3 | A | 1801[A] | SCD | CP8-CPA-CPB-O7 |
| 3 | C | 2801[A] | SCD | CP8-CPA-CPB-O7 |
| 4 | A | 1802[B] | MCD | P2-O6-P1-O12 |
| 5 | C | 2800 | B12 | C55-C56-C57-O58 |
| 4 | A | 1802[B] | MCD | CPS-CS1-CS2-CS4 |
| 3 | C | 2801[A] | SCD | P2-O6-P1-O11 |
| 5 | A | 1800 | B12 | C2P-O3-P-O4 |
| 5 | A | 1800 | B12 | C2P-O3-P-O5 |
| 5 | C | 2800 | B12 | C2P-O3-P-O4 |
| 5 | C | 2800 | B12 | C2P-O3-P-O5 |
| 5 | C | 2800 | B12 | C55-C56-C57-N59 |
| 5 | C | 2800 | B12 | C30-C31-C32-N33 |
| 5 | A | 1800 | B12 | C30-C31-C32-N33 |
| 3 | A | 1801[A] | SCD | CS2-CS3-CS4-OS4 |
| 5 | C | 2800 | B12 | C30-C31-C32-O34 |
| 3 | C | 2801[A] | SCD | CS2-CS3-CS4-OS5 |

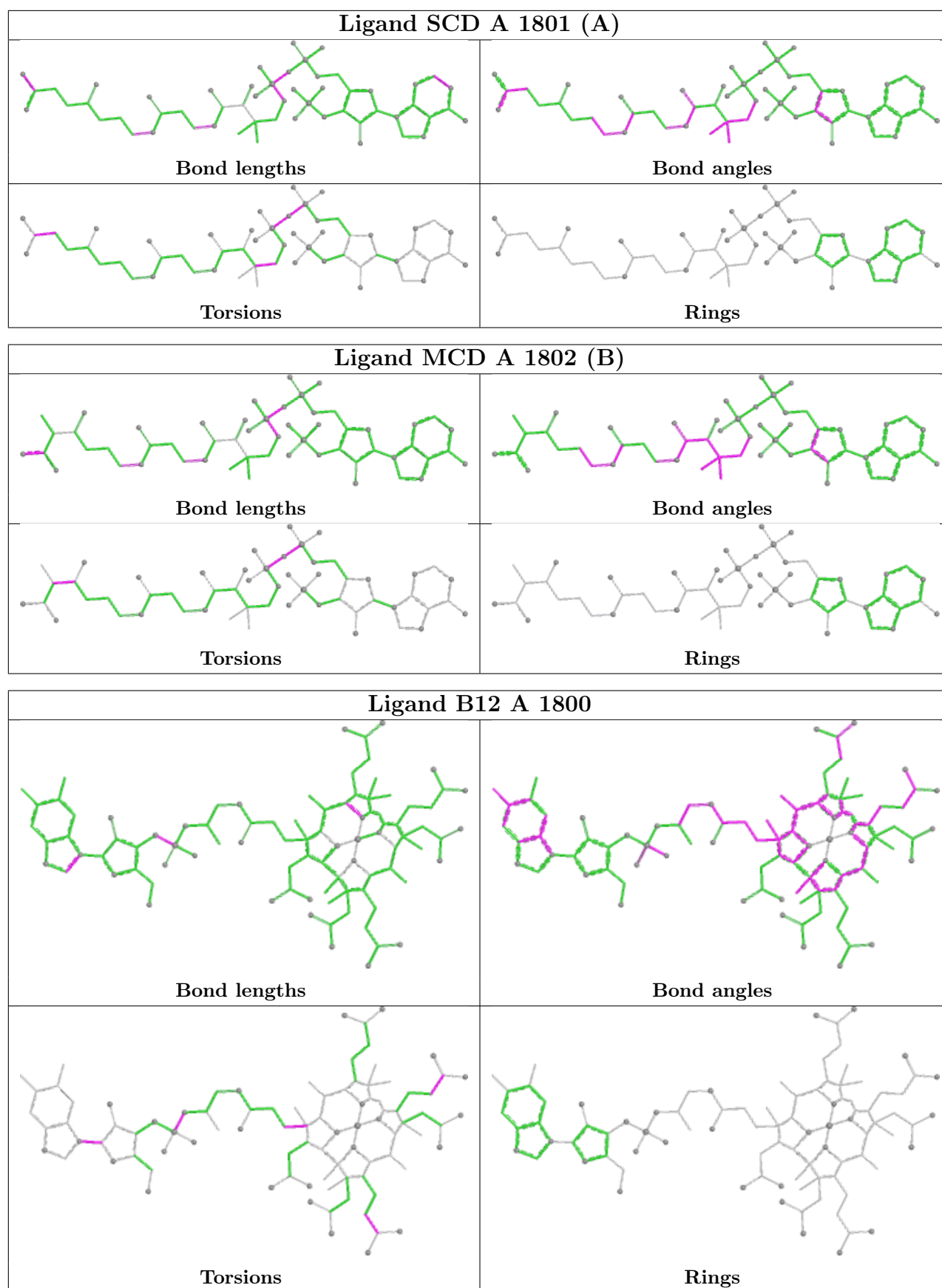
There are no ring outliers.

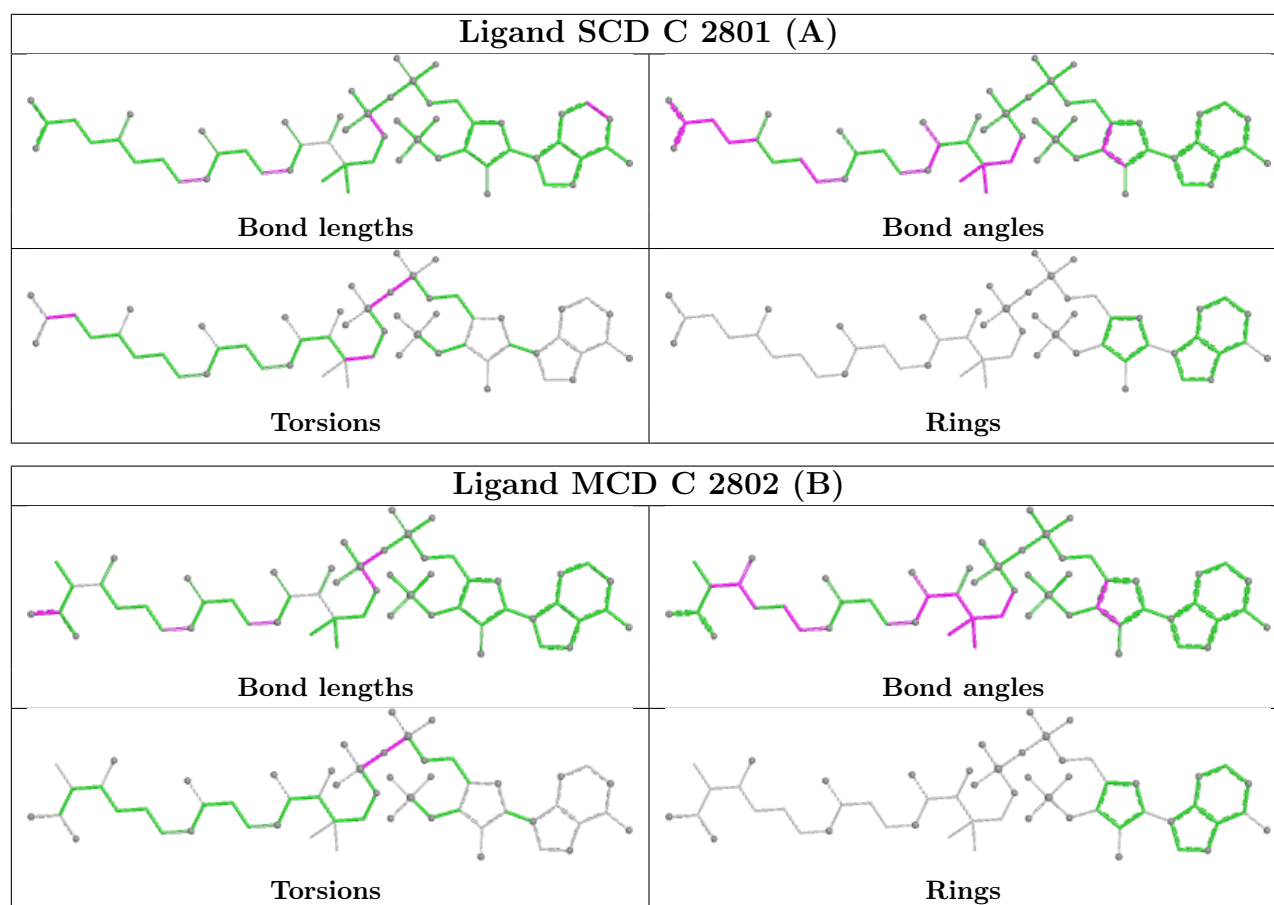
8 monomers are involved in 44 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 5 | C | 2800 | B12 | 16 | 0 |
| 3 | A | 1801[A] | SCD | 2 | 0 |
| 4 | A | 1802[B] | MCD | 3 | 0 |
| 5 | A | 1800 | B12 | 17 | 0 |
| 6 | B | 3002 | GOL | 1 | 0 |
| 6 | D | 3004 | GOL | 2 | 0 |
| 3 | C | 2801[A] | SCD | 1 | 0 |
| 4 | C | 2802[B] | MCD | 2 | 0 |

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







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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 725/727 (99%) | 0.14 | 12 (1%) 69 66 | 17, 36, 60, 80 | 0 |
| 1 | C | 725/727 (99%) | 0.34 | 29 (4%) 42 39 | 17, 36, 60, 81 | 0 |
| 2 | B | 619/637 (97%) | 0.69 | 46 (7%) 20 18 | 24, 49, 73, 89 | 0 |
| 2 | D | 619/637 (97%) | 0.90 | 74 (11%) 9 6 | 26, 50, 73, 89 | 0 |
| All | All | 2688/2728 (98%) | 0.50 | 161 (5%) 27 24 | 17, 42, 70, 89 | 0 |

All (161) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 20 | THR | 5.1 |
| 1 | C | 23 | ARG | 4.6 |
| 2 | B | 170 | TYR | 4.0 |
| 1 | C | 576 | ASN | 3.9 |
| 2 | D | 146 | ALA | 3.7 |
| 1 | C | 501 | ALA | 3.6 |
| 2 | D | 183 | TYR | 3.5 |
| 2 | B | 635 | GLY | 3.5 |
| 1 | C | 728 | ALA | 3.5 |
| 1 | C | 9 | SER | 3.4 |
| 1 | C | 25 | PHE | 3.3 |
| 2 | D | 182 | VAL | 3.3 |
| 2 | D | 638 | LYS | 3.3 |
| 1 | C | 16 | PRO | 3.1 |
| 2 | B | 183 | TYR | 3.1 |
| 2 | D | 126 | LEU | 3.1 |
| 2 | B | 179 | LEU | 3.0 |
| 2 | D | 637 | ALA | 3.0 |
| 1 | C | 7 | PHE | 2.9 |
| 2 | D | 140 | VAL | 2.9 |
| 1 | C | 27 | GLU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | B | 20 | THR | 2.9 |
| 2 | D | 25 | GLY | 2.8 |
| 2 | D | 170 | TYR | 2.8 |
| 2 | B | 106 | ALA | 2.8 |
| 2 | D | 227 | PHE | 2.8 |
| 2 | B | 155 | SER | 2.8 |
| 2 | B | 195 | LEU | 2.8 |
| 2 | B | 612 | LEU | 2.8 |
| 1 | C | 21 | ALA | 2.8 |
| 2 | D | 190 | ALA | 2.8 |
| 2 | D | 145 | ILE | 2.7 |
| 1 | C | 486 | SER | 2.7 |
| 2 | D | 427 | GLY | 2.7 |
| 2 | D | 195 | LEU | 2.7 |
| 2 | B | 423 | VAL | 2.7 |
| 1 | C | 14 | ASN | 2.7 |
| 2 | B | 487 | GLY | 2.7 |
| 2 | D | 180 | VAL | 2.7 |
| 2 | D | 272 | THR | 2.7 |
| 2 | D | 164 | VAL | 2.7 |
| 2 | D | 217 | LEU | 2.7 |
| 2 | D | 220 | TRP | 2.7 |
| 2 | B | 194 | ALA | 2.6 |
| 2 | B | 638 | LYS | 2.6 |
| 2 | D | 151 | ASP | 2.6 |
| 2 | D | 218 | GLY | 2.6 |
| 2 | D | 193 | LEU | 2.6 |
| 1 | C | 19 | ALA | 2.6 |
| 1 | A | 576 | ASN | 2.6 |
| 2 | D | 192 | ASP | 2.6 |
| 1 | A | 595 | GLY | 2.6 |
| 1 | A | 726 | LEU | 2.6 |
| 2 | D | 312 | GLY | 2.6 |
| 2 | D | 307 | ILE | 2.6 |
| 2 | D | 276 | ALA | 2.5 |
| 2 | B | 427 | GLY | 2.5 |
| 2 | B | 182 | VAL | 2.5 |
| 2 | D | 93 | PHE | 2.5 |
| 2 | B | 118 | GLU | 2.5 |
| 1 | C | 726 | LEU | 2.5 |
| 2 | B | 207 | LEU | 2.5 |
| 2 | D | 179 | LEU | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | D | 305 | ALA | 2.5 |
| 2 | B | 197 | LEU | 2.5 |
| 1 | C | 543 | ALA | 2.5 |
| 2 | B | 432 | ALA | 2.5 |
| 2 | B | 602 | PHE | 2.4 |
| 2 | B | 124 | ALA | 2.4 |
| 2 | D | 487 | GLY | 2.4 |
| 2 | D | 507 | VAL | 2.4 |
| 2 | D | 191 | LYS | 2.4 |
| 2 | D | 202 | ILE | 2.4 |
| 2 | B | 147 | PRO | 2.4 |
| 2 | B | 609 | ALA | 2.4 |
| 2 | D | 89 | GLY | 2.4 |
| 2 | D | 260 | ALA | 2.4 |
| 2 | B | 311 | PHE | 2.4 |
| 2 | B | 149 | HIS | 2.4 |
| 2 | D | 230 | ASP | 2.3 |
| 2 | B | 161 | MET | 2.3 |
| 2 | B | 636 | VAL | 2.3 |
| 2 | D | 209 | GLY | 2.3 |
| 2 | D | 194 | ALA | 2.3 |
| 1 | A | 92 | PHE | 2.3 |
| 1 | C | 574 | VAL | 2.3 |
| 2 | D | 150 | LEU | 2.3 |
| 2 | D | 188 | LYS | 2.3 |
| 1 | C | 274 | GLY | 2.3 |
| 2 | D | 161 | MET | 2.3 |
| 2 | D | 184 | GLU | 2.3 |
| 2 | D | 310 | VAL | 2.3 |
| 2 | D | 433 | VAL | 2.3 |
| 2 | B | 190 | ALA | 2.3 |
| 2 | B | 447 | ALA | 2.3 |
| 2 | D | 253 | ALA | 2.3 |
| 2 | D | 273 | ALA | 2.3 |
| 2 | D | 318 | ARG | 2.2 |
| 2 | D | 176 | ALA | 2.2 |
| 2 | D | 606 | ALA | 2.2 |
| 1 | C | 430 | VAL | 2.2 |
| 2 | D | 216 | VAL | 2.2 |
| 2 | D | 426 | LEU | 2.2 |
| 2 | D | 438 | VAL | 2.2 |
| 2 | D | 96 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 438 | GLU | 2.2 |
| 1 | C | 30 | ALA | 2.2 |
| 2 | B | 176 | ALA | 2.2 |
| 2 | D | 124 | ALA | 2.2 |
| 2 | D | 357 | SER | 2.2 |
| 2 | D | 634 | LEU | 2.2 |
| 2 | D | 313 | VAL | 2.2 |
| 2 | B | 373 | ASP | 2.2 |
| 1 | C | 671 | GLU | 2.2 |
| 2 | B | 576 | GLN | 2.2 |
| 1 | C | 29 | ALA | 2.2 |
| 2 | B | 241 | TYR | 2.2 |
| 2 | B | 227 | PHE | 2.2 |
| 2 | D | 311 | PHE | 2.2 |
| 1 | A | 474 | HIS | 2.2 |
| 1 | C | 592 | GLN | 2.2 |
| 1 | A | 9 | SER | 2.2 |
| 2 | B | 175 | ALA | 2.2 |
| 2 | D | 91 | ALA | 2.2 |
| 1 | C | 517 | TRP | 2.1 |
| 2 | D | 158 | LEU | 2.1 |
| 1 | C | 694 | ASP | 2.1 |
| 2 | D | 157 | VAL | 2.1 |
| 2 | D | 147 | PRO | 2.1 |
| 2 | D | 354 | GLY | 2.1 |
| 1 | A | 728 | ALA | 2.1 |
| 2 | B | 274 | THR | 2.1 |
| 2 | B | 171 | ASP | 2.1 |
| 2 | D | 201 | PRO | 2.1 |
| 2 | D | 267 | VAL | 2.1 |
| 2 | B | 264 | ARG | 2.1 |
| 2 | D | 274 | THR | 2.1 |
| 2 | B | 174 | ALA | 2.1 |
| 1 | C | 502 | GLU | 2.1 |
| 2 | D | 323 | ASN | 2.1 |
| 2 | D | 153 | VAL | 2.1 |
| 1 | A | 155 | GLY | 2.1 |
| 2 | B | 186 | SER | 2.1 |
| 2 | D | 121 | THR | 2.1 |
| 1 | A | 4 | LEU | 2.1 |
| 1 | C | 474 | HIS | 2.1 |
| 2 | D | 224 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 187 | ASP | 2.1 |
| 1 | C | 17 | VAL | 2.1 |
| 2 | B | 185 | ARG | 2.1 |
| 2 | B | 230 | ASP | 2.0 |
| 2 | B | 189 | PRO | 2.0 |
| 1 | C | 35 | GLY | 2.0 |
| 1 | A | 575 | LYS | 2.0 |
| 1 | C | 491 | GLU | 2.0 |
| 2 | B | 434 | MET | 2.0 |
| 2 | B | 587 | ALA | 2.0 |
| 2 | B | 606 | ALA | 2.0 |
| 2 | D | 320 | ALA | 2.0 |
| 2 | D | 197 | LEU | 2.0 |
| 1 | A | 5 | PRO | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

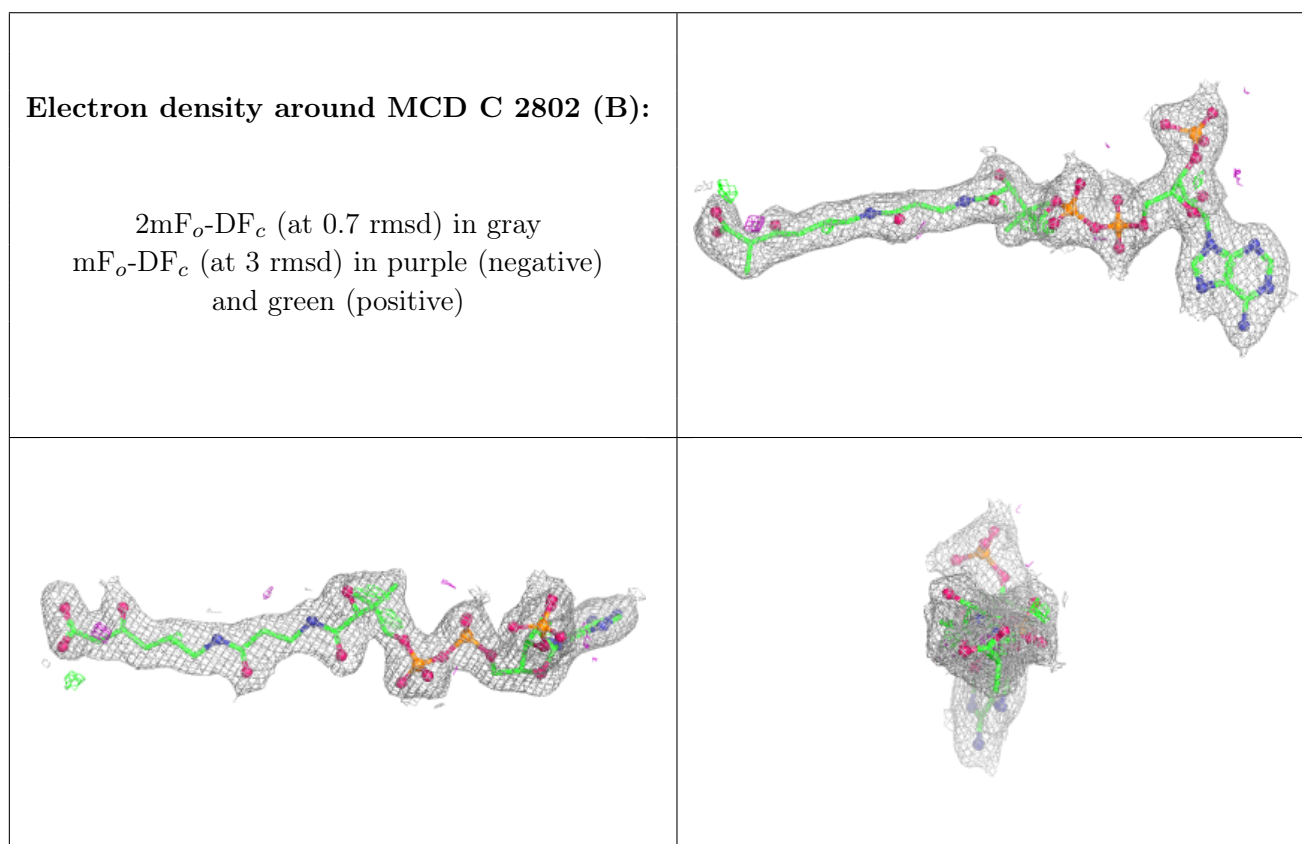
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 6 | GOL | D | 3004 | 6/6 | 0.48 | 0.29 | 84,84,85,86 | 0 |
| 6 | GOL | D | 3003 | 6/6 | 0.51 | 0.25 | 94,95,95,95 | 0 |
| 6 | GOL | B | 3001 | 6/6 | 0.74 | 0.23 | 95,95,95,95 | 0 |
| 6 | GOL | B | 3002 | 6/6 | 0.79 | 0.36 | 82,83,84,84 | 0 |
| 4 | MCD | C | 2802[B] | 55/55 | 0.95 | 0.08 | 19,24,35,37 | 55 |
| 5 | B12 | A | 1800 | 91/91 | 0.95 | 0.07 | 16,27,34,37 | 0 |
| 3 | SCD | A | 1801[A] | 55/55 | 0.96 | 0.07 | 15,22,26,27 | 55 |
| 3 | SCD | C | 2801[A] | 55/55 | 0.96 | 0.07 | 15,21,27,28 | 55 |
| 4 | MCD | A | 1802[B] | 55/55 | 0.96 | 0.07 | 21,24,36,39 | 55 |

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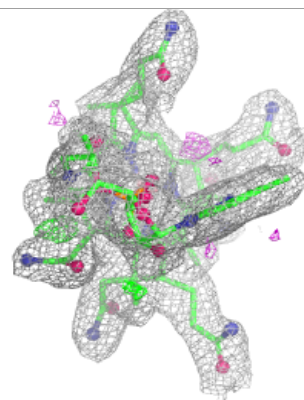
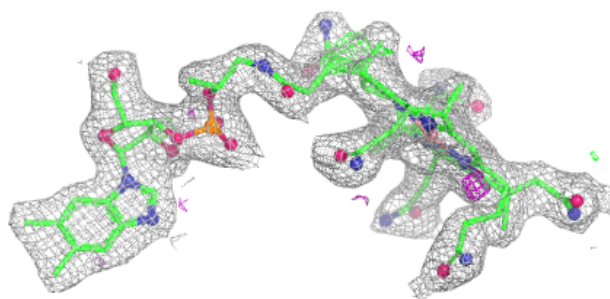
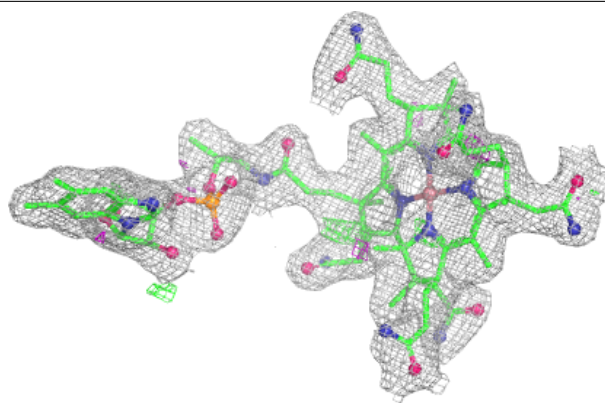
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5 | B12 | C | 2800 | 91/91 | 0.97 | 0.07 | 18,26,32,36 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

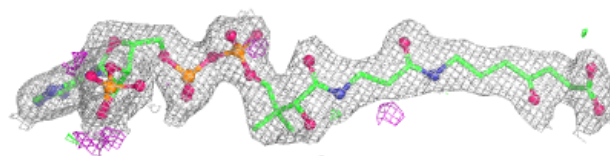
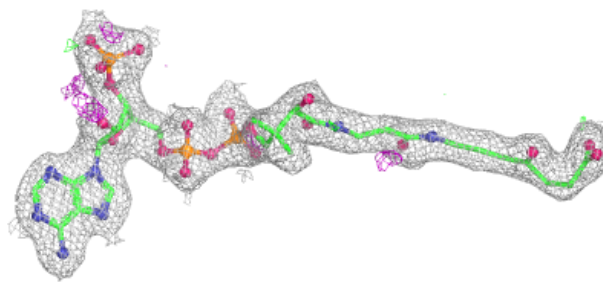


Electron density around B12 A 1800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

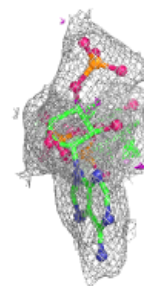
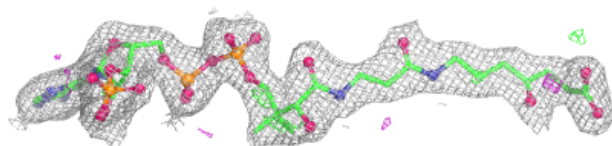
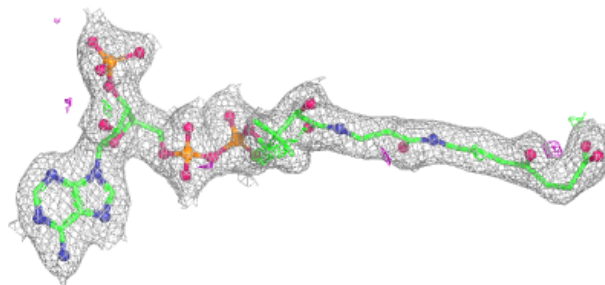
**Electron density around SCD A 1801 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

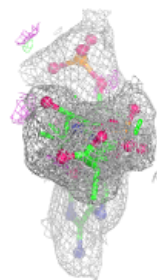
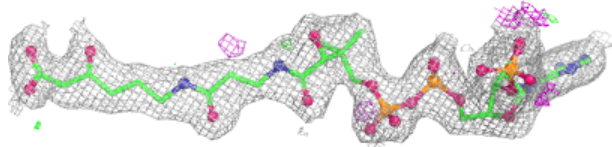
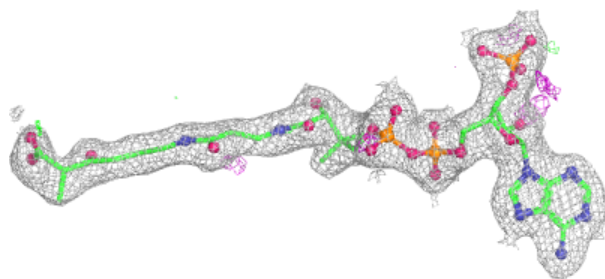


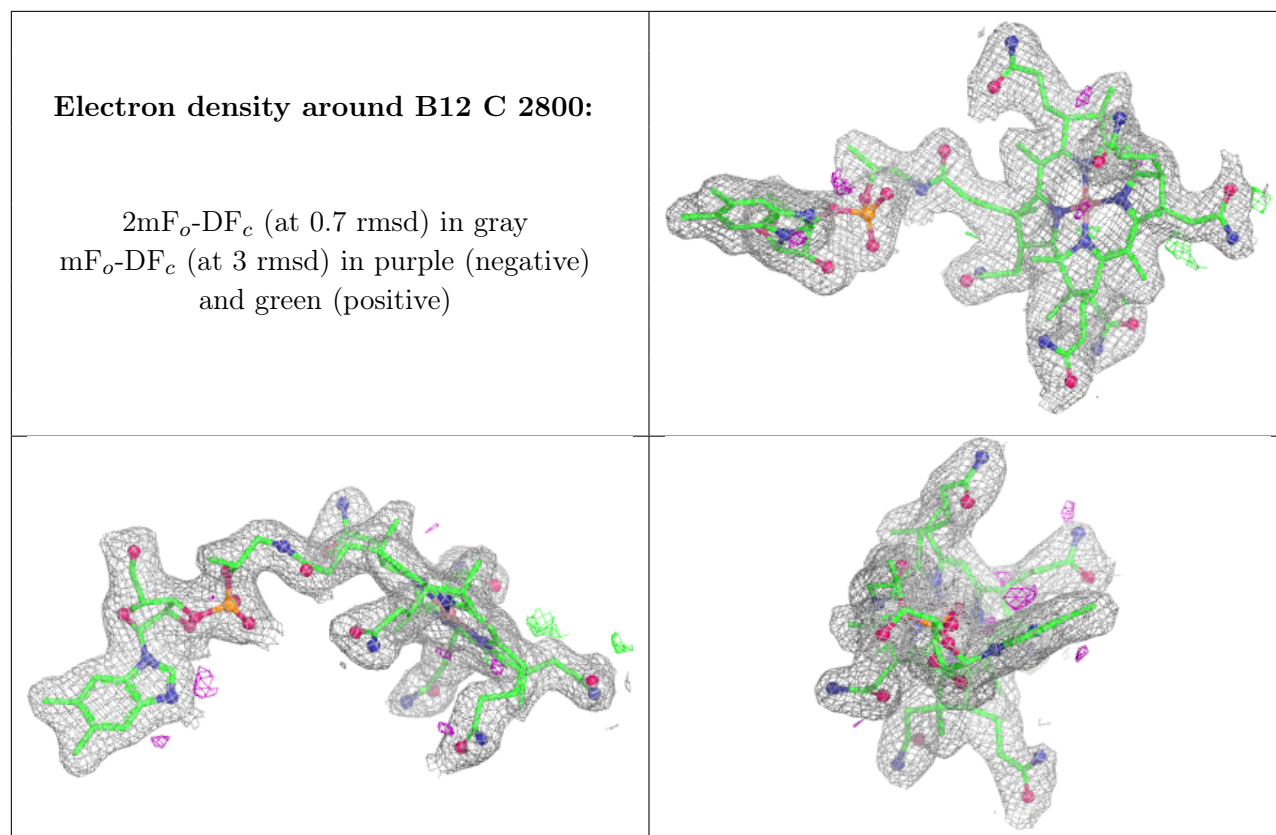
Electron density around SCD C 2801 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MCD A 1802 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.