



Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 11:04 am BST

PDB ID : 8PPK
EMDB ID : EMD-17804
Title : Bat-Hp-CoV Nsp1 and eIF1 bound to the human 40S small ribosomal subunit
Authors : Schubert, K.; Karousis, E.D.; Ban, I.; Lapointe, C.P.; Leibundgut, M.; Baeumlin, E.; Kummerant, E.; Scaiola, A.; Schoenhut, T.; Ziegelmueller, J.; Puglisi, J.D.; Muehlemann, O.; Ban, N.
Deposited on : 2023-07-07
Resolution : 2.98 Å(reported)
Based on initial models : 6ZOL, 6ZOK

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 79548 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Eukaryotic translation initiation factor 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | p | 85 | 691 | 438 | 125 | 126 | 2 | 0 | 0 |

- Molecule 2 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 2 | 2 | 1771 | 37855 | 16922 | 6786 | 12376 | 1771 | 0 | 0 |

- Molecule 3 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | A | 216 | 1708 | 1085 | 299 | 316 | 8 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | B | 224 | 1815 | 1152 | 328 | 321 | 14 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | C | 223 | 1741 | 1124 | 300 | 307 | 10 | 1 | 0 |

- Molecule 6 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | D | 225 | 1752 | 1117 | 315 | 313 | 7 | 0 | 0 |

- Molecule 7 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | E | 262 | 2076 | 1324 | 386 | 358 | 8 | 0 | 0 |

- Molecule 8 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | F | 192 | 1517 | 948 | 287 | 275 | 7 | 0 | 0 |

- Molecule 9 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | G | 240 | 1945 | 1212 | 393 | 333 | 7 | 0 | 0 |

- Molecule 10 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | H | 189 | 1523 | 972 | 280 | 270 | 1 | 0 | 0 |

- Molecule 11 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | I | 205 | 1682 | 1056 | 331 | 290 | 5 | 0 | 0 |

- Molecule 12 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | J | 180 | 1499 | 955 | 300 | 242 | 2 | 0 | 0 |

- Molecule 13 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | K | 97 | 816 | 533 | 144 | 133 | 6 | 0 | 0 |

- Molecule 14 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 14 | L | 155 | 1267 | 807 | 237 | 217 | 6 | 0 | 0 |

- Molecule 15 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 15 | M | 123 | 953 | 598 | 169 | 177 | 9 | 0 | 0 |

- Molecule 16 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 16 | N | 149 | 1202 | 770 | 228 | 203 | 1 | 0 | 0 |

- Molecule 17 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 17 | O | 135 | 1010 | 618 | 198 | 188 | 6 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| O | 138 | IAS | ASP | modified residue | UNP P62263 |

- Molecule 18 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 18 | P | 124 | 1016 | 644 | 192 | 173 | 7 | 0 | 0 |

- Molecule 19 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 19 | Q | 142 | 1128 | 717 | 213 | 195 | 3 | 0 | 0 |

- Molecule 20 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 20 | R | 134 | 1082 | 680 | 201 | 197 | 4 | 0 | 0 |

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 21 | S | 145 | 1200 | 753 | 242 | 204 | 1 | 0 | 0 |

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 22 | T | 144 | 1123 | 704 | 217 | 199 | 3 | 0 | 0 |

- Molecule 23 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 23 | U | 101 | 803 | 504 | 153 | 142 | 4 | 0 | 0 |

- Molecule 24 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 24 | V | 83 | 639 | 395 | 117 | 122 | 5 | 0 | 0 |

- Molecule 25 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 25 | W | 129 | 1034 | 659 | 193 | 176 | 6 | 0 | 0 |

- Molecule 26 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 26 | X | 141 | 1099 | 693 | 219 | 184 | 3 | 0 | 0 |

- Molecule 27 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | Y | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1014 | 641 | 198 | 170 | 5 | | |

- Molecule 28 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | Z | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 574 | 368 | 104 | 101 | 1 | | |

- Molecule 29 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | a | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 507 | 170 | 132 | 5 | | |

- Molecule 30 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | b | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 650 | 408 | 121 | 114 | 7 | | |

- Molecule 31 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31 | c | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 512 | 311 | 103 | 96 | 2 | | |

- Molecule 32 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32 | d | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 458 | 286 | 94 | 73 | 5 | | |

- Molecule 33 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33 | e | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 467 | 290 | 102 | 74 | 1 | | |

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 34 | f | 74 | 610 | 385 | 117 | 101 | 7 | 0 | 0 |

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 35 | g | 314 | 2440 | 1537 | 425 | 466 | 12 | 0 | 0 |

- Molecule 36 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 36 | h | 25 | 239 | 145 | 64 | 27 | 3 | 0 | 0 |

- Molecule 37 is a protein called Nsp1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 37 | j | 174 | 1363 | 867 | 239 | 253 | 4 | 0 | 0 |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|----------------|
| j | -13 | MET | - | initiating methionine | UNP A0A088DIE1 |
| j | -12 | HIS | - | expression tag | UNP A0A088DIE1 |
| j | -11 | HIS | - | expression tag | UNP A0A088DIE1 |
| j | -10 | HIS | - | expression tag | UNP A0A088DIE1 |
| j | -9 | HIS | - | expression tag | UNP A0A088DIE1 |
| j | -8 | HIS | - | expression tag | UNP A0A088DIE1 |
| j | -7 | HIS | - | expression tag | UNP A0A088DIE1 |
| j | -6 | GLU | - | expression tag | UNP A0A088DIE1 |
| j | -5 | ASN | - | expression tag | UNP A0A088DIE1 |
| j | -4 | LEU | - | expression tag | UNP A0A088DIE1 |
| j | -3 | TYR | - | expression tag | UNP A0A088DIE1 |
| j | -2 | PHE | - | expression tag | UNP A0A088DIE1 |
| j | -1 | GLN | - | expression tag | UNP A0A088DIE1 |
| j | 0 | SER | - | expression tag | UNP A0A088DIE1 |

- Molecule 38 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|--------------------|---------|
| 38 | 2 | 108 | Total X 108 108 | 0 |
| 38 | G | 1 | Total X 1 1 | 0 |
| 38 | H | 1 | Total X 1 1 | 0 |
| 38 | I | 1 | Total X 1 1 | 0 |
| 38 | J | 1 | Total X 1 1 | 0 |
| 38 | L | 1 | Total X 1 1 | 0 |
| 38 | N | 1 | Total X 1 1 | 0 |
| 38 | O | 2 | Total X 2 2 | 0 |
| 38 | X | 1 | Total X 1 1 | 0 |

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|---------------------|---------|
| 39 | 2 | 110 | Total Mg 110 110 | 0 |
| 39 | X | 1 | Total Mg 1 1 | 0 |

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 40 | a | 1 | Total Zn 1 1 | 0 |
| 40 | d | 1 | Total Zn 1 1 | 0 |
| 40 | f | 1 | Total Zn 1 1 | 0 |

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

| Property | Value | Source |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 98750 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 60 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

92 non-standard protein/DNA/RNA residues 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 | $\# Z > 2$ |
| 2 | PSU | 2 | 1244 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.83 | 3 (13%) |
| 2 | OMU | 2 | 1442 | 2,39 | 19,22,23 | 1.23 | 2 (10%) | 26,31,34 | 1.70 | 4 (15%) |
| 2 | MA6 | 2 | 1850 | 2 | 18,26,27 | 1.09 | 1 (5%) | 19,38,41 | 1.94 | 3 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | PSU | 2 | 105 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.90 | 3 (13%) |
| 2 | PSU | 2 | 1177 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.87 | 3 (13%) |
| 2 | PSU | 2 | 572 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.93 | 3 (13%) |
| 2 | OMU | 2 | 1326 | 2,39 | 19,22,23 | 1.19 | 2 (10%) | 26,31,34 | 1.72 | 5 (19%) |
| 2 | OMG | 2 | 509 | 2,39 | 18,26,27 | 0.95 | 1 (5%) | 19,38,41 | 1.09 | 2 (10%) |
| 2 | A2M | 2 | 99 | 2,39 | 18,25,26 | 1.05 | 1 (5%) | 18,36,39 | 1.20 | 2 (11%) |
| 2 | B8N | 2 | 1248 | 2 | 24,29,30 | 1.29 | 3 (12%) | 29,42,45 | 1.26 | 3 (10%) |
| 2 | PSU | 2 | 1445 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 2 | OMU | 2 | 116 | 2 | 19,22,23 | 1.21 | 3 (15%) | 26,31,34 | 1.70 | 4 (15%) |
| 2 | 6MZ | 2 | 1832 | 2,39 | 18,25,26 | 0.91 | 1 (5%) | 16,36,39 | 1.76 | 3 (18%) |
| 2 | OMG | 2 | 1328 | 2 | 18,26,27 | 0.93 | 1 (5%) | 19,38,41 | 1.07 | 2 (10%) |
| 2 | OMU | 2 | 627 | 2 | 19,22,23 | 1.20 | 2 (10%) | 26,31,34 | 1.67 | 5 (19%) |
| 2 | PSU | 2 | 1367 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 2 | PSU | 2 | 119 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.90 | 3 (13%) |
| 24 | AME | V | 1 | 24 | 9,10,11 | 0.47 | 0 | 9,11,13 | 0.88 | 1 (11%) |
| 2 | OMC | 2 | 174 | 2,39 | 19,22,23 | 0.82 | 0 | 26,31,34 | 0.79 | 0 |
| 2 | PSU | 2 | 814 | 2 | 18,21,22 | 1.37 | 2 (11%) | 22,30,33 | 1.89 | 3 (13%) |
| 2 | A2M | 2 | 159 | 2 | 18,25,26 | 1.07 | 1 (5%) | 18,36,39 | 1.18 | 2 (11%) |
| 26 | HY3 | X | 62 | 26 | 6,8,9 | 2.16 | 1 (16%) | 5,10,12 | 1.16 | 1 (20%) |
| 2 | PSU | 2 | 686 | 2 | 18,21,22 | 1.33 | 2 (11%) | 22,30,33 | 1.93 | 4 (18%) |
| 2 | OMC | 2 | 1703 | 2 | 19,22,23 | 0.83 | 0 | 26,31,34 | 0.89 | 1 (3%) |
| 2 | PSU | 2 | 1625 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.89 | 3 (13%) |
| 2 | PSU | 2 | 651 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.92 | 4 (18%) |
| 2 | A2M | 2 | 468 | 2 | 18,25,26 | 1.02 | 1 (5%) | 18,36,39 | 1.27 | 2 (11%) |
| 2 | G7M | 2 | 1639 | 2 | 20,26,27 | 2.96 | 7 (35%) | 17,39,42 | 1.00 | 1 (5%) |
| 2 | PSU | 2 | 649 | 2 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.90 | 4 (18%) |
| 2 | PSU | 2 | 815 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.90 | 3 (13%) |
| 2 | PSU | 2 | 1692 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.90 | 3 (13%) |
| 2 | A2M | 2 | 590 | 2 | 18,25,26 | 1.02 | 1 (5%) | 18,36,39 | 1.20 | 2 (11%) |
| 2 | PSU | 2 | 36 | 2 | 18,21,22 | 1.37 | 2 (11%) | 22,30,33 | 1.95 | 3 (13%) |
| 22 | NMM | T | 67 | 22 | 9,11,12 | 0.59 | 0 | 6,12,14 | 0.55 | 0 |
| 2 | A2M | 2 | 166 | 2 | 18,25,26 | 1.02 | 1 (5%) | 18,36,39 | 1.26 | 2 (11%) |
| 2 | PSU | 2 | 109 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 2 | PSU | 2 | 93 | 2 | 18,21,22 | 1.38 | 2 (11%) | 22,30,33 | 1.95 | 3 (13%) |
| 2 | PSU | 2 | 1081 | 2 | 18,21,22 | 1.38 | 3 (16%) | 22,30,33 | 1.88 | 3 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | PSU | 2 | 863 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.88 | 3 (13%) |
| 2 | PSU | 2 | 1347 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.89 | 3 (13%) |
| 2 | PSU | 2 | 1643 | 2,39 | 18,21,22 | 1.37 | 2 (11%) | 22,30,33 | 1.87 | 3 (13%) |
| 2 | PSU | 2 | 1045 | 2 | 18,21,22 | 1.33 | 2 (11%) | 22,30,33 | 1.89 | 3 (13%) |
| 2 | PSU | 2 | 406 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 2 | PSU | 2 | 34 | 2 | 18,21,22 | 1.37 | 2 (11%) | 22,30,33 | 1.95 | 3 (13%) |
| 2 | PSU | 2 | 1238 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.86 | 3 (13%) |
| 2 | OMU | 2 | 1288 | 2 | 19,22,23 | 1.22 | 3 (15%) | 26,31,34 | 1.69 | 4 (15%) |
| 2 | OMU | 2 | 172 | 2 | 19,22,23 | 1.21 | 2 (10%) | 26,31,34 | 1.73 | 5 (19%) |
| 2 | PSU | 2 | 609 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.87 | 3 (13%) |
| 2 | PSU | 2 | 866 | 2 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.93 | 4 (18%) |
| 2 | OMG | 2 | 1447 | 2 | 18,26,27 | 0.94 | 1 (5%) | 19,38,41 | 1.07 | 2 (10%) |
| 2 | MA6 | 2 | 1851 | 2 | 18,26,27 | 1.09 | 2 (11%) | 19,38,41 | 1.97 | 3 (15%) |
| 2 | OMG | 2 | 644 | 2 | 18,26,27 | 0.95 | 1 (5%) | 19,38,41 | 1.10 | 2 (10%) |
| 2 | OMG | 2 | 1490 | 2,39 | 18,26,27 | 0.94 | 1 (5%) | 19,38,41 | 1.08 | 2 (10%) |
| 2 | OMG | 2 | 683 | 2 | 18,26,27 | 0.93 | 1 (5%) | 19,38,41 | 1.07 | 2 (10%) |
| 2 | A2M | 2 | 1031 | 2 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.24 | 2 (11%) |
| 2 | OMG | 2 | 601 | 2 | 18,26,27 | 0.91 | 1 (5%) | 19,38,41 | 1.09 | 2 (10%) |
| 2 | OMC | 2 | 517 | 2 | 19,22,23 | 0.82 | 0 | 26,31,34 | 0.82 | 0 |
| 2 | A2M | 2 | 1383 | 2 | 18,25,26 | 1.04 | 1 (5%) | 18,36,39 | 1.28 | 2 (11%) |
| 2 | PSU | 2 | 822 | 2 | 18,21,22 | 1.37 | 2 (11%) | 22,30,33 | 1.94 | 4 (18%) |
| 2 | 4AC | 2 | 1337 | 2 | 21,24,25 | 1.10 | 2 (9%) | 29,34,37 | 1.02 | 2 (6%) |
| 2 | OMU | 2 | 799 | 2 | 19,22,23 | 1.21 | 3 (15%) | 26,31,34 | 1.72 | 5 (19%) |
| 2 | PSU | 2 | 1232 | 2 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.92 | 4 (18%) |
| 2 | PSU | 2 | 1174 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.89 | 3 (13%) |
| 2 | PSU | 2 | 681 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.92 | 3 (13%) |
| 2 | OMU | 2 | 354 | 2 | 19,22,23 | 1.22 | 3 (15%) | 26,31,34 | 1.72 | 5 (19%) |
| 2 | OMU | 2 | 1804 | 2 | 19,22,23 | 1.21 | 3 (15%) | 26,31,34 | 1.71 | 4 (15%) |
| 2 | PSU | 2 | 1136 | 2 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 2 | OMU | 2 | 121 | 2 | 19,22,23 | 1.21 | 3 (15%) | 26,31,34 | 1.69 | 5 (19%) |
| 2 | A2M | 2 | 512 | 2 | 18,25,26 | 1.00 | 1 (5%) | 18,36,39 | 1.20 | 2 (11%) |
| 2 | OMU | 2 | 428 | 2 | 19,22,23 | 1.19 | 3 (15%) | 26,31,34 | 1.71 | 5 (19%) |
| 2 | A2M | 2 | 484 | 2 | 18,25,26 | 0.99 | 1 (5%) | 18,36,39 | 1.23 | 2 (11%) |
| 2 | OMG | 2 | 436 | 2 | 18,26,27 | 0.93 | 1 (5%) | 19,38,41 | 1.10 | 2 (10%) |
| 2 | PSU | 2 | 218 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.88 | 3 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | PSU | 2 | 966 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.88 | 3 (13%) |
| 2 | PSU | 2 | 1046 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.86 | 3 (13%) |
| 2 | OMC | 2 | 1272 | 2 | 19,22,23 | 0.83 | 0 | 26,31,34 | 0.89 | 1 (3%) |
| 17 | IAS | O | 138 | 17 | 6,7,8 | 0.97 | 0 | 6,8,10 | 1.32 | 1 (16%) |
| 2 | PSU | 2 | 1004 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.89 | 3 (13%) |
| 2 | PSU | 2 | 296 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.90 | 3 (13%) |
| 2 | OMC | 2 | 797 | 2 | 19,22,23 | 0.82 | 0 | 26,31,34 | 0.87 | 1 (3%) |
| 2 | A2M | 2 | 668 | 2,39 | 18,25,26 | 0.96 | 1 (5%) | 18,36,39 | 1.35 | 2 (11%) |
| 2 | A2M | 2 | 1678 | 2 | 18,25,26 | 1.01 | 1 (5%) | 18,36,39 | 1.26 | 2 (11%) |
| 2 | PSU | 2 | 801 | 2 | 18,21,22 | 1.36 | 2 (11%) | 22,30,33 | 1.91 | 3 (13%) |
| 2 | 4AC | 2 | 1842 | 2 | 21,24,25 | 1.11 | 2 (9%) | 29,34,37 | 1.23 | 3 (10%) |
| 2 | PSU | 2 | 210 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.87 | 3 (13%) |
| 2 | A2M | 2 | 27 | 2,39 | 18,25,26 | 1.04 | 1 (5%) | 18,36,39 | 1.15 | 2 (11%) |
| 3 | SAC | A | 2 | 3 | 7,8,9 | 0.52 | 0 | 8,9,11 | 0.86 | 1 (12%) |
| 21 | SAC | S | 2 | 21 | 7,8,9 | 0.53 | 0 | 8,9,11 | 0.91 | 1 (12%) |
| 2 | PSU | 2 | 1056 | 2 | 18,21,22 | 1.35 | 2 (11%) | 22,30,33 | 1.88 | 3 (13%) |
| 2 | A2M | 2 | 576 | 2 | 18,25,26 | 0.98 | 1 (5%) | 18,36,39 | 1.22 | 2 (11%) |
| 2 | OMC | 2 | 1391 | 2 | 19,22,23 | 0.81 | 0 | 26,31,34 | 0.83 | 0 |
| 2 | OMC | 2 | 462 | 2 | 19,22,23 | 0.81 | 0 | 26,31,34 | 0.81 | 0 |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | PSU | 2 | 1244 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | 2 | 1442 | 2,39 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | MA6 | 2 | 1850 | 2 | - | 0/7/29/30 | 0/3/3/3 |
| 2 | PSU | 2 | 105 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1177 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 572 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | 2 | 1326 | 2,39 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 509 | 2,39 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 99 | 2,39 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | B8N | 2 | 1248 | 2 | - | 4/16/34/35 | 0/2/2/2 |
| 2 | PSU | 2 | 1445 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | 2 | 116 | 2 | - | 1/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 2 | 6MZ | 2 | 1832 | 2,39 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 1328 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | 2 | 627 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | PSU | 2 | 1367 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 119 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | AME | V | 1 | 24 | - | 2/9/10/12 | - |
| 2 | OMC | 2 | 174 | 2,39 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | 2 | 814 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | 2 | 159 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | HY3 | X | 62 | 26 | - | 1/1/12/14 | 0/1/1/1 |
| 2 | PSU | 2 | 686 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | 2 | 1703 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | PSU | 2 | 1625 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 651 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | 2 | 468 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | G7M | 2 | 1639 | 2 | - | 0/3/25/26 | 0/3/3/3 |
| 2 | PSU | 2 | 649 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 815 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1692 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | 2 | 590 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | 2 | 36 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | NMM | T | 67 | 22 | - | 0/9/11/13 | - |
| 2 | A2M | 2 | 166 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | 2 | 109 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 93 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1081 | 2 | - | 1/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 863 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1347 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1643 | 2,39 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1045 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 406 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 34 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1238 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | 2 | 1288 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMU | 2 | 172 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | 2 | 609 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 866 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | 2 | 1447 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | MA6 | 2 | 1851 | 2 | - | 1/7/29/30 | 0/3/3/3 |
| 2 | OMG | 2 | 644 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 1490 | 2,39 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 683 | 2 | - | 1/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | A2M | 2 | 1031 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 601 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 517 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 1383 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | 2 | 822 | 2 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | 4AC | 2 | 1337 | 2 | - | 2/11/29/30 | 0/2/2/2 |
| 2 | OMU | 2 | 799 | 2 | - | 2/9/27/28 | 0/2/2/2 |
| 2 | PSU | 2 | 1232 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1174 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 681 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | 2 | 354 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | OMU | 2 | 1804 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | PSU | 2 | 1136 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMU | 2 | 121 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 512 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | OMU | 2 | 428 | 2 | - | 4/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 484 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 436 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | 2 | 218 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 966 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 1046 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | 2 | 1272 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 17 | IAS | O | 138 | 17 | - | 1/7/7/8 | - |
| 2 | PSU | 2 | 1004 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 296 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMC | 2 | 797 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 668 | 2,39 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 1678 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | 2 | 801 | 2 | - | 1/7/25/26 | 0/2/2/2 |
| 2 | 4AC | 2 | 1842 | 2 | - | 2/11/29/30 | 0/2/2/2 |
| 2 | PSU | 2 | 210 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | 2 | 27 | 2,39 | - | 0/5/27/28 | 0/3/3/3 |
| 3 | SAC | A | 2 | 3 | - | 1/7/8/10 | - |
| 21 | SAC | S | 2 | 21 | - | 0/7/8/10 | - |
| 2 | PSU | 2 | 1056 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | A2M | 2 | 576 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 1391 | 2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | OMC | 2 | 462 | 2 | - | 0/9/27/28 | 0/2/2/2 |

All (150) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | 2 | 1639 | G7M | C5-C4 | 7.37 | 1.53 | 1.39 |
| 2 | 2 | 1639 | G7M | O6-C6 | 7.18 | 1.37 | 1.23 |
| 26 | X | 62 | HY3 | C3-CA | -4.94 | 1.50 | 1.55 |
| 2 | 2 | 1639 | G7M | C2-N2 | 4.43 | 1.44 | 1.34 |
| 2 | 2 | 1639 | G7M | C2-N1 | 3.80 | 1.47 | 1.37 |
| 2 | 2 | 1639 | G7M | C8-N9 | 3.48 | 1.39 | 1.33 |
| 2 | 2 | 1850 | MA6 | C5-N7 | 3.35 | 1.51 | 1.39 |
| 2 | 2 | 1851 | MA6 | C5-N7 | 3.35 | 1.51 | 1.39 |
| 2 | 2 | 1639 | G7M | C2-N3 | 3.28 | 1.41 | 1.33 |
| 2 | 2 | 1248 | B8N | C4-N3 | -3.18 | 1.34 | 1.40 |
| 2 | 2 | 1625 | PSU | C6-C5 | 3.16 | 1.39 | 1.35 |
| 2 | 2 | 210 | PSU | C6-C5 | 3.16 | 1.39 | 1.35 |
| 2 | 2 | 801 | PSU | C6-C5 | 3.15 | 1.39 | 1.35 |
| 2 | 2 | 1238 | PSU | C6-C5 | 3.15 | 1.39 | 1.35 |
| 2 | 2 | 1639 | G7M | C6-N1 | 3.12 | 1.42 | 1.37 |
| 2 | 2 | 1643 | PSU | C6-C5 | 3.11 | 1.38 | 1.35 |
| 2 | 2 | 1445 | PSU | C6-C5 | 3.11 | 1.38 | 1.35 |
| 2 | 2 | 609 | PSU | C6-C5 | 3.10 | 1.38 | 1.35 |
| 2 | 2 | 218 | PSU | C6-C5 | 3.09 | 1.38 | 1.35 |
| 2 | 2 | 296 | PSU | C6-C5 | 3.09 | 1.38 | 1.35 |
| 2 | 2 | 651 | PSU | C6-C5 | 3.08 | 1.38 | 1.35 |
| 2 | 2 | 866 | PSU | C6-C5 | 3.07 | 1.38 | 1.35 |
| 2 | 2 | 1232 | PSU | C6-C5 | 3.06 | 1.38 | 1.35 |
| 2 | 2 | 1174 | PSU | C6-C5 | 3.06 | 1.38 | 1.35 |
| 2 | 2 | 1692 | PSU | C6-C5 | 3.06 | 1.38 | 1.35 |
| 2 | 2 | 966 | PSU | C6-C5 | 3.05 | 1.38 | 1.35 |
| 2 | 2 | 105 | PSU | C6-C5 | 3.03 | 1.38 | 1.35 |
| 2 | 2 | 814 | PSU | C6-C5 | 3.02 | 1.38 | 1.35 |
| 2 | 2 | 109 | PSU | C6-C5 | 3.02 | 1.38 | 1.35 |
| 2 | 2 | 1248 | B8N | C6-C5 | 3.02 | 1.39 | 1.34 |
| 2 | 2 | 863 | PSU | C6-C5 | 3.02 | 1.38 | 1.35 |
| 2 | 2 | 1056 | PSU | C6-C5 | 3.01 | 1.38 | 1.35 |
| 2 | 2 | 93 | PSU | C6-C5 | 3.00 | 1.38 | 1.35 |
| 2 | 2 | 1244 | PSU | C6-C5 | 3.00 | 1.38 | 1.35 |
| 2 | 2 | 1177 | PSU | C6-C5 | 3.00 | 1.38 | 1.35 |
| 2 | 2 | 815 | PSU | C6-C5 | 2.99 | 1.38 | 1.35 |
| 2 | 2 | 1367 | PSU | C6-C5 | 2.99 | 1.38 | 1.35 |
| 2 | 2 | 1046 | PSU | C6-C5 | 2.98 | 1.38 | 1.35 |
| 2 | 2 | 1004 | PSU | C6-C5 | 2.98 | 1.38 | 1.35 |
| 2 | 2 | 1842 | 4AC | C4-N4 | -2.97 | 1.35 | 1.39 |
| 2 | 2 | 1081 | PSU | C6-C5 | 2.97 | 1.38 | 1.35 |
| 2 | 2 | 572 | PSU | C6-C5 | 2.97 | 1.38 | 1.35 |
| 2 | 2 | 1347 | PSU | C6-C5 | 2.96 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | 2 | 681 | PSU | C6-C5 | 2.95 | 1.38 | 1.35 |
| 2 | 2 | 1337 | 4AC | C4-N4 | -2.95 | 1.35 | 1.39 |
| 2 | 2 | 119 | PSU | C6-C5 | 2.95 | 1.38 | 1.35 |
| 2 | 2 | 36 | PSU | C6-C5 | 2.94 | 1.38 | 1.35 |
| 2 | 2 | 406 | PSU | C6-C5 | 2.93 | 1.38 | 1.35 |
| 2 | 2 | 686 | PSU | C6-C5 | 2.93 | 1.38 | 1.35 |
| 2 | 2 | 34 | PSU | C6-C5 | 2.91 | 1.38 | 1.35 |
| 2 | 2 | 822 | PSU | C6-C5 | 2.89 | 1.38 | 1.35 |
| 2 | 2 | 36 | PSU | C4-N3 | -2.87 | 1.33 | 1.38 |
| 2 | 2 | 649 | PSU | C6-C5 | 2.87 | 1.38 | 1.35 |
| 2 | 2 | 1045 | PSU | C6-C5 | 2.86 | 1.38 | 1.35 |
| 2 | 2 | 1136 | PSU | C6-C5 | 2.84 | 1.38 | 1.35 |
| 2 | 2 | 34 | PSU | C4-N3 | -2.84 | 1.33 | 1.38 |
| 2 | 2 | 93 | PSU | C4-N3 | -2.80 | 1.33 | 1.38 |
| 2 | 2 | 1136 | PSU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 2 | 2 | 1347 | PSU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 2 | 2 | 1081 | PSU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 2 | 2 | 649 | PSU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 2 | 2 | 406 | PSU | C4-N3 | -2.78 | 1.33 | 1.38 |
| 2 | 2 | 572 | PSU | C4-N3 | -2.78 | 1.33 | 1.38 |
| 2 | 2 | 1045 | PSU | C4-N3 | -2.77 | 1.33 | 1.38 |
| 2 | 2 | 119 | PSU | C4-N3 | -2.77 | 1.33 | 1.38 |
| 2 | 2 | 681 | PSU | C4-N3 | -2.77 | 1.33 | 1.38 |
| 2 | 2 | 1367 | PSU | C4-N3 | -2.76 | 1.33 | 1.38 |
| 2 | 2 | 815 | PSU | C4-N3 | -2.76 | 1.33 | 1.38 |
| 2 | 2 | 651 | PSU | C4-N3 | -2.75 | 1.33 | 1.38 |
| 2 | 2 | 609 | PSU | C4-N3 | -2.75 | 1.33 | 1.38 |
| 2 | 2 | 814 | PSU | C4-N3 | -2.75 | 1.33 | 1.38 |
| 2 | 2 | 1177 | PSU | C4-N3 | -2.74 | 1.33 | 1.38 |
| 2 | 2 | 966 | PSU | C4-N3 | -2.74 | 1.33 | 1.38 |
| 2 | 2 | 1004 | PSU | C4-N3 | -2.74 | 1.33 | 1.38 |
| 2 | 2 | 296 | PSU | C4-N3 | -2.74 | 1.33 | 1.38 |
| 2 | 2 | 863 | PSU | C4-N3 | -2.73 | 1.33 | 1.38 |
| 2 | 2 | 105 | PSU | C4-N3 | -2.73 | 1.33 | 1.38 |
| 2 | 2 | 822 | PSU | C4-N3 | -2.73 | 1.33 | 1.38 |
| 2 | 2 | 1692 | PSU | C4-N3 | -2.72 | 1.33 | 1.38 |
| 2 | 2 | 1174 | PSU | C4-N3 | -2.72 | 1.33 | 1.38 |
| 2 | 2 | 1445 | PSU | C4-N3 | -2.71 | 1.33 | 1.38 |
| 2 | 2 | 801 | PSU | C4-N3 | -2.71 | 1.33 | 1.38 |
| 2 | 2 | 1643 | PSU | C4-N3 | -2.70 | 1.33 | 1.38 |
| 2 | 2 | 1056 | PSU | C4-N3 | -2.70 | 1.33 | 1.38 |
| 2 | 2 | 109 | PSU | C4-N3 | -2.69 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | 2 | 1625 | PSU | C4-N3 | -2.69 | 1.33 | 1.38 |
| 2 | 2 | 866 | PSU | C4-N3 | -2.68 | 1.33 | 1.38 |
| 2 | 2 | 686 | PSU | C4-N3 | -2.68 | 1.33 | 1.38 |
| 2 | 2 | 1046 | PSU | C4-N3 | -2.67 | 1.33 | 1.38 |
| 2 | 2 | 1232 | PSU | C4-N3 | -2.67 | 1.33 | 1.38 |
| 2 | 2 | 218 | PSU | C4-N3 | -2.66 | 1.33 | 1.38 |
| 2 | 2 | 1244 | PSU | C4-N3 | -2.66 | 1.33 | 1.38 |
| 2 | 2 | 1238 | PSU | C4-N3 | -2.66 | 1.33 | 1.38 |
| 2 | 2 | 644 | OMG | C6-N1 | -2.65 | 1.33 | 1.37 |
| 2 | 2 | 210 | PSU | C4-N3 | -2.65 | 1.33 | 1.38 |
| 2 | 2 | 172 | OMU | C4-N3 | -2.63 | 1.33 | 1.38 |
| 2 | 2 | 509 | OMG | C6-N1 | -2.62 | 1.34 | 1.37 |
| 2 | 2 | 1442 | OMU | C4-N3 | -2.59 | 1.33 | 1.38 |
| 2 | 2 | 116 | OMU | C4-N3 | -2.58 | 1.33 | 1.38 |
| 2 | 2 | 121 | OMU | C4-N3 | -2.58 | 1.33 | 1.38 |
| 2 | 2 | 354 | OMU | C4-N3 | -2.57 | 1.34 | 1.38 |
| 2 | 2 | 428 | OMU | C4-N3 | -2.55 | 1.34 | 1.38 |
| 2 | 2 | 436 | OMG | C6-N1 | -2.54 | 1.34 | 1.37 |
| 2 | 2 | 683 | OMG | C6-N1 | -2.53 | 1.34 | 1.37 |
| 2 | 2 | 159 | A2M | C5-C4 | 2.53 | 1.47 | 1.40 |
| 2 | 2 | 1490 | OMG | C6-N1 | -2.52 | 1.34 | 1.37 |
| 2 | 2 | 1288 | OMU | C4-N3 | -2.51 | 1.34 | 1.38 |
| 2 | 2 | 1328 | OMG | C6-N1 | -2.50 | 1.34 | 1.37 |
| 2 | 2 | 627 | OMU | C4-N3 | -2.49 | 1.34 | 1.38 |
| 2 | 2 | 799 | OMU | C4-N3 | -2.48 | 1.34 | 1.38 |
| 2 | 2 | 99 | A2M | C5-C4 | 2.48 | 1.47 | 1.40 |
| 2 | 2 | 1326 | OMU | C4-N3 | -2.47 | 1.34 | 1.38 |
| 2 | 2 | 27 | A2M | C5-C4 | 2.47 | 1.47 | 1.40 |
| 2 | 2 | 590 | A2M | C5-C4 | 2.47 | 1.47 | 1.40 |
| 2 | 2 | 1447 | OMG | C6-N1 | -2.46 | 1.34 | 1.37 |
| 2 | 2 | 601 | OMG | C6-N1 | -2.45 | 1.34 | 1.37 |
| 2 | 2 | 1804 | OMU | C4-N3 | -2.45 | 1.34 | 1.38 |
| 2 | 2 | 1248 | B8N | C2-N3 | -2.44 | 1.34 | 1.38 |
| 2 | 2 | 484 | A2M | C5-C4 | 2.39 | 1.47 | 1.40 |
| 2 | 2 | 1678 | A2M | C5-C4 | 2.38 | 1.47 | 1.40 |
| 2 | 2 | 1383 | A2M | C5-C4 | 2.38 | 1.47 | 1.40 |
| 2 | 2 | 1832 | 6MZ | C5-C4 | 2.37 | 1.47 | 1.40 |
| 2 | 2 | 166 | A2M | C5-C4 | 2.36 | 1.47 | 1.40 |
| 2 | 2 | 468 | A2M | C5-C4 | 2.35 | 1.47 | 1.40 |
| 2 | 2 | 576 | A2M | C5-C4 | 2.35 | 1.47 | 1.40 |
| 2 | 2 | 512 | A2M | C5-C4 | 2.34 | 1.47 | 1.40 |
| 2 | 2 | 1031 | A2M | C5-C4 | 2.32 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | 2 | 668 | A2M | C5-C4 | 2.32 | 1.47 | 1.40 |
| 2 | 2 | 1842 | 4AC | C7-N4 | -2.30 | 1.32 | 1.37 |
| 2 | 2 | 354 | OMU | C2-N3 | -2.28 | 1.33 | 1.38 |
| 2 | 2 | 428 | OMU | C2-N3 | -2.24 | 1.34 | 1.38 |
| 2 | 2 | 121 | OMU | C2-N3 | -2.23 | 1.34 | 1.38 |
| 2 | 2 | 116 | OMU | C2-N3 | -2.23 | 1.34 | 1.38 |
| 2 | 2 | 1442 | OMU | C2-N3 | -2.22 | 1.34 | 1.38 |
| 2 | 2 | 172 | OMU | C2-N3 | -2.22 | 1.34 | 1.38 |
| 2 | 2 | 1326 | OMU | C2-N3 | -2.17 | 1.34 | 1.38 |
| 2 | 2 | 1337 | 4AC | C7-N4 | -2.14 | 1.33 | 1.37 |
| 2 | 2 | 1804 | OMU | C2-N3 | -2.14 | 1.34 | 1.38 |
| 2 | 2 | 799 | OMU | C2-N3 | -2.13 | 1.34 | 1.38 |
| 2 | 2 | 1851 | MA6 | C4-N3 | -2.10 | 1.32 | 1.35 |
| 2 | 2 | 1288 | OMU | C2-N3 | -2.10 | 1.34 | 1.38 |
| 2 | 2 | 121 | OMU | C5-C4 | -2.08 | 1.39 | 1.43 |
| 2 | 2 | 627 | OMU | C2-N3 | -2.07 | 1.34 | 1.38 |
| 2 | 2 | 1288 | OMU | C2-N1 | 2.07 | 1.41 | 1.38 |
| 2 | 2 | 1081 | PSU | C2-N3 | -2.07 | 1.34 | 1.37 |
| 2 | 2 | 354 | OMU | C5-C4 | -2.06 | 1.39 | 1.43 |
| 2 | 2 | 428 | OMU | C5-C4 | -2.06 | 1.39 | 1.43 |
| 2 | 2 | 116 | OMU | C5-C4 | -2.04 | 1.39 | 1.43 |
| 2 | 2 | 1804 | OMU | C2-N1 | 2.02 | 1.41 | 1.38 |
| 2 | 2 | 799 | OMU | C5-C4 | -2.02 | 1.39 | 1.43 |

All (245) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2 | 2 | 822 | PSU | N1-C2-N3 | 6.21 | 122.16 | 115.13 |
| 2 | 2 | 36 | PSU | N1-C2-N3 | 6.13 | 122.07 | 115.13 |
| 2 | 2 | 34 | PSU | N1-C2-N3 | 6.13 | 122.07 | 115.13 |
| 2 | 2 | 93 | PSU | N1-C2-N3 | 6.11 | 122.05 | 115.13 |
| 2 | 2 | 572 | PSU | N1-C2-N3 | 6.11 | 122.05 | 115.13 |
| 2 | 2 | 681 | PSU | N1-C2-N3 | 6.09 | 122.03 | 115.13 |
| 2 | 2 | 1232 | PSU | N1-C2-N3 | 6.08 | 122.02 | 115.13 |
| 2 | 2 | 651 | PSU | N1-C2-N3 | 6.07 | 122.01 | 115.13 |
| 2 | 2 | 406 | PSU | N1-C2-N3 | 6.06 | 122.00 | 115.13 |
| 2 | 2 | 105 | PSU | N1-C2-N3 | 6.06 | 121.99 | 115.13 |
| 2 | 2 | 1445 | PSU | N1-C2-N3 | 6.05 | 121.99 | 115.13 |
| 2 | 2 | 866 | PSU | N1-C2-N3 | 6.05 | 121.98 | 115.13 |
| 2 | 2 | 1136 | PSU | N1-C2-N3 | 6.03 | 121.96 | 115.13 |
| 2 | 2 | 1692 | PSU | N1-C2-N3 | 6.03 | 121.96 | 115.13 |
| 2 | 2 | 296 | PSU | N1-C2-N3 | 6.02 | 121.96 | 115.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2 | 2 | 815 | PSU | N1-C2-N3 | 6.02 | 121.95 | 115.13 |
| 2 | 2 | 686 | PSU | N1-C2-N3 | 6.01 | 121.94 | 115.13 |
| 2 | 2 | 119 | PSU | N1-C2-N3 | 6.01 | 121.94 | 115.13 |
| 2 | 2 | 1625 | PSU | N1-C2-N3 | 6.00 | 121.93 | 115.13 |
| 2 | 2 | 109 | PSU | N1-C2-N3 | 6.00 | 121.93 | 115.13 |
| 2 | 2 | 1367 | PSU | N1-C2-N3 | 6.00 | 121.92 | 115.13 |
| 2 | 2 | 649 | PSU | N1-C2-N3 | 5.99 | 121.92 | 115.13 |
| 2 | 2 | 801 | PSU | N1-C2-N3 | 5.98 | 121.91 | 115.13 |
| 2 | 2 | 1238 | PSU | N1-C2-N3 | 5.98 | 121.91 | 115.13 |
| 2 | 2 | 1643 | PSU | N1-C2-N3 | 5.98 | 121.91 | 115.13 |
| 2 | 2 | 218 | PSU | N1-C2-N3 | 5.98 | 121.90 | 115.13 |
| 2 | 2 | 1004 | PSU | N1-C2-N3 | 5.98 | 121.90 | 115.13 |
| 2 | 2 | 966 | PSU | N1-C2-N3 | 5.96 | 121.88 | 115.13 |
| 2 | 2 | 1045 | PSU | N1-C2-N3 | 5.96 | 121.88 | 115.13 |
| 2 | 2 | 1056 | PSU | N1-C2-N3 | 5.95 | 121.88 | 115.13 |
| 2 | 2 | 1347 | PSU | N1-C2-N3 | 5.95 | 121.88 | 115.13 |
| 2 | 2 | 609 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 2 | 2 | 814 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 2 | 2 | 210 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 2 | 2 | 863 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 2 | 2 | 1174 | PSU | N1-C2-N3 | 5.95 | 121.87 | 115.13 |
| 2 | 2 | 1046 | PSU | N1-C2-N3 | 5.94 | 121.86 | 115.13 |
| 2 | 2 | 1177 | PSU | N1-C2-N3 | 5.94 | 121.86 | 115.13 |
| 2 | 2 | 1244 | PSU | N1-C2-N3 | 5.88 | 121.80 | 115.13 |
| 2 | 2 | 1081 | PSU | N1-C2-N3 | 5.87 | 121.78 | 115.13 |
| 2 | 2 | 1850 | MA6 | C4-C5-N7 | -5.67 | 103.49 | 109.40 |
| 2 | 2 | 1851 | MA6 | C4-C5-N7 | -5.51 | 103.66 | 109.40 |
| 2 | 2 | 1832 | 6MZ | C2-N1-C6 | 5.46 | 121.27 | 116.59 |
| 2 | 2 | 1326 | OMU | C4-N3-C2 | -4.57 | 120.56 | 126.58 |
| 2 | 2 | 799 | OMU | C4-N3-C2 | -4.56 | 120.56 | 126.58 |
| 2 | 2 | 172 | OMU | C4-N3-C2 | -4.51 | 120.62 | 126.58 |
| 2 | 2 | 428 | OMU | C4-N3-C2 | -4.51 | 120.63 | 126.58 |
| 2 | 2 | 1442 | OMU | C4-N3-C2 | -4.50 | 120.64 | 126.58 |
| 2 | 2 | 627 | OMU | C4-N3-C2 | -4.49 | 120.66 | 126.58 |
| 2 | 2 | 1851 | MA6 | N3-C2-N1 | -4.46 | 121.70 | 128.68 |
| 2 | 2 | 121 | OMU | C4-N3-C2 | -4.43 | 120.73 | 126.58 |
| 2 | 2 | 1804 | OMU | C4-N3-C2 | -4.41 | 120.76 | 126.58 |
| 2 | 2 | 1842 | 4AC | N4-C4-N3 | 4.40 | 121.24 | 113.85 |
| 2 | 2 | 116 | OMU | C4-N3-C2 | -4.39 | 120.78 | 126.58 |
| 2 | 2 | 1288 | OMU | C4-N3-C2 | -4.39 | 120.79 | 126.58 |
| 2 | 2 | 354 | OMU | C4-N3-C2 | -4.38 | 120.80 | 126.58 |
| 2 | 2 | 1850 | MA6 | N3-C2-N1 | -4.32 | 121.93 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1851 | MA6 | C1'-N9-C4 | -4.27 | 119.14 | 126.64 |
| 2 | 2 | 799 | OMU | N3-C2-N1 | 4.19 | 120.46 | 114.89 |
| 2 | 2 | 116 | OMU | N3-C2-N1 | 4.16 | 120.41 | 114.89 |
| 2 | 2 | 627 | OMU | N3-C2-N1 | 4.15 | 120.40 | 114.89 |
| 2 | 2 | 93 | PSU | C4-N3-C2 | -4.15 | 120.36 | 126.34 |
| 2 | 2 | 172 | OMU | N3-C2-N1 | 4.15 | 120.39 | 114.89 |
| 2 | 2 | 1442 | OMU | N3-C2-N1 | 4.14 | 120.38 | 114.89 |
| 2 | 2 | 1326 | OMU | N3-C2-N1 | 4.12 | 120.36 | 114.89 |
| 2 | 2 | 34 | PSU | C4-N3-C2 | -4.12 | 120.41 | 126.34 |
| 2 | 2 | 121 | OMU | N3-C2-N1 | 4.10 | 120.33 | 114.89 |
| 2 | 2 | 1804 | OMU | N3-C2-N1 | 4.10 | 120.33 | 114.89 |
| 2 | 2 | 354 | OMU | N3-C2-N1 | 4.09 | 120.32 | 114.89 |
| 2 | 2 | 686 | PSU | C4-N3-C2 | -4.09 | 120.44 | 126.34 |
| 2 | 2 | 36 | PSU | C4-N3-C2 | -4.07 | 120.47 | 126.34 |
| 2 | 2 | 866 | PSU | C4-N3-C2 | -4.07 | 120.48 | 126.34 |
| 2 | 2 | 428 | OMU | N3-C2-N1 | 4.06 | 120.29 | 114.89 |
| 2 | 2 | 1232 | PSU | C4-N3-C2 | -4.02 | 120.54 | 126.34 |
| 2 | 2 | 681 | PSU | C4-N3-C2 | -4.02 | 120.55 | 126.34 |
| 2 | 2 | 801 | PSU | C4-N3-C2 | -4.02 | 120.55 | 126.34 |
| 2 | 2 | 651 | PSU | C4-N3-C2 | -4.01 | 120.56 | 126.34 |
| 2 | 2 | 649 | PSU | C4-N3-C2 | -4.00 | 120.57 | 126.34 |
| 2 | 2 | 1288 | OMU | N3-C2-N1 | 3.99 | 120.19 | 114.89 |
| 2 | 2 | 572 | PSU | C4-N3-C2 | -3.99 | 120.58 | 126.34 |
| 2 | 2 | 1136 | PSU | C4-N3-C2 | -3.99 | 120.58 | 126.34 |
| 2 | 2 | 109 | PSU | C4-N3-C2 | -3.99 | 120.59 | 126.34 |
| 2 | 2 | 1367 | PSU | C4-N3-C2 | -3.98 | 120.60 | 126.34 |
| 2 | 2 | 815 | PSU | C4-N3-C2 | -3.98 | 120.60 | 126.34 |
| 2 | 2 | 1347 | PSU | C4-N3-C2 | -3.98 | 120.60 | 126.34 |
| 2 | 2 | 1045 | PSU | C4-N3-C2 | -3.97 | 120.61 | 126.34 |
| 2 | 2 | 1445 | PSU | C4-N3-C2 | -3.96 | 120.63 | 126.34 |
| 2 | 2 | 406 | PSU | C4-N3-C2 | -3.95 | 120.65 | 126.34 |
| 2 | 2 | 105 | PSU | C4-N3-C2 | -3.95 | 120.65 | 126.34 |
| 2 | 2 | 1692 | PSU | C4-N3-C2 | -3.94 | 120.66 | 126.34 |
| 2 | 2 | 1850 | MA6 | C1'-N9-C4 | -3.94 | 119.72 | 126.64 |
| 2 | 2 | 119 | PSU | C4-N3-C2 | -3.93 | 120.67 | 126.34 |
| 2 | 2 | 1174 | PSU | C4-N3-C2 | -3.93 | 120.68 | 126.34 |
| 2 | 2 | 296 | PSU | C4-N3-C2 | -3.92 | 120.69 | 126.34 |
| 2 | 2 | 814 | PSU | C4-N3-C2 | -3.91 | 120.70 | 126.34 |
| 2 | 2 | 1056 | PSU | C4-N3-C2 | -3.90 | 120.72 | 126.34 |
| 2 | 2 | 1625 | PSU | C4-N3-C2 | -3.90 | 120.72 | 126.34 |
| 2 | 2 | 1081 | PSU | C4-N3-C2 | -3.90 | 120.72 | 126.34 |
| 2 | 2 | 609 | PSU | C4-N3-C2 | -3.89 | 120.73 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2 | 2 | 1177 | PSU | C4-N3-C2 | -3.89 | 120.73 | 126.34 |
| 2 | 2 | 966 | PSU | C4-N3-C2 | -3.89 | 120.74 | 126.34 |
| 2 | 2 | 863 | PSU | C4-N3-C2 | -3.87 | 120.76 | 126.34 |
| 2 | 2 | 210 | PSU | C4-N3-C2 | -3.86 | 120.77 | 126.34 |
| 2 | 2 | 1004 | PSU | C4-N3-C2 | -3.86 | 120.78 | 126.34 |
| 2 | 2 | 1643 | PSU | C4-N3-C2 | -3.85 | 120.79 | 126.34 |
| 2 | 2 | 822 | PSU | C4-N3-C2 | -3.85 | 120.80 | 126.34 |
| 2 | 2 | 1238 | PSU | C4-N3-C2 | -3.82 | 120.83 | 126.34 |
| 2 | 2 | 218 | PSU | C4-N3-C2 | -3.79 | 120.87 | 126.34 |
| 2 | 2 | 822 | PSU | O2-C2-N1 | -3.79 | 118.62 | 122.79 |
| 2 | 2 | 1046 | PSU | C4-N3-C2 | -3.76 | 120.92 | 126.34 |
| 2 | 2 | 1244 | PSU | C4-N3-C2 | -3.70 | 121.01 | 126.34 |
| 2 | 2 | 34 | PSU | O2-C2-N1 | -3.65 | 118.77 | 122.79 |
| 2 | 2 | 428 | OMU | C5-C4-N3 | 3.63 | 120.27 | 114.84 |
| 2 | 2 | 1326 | OMU | C5-C4-N3 | 3.62 | 120.25 | 114.84 |
| 2 | 2 | 1288 | OMU | C5-C4-N3 | 3.60 | 120.23 | 114.84 |
| 2 | 2 | 1442 | OMU | C5-C4-N3 | 3.60 | 120.22 | 114.84 |
| 2 | 2 | 172 | OMU | C5-C4-N3 | 3.59 | 120.22 | 114.84 |
| 2 | 2 | 93 | PSU | O2-C2-N1 | -3.59 | 118.83 | 122.79 |
| 2 | 2 | 121 | OMU | C5-C4-N3 | 3.56 | 120.16 | 114.84 |
| 2 | 2 | 354 | OMU | C5-C4-N3 | 3.55 | 120.16 | 114.84 |
| 2 | 2 | 1804 | OMU | C5-C4-N3 | 3.54 | 120.13 | 114.84 |
| 2 | 2 | 218 | PSU | O2-C2-N1 | -3.53 | 118.90 | 122.79 |
| 2 | 2 | 686 | PSU | O2-C2-N1 | -3.52 | 118.92 | 122.79 |
| 2 | 2 | 36 | PSU | O2-C2-N1 | -3.51 | 118.93 | 122.79 |
| 2 | 2 | 1046 | PSU | O2-C2-N1 | -3.50 | 118.94 | 122.79 |
| 2 | 2 | 116 | OMU | C5-C4-N3 | 3.50 | 120.07 | 114.84 |
| 2 | 2 | 627 | OMU | C5-C4-N3 | 3.48 | 120.05 | 114.84 |
| 2 | 2 | 1004 | PSU | O2-C2-N1 | -3.48 | 118.96 | 122.79 |
| 2 | 2 | 1445 | PSU | O2-C2-N1 | -3.47 | 118.97 | 122.79 |
| 2 | 2 | 1056 | PSU | O2-C2-N1 | -3.46 | 118.98 | 122.79 |
| 2 | 2 | 109 | PSU | O2-C2-N1 | -3.46 | 118.98 | 122.79 |
| 2 | 2 | 799 | OMU | C5-C4-N3 | 3.46 | 120.01 | 114.84 |
| 2 | 2 | 572 | PSU | O2-C2-N1 | -3.45 | 118.99 | 122.79 |
| 2 | 2 | 210 | PSU | O2-C2-N1 | -3.44 | 119.01 | 122.79 |
| 2 | 2 | 1367 | PSU | O2-C2-N1 | -3.44 | 119.01 | 122.79 |
| 2 | 2 | 296 | PSU | O2-C2-N1 | -3.43 | 119.01 | 122.79 |
| 2 | 2 | 863 | PSU | O2-C2-N1 | -3.43 | 119.01 | 122.79 |
| 2 | 2 | 1232 | PSU | O2-C2-N1 | -3.43 | 119.02 | 122.79 |
| 2 | 2 | 866 | PSU | O2-C2-N1 | -3.42 | 119.02 | 122.79 |
| 2 | 2 | 1136 | PSU | O2-C2-N1 | -3.42 | 119.03 | 122.79 |
| 2 | 2 | 1174 | PSU | O2-C2-N1 | -3.41 | 119.03 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2 | 2 | 406 | PSU | O2-C2-N1 | -3.40 | 119.04 | 122.79 |
| 2 | 2 | 1692 | PSU | O2-C2-N1 | -3.40 | 119.05 | 122.79 |
| 2 | 2 | 651 | PSU | O2-C2-N1 | -3.39 | 119.05 | 122.79 |
| 2 | 2 | 105 | PSU | O2-C2-N1 | -3.38 | 119.07 | 122.79 |
| 2 | 2 | 681 | PSU | O2-C2-N1 | -3.38 | 119.07 | 122.79 |
| 2 | 2 | 966 | PSU | O2-C2-N1 | -3.38 | 119.07 | 122.79 |
| 2 | 2 | 814 | PSU | O2-C2-N1 | -3.38 | 119.07 | 122.79 |
| 2 | 2 | 119 | PSU | O2-C2-N1 | -3.37 | 119.08 | 122.79 |
| 2 | 2 | 1625 | PSU | O2-C2-N1 | -3.36 | 119.09 | 122.79 |
| 2 | 2 | 1238 | PSU | O2-C2-N1 | -3.35 | 119.10 | 122.79 |
| 2 | 2 | 801 | PSU | O2-C2-N1 | -3.35 | 119.10 | 122.79 |
| 2 | 2 | 815 | PSU | O2-C2-N1 | -3.34 | 119.11 | 122.79 |
| 2 | 2 | 1643 | PSU | O2-C2-N1 | -3.34 | 119.11 | 122.79 |
| 2 | 2 | 649 | PSU | O2-C2-N1 | -3.33 | 119.12 | 122.79 |
| 2 | 2 | 1244 | PSU | O2-C2-N1 | -3.32 | 119.14 | 122.79 |
| 2 | 2 | 609 | PSU | O2-C2-N1 | -3.31 | 119.14 | 122.79 |
| 2 | 2 | 1177 | PSU | O2-C2-N1 | -3.31 | 119.15 | 122.79 |
| 2 | 2 | 1045 | PSU | O2-C2-N1 | -3.30 | 119.16 | 122.79 |
| 2 | 2 | 1248 | B8N | C4-N3-C2 | -3.28 | 121.31 | 125.46 |
| 2 | 2 | 1347 | PSU | O2-C2-N1 | -3.28 | 119.18 | 122.79 |
| 2 | 2 | 1337 | 4AC | N4-C4-N3 | 3.26 | 119.32 | 113.85 |
| 2 | 2 | 576 | A2M | N3-C2-N1 | -3.22 | 123.64 | 128.68 |
| 2 | 2 | 1678 | A2M | N3-C2-N1 | -3.22 | 123.65 | 128.68 |
| 2 | 2 | 1031 | A2M | N3-C2-N1 | -3.21 | 123.66 | 128.68 |
| 2 | 2 | 590 | A2M | N3-C2-N1 | -3.21 | 123.66 | 128.68 |
| 2 | 2 | 166 | A2M | N3-C2-N1 | -3.19 | 123.69 | 128.68 |
| 2 | 2 | 1081 | PSU | O2-C2-N1 | -3.17 | 119.31 | 122.79 |
| 2 | 2 | 1383 | A2M | N3-C2-N1 | -3.15 | 123.75 | 128.68 |
| 2 | 2 | 512 | A2M | N3-C2-N1 | -3.15 | 123.75 | 128.68 |
| 2 | 2 | 668 | A2M | N3-C2-N1 | -3.12 | 123.80 | 128.68 |
| 2 | 2 | 468 | A2M | N3-C2-N1 | -3.11 | 123.81 | 128.68 |
| 2 | 2 | 428 | OMU | O4-C4-C5 | -3.10 | 119.71 | 125.16 |
| 2 | 2 | 484 | A2M | N3-C2-N1 | -3.09 | 123.85 | 128.68 |
| 2 | 2 | 1326 | OMU | O4-C4-C5 | -3.07 | 119.76 | 125.16 |
| 2 | 2 | 799 | OMU | O4-C4-C5 | -3.06 | 119.78 | 125.16 |
| 2 | 2 | 354 | OMU | O4-C4-C5 | -3.05 | 119.80 | 125.16 |
| 2 | 2 | 1639 | G7M | C2-N1-C6 | -3.01 | 119.55 | 125.10 |
| 2 | 2 | 1288 | OMU | O4-C4-C5 | -2.99 | 119.91 | 125.16 |
| 2 | 2 | 1832 | 6MZ | N3-C2-N1 | -2.99 | 124.01 | 128.68 |
| 2 | 2 | 1248 | B8N | N3-C2-N1 | 2.98 | 120.97 | 116.76 |
| 2 | 2 | 121 | OMU | O4-C4-C5 | -2.98 | 119.91 | 125.16 |
| 2 | 2 | 1804 | OMU | O4-C4-C5 | -2.98 | 119.92 | 125.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 116 | OMU | O4-C4-C5 | -2.98 | 119.92 | 125.16 |
| 2 | 2 | 172 | OMU | O4-C4-C5 | -2.96 | 119.95 | 125.16 |
| 2 | 2 | 627 | OMU | O4-C4-C5 | -2.92 | 120.02 | 125.16 |
| 2 | 2 | 27 | A2M | N3-C2-N1 | -2.91 | 124.13 | 128.68 |
| 2 | 2 | 99 | A2M | N3-C2-N1 | -2.88 | 124.17 | 128.68 |
| 2 | 2 | 99 | A2M | C4-C5-N7 | -2.87 | 106.40 | 109.40 |
| 2 | 2 | 1442 | OMU | O4-C4-C5 | -2.86 | 120.14 | 125.16 |
| 2 | 2 | 159 | A2M | C4-C5-N7 | -2.84 | 106.44 | 109.40 |
| 2 | 2 | 27 | A2M | C4-C5-N7 | -2.83 | 106.45 | 109.40 |
| 2 | 2 | 159 | A2M | N3-C2-N1 | -2.82 | 124.27 | 128.68 |
| 2 | 2 | 484 | A2M | C4-C5-N7 | -2.75 | 106.53 | 109.40 |
| 2 | 2 | 1383 | A2M | C4-C5-N7 | -2.73 | 106.55 | 109.40 |
| 2 | 2 | 668 | A2M | C4-C5-N7 | -2.71 | 106.58 | 109.40 |
| 2 | 2 | 166 | A2M | C4-C5-N7 | -2.70 | 106.59 | 109.40 |
| 2 | 2 | 1031 | A2M | C4-C5-N7 | -2.70 | 106.59 | 109.40 |
| 2 | 2 | 468 | A2M | C4-C5-N7 | -2.67 | 106.62 | 109.40 |
| 2 | 2 | 512 | A2M | C4-C5-N7 | -2.62 | 106.67 | 109.40 |
| 2 | 2 | 1678 | A2M | C4-C5-N7 | -2.60 | 106.69 | 109.40 |
| 17 | O | 138 | IAS | OD1-CG-CB | -2.55 | 118.01 | 125.43 |
| 2 | 2 | 576 | A2M | C4-C5-N7 | -2.54 | 106.75 | 109.40 |
| 24 | V | 1 | AME | O-C-CA | -2.53 | 118.14 | 124.78 |
| 2 | 2 | 590 | A2M | C4-C5-N7 | -2.51 | 106.78 | 109.40 |
| 21 | S | 2 | SAC | O-C-CA | -2.45 | 118.35 | 124.78 |
| 2 | 2 | 1842 | 4AC | C6-C5-C4 | 2.43 | 119.94 | 116.96 |
| 2 | 2 | 1337 | 4AC | C6-C5-C4 | 2.38 | 119.88 | 116.96 |
| 2 | 2 | 436 | OMG | C5-C6-N1 | 2.36 | 118.12 | 113.95 |
| 2 | 2 | 644 | OMG | C5-C6-N1 | 2.35 | 118.11 | 113.95 |
| 2 | 2 | 601 | OMG | C5-C6-N1 | 2.35 | 118.10 | 113.95 |
| 2 | 2 | 1328 | OMG | C8-N7-C5 | 2.33 | 107.43 | 102.99 |
| 2 | 2 | 644 | OMG | C8-N7-C5 | 2.33 | 107.42 | 102.99 |
| 3 | A | 2 | SAC | O-C-CA | -2.32 | 118.70 | 124.78 |
| 2 | 2 | 1328 | OMG | C5-C6-N1 | 2.32 | 118.04 | 113.95 |
| 2 | 2 | 1490 | OMG | C5-C6-N1 | 2.31 | 118.04 | 113.95 |
| 2 | 2 | 436 | OMG | C8-N7-C5 | 2.31 | 107.39 | 102.99 |
| 2 | 2 | 683 | OMG | C8-N7-C5 | 2.31 | 107.38 | 102.99 |
| 2 | 2 | 509 | OMG | C5-C6-N1 | 2.30 | 118.02 | 113.95 |
| 2 | 2 | 509 | OMG | C8-N7-C5 | 2.30 | 107.37 | 102.99 |
| 2 | 2 | 1326 | OMU | O2-C2-N1 | -2.29 | 119.74 | 122.79 |
| 2 | 2 | 601 | OMG | C8-N7-C5 | 2.29 | 107.34 | 102.99 |
| 2 | 2 | 428 | OMU | O2-C2-N1 | -2.27 | 119.77 | 122.79 |
| 2 | 2 | 1447 | OMG | C5-C6-N1 | 2.27 | 117.96 | 113.95 |
| 2 | 2 | 1842 | 4AC | C5-C4-N4 | -2.27 | 118.98 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 2 | 683 | OMG | C5-C6-N1 | 2.26 | 117.95 | 113.95 |
| 26 | X | 62 | HY3 | O-C-CA | -2.26 | 118.54 | 124.83 |
| 2 | 2 | 1490 | OMG | C8-N7-C5 | 2.25 | 107.28 | 102.99 |
| 2 | 2 | 1447 | OMG | C8-N7-C5 | 2.24 | 107.25 | 102.99 |
| 2 | 2 | 121 | OMU | O2-C2-N1 | -2.18 | 119.88 | 122.79 |
| 2 | 2 | 1272 | OMC | O2-C2-N3 | -2.18 | 118.79 | 122.33 |
| 2 | 2 | 172 | OMU | O2-C2-N1 | -2.18 | 119.89 | 122.79 |
| 2 | 2 | 1248 | B8N | C5-C4-N3 | 2.16 | 120.18 | 116.17 |
| 2 | 2 | 1832 | 6MZ | C4-C5-N7 | -2.13 | 107.17 | 109.40 |
| 2 | 2 | 354 | OMU | O2-C2-N1 | -2.12 | 119.97 | 122.79 |
| 2 | 2 | 1703 | OMC | O2-C2-N3 | -2.11 | 118.89 | 122.33 |
| 2 | 2 | 822 | PSU | O4'-C1'-C2' | 2.11 | 108.12 | 105.14 |
| 2 | 2 | 797 | OMC | O2-C2-N3 | -2.09 | 118.93 | 122.33 |
| 2 | 2 | 866 | PSU | C5-C6-N1 | -2.07 | 119.00 | 122.11 |
| 2 | 2 | 799 | OMU | O2-C2-N1 | -2.06 | 120.05 | 122.79 |
| 2 | 2 | 627 | OMU | O2-C2-N1 | -2.05 | 120.06 | 122.79 |
| 2 | 2 | 649 | PSU | C5-C6-N1 | -2.04 | 119.04 | 122.11 |
| 2 | 2 | 651 | PSU | C5-C6-N1 | -2.03 | 119.06 | 122.11 |
| 2 | 2 | 1232 | PSU | C5-C6-N1 | -2.01 | 119.09 | 122.11 |
| 2 | 2 | 686 | PSU | C5-C6-N1 | -2.01 | 119.09 | 122.11 |

There are no chirality outliers.

All (53) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | 2 | 428 | OMU | C2'-C1'-N1-C2 |
| 2 | 2 | 428 | OMU | C2'-C1'-N1-C6 |
| 2 | 2 | 644 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 644 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 668 | A2M | C1'-C2'-O2'-CM' |
| 2 | 2 | 1248 | B8N | N34-C33-C34-O35 |
| 2 | 2 | 1337 | 4AC | O7-C7-N4-C4 |
| 2 | 2 | 1337 | 4AC | CM7-C7-N4-C4 |
| 2 | 2 | 1842 | 4AC | N3-C4-N4-C7 |
| 2 | 2 | 1842 | 4AC | C5-C4-N4-C7 |
| 2 | 2 | 512 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 668 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 668 | A2M | C3'-C4'-C5'-O5' |
| 24 | V | 1 | AME | CT2-CT1-N-CA |
| 24 | V | 1 | AME | OT-CT1-N-CA |
| 2 | 2 | 1248 | B8N | N34-C33-C34-O36 |
| 2 | 2 | 512 | A2M | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | 2 | 576 | A2M | C3'-C4'-C5'-O5' |
| 2 | 2 | 1447 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 509 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 799 | OMU | C4'-C5'-O5'-P |
| 2 | 2 | 99 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 576 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 509 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 1447 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 627 | OMU | C4'-C5'-O5'-P |
| 2 | 2 | 1851 | MA6 | C4'-C5'-O5'-P |
| 2 | 2 | 822 | PSU | C3'-C4'-C5'-O5' |
| 3 | A | 2 | SAC | C-CA-N-C1A |
| 2 | 2 | 354 | OMU | C3'-C2'-O2'-CM2 |
| 2 | 2 | 484 | A2M | C3'-C2'-O2'-CM' |
| 2 | 2 | 1248 | B8N | C32-C33-C34-O36 |
| 2 | 2 | 1248 | B8N | C32-C33-C34-O35 |
| 2 | 2 | 644 | OMG | C4'-C5'-O5'-P |
| 2 | 2 | 1703 | OMC | C3'-C4'-C5'-O5' |
| 2 | 2 | 576 | A2M | C3'-C2'-O2'-CM' |
| 2 | 2 | 428 | OMU | O4'-C1'-N1-C6 |
| 2 | 2 | 801 | PSU | O4'-C1'-C5-C4 |
| 2 | 2 | 509 | OMG | C3'-C2'-O2'-CM2 |
| 2 | 2 | 512 | A2M | C3'-C2'-O2'-CM' |
| 2 | 2 | 797 | OMC | C3'-C2'-O2'-CM2 |
| 2 | 2 | 1272 | OMC | C3'-C2'-O2'-CM2 |
| 2 | 2 | 1391 | OMC | C3'-C2'-O2'-CM2 |
| 2 | 2 | 822 | PSU | O4'-C4'-C5'-O5' |
| 2 | 2 | 484 | A2M | C1'-C2'-O2'-CM' |
| 2 | 2 | 428 | OMU | O4'-C1'-N1-C2 |
| 26 | X | 62 | HY3 | O-C-CA-C3 |
| 2 | 2 | 116 | OMU | O4'-C4'-C5'-O5' |
| 2 | 2 | 799 | OMU | O4'-C4'-C5'-O5' |
| 17 | O | 138 | IAS | CA-CB-CG-OD1 |
| 2 | 2 | 683 | OMG | C3'-C2'-O2'-CM2 |
| 2 | 2 | 99 | A2M | C3'-C4'-C5'-O5' |
| 2 | 2 | 1081 | PSU | C4'-C5'-O5'-P |

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 117 are unknown and 114 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-17804. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

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

6 Map analysis

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

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit

This section was not generated.