



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2018 – 03:33 PM EST

PDB ID : 5NB4
Title : Atomic resolution structure of C-phycoerythrin from marine cyanobacterium
Phormidium sp. A09DM at pH 7.5
Authors : Sonani, R.R.; Roszak, A.W.; Ortmann de Percin Northumberland, C.;
Madamwar, D.; Cogdell, R.J.
Deposited on : 2017-03-01
Resolution : 1.14 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

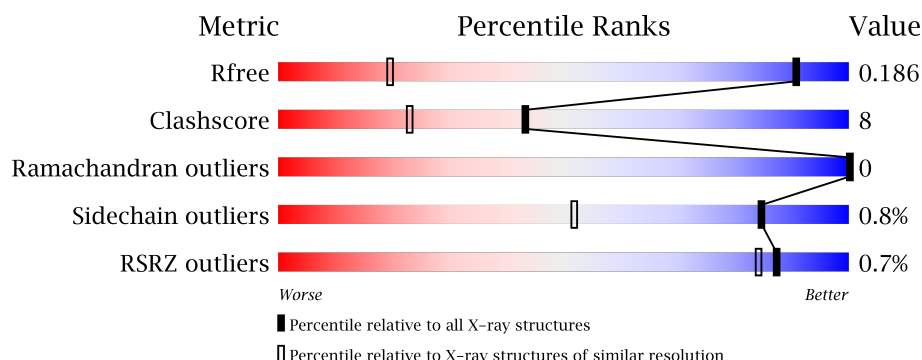
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.14 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.




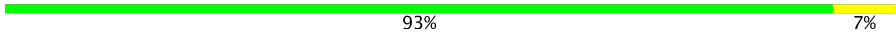


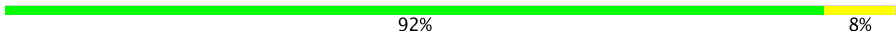
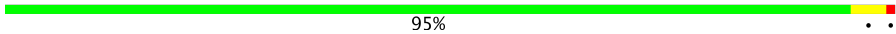

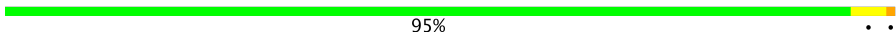











| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R_{free} | 100719 | 1078 (1.18-1.10) |
| Clashscore | 112137 | 1123 (1.18-1.10) |
| Ramachandran outliers | 110173 | 1074 (1.18-1.10) |
| Sidechain outliers | 110143 | 1071 (1.18-1.10) |
| RSRZ outliers | 101464 | 1082 (1.18-1.10) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 164 | <div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div> <div>92% 7% .</div> |
| 1 | B | 164 | <div> <div style="width: 94%;"></div> <div style="width: 6%;"></div> <div style="width: 0%;"></div> </div> <div>94% 6%</div> |
| 1 | C | 164 | <div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> <div style="width: 0%;"></div> </div> <div>91% 9%</div> |
| 1 | D | 164 | <div> <div style="width: 95%;"></div> <div style="width: 5%;"></div> <div style="width: 0%;"></div> </div> <div>95% 5%</div> |
| 1 | E | 164 | <div> <div style="width: 94%;"></div> <div style="width: 6%;"></div> <div style="width: 0%;"></div> </div> <div>94% 6%</div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1 | F | 164 |  |
| 1 | G | 164 |  |
| 1 | H | 164 |  |
| 1 | I | 164 |  |
| 1 | J | 164 |  |
| 1 | K | 164 |  |
| 1 | L | 164 |  |
| 2 | M | 184 |  |
| 2 | N | 184 |  |
| 2 | O | 184 |  |
| 2 | P | 184 |  |
| 2 | Q | 184 |  |
| 2 | R | 184 |  |
| 2 | S | 184 |  |
| 2 | T | 184 |  |
| 2 | U | 184 |  |
| 2 | V | 184 |  |
| 2 | W | 184 |  |
| 2 | X | 184 |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | PI | A | 204 | - | - | X | - |
| 5 | PI | H | 203 | - | - | X | - |
| 5 | PI | M | 205 | - | - | - | X |
| 5 | PI | N | 204 | - | - | - | X |
| 5 | PI | P | 205 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | PI | Q | 205 | - | - | - | X |
| 5 | PI | S | 205 | - | - | - | X |
| 5 | PI | U | 205 | - | - | - | X |
| 5 | PI | V | 205 | - | - | - | X |
| 5 | PI | W | 205 | - | - | - | X |
| 5 | PI | X | 205 | - | - | - | X |
| 6 | NA | N | 205 | - | - | - | X |
| 6 | NA | S | 206 | - | - | - | X |
| 6 | NA | W | 206 | - | - | - | X |
| 7 | MPD | B | 203 | - | - | - | X |
| 7 | MPD | M | 204 | - | - | - | X |
| 7 | MPD | O | 204 | - | - | X | X |
| 7 | MPD | P | 204 | - | - | X | X |
| 7 | MPD | Q | 204 | - | - | X | X |
| 7 | MPD | R | 204 | - | - | X | X |
| 7 | MPD | S | 204 | - | - | X | X |
| 7 | MPD | U | 204 | - | - | X | X |
| 7 | MPD | W | 204 | - | - | X | X |
| 7 | MPD | X | 204 | - | - | X | - |
| 8 | MRD | T | 204 | - | - | X | X |
| 8 | MRD | V | 204 | - | - | X | X |

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 43607 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 Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,P hycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 164 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1300 | 812 | 229 | 252 | 7 | | | |
| 1 | B | 164 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 1292 | 805 | 227 | 253 | 7 | | | |
| 1 | C | 164 | Total | C | N | O | S | 0 | 9 | 0 |
| | | | 1298 | 810 | 227 | 254 | 7 | | | |
| 1 | D | 164 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1314 | 822 | 233 | 252 | 7 | | | |
| 1 | E | 164 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 1292 | 805 | 227 | 253 | 7 | | | |
| 1 | F | 164 | Total | C | N | O | S | 0 | 11 | 0 |
| | | | 1316 | 820 | 230 | 259 | 7 | | | |
| 1 | G | 164 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 1301 | 811 | 228 | 255 | 7 | | | |
| 1 | H | 164 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1316 | 820 | 231 | 258 | 7 | | | |
| 1 | I | 164 | Total | C | N | O | S | 0 | 12 | 0 |
| | | | 1315 | 823 | 229 | 256 | 7 | | | |
| 1 | J | 164 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1306 | 816 | 228 | 255 | 7 | | | |
| 1 | K | 164 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1304 | 813 | 228 | 256 | 7 | | | |
| 1 | L | 164 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 1300 | 811 | 230 | 252 | 7 | | | |

- Molecule 2 is a protein called Phycoerythrin Beta subunit,Phycoerythrin Beta subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2 | M | 184 | Total | C | N | O | S | 0 | 12 | 0 |
| | | | 1416 | 876 | 254 | 273 | 13 | | | |
| 2 | N | 184 | Total | C | N | O | S | 0 | 12 | 0 |
| | | | 1411 | 868 | 252 | 277 | 14 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|---------|-------|
| 2 | O | 184 | Total 1400 | C 867 | N 252 | O 268 | S 13 | 0 | 9 | 0 |
| 2 | P | 184 | Total 1401 | C 865 | N 249 | O 273 | S 14 | 0 | 11 | 0 |
| 2 | Q | 184 | Total 1394 | C 862 | N 248 | O 271 | S 13 | 0 | 10 | 0 |
| 2 | R | 184 | Total 1402 | C 867 | N 251 | O 271 | S 13 | 0 | 10 | 0 |
| 2 | S | 184 | Total 1410 | C 870 | N 251 | O 275 | S 14 | 0 | 12 | 0 |
| 2 | T | 184 | Total 1407 | C 871 | N 247 | O 276 | S 13 | 0 | 12 | 0 |
| 2 | U | 184 | Total 1441 | C 892 | N 257 | O 279 | S 13 | 0 | 16 | 0 |
| 2 | V | 184 | Total 1437 | C 888 | N 255 | O 280 | S 14 | 0 | 16 | 0 |
| 2 | W | 184 | Total 1423 | C 880 | N 251 | O 278 | S 14 | 0 | 15 | 0 |
| 2 | X | 184 | Total 1401 | C 865 | N 251 | O 272 | S 13 | 0 | 11 | 0 |

- # PEB

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 43 | 33 | 4 | 6 | | |



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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 3 | A | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | B | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | B | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | C | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | C | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | D | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | D | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | E | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | E | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | F | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | F | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | G | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | G | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | H | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | H | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | I | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | I | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | J | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | J | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | K | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | K | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |

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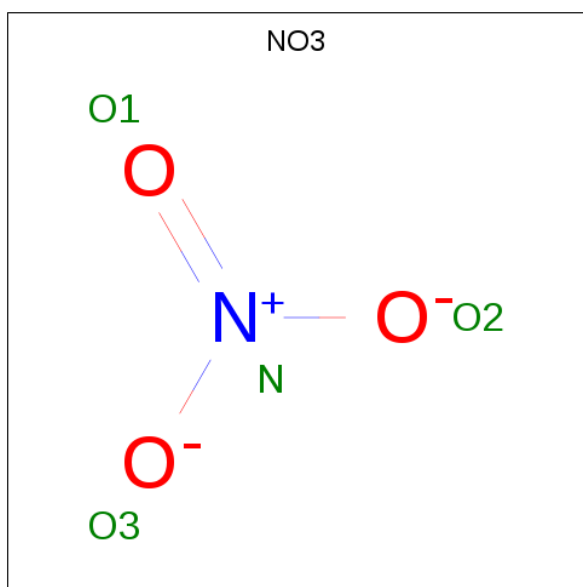
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 3 | L | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | L | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | M | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | M | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | M | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | N | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | N | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | N | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | O | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | O | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | O | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | P | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | P | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | P | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | Q | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | Q | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | Q | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | R | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | R | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | R | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | S | 1 | Total 49 | C 37 | N 4 | O 8 | 0 | 1 |

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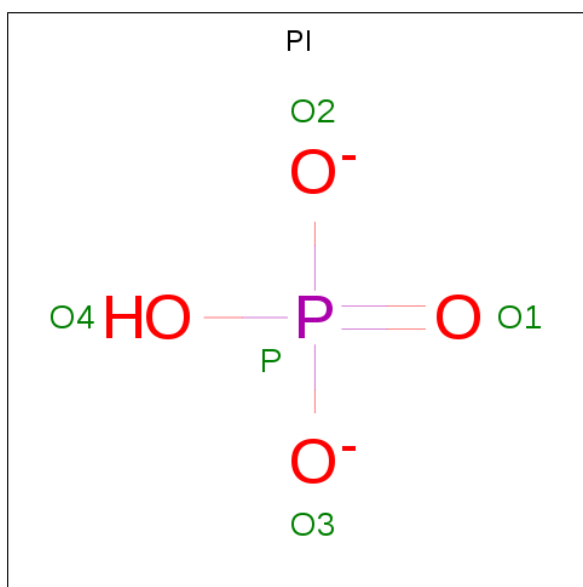
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 3 | S | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | S | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | T | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | T | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | T | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | U | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | U | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | U | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | V | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | V | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | V | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | W | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | W | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | W | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | X | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | X | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |
| 3 | X | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | 0 |

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | A | 1 | Total | N | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 4 | C | 1 | Total | N | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 4 | D | 1 | Total | N | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 4 | I | 1 | Total | N | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 4 | J | 1 | Total | N | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 4 | L | 1 | Total | N | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |

- Molecule 5 is HYDROGENPHOSPHATE ION (three-letter code: PI) (formula: HO₄P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5 | A | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | B | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | C | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | D | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | E | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | F | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | G | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | H | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | I | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | J | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | K | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | L | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | M | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | N | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5 | O | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | P | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | Q | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | R | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | S | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | T | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | U | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | V | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | W | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | X | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

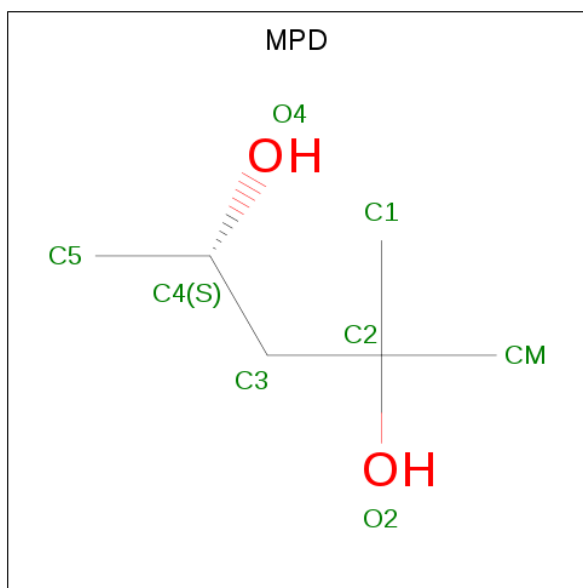
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6 | G | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | J | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | D | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | K | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | E | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | H | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | B | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | I | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | C | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6 | V | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | W | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | N | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | L | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | S | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | F | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



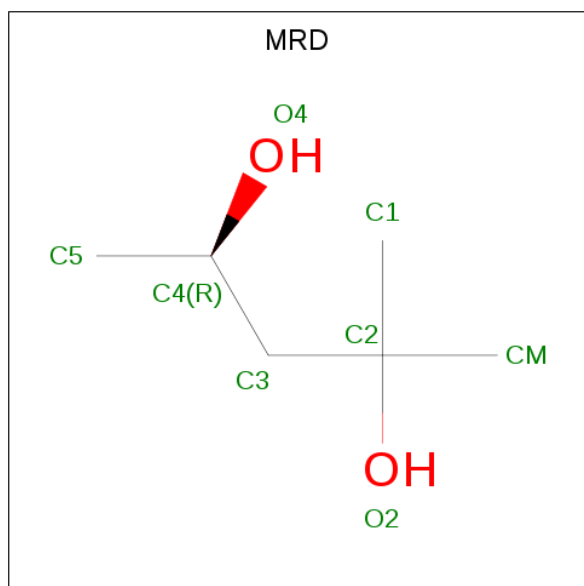
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | M | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | O | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | P | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7 | Q | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | R | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | S | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | U | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | W | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 7 | X | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8 | T | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 8 | V | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 9 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 9 | A | 356 | Total | O | 0 | 0 |
| | | | 356 | 356 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 9 | B | 312 | Total 312 | O 312 | 0 | 0 |
| 9 | C | 341 | Total 341 | O 341 | 0 | 0 |
| 9 | D | 363 | Total 363 | O 363 | 0 | 0 |
| 9 | E | 319 | Total 319 | O 319 | 0 | 0 |
| 9 | F | 345 | Total 345 | O 345 | 0 | 0 |
| 9 | G | 350 | Total 350 | O 350 | 0 | 0 |
| 9 | H | 324 | Total 324 | O 324 | 0 | 0 |
| 9 | I | 351 | Total 351 | O 351 | 0 | 0 |
| 9 | J | 345 | Total 345 | O 345 | 0 | 0 |
| 9 | K | 319 | Total 319 | O 319 | 0 | 0 |
| 9 | L | 355 | Total 355 | O 355 | 0 | 0 |
| 9 | M | 362 | Total 362 | O 362 | 0 | 0 |
| 9 | N | 359 | Total 359 | O 359 | 0 | 0 |
| 9 | O | 362 | Total 362 | O 362 | 0 | 0 |
| 9 | P | 330 | Total 330 | O 330 | 0 | 0 |
| 9 | Q | 322 | Total 322 | O 322 | 0 | 0 |
| 9 | R | 297 | Total 297 | O 297 | 0 | 0 |
| 9 | S | 318 | Total 318 | O 318 | 0 | 0 |
| 9 | T | 312 | Total 312 | O 312 | 0 | 0 |
| 9 | U | 340 | Total 340 | O 340 | 0 | 0 |
| 9 | V | 361 | Total 361 | O 361 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 9 | W | 368 | Total | O | 0 | 0 |
| | | | 368 | 368 | | |
| 9 | X | 357 | Total | O | 0 | 0 |
| | | | 357 | 357 | | |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

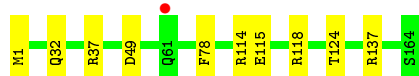
- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain A: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain B: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain C: 



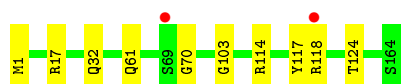
- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain D: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain E: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain F: 86% 13%



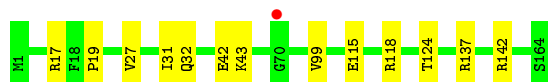
- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain G: 93% 7%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain H: 92% 8%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain I: 91% 8%



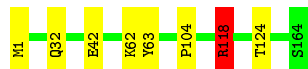
- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain J: 92% 8%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain K: 95%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain L:  92% 7% .




- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain M:  95% . .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain N:  90% 8% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain O:  91% 7% .



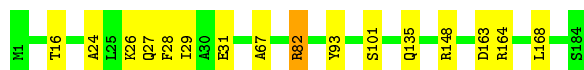
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain P:  91% 8% .

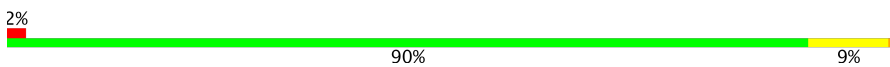


- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain Q:  91% 8% .

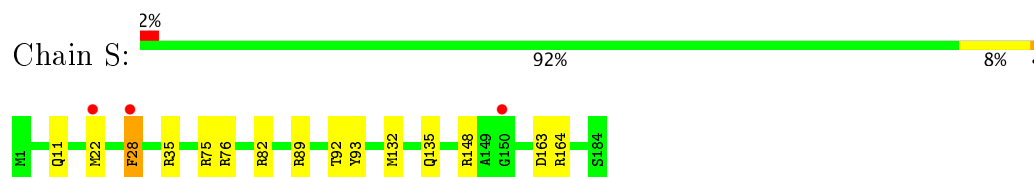


- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

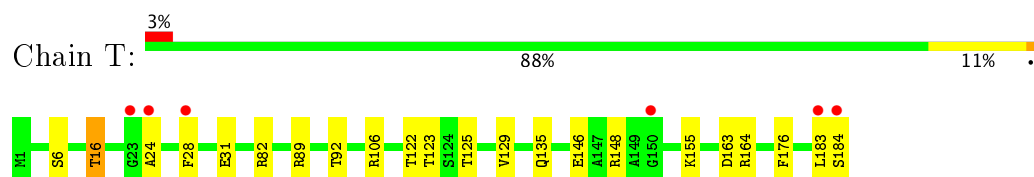
Chain R:  90% 9% .



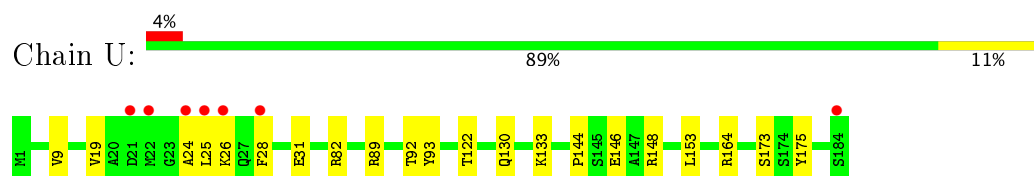
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



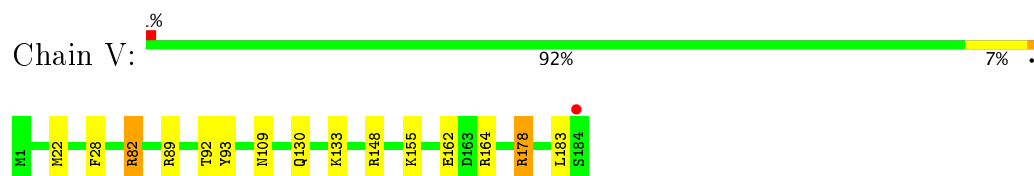
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



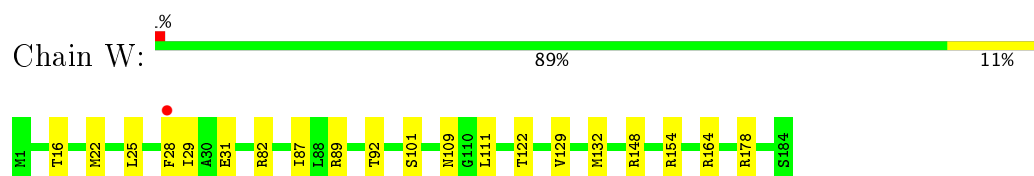
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



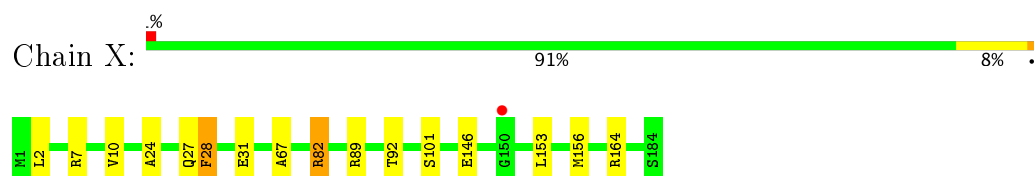
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



4 Data and refinement statistics

| Property | Value | Source |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 109.05Å 109.09Å 117.37Å 78.78° 82.32° 60.26° | Depositor |
| Resolution (Å) | 94.62 – 1.14 94.59 – 1.14 | Depositor EDS |
| % Data completeness (in resolution range) | 93.8 (94.62-1.14) 88.3 (94.59-1.14) | Depositor EDS |
| R_{merge} | 0.04 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.80 (at 1.14Å) | Xtriage |
| Refinement program | REFMAC 5.8.0158 | Depositor |
| R, R_{free} | 0.147 , 0.184 0.149 , 0.186 | Depositor DCC |
| R_{free} test set | 79188 reflections (5.29%) | DCC |
| Wilson B-factor (Å ²) | 10.8 | Xtriage |
| Anisotropy | 0.255 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 60.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.014 for h-k,-k,-l | Xtriage |
| F_o, F_c correlation | 0.97 | EDS |
| Total number of atoms | 43607 | wwPDB-VP |
| Average B, all atoms (Å ²) | 17.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, NA, MEN, MRD, PI, PEB, NO3

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 | 0.85 | 1/1344 (0.1%) | 0.99 | 7/1816 (0.4%) |
| 1 | B | 0.74 | 0/1327 | 0.92 | 6/1795 (0.3%) |
| 1 | C | 0.80 | 1/1336 (0.1%) | 0.90 | 2/1806 (0.1%) |
| 1 | D | 0.76 | 0/1364 | 0.90 | 1/1841 (0.1%) |
| 1 | E | 0.74 | 1/1327 (0.1%) | 0.88 | 1/1795 (0.1%) |
| 1 | F | 0.82 | 0/1354 | 0.92 | 2/1830 (0.1%) |
| 1 | G | 0.77 | 2/1336 (0.1%) | 0.92 | 2/1806 (0.1%) |
| 1 | H | 0.70 | 0/1354 | 0.88 | 5/1830 (0.3%) |
| 1 | I | 0.79 | 0/1365 | 0.92 | 4/1843 (0.2%) |
| 1 | J | 0.79 | 1/1344 (0.1%) | 0.92 | 5/1817 (0.3%) |
| 1 | K | 0.81 | 0/1342 | 1.01 | 4/1814 (0.2%) |
| 1 | L | 0.81 | 1/1338 (0.1%) | 0.98 | 10/1808 (0.6%) |
| 2 | M | 0.82 | 0/1455 | 0.96 | 5/1959 (0.3%) |
| 2 | N | 0.76 | 0/1439 | 1.00 | 9/1937 (0.5%) |
| 2 | O | 0.74 | 0/1427 | 1.00 | 9/1921 (0.5%) |
| 2 | P | 0.84 | 1/1434 (0.1%) | 1.00 | 6/1933 (0.3%) |
| 2 | Q | 0.75 | 0/1427 | 0.95 | 6/1925 (0.3%) |
| 2 | R | 0.73 | 0/1432 | 0.92 | 2/1929 (0.1%) |
| 2 | S | 0.72 | 0/1443 | 1.05 | 8/1945 (0.4%) |
| 2 | T | 0.71 | 0/1442 | 0.91 | 3/1942 (0.2%) |
| 2 | U | 0.82 | 0/1488 | 0.99 | 5/2002 (0.2%) |
| 2 | V | 0.79 | 0/1478 | 0.89 | 5/1989 (0.3%) |
| 2 | W | 0.77 | 0/1464 | 0.92 | 3/1971 (0.2%) |
| 2 | X | 0.73 | 0/1437 | 0.94 | 3/1937 (0.2%) |
| All | All | 0.77 | 8/33497 (0.0%) | 0.95 | 113/45191 (0.3%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | C | 54 | GLU | CD-OE2 | -8.60 | 1.16 | 1.25 |
| 1 | A | 54 | GLU | CD-OE2 | -6.46 | 1.18 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | J | 54 | GLU | CD-OE2 | -6.04 | 1.19 | 1.25 |
| 1 | L | 54 | GLU | CD-OE2 | -5.53 | 1.19 | 1.25 |
| 1 | G | 39 | GLU | CD-OE2 | -5.51 | 1.19 | 1.25 |
| 1 | E | 117 | TYR | CG-CD1 | 5.44 | 1.46 | 1.39 |
| 2 | P | 60 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 1 | G | 131 | LEU | C-O | 5.04 | 1.32 | 1.23 |

All (113) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|--------|-------------|----------|
| 2 | S | 82[A] | ARG | NE-CZ-NH2 | -11.16 | 114.72 | 120.30 |
| 2 | S | 82[B] | ARG | NE-CZ-NH2 | -11.16 | 114.72 | 120.30 |
| 2 | O | 164 | ARG | NE-CZ-NH1 | 10.87 | 125.73 | 120.30 |
| 1 | K | 118[A] | ARG | NE-CZ-NH2 | -9.68 | 115.46 | 120.30 |
| 1 | K | 118[B] | ARG | NE-CZ-NH2 | -9.68 | 115.46 | 120.30 |
| 2 | N | 163 | ASP | CB-CG-OD1 | 9.63 | 126.97 | 118.30 |
| 1 | K | 118[A] | ARG | NE-CZ-NH1 | 9.46 | 125.03 | 120.30 |
| 1 | K | 118[B] | ARG | NE-CZ-NH1 | 9.46 | 125.03 | 120.30 |
| 2 | P | 164 | ARG | NE-CZ-NH1 | 9.41 | 125.00 | 120.30 |
| 2 | S | 82[A] | ARG | NE-CZ-NH1 | 9.33 | 124.96 | 120.30 |
| 2 | S | 82[B] | ARG | NE-CZ-NH1 | 9.33 | 124.96 | 120.30 |
| 2 | U | 164 | ARG | NE-CZ-NH1 | 9.14 | 124.87 | 120.30 |
| 2 | S | 163 | ASP | CB-CG-OD1 | 8.93 | 126.34 | 118.30 |
| 2 | X | 82[A] | ARG | NE-CZ-NH2 | -8.84 | 115.88 | 120.30 |
| 2 | X | 82[B] | ARG | NE-CZ-NH2 | -8.84 | 115.88 | 120.30 |
| 2 | V | 164 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 1 | D | 142 | ARG | NE-CZ-NH1 | 7.93 | 124.27 | 120.30 |
| 1 | J | 37 | ARG | NE-CZ-NH2 | -7.72 | 116.44 | 120.30 |
| 2 | T | 163 | ASP | CB-CG-OD1 | 7.58 | 125.12 | 118.30 |
| 2 | O | 89 | ARG | NE-CZ-NH2 | -7.54 | 116.53 | 120.30 |
| 2 | P | 164 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 1 | F | 84 | ARG | NE-CZ-NH2 | -7.37 | 116.61 | 120.30 |
| 2 | Q | 82[A] | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 2 | Q | 82[B] | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 2 | R | 154 | ARG | NE-CZ-NH2 | -7.31 | 116.64 | 120.30 |
| 2 | U | 164 | ARG | NE-CZ-NH2 | -7.24 | 116.68 | 120.30 |
| 1 | L | 95 | TYR | CB-CG-CD1 | 7.13 | 125.28 | 121.00 |
| 2 | P | 34 | ARG | NE-CZ-NH2 | -7.08 | 116.76 | 120.30 |
| 1 | I | 37 | ARG | NE-CZ-NH2 | -6.98 | 116.81 | 120.30 |
| 2 | O | 82[A] | ARG | NE-CZ-NH2 | -6.97 | 116.81 | 120.30 |
| 2 | O | 82[B] | ARG | NE-CZ-NH2 | -6.97 | 116.81 | 120.30 |
| 2 | O | 164 | ARG | NE-CZ-NH2 | -6.83 | 116.89 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1 | A | 142 | ARG | NE-CZ-NH1 | 6.77 | 123.69 | 120.30 |
| 2 | W | 154 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 1 | H | 137 | ARG | NE-CZ-NH2 | -6.76 | 116.92 | 120.30 |
| 2 | S | 93 | TYR | CB-CG-CD1 | 6.74 | 125.04 | 121.00 |
| 1 | A | 37 | ARG | NE-CZ-NH2 | -6.73 | 116.94 | 120.30 |
| 2 | N | 22[A] | MET | CG-SD-CE | 6.71 | 110.94 | 100.20 |
| 2 | N | 22[B] | MET | CG-SD-CE | 6.71 | 110.94 | 100.20 |
| 2 | Q | 163 | ASP | CB-CG-OD1 | 6.69 | 124.32 | 118.30 |
| 2 | O | 89 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 2 | N | 164 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | C | 142 | ARG | NE-CZ-NH2 | -6.42 | 117.09 | 120.30 |
| 2 | M | 82[A] | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |
| 2 | M | 82[B] | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |
| 2 | M | 82[C] | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |
| 2 | O | 106 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 1 | L | 114 | ARG | NE-CZ-NH1 | 6.29 | 123.45 | 120.30 |
| 1 | B | 37 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 2 | W | 164 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 2 | X | 164 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 2 | N | 89 | ARG | NE-CZ-NH2 | -6.13 | 117.23 | 120.30 |
| 2 | Q | 164 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 2 | V | 93 | TYR | CB-CG-CD1 | 6.06 | 124.64 | 121.00 |
| 1 | J | 95 | TYR | CB-CG-CD2 | -6.05 | 117.37 | 121.00 |
| 2 | S | 93 | TYR | CB-CG-CD2 | -6.03 | 117.38 | 121.00 |
| 1 | H | 142 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 2 | N | 21 | ASP | CB-CG-OD1 | 5.87 | 123.58 | 118.30 |
| 2 | R | 154 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 2 | U | 175 | TYR | CZ-CE2-CD2 | -5.81 | 114.57 | 119.80 |
| 2 | M | 93 | TYR | CB-CG-CD1 | 5.79 | 124.47 | 121.00 |
| 1 | B | 78 | PHE | CB-CG-CD2 | -5.77 | 116.76 | 120.80 |
| 2 | O | 93 | TYR | CB-CG-CD1 | 5.74 | 124.44 | 121.00 |
| 2 | N | 82[A] | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 2 | N | 82[B] | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 1 | A | 137 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 1 | B | 78 | PHE | CB-CG-CD1 | 5.65 | 124.76 | 120.80 |
| 2 | O | 154 | ARG | NE-CZ-NH1 | 5.56 | 123.08 | 120.30 |
| 1 | H | 142 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | C | 142 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 2 | P | 82[A] | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 2 | P | 82[B] | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 2 | V | 82[A] | ARG | NE-CZ-NH2 | -5.47 | 117.57 | 120.30 |
| 2 | V | 82[B] | ARG | NE-CZ-NH2 | -5.47 | 117.57 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | B | 137 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 2 | P | 34 | ARG | CG-CD-NE | -5.46 | 100.34 | 111.80 |
| 1 | L | 142 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | J | 95 | TYR | CB-CG-CD1 | 5.33 | 124.20 | 121.00 |
| 2 | W | 164 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 1 | J | 142 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 2 | M | 127 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | L | 78 | PHE | CB-CG-CD2 | -5.30 | 117.09 | 120.80 |
| 1 | G | 37 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | F | 84 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 2 | Q | 93 | TYR | CB-CG-CD2 | -5.28 | 117.83 | 121.00 |
| 2 | S | 164 | ARG | NE-CZ-NH1 | 5.25 | 122.93 | 120.30 |
| 2 | N | 154 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | A | 95 | TYR | CB-CG-CD1 | 5.24 | 124.14 | 121.00 |
| 1 | A | 114[A] | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 1 | A | 114[B] | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 1 | G | 49 | ASP | CB-CG-OD1 | 5.22 | 122.99 | 118.30 |
| 1 | H | 137 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 1 | L | 78 | PHE | CB-CG-CD1 | 5.20 | 124.44 | 120.80 |
| 2 | U | 93 | TYR | CB-CG-CD2 | -5.19 | 117.89 | 121.00 |
| 1 | E | 17 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 1 | B | 114 | ARG | NE-CZ-NH2 | -5.15 | 117.72 | 120.30 |
| 2 | U | 93 | TYR | CB-CG-CD1 | 5.14 | 124.09 | 121.00 |
| 1 | I | 137 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 2 | V | 133 | LYS | CD-CE-NZ | -5.10 | 99.96 | 111.70 |
| 2 | T | 106 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | J | 17 | ARG | NE-CZ-NH1 | 5.07 | 122.84 | 120.30 |
| 1 | L | 118[A] | ARG | NE-CZ-NH2 | 5.07 | 122.84 | 120.30 |
| 1 | L | 118[B] | ARG | NE-CZ-NH2 | 5.07 | 122.84 | 120.30 |
| 1 | L | 118[C] | ARG | NE-CZ-NH2 | 5.07 | 122.84 | 120.30 |
| 1 | H | 17 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 2 | Q | 164 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 2 | T | 164 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 1 | B | 49 | ASP | CB-CG-OD1 | 5.02 | 122.82 | 118.30 |
| 1 | A | 142 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 1 | I | 118[A] | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | I | 118[B] | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | L | 1[A] | MET | CG-SD-CE | 5.01 | 108.22 | 100.20 |
| 1 | L | 1[B] | MET | CG-SD-CE | 5.01 | 108.22 | 100.20 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1300 | 0 | 1313 | 27 | 0 |
| 1 | B | 1292 | 0 | 1289 | 11 | 0 |
| 1 | C | 1298 | 0 | 1301 | 17 | 0 |
| 1 | D | 1314 | 0 | 1339 | 21 | 0 |
| 1 | E | 1292 | 0 | 1289 | 12 | 0 |
| 1 | F | 1316 | 0 | 1314 | 35 | 0 |
| 1 | G | 1301 | 0 | 1300 | 19 | 0 |
| 1 | H | 1316 | 0 | 1316 | 20 | 0 |
| 1 | I | 1315 | 0 | 1334 | 17 | 0 |
| 1 | J | 1306 | 0 | 1311 | 15 | 0 |
| 1 | K | 1304 | 0 | 1305 | 22 | 0 |
| 1 | L | 1300 | 0 | 1307 | 15 | 0 |
| 2 | M | 1416 | 0 | 1462 | 11 | 0 |
| 2 | N | 1411 | 0 | 1444 | 16 | 0 |
| 2 | O | 1400 | 0 | 1443 | 16 | 0 |
| 2 | P | 1401 | 0 | 1432 | 14 | 0 |
| 2 | Q | 1394 | 0 | 1428 | 27 | 0 |
| 2 | R | 1402 | 0 | 1439 | 30 | 0 |
| 2 | S | 1410 | 0 | 1439 | 20 | 0 |
| 2 | T | 1407 | 0 | 1443 | 27 | 0 |
| 2 | U | 1441 | 0 | 1488 | 25 | 0 |
| 2 | V | 1437 | 0 | 1476 | 18 | 0 |
| 2 | W | 1423 | 0 | 1466 | 29 | 0 |
| 2 | X | 1401 | 0 | 1437 | 21 | 0 |
| 3 | A | 86 | 0 | 74 | 2 | 0 |
| 3 | B | 86 | 0 | 74 | 1 | 0 |
| 3 | C | 86 | 0 | 74 | 2 | 0 |
| 3 | D | 86 | 0 | 74 | 1 | 0 |
| 3 | E | 86 | 0 | 74 | 2 | 0 |
| 3 | F | 86 | 0 | 74 | 3 | 0 |
| 3 | G | 86 | 0 | 74 | 2 | 0 |
| 3 | H | 86 | 0 | 74 | 2 | 0 |
| 3 | I | 86 | 0 | 74 | 1 | 0 |
| 3 | J | 86 | 0 | 74 | 1 | 0 |
| 3 | K | 86 | 0 | 74 | 1 | 0 |
| 3 | L | 86 | 0 | 74 | 2 | 0 |
| 3 | M | 129 | 0 | 110 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | N | 129 | 0 | 110 | 6 | 0 |
| 3 | O | 129 | 0 | 110 | 6 | 0 |
| 3 | P | 129 | 0 | 110 | 6 | 0 |
| 3 | Q | 129 | 0 | 110 | 8 | 0 |
| 3 | R | 129 | 0 | 111 | 10 | 0 |
| 3 | S | 135 | 0 | 87 | 3 | 0 |
| 3 | T | 129 | 0 | 110 | 8 | 0 |
| 3 | U | 129 | 0 | 110 | 6 | 0 |
| 3 | V | 129 | 0 | 110 | 5 | 0 |
| 3 | W | 129 | 0 | 110 | 6 | 0 |
| 3 | X | 129 | 0 | 110 | 8 | 0 |
| 4 | A | 4 | 0 | 0 | 1 | 0 |
| 4 | C | 4 | 0 | 0 | 0 | 0 |
| 4 | D | 4 | 0 | 0 | 0 | 0 |
| 4 | I | 4 | 0 | 0 | 1 | 0 |
| 4 | J | 4 | 0 | 0 | 0 | 0 |
| 4 | L | 4 | 0 | 0 | 1 | 0 |
| 5 | A | 5 | 0 | 0 | 11 | 0 |
| 5 | B | 5 | 0 | 0 | 0 | 0 |
| 5 | C | 5 | 0 | 0 | 1 | 0 |
| 5 | D | 5 | 0 | 0 | 1 | 0 |
| 5 | E | 5 | 0 | 0 | 0 | 0 |
| 5 | F | 5 | 0 | 0 | 1 | 0 |
| 5 | G | 5 | 0 | 0 | 0 | 0 |
| 5 | H | 5 | 0 | 0 | 2 | 0 |
| 5 | I | 5 | 0 | 0 | 0 | 0 |
| 5 | J | 5 | 0 | 0 | 0 | 0 |
| 5 | K | 5 | 0 | 0 | 1 | 0 |
| 5 | L | 5 | 0 | 0 | 0 | 0 |
| 5 | M | 5 | 0 | 0 | 0 | 0 |
| 5 | N | 5 | 0 | 0 | 0 | 0 |
| 5 | O | 5 | 0 | 0 | 0 | 0 |
| 5 | P | 5 | 0 | 0 | 0 | 0 |
| 5 | Q | 5 | 0 | 0 | 0 | 0 |
| 5 | R | 5 | 0 | 0 | 0 | 0 |
| 5 | S | 5 | 0 | 0 | 0 | 0 |
| 5 | T | 5 | 0 | 0 | 0 | 0 |
| 5 | U | 5 | 0 | 0 | 0 | 0 |
| 5 | V | 5 | 0 | 0 | 0 | 0 |
| 5 | W | 5 | 0 | 0 | 0 | 0 |
| 5 | X | 5 | 0 | 0 | 0 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 6 | C | 1 | 0 | 0 | 0 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| 6 | E | 1 | 0 | 0 | 0 | 0 |
| 6 | F | 1 | 0 | 0 | 0 | 0 |
| 6 | G | 1 | 0 | 0 | 0 | 0 |
| 6 | H | 1 | 0 | 0 | 0 | 0 |
| 6 | I | 1 | 0 | 0 | 0 | 0 |
| 6 | J | 1 | 0 | 0 | 0 | 0 |
| 6 | K | 1 | 0 | 0 | 0 | 0 |
| 6 | L | 1 | 0 | 0 | 0 | 0 |
| 6 | N | 1 | 0 | 0 | 0 | 0 |
| 6 | S | 1 | 0 | 0 | 0 | 0 |
| 6 | V | 1 | 0 | 0 | 0 | 0 |
| 6 | W | 1 | 0 | 0 | 0 | 0 |
| 7 | B | 8 | 0 | 14 | 5 | 0 |
| 7 | M | 8 | 0 | 12 | 4 | 0 |
| 7 | O | 8 | 0 | 10 | 9 | 0 |
| 7 | P | 8 | 0 | 11 | 6 | 0 |
| 7 | Q | 8 | 0 | 11 | 11 | 0 |
| 7 | R | 8 | 0 | 14 | 15 | 0 |
| 7 | S | 8 | 0 | 14 | 8 | 0 |
| 7 | U | 8 | 0 | 12 | 8 | 0 |
| 7 | W | 8 | 0 | 11 | 7 | 0 |
| 7 | X | 8 | 0 | 14 | 8 | 0 |
| 8 | T | 8 | 0 | 11 | 10 | 0 |
| 8 | V | 8 | 0 | 11 | 10 | 0 |
| 9 | A | 356 | 0 | 0 | 8 | 0 |
| 9 | B | 312 | 0 | 0 | 10 | 0 |
| 9 | C | 341 | 0 | 0 | 9 | 0 |
| 9 | D | 363 | 0 | 0 | 15 | 1 |
| 9 | E | 319 | 0 | 0 | 8 | 0 |
| 9 | F | 345 | 0 | 0 | 27 | 0 |
| 9 | G | 350 | 0 | 0 | 11 | 0 |
| 9 | H | 324 | 0 | 0 | 11 | 0 |
| 9 | I | 351 | 0 | 0 | 15 | 0 |
| 9 | J | 345 | 0 | 0 | 12 | 0 |
| 9 | K | 319 | 0 | 0 | 9 | 0 |
| 9 | L | 355 | 0 | 0 | 6 | 0 |
| 9 | M | 362 | 0 | 0 | 2 | 1 |
| 9 | N | 359 | 0 | 0 | 6 | 1 |
| 9 | O | 362 | 0 | 0 | 7 | 1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | P | 330 | 0 | 0 | 5 | 0 |
| 9 | Q | 322 | 0 | 0 | 11 | 0 |
| 9 | R | 297 | 0 | 0 | 11 | 1 |
| 9 | S | 318 | 0 | 0 | 9 | 0 |
| 9 | T | 312 | 0 | 0 | 13 | 1 |
| 9 | U | 340 | 0 | 0 | 17 | 0 |
| 9 | V | 361 | 0 | 0 | 5 | 0 |
| 9 | W | 368 | 0 | 0 | 13 | 1 |
| 9 | X | 357 | 0 | 0 | 11 | 1 |
| All | All | 43607 | 0 | 35446 | 544 | 4 |

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 8.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:V:28[A]:PHE:CE1 | 8:V:204:MRD:H5C2 | 1.27 | 1.59 |
| 2:V:28[A]:PHE:CD1 | 8:V:204:MRD:C5 | 1.83 | 1.57 |
| 2:V:28[A]:PHE:CD1 | 8:V:204:MRD:H5C2 | 1.03 | 1.56 |
| 2:X:28[A]:PHE:HE2 | 7:X:204:MPD:C1 | 1.18 | 1.54 |
| 2:O:28[B]:PHE:CD1 | 7:O:204:MPD:C5 | 1.76 | 1.51 |
| 2:Q:28[A]:PHE:CD1 | 7:Q:204:MPD:H4 | 1.53 | 1.42 |
| 2:Q:28[A]:PHE:CE1 | 7:Q:204:MPD:H4 | 1.56 | 1.40 |
| 2:X:28[A]:PHE:CE2 | 7:X:204:MPD:C1 | 2.01 | 1.40 |
| 2:X:28[A]:PHE:CE2 | 7:X:204:MPD:H12 | 1.57 | 1.39 |
| 1:A:114[B]:ARG:HG2 | 5:A:204:PI:P | 1.62 | 1.38 |
| 2:S:28[A]:PHE:HE2 | 7:S:204:MPD:C1 | 1.39 | 1.33 |
| 1:K:118[B]:ARG:NE | 9:K:303:HOH:O | 1.57 | 1.32 |
| 2:S:28[A]:PHE:CE2 | 7:S:204:MPD:C1 | 2.16 | 1.27 |
| 2:N:109[A]:ASN:ND2 | 9:N:301:HOH:O | 1.64 | 1.26 |
| 2:O:28[B]:PHE:HD1 | 7:O:204:MPD:C5 | 1.20 | 1.26 |
| 1:A:114[B]:ARG:HD2 | 5:A:204:PI:O4 | 1.14 | 1.24 |
| 2:Q:28[A]:PHE:CE1 | 7:Q:204:MPD:C4 | 2.16 | 1.23 |
| 2:S:11[B]:GLN:NE2 | 9:S:304:HOH:O | 1.68 | 1.23 |
| 7:B:203:MPD:H52 | 9:B:311:HOH:O | 1.33 | 1.23 |
| 5:K:203:PI:O3 | 9:K:302:HOH:O | 1.53 | 1.21 |
| 2:R:28[A]:PHE:HE2 | 7:R:204:MPD:C1 | 1.53 | 1.21 |
| 2:T:28[A]:PHE:CE1 | 8:T:204:MRD:H4 | 1.75 | 1.21 |
| 2:V:28[A]:PHE:CE1 | 8:V:204:MRD:C5 | 2.07 | 1.20 |
| 1:K:118[B]:ARG:CZ | 9:K:303:HOH:O | 1.85 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 2:S:11[A]:GLN:OE1 | 9:S:303:HOH:O | 1.58 | 1.20 |
| 2:N:31[B]:GLU:HG3 | 9:N:311:HOH:O | 1.41 | 1.19 |
| 1:B:115[A]:GLU:OE1 | 9:M:301:HOH:O | 1.60 | 1.19 |
| 9:D:511:HOH:O | 7:P:204:MPD:H32 | 1.01 | 1.19 |
| 1:C:32[A]:GLN:HG3 | 1:F:32[A]:GLN:HG3 | 1.20 | 1.19 |
| 2:T:28[A]:PHE:CD1 | 8:T:204:MRD:H4 | 1.78 | 1.18 |
| 2:W:31[B]:GLU:HG3 | 9:W:364:HOH:O | 1.41 | 1.18 |
| 2:V:28[A]:PHE:HD1 | 8:V:204:MRD:C5 | 1.30 | 1.17 |
| 1:A:114[B]:ARG:CG | 5:A:204:PI:P | 2.33 | 1.17 |
| 2:Q:31[B]:GLU:HG3 | 9:Q:307:HOH:O | 1.45 | 1.16 |
| 7:B:203:MPD:C4 | 9:B:311:HOH:O | 1.93 | 1.15 |
| 2:R:28[A]:PHE:CD2 | 7:R:204:MPD:H52 | 1.80 | 1.15 |
| 1:I:32[A]:GLN:HG3 | 1:L:32[A]:GLN:HG3 | 1.17 | 1.14 |
| 1:A:114[B]:ARG:CD | 5:A:204:PI:O4 | 1.94 | 1.14 |
| 1:H:32[A]:GLN:HG3 | 1:K:32[A]:GLN:HG3 | 1.25 | 1.14 |
| 2:R:28[A]:PHE:CE2 | 7:R:204:MPD:C1 | 2.31 | 1.14 |
| 1:B:32[A]:GLN:HG3 | 1:E:32[A]:GLN:HG3 | 1.24 | 1.14 |
| 7:U:204:MPD:H31 | 9:U:317:HOH:O | 0.97 | 1.14 |
| 1:L:62[A]:LYS:NZ | 9:L:304:HOH:O | 1.81 | 1.13 |
| 2:P:109[B]:ASN:ND2 | 9:P:301:HOH:O | 1.69 | 1.12 |
| 1:A:32[A]:GLN:HG3 | 1:D:32[A]:GLN:HG3 | 1.25 | 1.12 |
| 1:H:118[B]:ARG:NH2 | 9:H:304:HOH:O | 1.82 | 1.12 |
| 1:K:118[B]:ARG:NH2 | 9:K:303:HOH:O | 1.80 | 1.12 |
| 2:U:130[B]:GLN:OE1 | 9:U:302:HOH:O | 1.65 | 1.12 |
| 1:A:114[B]:ARG:HG2 | 5:A:204:PI:O2 | 1.48 | 1.11 |
| 1:F:118[B]:ARG:NH2 | 9:F:303:HOH:O | 1.80 | 1.10 |
| 2:R:28[A]:PHE:HD2 | 7:R:204:MPD:C5 | 1.65 | 1.09 |
| 1:C:118[B]:ARG:HD3 | 9:E:354:HOH:O | 1.51 | 1.09 |
| 2:W:28[A]:PHE:CE1 | 7:W:204:MPD:H4 | 1.89 | 1.08 |
| 1:J:124[A]:THR:HG21 | 9:J:312:HOH:O | 1.51 | 1.08 |
| 7:B:203:MPD:C5 | 9:B:311:HOH:O | 1.87 | 1.07 |
| 1:G:115[C]:GLU:OE1 | 2:U:82[C]:ARG:NH2 | 1.87 | 1.07 |
| 1:C:32[A]:GLN:HG3 | 1:F:32[A]:GLN:CG | 1.83 | 1.07 |
| 8:V:204:MRD:O4 | 9:V:301:HOH:O | 1.72 | 1.06 |
| 2:R:28[A]:PHE:HE2 | 7:R:204:MPD:H12 | 1.16 | 1.06 |
| 1:C:32[A]:GLN:CG | 1:F:32[A]:GLN:HG3 | 1.85 | 1.06 |
| 2:P:28[A]:PHE:CD1 | 7:P:204:MPD:H4 | 1.91 | 1.06 |
| 7:O:204:MPD:O4 | 7:O:204:MPD:HM1 | 1.50 | 1.06 |
| 2:U:130[A]:GLN:NE2 | 9:U:301:HOH:O | 1.86 | 1.06 |
| 2:R:28[A]:PHE:CE2 | 7:R:204:MPD:H12 | 1.91 | 1.05 |
| 2:R:28[A]:PHE:HD2 | 7:R:204:MPD:H52 | 1.09 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:O:204:MPD:CM | 7:O:204:MPD:O4 | 2.05 | 1.04 |
| 2:X:28[A]:PHE:CE2 | 7:X:204:MPD:H11 | 1.89 | 1.04 |
| 2:V:130[A]:GLN:OE1 | 9:V:302:HOH:O | 1.75 | 1.04 |
| 2:W:122[A]:THR:HG22 | 9:W:491:HOH:O | 1.56 | 1.04 |
| 2:U:130[A]:GLN:NE2 | 9:U:303:HOH:O | 1.81 | 1.04 |
| 2:W:28[A]:PHE:CD1 | 7:W:204:MPD:H4 | 1.92 | 1.03 |
| 1:A:32[A]:GLN:HG3 | 1:D:32[A]:GLN:CG | 1.88 | 1.03 |
| 1:D:114[B]:ARG:NH2 | 9:D:306:HOH:O | 1.89 | 1.03 |
| 1:I:32[A]:GLN:CG | 1:L:32[A]:GLN:HG3 | 1.89 | 1.02 |
| 1:I:32[A]:GLN:HG3 | 1:L:32[A]:GLN:CG | 1.90 | 1.02 |
| 1:C:42[A]:GLU:OE2 | 9:C:303:HOH:O | 1.76 | 1.01 |
| 1:B:32[A]:GLN:HG3 | 1:E:32[A]:GLN:CG | 1.90 | 1.01 |
| 9:G:397:HOH:O | 1:L:124[A]:THR:HG21 | 1.60 | 1.01 |
| 2:O:130[A]:GLN:OE1 | 9:O:301:HOH:O | 1.78 | 1.01 |
| 1:B:32[A]:GLN:CG | 1:E:32[A]:GLN:HG3 | 1.90 | 0.99 |
| 2:S:28[A]:PHE:CE2 | 7:S:204:MPD:H12 | 1.93 | 0.99 |
| 2:V:28[A]:PHE:HD1 | 8:V:204:MRD:H5C3 | 1.27 | 0.99 |
| 1:A:32[A]:GLN:CG | 1:D:32[A]:GLN:HG3 | 1.92 | 0.99 |
| 2:Q:28[A]:PHE:CD1 | 9:Q:316:HOH:O | 2.15 | 0.99 |
| 2:N:82[B]:ARG:NH1 | 9:N:302:HOH:O | 1.96 | 0.97 |
| 1:K:42[A]:GLU:CG | 2:W:22[A]:MET:HG3 | 1.94 | 0.97 |
| 1:H:115[A]:GLU:OE2 | 9:H:303:HOH:O | 1.80 | 0.97 |
| 2:M:28[A]:PHE:CD1 | 7:M:204:MPD:H4 | 2.00 | 0.97 |
| 9:I:579:HOH:O | 3:X:187:PEB:HAD1 | 1.63 | 0.96 |
| 2:U:130[A]:GLN:OE1 | 9:U:303:HOH:O | 1.83 | 0.96 |
| 2:X:24:ALA:HB3 | 9:X:307:HOH:O | 1.65 | 0.96 |
| 2:M:28[A]:PHE:CE1 | 7:M:204:MPD:H4 | 2.00 | 0.96 |
| 1:H:32[A]:GLN:HG3 | 1:K:32[A]:GLN:CG | 1.96 | 0.95 |
| 2:S:28[A]:PHE:HE2 | 7:S:204:MPD:H13 | 1.29 | 0.95 |
| 2:X:28[A]:PHE:HE2 | 7:X:204:MPD:H12 | 0.78 | 0.95 |
| 1:A:118[B]:ARG:HD2 | 9:F:377:HOH:O | 1.67 | 0.94 |
| 1:I:124[A]:THR:HG21 | 9:I:367:HOH:O | 1.65 | 0.93 |
| 2:P:28[A]:PHE:CE1 | 7:P:204:MPD:H4 | 2.02 | 0.93 |
| 2:S:28[A]:PHE:CE2 | 7:S:204:MPD:H11 | 2.02 | 0.93 |
| 2:Q:28[A]:PHE:CE1 | 9:Q:316:HOH:O | 2.21 | 0.93 |
| 1:C:124[A]:THR:HG21 | 9:C:428:HOH:O | 1.66 | 0.93 |
| 9:G:321:HOH:O | 1:L:118[B]:ARG:HD2 | 1.69 | 0.93 |
| 2:Q:28[A]:PHE:HE1 | 7:Q:204:MPD:HO4 | 1.16 | 0.93 |
| 1:G:120:LEU:HA | 9:G:313:HOH:O | 1.67 | 0.93 |
| 2:Q:28[A]:PHE:HE1 | 7:Q:204:MPD:O4 | 1.52 | 0.93 |
| 1:D:114[B]:ARG:HG3 | 1:D:114[B]:ARG:HH11 | 1.34 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:H:32[A]:GLN:CG | 1:K:32[A]:GLN:HG3 | 1.98 | 0.92 |
| 9:S:463:HOH:O | 2:T:16:THR:HB | 1.69 | 0.92 |
| 1:B:124[A]:THR:HG21 | 9:B:371:HOH:O | 1.70 | 0.92 |
| 2:T:28[A]:PHE:CE1 | 8:T:204:MRD:C4 | 2.45 | 0.91 |
| 2:Q:28[A]:PHE:HE1 | 7:Q:204:MPD:C4 | 1.62 | 0.91 |
| 1:K:124[A]:THR:HG21 | 9:K:398:HOH:O | 1.68 | 0.91 |
| 2:Q:28[A]:PHE:HD1 | 7:Q:204:MPD:H4 | 1.36 | 0.91 |
| 1:F:62[A]:LYS:NZ | 9:F:305:HOH:O | 2.03 | 0.90 |
| 2:V:28[A]:PHE:CD1 | 8:V:204:MRD:H5C3 | 2.01 | 0.90 |
| 1:D:114[B]:ARG:HG3 | 1:D:114[B]:ARG:NH1 | 1.86 | 0.90 |
| 1:D:33:ARG:HB2 | 9:D:506:HOH:O | 1.71 | 0.90 |
| 2:N:31[B]:GLU:CG | 9:N:311:HOH:O | 2.04 | 0.90 |
| 1:K:124[A]:THR:CG2 | 9:K:398:HOH:O | 2.20 | 0.90 |
| 7:R:204:MPD:H12 | 7:R:204:MPD:H52 | 1.55 | 0.89 |
| 2:N:16[B]:THR:HG21 | 9:N:440:HOH:O | 1.72 | 0.89 |
| 1:G:118[A]:ARG:NE | 9:G:304:HOH:O | 2.04 | 0.89 |
| 1:J:124[A]:THR:CG2 | 9:J:312:HOH:O | 2.11 | 0.89 |
| 2:O:141[B]:LYS:NZ | 9:O:302:HOH:O | 1.99 | 0.89 |
| 2:S:22[B]:MET:HA | 2:S:22[B]:MET:HE2 | 1.55 | 0.88 |
| 1:G:124[A]:THR:HG23 | 4:L:203:NO3:O2 | 1.73 | 0.88 |
| 1:K:118[A]:ARG:HD3 | 9:K:389:HOH:O | 1.74 | 0.88 |
| 3:R:188:PEB:HBA1 | 9:R:330:HOH:O | 1.74 | 0.88 |
| 7:Q:204:MPD:HM2 | 9:Q:500:HOH:O | 1.74 | 0.87 |
| 1:F:78:PHE:HA | 9:F:513:HOH:O | 1.70 | 0.87 |
| 2:P:28[A]:PHE:CE1 | 7:P:204:MPD:C4 | 2.55 | 0.87 |
| 1:H:118[A]:ARG:NH2 | 9:H:305:HOH:O | 1.99 | 0.87 |
| 1:J:32[B]:GLN:NE2 | 9:J:304:HOH:O | 2.08 | 0.87 |
| 7:W:204:MPD:O4 | 9:W:302:HOH:O | 1.92 | 0.87 |
| 2:T:146[B]:GLU:OE1 | 9:T:302:HOH:O | 1.92 | 0.87 |
| 2:R:170:ALA:HB2 | 9:R:498:HOH:O | 1.74 | 0.86 |
| 1:A:132:SER:HB2 | 9:A:390:HOH:O | 1.74 | 0.86 |
| 1:A:118[B]:ARG:CD | 9:F:377:HOH:O | 2.18 | 0.86 |
| 2:S:22[B]:MET:HA | 2:S:22[B]:MET:CE | 2.05 | 0.86 |
| 2:X:2:LEU:HD13 | 9:X:302:HOH:O | 1.74 | 0.86 |
| 2:W:122[A]:THR:CG2 | 9:W:491:HOH:O | 2.18 | 0.86 |
| 1:F:118[A]:ARG:NE | 9:F:304:HOH:O | 1.96 | 0.85 |
| 2:X:156:MET:HB3 | 9:X:322:HOH:O | 1.75 | 0.85 |
| 2:M:67:ALA:HB2 | 2:N:16[B]:THR:HG22 | 1.59 | 0.85 |
| 1:D:124[A]:THR:HG21 | 9:D:459:HOH:O | 1.77 | 0.84 |
| 1:J:118[A]:ARG:HD2 | 9:J:333:HOH:O | 1.78 | 0.84 |
| 1:F:39:GLU:O | 1:F:42[A]:GLU:HG3 | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:T:129:VAL:HG13 | 9:T:467:HOH:O | 1.78 | 0.83 |
| 2:R:28[A]:PHE:CE2 | 7:R:204:MPD:H11 | 2.11 | 0.83 |
| 7:R:204:MPD:C1 | 7:R:204:MPD:H52 | 2.08 | 0.83 |
| 2:R:28[A]:PHE:CD2 | 7:R:204:MPD:C5 | 2.51 | 0.83 |
| 2:W:28[A]:PHE:CE1 | 7:W:204:MPD:C4 | 2.58 | 0.83 |
| 2:U:130[B]:GLN:CD | 9:U:302:HOH:O | 2.06 | 0.83 |
| 1:A:114[B]:ARG:HG2 | 5:A:204:PI:O1 | 1.77 | 0.82 |
| 2:Q:28[A]:PHE:CD1 | 7:Q:204:MPD:C4 | 2.48 | 0.82 |
| 1:A:114[B]:ARG:CD | 5:A:204:PI:P | 2.67 | 0.81 |
| 1:D:113:GLN:HE21 | 1:D:114[B]:ARG:HH12 | 1.23 | 0.81 |
| 9:D:511:HOH:O | 7:P:204:MPD:C3 | 1.77 | 0.81 |
| 2:W:111:LEU:HD21 | 9:W:344:HOH:O | 1.79 | 0.81 |
| 2:U:130[A]:GLN:CD | 9:U:301:HOH:O | 2.12 | 0.81 |
| 1:H:43[B]:LYS:NZ | 9:H:306:HOH:O | 2.01 | 0.81 |
| 2:S:28[A]:PHE:CD2 | 7:S:204:MPD:C1 | 2.64 | 0.81 |
| 2:M:82[C]:ARG:NH1 | 9:M:302:HOH:O | 2.14 | 0.80 |
| 1:H:118[B]:ARG:CD | 9:J:383:HOH:O | 2.29 | 0.80 |
| 1:I:154:ALA:HB1 | 9:I:458:HOH:O | 1.80 | 0.80 |
| 3:R:188:PEB:CBA | 9:R:330:HOH:O | 2.27 | 0.80 |
| 1:D:114[B]:ARG:CG | 1:D:114[B]:ARG:HH11 | 1.93 | 0.79 |
| 2:P:28[A]:PHE:HD1 | 7:P:204:MPD:H4 | 1.46 | 0.78 |
| 1:D:114[C]:ARG:HG3 | 5:D:204:PI:O4 | 1.84 | 0.77 |
| 1:K:42[A]:GLU:HG2 | 2:W:22[A]:MET:HG3 | 1.66 | 0.76 |
| 1:H:99:VAL:HG13 | 9:T:335:HOH:O | 1.84 | 0.76 |
| 2:P:16:THR:HG23 | 2:Q:67:ALA:HB2 | 1.66 | 0.76 |
| 2:W:31[B]:GLU:CG | 9:W:364:HOH:O | 2.14 | 0.76 |
| 1:B:124[A]:THR:CG2 | 9:B:371:HOH:O | 2.30 | 0.76 |
| 4:A:203:NO3:O2 | 1:F:118[A]:ARG:NH2 | 2.19 | 0.76 |
| 1:F:124[A]:THR:HG21 | 9:F:474:HOH:O | 1.86 | 0.76 |
| 2:S:28[A]:PHE:CD2 | 7:S:204:MPD:H12 | 2.21 | 0.76 |
| 9:I:390:HOH:O | 1:K:118[B]:ARG:HD2 | 1.86 | 0.75 |
| 2:P:82[A]:ARG:NH1 | 3:P:186:PEB:O2C | 2.16 | 0.75 |
| 1:B:118[A]:ARG:NH2 | 9:B:303:HOH:O | 2.04 | 0.75 |
| 3:R:187:PEB:HBA2 | 9:R:354:HOH:O | 1.87 | 0.75 |
| 2:M:28[A]:PHE:CE1 | 7:M:204:MPD:C4 | 2.66 | 0.75 |
| 2:N:83:ASP:HB3 | 9:N:320:HOH:O | 1.86 | 0.75 |
| 2:Q:31[B]:GLU:CG | 9:Q:307:HOH:O | 2.14 | 0.75 |
| 7:B:203:MPD:H4 | 9:B:311:HOH:O | 1.70 | 0.75 |
| 2:T:28[A]:PHE:HD1 | 8:T:204:MRD:H4 | 1.44 | 0.74 |
| 2:V:28[A]:PHE:CE1 | 8:V:204:MRD:C4 | 2.50 | 0.74 |
| 3:Q:187:PEB:HMB2 | 3:Q:187:PEB:HNA | 1.53 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:U:89:ARG:O | 2:U:92[B]:THR:HG22 | 1.88 | 0.74 |
| 1:A:114[B]:ARG:CG | 5:A:204:PI:O2 | 2.32 | 0.73 |
| 1:F:78:PHE:HD1 | 9:F:503:HOH:O | 1.70 | 0.73 |
| 2:W:87:ILE:HD11 | 9:W:344:HOH:O | 1.87 | 0.73 |
| 1:F:115[B]:GLU:HG3 | 1:F:118[B]:ARG:NH2 | 2.04 | 0.72 |
| 1:G:62[B]:LYS:NZ | 9:G:305:HOH:O | 2.22 | 0.72 |
| 1:A:118[A]:ARG:NH2 | 9:A:303:HOH:O | 1.84 | 0.72 |
| 1:F:115[B]:GLU:HG3 | 1:F:118[B]:ARG:HH22 | 1.55 | 0.72 |
| 1:I:87[B]:LYS:NZ | 9:I:304:HOH:O | 2.19 | 0.72 |
| 2:R:129:VAL:HG11 | 9:R:320:HOH:O | 1.90 | 0.72 |
| 1:F:81:LYS:HB2 | 9:F:513:HOH:O | 1.88 | 0.72 |
| 3:T:187:PEB:HMB2 | 3:T:187:PEB:HNA | 1.55 | 0.72 |
| 1:A:114[B]:ARG:CG | 5:A:204:PI:O1 | 2.32 | 0.72 |
| 1:B:118[B]:ARG:NE | 9:D:307:HOH:O | 2.22 | 0.72 |
| 1:F:91:ARG:HG2 | 9:F:350:HOH:O | 1.90 | 0.71 |
| 2:V:82[A]:ARG:NH1 | 3:V:186:PEB:O2C | 2.23 | 0.71 |
| 3:O:187:PEB:HNA | 3:O:187:PEB:HMB2 | 1.55 | 0.71 |
| 1:I:159:ALA:HB3 | 9:I:309:HOH:O | 1.88 | 0.71 |
| 3:N:187:PEB:HMB2 | 3:N:187:PEB:HNA | 1.56 | 0.71 |
| 1:I:118[B]:ARG:HD2 | 9:K:325:HOH:O | 1.91 | 0.71 |
| 1:H:118[B]:ARG:HD2 | 9:J:383:HOH:O | 1.90 | 0.70 |
| 2:X:153:LEU:HD22 | 9:X:436:HOH:O | 1.90 | 0.70 |
| 2:R:180:ILE:HG13 | 9:R:320:HOH:O | 1.92 | 0.70 |
| 2:T:28[A]:PHE:HE1 | 8:T:204:MRD:C4 | 1.75 | 0.70 |
| 1:A:124[A]:THR:HG21 | 9:A:486:HOH:O | 1.90 | 0.70 |
| 1:K:118[A]:ARG:CD | 9:K:389:HOH:O | 2.36 | 0.70 |
| 9:I:390:HOH:O | 1:K:118[B]:ARG:CD | 2.37 | 0.70 |
| 5:F:203:PI:O4 | 9:F:301:HOH:O | 0.70 | 0.70 |
| 1:G:118[B]:ARG:CD | 9:L:318:HOH:O | 2.40 | 0.70 |
| 3:W:187:PEB:HNA | 3:W:187:PEB:HMB2 | 1.56 | 0.70 |
| 2:X:82[A]:ARG:NH1 | 3:X:186:PEB:O2C | 2.23 | 0.70 |
| 1:H:118[B]:ARG:HD3 | 9:J:383:HOH:O | 1.89 | 0.69 |
| 9:G:397:HOH:O | 1:L:124[A]:THR:CG2 | 2.30 | 0.69 |
| 2:O:89:ARG:O | 2:O:92[A]:THR:HG22 | 1.92 | 0.69 |
| 1:F:120:LEU:HD22 | 9:F:502:HOH:O | 1.94 | 0.68 |
| 1:F:54[B]:GLU:HG2 | 9:F:461:HOH:O | 1.93 | 0.67 |
| 1:F:89:TYR:HB2 | 9:F:532:HOH:O | 1.93 | 0.67 |
| 2:W:28[A]:PHE:HD1 | 7:W:204:MPD:H4 | 1.54 | 0.67 |
| 2:W:109[B]:ASN:OD1 | 9:W:303:HOH:O | 2.13 | 0.67 |
| 1:G:118[B]:ARG:HD3 | 9:L:318:HOH:O | 1.94 | 0.67 |
| 2:S:28[A]:PHE:CD2 | 7:S:204:MPD:H11 | 2.28 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:I:124[A]:THR:CG2 | 9:I:367:HOH:O | 2.32 | 0.67 |
| 2:P:65:ILE:O | 9:P:302:HOH:O | 2.13 | 0.67 |
| 3:S:187:PEB:HMB2 | 3:S:187:PEB:HNA | 1.60 | 0.67 |
| 2:R:155[B]:LYS:HA | 2:R:155[B]:LYS:HE2 | 1.77 | 0.66 |
| 2:O:82[A]:ARG:NH1 | 3:O:186:PEB:O2C | 2.23 | 0.66 |
| 3:M:187:PEB:HNA | 3:M:187:PEB:HMB2 | 1.60 | 0.66 |
| 2:P:74:ASN:HA | 9:P:329:HOH:O | 1.95 | 0.66 |
| 2:W:16[B]:THR:HG21 | 9:W:354:HOH:O | 1.95 | 0.66 |
| 9:A:307:HOH:O | 2:O:82[B]:ARG:HD3 | 1.94 | 0.66 |
| 2:T:82:ARG:NH1 | 3:T:186:PEB:O2C | 2.27 | 0.66 |
| 1:K:42[A]:GLU:HG2 | 2:W:22[A]:MET:CG | 2.25 | 0.66 |
| 2:O:130[B]:GLN:OE1 | 9:O:303:HOH:O | 2.13 | 0.66 |
| 1:G:28:GLN:HG2 | 9:S:503:HOH:O | 1.96 | 0.66 |
| 3:X:187:PEB:HMB2 | 3:X:187:PEB:HNA | 1.61 | 0.65 |
| 3:U:187:PEB:HNA | 3:U:187:PEB:HMB2 | 1.60 | 0.65 |
| 3:P:187:PEB:HMB2 | 3:P:187:PEB:HNA | 1.60 | 0.65 |
| 2:R:28[A]:PHE:CE2 | 7:R:204:MPD:H52 | 2.30 | 0.65 |
| 2:R:38:ALA:HA | 9:R:354:HOH:O | 1.97 | 0.65 |
| 2:S:89:ARG:O | 2:S:92[B]:THR:HG22 | 1.96 | 0.65 |
| 1:K:42[A]:GLU:HG3 | 2:W:22[A]:MET:HG3 | 1.77 | 0.65 |
| 2:N:89:ARG:O | 2:N:92[A]:THR:HG22 | 1.97 | 0.64 |
| 1:H:124[A]:THR:HG21 | 9:H:422:HOH:O | 1.98 | 0.64 |
| 2:T:148:ARG:NH1 | 9:T:305:HOH:O | 2.29 | 0.64 |
| 2:V:89:ARG:O | 2:V:92[B]:THR:HG22 | 1.97 | 0.64 |
| 7:O:204:MPD:HM1 | 7:O:204:MPD:HO4 | 1.63 | 0.64 |
| 5:H:203:PI:O2 | 9:H:301:HOH:O | 0.64 | 0.64 |
| 1:E:118[B]:ARG:NH2 | 9:E:307:HOH:O | 2.26 | 0.64 |
| 1:H:27:VAL:HG12 | 9:T:505:HOH:O | 1.98 | 0.64 |
| 2:U:122[A]:THR:HG22 | 9:U:528:HOH:O | 1.96 | 0.64 |
| 1:A:118[A]:ARG:NH1 | 9:A:304:HOH:O | 2.29 | 0.64 |
| 2:R:155[B]:LYS:CA | 2:R:155[B]:LYS:HE2 | 2.28 | 0.64 |
| 7:U:204:MPD:O4 | 7:U:204:MPD:HM1 | 1.97 | 0.64 |
| 1:F:131:LEU:HB3 | 9:F:347:HOH:O | 1.98 | 0.63 |
| 8:T:204:MRD:H5C3 | 8:T:204:MRD:O2 | 1.97 | 0.63 |
| 1:E:118[A]:ARG:NH2 | 9:E:305:HOH:O | 2.12 | 0.63 |
| 2:S:76:ARG:NH2 | 9:S:305:HOH:O | 2.25 | 0.63 |
| 1:H:31:ILE:HD11 | 9:T:505:HOH:O | 1.97 | 0.63 |
| 2:U:146:GLU:OE2 | 2:U:153[A]:LEU:HD22 | 1.99 | 0.63 |
| 3:V:187:PEB:HMB2 | 3:V:187:PEB:HNA | 1.63 | 0.63 |
| 2:M:28[A]:PHE:HD1 | 7:M:204:MPD:H4 | 1.60 | 0.63 |
| 2:W:22[A]:MET:SD | 2:W:25:LEU:HD12 | 2.38 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:U:204:MPD:C3 | 9:U:317:HOH:O | 1.79 | 0.63 |
| 3:A:167:PEB:HMB2 | 3:A:167:PEB:HNA | 1.64 | 0.62 |
| 1:F:77:THR:HG22 | 9:F:503:HOH:O | 2.00 | 0.62 |
| 2:X:89:ARG:O | 2:X:92[B]:THR:HG22 | 1.99 | 0.62 |
| 2:V:28[A]:PHE:HE1 | 8:V:204:MRD:C4 | 1.70 | 0.62 |
| 2:U:82[A]:ARG:NH1 | 3:U:186:PEB:O2C | 2.24 | 0.62 |
| 2:W:28[A]:PHE:HE1 | 7:W:204:MPD:C4 | 1.88 | 0.62 |
| 3:Q:186:PEB:HMB2 | 3:Q:186:PEB:HNA | 1.65 | 0.62 |
| 2:X:28[A]:PHE:CD2 | 7:X:204:MPD:H12 | 2.30 | 0.61 |
| 3:J:167:PEB:HNA | 3:J:167:PEB:HMB2 | 1.65 | 0.61 |
| 3:R:187:PEB:HNA | 3:R:187:PEB:HMB2 | 1.66 | 0.61 |
| 1:J:33:ARG:HB2 | 9:S:503:HOH:O | 2.01 | 0.61 |
| 1:A:128:VAL:HG12 | 9:A:390:HOH:O | 2.00 | 0.61 |
| 2:T:89:ARG:O | 2:T:92[B]:THR:HG22 | 2.01 | 0.61 |
| 9:B:326:HOH:O | 1:D:118[B]:ARG:HD3 | 2.01 | 0.60 |
| 2:X:28[A]:PHE:CD2 | 7:X:204:MPD:C1 | 2.78 | 0.60 |
| 2:O:141[B]:LYS:HE3 | 2:O:164:ARG:HB2 | 1.82 | 0.60 |
| 1:G:118[A]:ARG:CZ | 9:G:304:HOH:O | 2.48 | 0.60 |
| 3:L:167:PEB:HNA | 3:L:167:PEB:HMB2 | 1.66 | 0.60 |
| 1:J:102:THR:N | 9:J:305:HOH:O | 2.34 | 0.60 |
| 3:I:167:PEB:HMB2 | 3:I:167:PEB:HNA | 1.67 | 0.60 |
| 1:F:124[A]:THR:CG2 | 9:F:474:HOH:O | 2.48 | 0.60 |
| 1:D:114[B]:ARG:CZ | 9:D:301:HOH:O | 2.49 | 0.60 |
| 2:U:28[A]:PHE:CD2 | 7:U:204:MPD:H32 | 2.37 | 0.59 |
| 2:Q:16:THR:HG23 | 2:R:67:ALA:HB2 | 1.82 | 0.59 |
| 2:M:82[A]:ARG:NH1 | 3:M:186:PEB:O2C | 2.30 | 0.59 |
| 1:B:118[A]:ARG:NE | 9:B:303:HOH:O | 2.31 | 0.59 |
| 8:T:204:MRD:HMC2 | 9:T:517:HOH:O | 2.02 | 0.59 |
| 3:E:167:PEB:HMB2 | 3:E:167:PEB:HNA | 1.68 | 0.58 |
| 1:F:120:LEU:CD2 | 9:F:502:HOH:O | 2.51 | 0.58 |
| 1:I:156:LEU:HA | 9:I:309:HOH:O | 2.04 | 0.58 |
| 2:Q:168:LEU:HD11 | 9:Q:360:HOH:O | 2.04 | 0.58 |
| 1:G:118[B]:ARG:HD2 | 9:L:318:HOH:O | 2.04 | 0.58 |
| 3:G:167:PEB:HMB2 | 3:G:167:PEB:HNA | 1.68 | 0.58 |
| 1:J:114:ARG:HG3 | 9:J:473:HOH:O | 2.03 | 0.58 |
| 2:V:130[B]:GLN:NE2 | 9:V:303:HOH:O | 2.24 | 0.58 |
| 2:V:22[A]:MET:HE3 | 9:V:422:HOH:O | 2.03 | 0.58 |
| 2:N:82[A]:ARG:NH1 | 3:N:186:PEB:O2C | 2.26 | 0.58 |
| 1:G:115[C]:GLU:CD | 2:U:82[C]:ARG:NH2 | 2.55 | 0.58 |
| 1:G:118[B]:ARG:HD2 | 9:G:306:HOH:O | 2.03 | 0.58 |
| 2:N:22[A]:MET:CE | 2:N:25:LEU:HD12 | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:O:204:MPD:O4 | 7:O:204:MPD:HM2 | 2.00 | 0.58 |
| 2:T:6:SER:HB3 | 9:T:335:HOH:O | 2.04 | 0.57 |
| 2:W:89:ARG:O | 2:W:92[B]:THR:HG22 | 2.04 | 0.57 |
| 1:C:124[A]:THR:CG2 | 9:C:428:HOH:O | 2.37 | 0.57 |
| 2:U:9:VAL:HG23 | 9:U:369:HOH:O | 2.04 | 0.57 |
| 3:K:167:PEB:HNA | 3:K:167:PEB:HMB2 | 1.69 | 0.57 |
| 1:E:70:GLY:O | 9:E:306:HOH:O | 2.16 | 0.57 |
| 2:W:29:ILE:HD13 | 7:W:204:MPD:H52 | 1.87 | 0.57 |
| 3:H:167:PEB:HNA | 3:H:167:PEB:HMB2 | 1.70 | 0.57 |
| 1:A:118[B]:ARG:HD3 | 9:F:377:HOH:O | 1.96 | 0.57 |
| 1:I:115[B]:GLU:CD | 9:I:303:HOH:O | 2.43 | 0.56 |
| 2:R:28[A]:PHE:CD2 | 7:R:204:MPD:C1 | 2.87 | 0.56 |
| 7:U:204:MPD:C4 | 9:U:317:HOH:O | 2.35 | 0.56 |
| 7:B:203:MPD:C3 | 9:B:311:HOH:O | 2.38 | 0.56 |
| 1:I:118[B]:ARG:NH2 | 9:I:303:HOH:O | 2.35 | 0.56 |
| 2:X:153:LEU:HB2 | 9:X:436:HOH:O | 2.04 | 0.56 |
| 1:L:118[A]:ARG:NH1 | 9:L:307:HOH:O | 2.39 | 0.56 |
| 2:U:24:ALA:HB3 | 9:U:496:HOH:O | 2.06 | 0.56 |
| 2:W:82[A]:ARG:NH1 | 3:W:186:PEB:O1C | 2.36 | 0.56 |
| 3:B:167:PEB:HMB2 | 3:B:167:PEB:HNA | 1.71 | 0.55 |
| 8:T:204:MRD:C5 | 8:T:204:MRD:O2 | 2.54 | 0.55 |
| 5:H:203:PI:O4 | 9:H:307:HOH:O | 2.17 | 0.55 |
| 2:X:146:GLU:HA | 9:X:436:HOH:O | 2.05 | 0.55 |
| 2:R:52:ASP:HB2 | 9:R:330:HOH:O | 2.06 | 0.55 |
| 2:Q:82[A]:ARG:NH2 | 3:Q:186:PEB:O2C | 2.40 | 0.55 |
| 3:W:186:PEB:HNA | 3:W:186:PEB:HMB2 | 1.72 | 0.55 |
| 3:F:167:PEB:HMB2 | 3:F:167:PEB:HNA | 1.71 | 0.55 |
| 2:Q:29:ILE:HD13 | 7:Q:204:MPD:H52 | 1.89 | 0.55 |
| 1:A:114[B]:ARG:HG3 | 5:A:204:PI:O1 | 2.07 | 0.55 |
| 3:C:167:PEB:HMB2 | 3:C:167:PEB:HNA | 1.72 | 0.55 |
| 1:D:124[A]:THR:CG2 | 9:D:459:HOH:O | 2.46 | 0.55 |
| 1:H:124[A]:THR:CG2 | 9:H:422:HOH:O | 2.54 | 0.54 |
| 2:W:132:MET:HB2 | 9:W:307:HOH:O | 2.05 | 0.54 |
| 1:C:33:ARG:HG2 | 9:F:366:HOH:O | 2.08 | 0.54 |
| 1:I:30[B]:SER:OG | 7:U:204:MPD:H51 | 2.07 | 0.54 |
| 3:U:186:PEB:HMB2 | 3:U:186:PEB:HNA | 1.72 | 0.54 |
| 1:D:118[B]:ARG:HD2 | 9:D:388:HOH:O | 2.06 | 0.54 |
| 2:O:76:ARG:NH2 | 9:O:306:HOH:O | 2.40 | 0.54 |
| 2:V:178[B]:ARG:HG3 | 2:V:178[B]:ARG:NH2 | 2.22 | 0.54 |
| 1:G:118[A]:ARG:NH1 | 9:G:309:HOH:O | 2.40 | 0.53 |
| 2:T:146[B]:GLU:HG2 | 9:T:301:HOH:O | 2.06 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:T:186:PEB:HNA | 3:T:186:PEB:HMB2 | 1.74 | 0.53 |
| 1:D:114[C]:ARG:HG3 | 9:D:301:HOH:O | 2.07 | 0.53 |
| 2:R:28[B]:PHE:HA | 2:R:31[B]:GLU:HG2 | 1.89 | 0.53 |
| 3:R:186:PEB:HNA | 3:R:186:PEB:HMB2 | 1.73 | 0.53 |
| 2:T:176:PHE:HD1 | 9:T:467:HOH:O | 1.91 | 0.53 |
| 2:P:148:ARG:NH1 | 3:P:188:PEB:HND | 2.07 | 0.53 |
| 2:U:28[A]:PHE:CD2 | 7:U:204:MPD:C3 | 2.92 | 0.53 |
| 1:J:33:ARG:HD3 | 9:S:503:HOH:O | 2.08 | 0.52 |
| 2:R:179:VAL:HG12 | 9:R:320:HOH:O | 2.08 | 0.52 |
| 7:U:204:MPD:O4 | 7:U:204:MPD:CM | 2.58 | 0.52 |
| 2:U:148:ARG:NH1 | 3:U:188:PEB:HND | 2.07 | 0.52 |
| 2:Q:26:LYS:NZ | 9:Q:302:HOH:O | 2.42 | 0.52 |
| 2:R:163:ASP:HB3 | 9:R:443:HOH:O | 2.10 | 0.52 |
| 3:M:186:PEB:HNA | 3:M:186:PEB:HMB2 | 1.75 | 0.52 |
| 2:U:19:VAL:HG21 | 9:U:369:HOH:O | 2.10 | 0.52 |
| 2:R:82:ARG:NH1 | 3:R:186:PEB:O2C | 2.40 | 0.51 |
| 2:S:22[B]:MET:CE | 2:S:22[B]:MET:CA | 2.83 | 0.51 |
| 3:W:187:PEB:HMB2 | 3:W:187:PEB:NA | 2.25 | 0.51 |
| 2:X:28[A]:PHE:CD2 | 7:X:204:MPD:H11 | 2.41 | 0.51 |
| 1:C:5:VAL:HG11 | 7:O:204:MPD:H13 | 1.91 | 0.51 |
| 2:R:135:GLN:HG2 | 3:R:188:PEB:C1B | 2.41 | 0.51 |
| 3:N:186:PEB:HNA | 3:N:186:PEB:HMB2 | 1.74 | 0.51 |
| 2:R:28[A]:PHE:CD2 | 7:R:204:MPD:H12 | 2.41 | 0.51 |
| 1:A:128:VAL:CG1 | 9:A:390:HOH:O | 2.59 | 0.51 |
| 2:N:22[A]:MET:HE2 | 2:N:25:LEU:HD12 | 1.93 | 0.51 |
| 2:U:130[B]:GLN:HE21 | 2:U:130[B]:GLN:HA | 1.76 | 0.50 |
| 2:X:7:ARG:HA | 9:X:302:HOH:O | 2.10 | 0.50 |
| 3:P:186:PEB:HMB2 | 3:P:186:PEB:HNA | 1.77 | 0.50 |
| 3:O:186:PEB:HNA | 3:O:186:PEB:HMB2 | 1.75 | 0.50 |
| 3:S:188:PEB:HMB3 | 3:S:188:PEB:HNA | 1.76 | 0.50 |
| 2:T:148:ARG:NH1 | 3:T:188:PEB:HND | 2.10 | 0.50 |
| 1:A:118[A]:ARG:NH1 | 1:F:124[A]:THR:OG1 | 2.45 | 0.50 |
| 1:C:102:THR:N | 9:C:307:HOH:O | 2.41 | 0.50 |
| 2:T:31[A]:GLU:OE1 | 9:T:303:HOH:O | 2.20 | 0.50 |
| 1:C:114:ARG:HG3 | 9:C:413:HOH:O | 2.11 | 0.50 |
| 1:C:118[A]:ARG:NH1 | 1:E:124[A]:THR:OG1 | 2.45 | 0.50 |
| 2:W:101[A]:SER:HB2 | 9:W:322:HOH:O | 2.11 | 0.50 |
| 1:C:115[A]:GLU:HG3 | 5:C:204:PI:O1 | 2.12 | 0.49 |
| 3:D:167:PEB:HNA | 3:D:167:PEB:HMB2 | 1.76 | 0.49 |
| 1:D:114[B]:ARG:CZ | 9:D:306:HOH:O | 2.47 | 0.49 |
| 1:I:115[B]:GLU:OE2 | 9:I:303:HOH:O | 2.19 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 9:I:390:HOH:O | 1:K:118[B]:ARG:HD3 | 2.06 | 0.49 |
| 2:O:31:GLU:OE2 | 9:O:304:HOH:O | 2.19 | 0.49 |
| 2:Q:148:ARG:NH1 | 9:Q:303:HOH:O | 2.46 | 0.49 |
| 2:R:28[A]:PHE:CD2 | 7:R:204:MPD:H11 | 2.47 | 0.49 |
| 9:I:579:HOH:O | 1:L:24:LEU:HD12 | 2.11 | 0.49 |
| 9:H:372:HOH:O | 1:J:118[A]:ARG:HD3 | 2.12 | 0.49 |
| 3:X:188:PEB:HMB3 | 3:X:188:PEB:HNA | 1.76 | 0.49 |
| 1:C:32[A]:GLN:HG3 | 1:F:32[A]:GLN:HG2 | 1.86 | 0.49 |
| 1:F:102:THR:N | 9:F:308:HOH:O | 2.43 | 0.49 |
| 3:Q:188:PEB:HMB3 | 3:Q:188:PEB:HNA | 1.78 | 0.49 |
| 3:V:186:PEB:HMB2 | 3:V:186:PEB:HNA | 1.78 | 0.49 |
| 1:H:118[A]:ARG:NH1 | 1:J:124[A]:THR:OG1 | 2.46 | 0.49 |
| 3:R:188:PEB:HMB3 | 3:R:188:PEB:HNA | 1.77 | 0.49 |
| 9:I:579:HOH:O | 3:X:187:PEB:HMD1 | 2.12 | 0.49 |
| 1:B:118[B]:ARG:HD2 | 9:D:307:HOH:O | 2.13 | 0.49 |
| 1:F:54[B]:GLU:CG | 9:F:461:HOH:O | 2.55 | 0.49 |
| 1:C:118[A]:ARG:NH2 | 9:C:305:HOH:O | 2.36 | 0.48 |
| 1:D:113:GLN:HE21 | 1:D:114[B]:ARG:NH1 | 2.03 | 0.48 |
| 1:B:118[B]:ARG:CD | 9:D:307:HOH:O | 2.61 | 0.48 |
| 1:E:124[A]:THR:HG21 | 9:E:492:HOH:O | 2.13 | 0.48 |
| 2:Q:168:LEU:HD21 | 9:Q:360:HOH:O | 2.13 | 0.48 |
| 2:Q:101[A]:SER:HB2 | 9:Q:337:HOH:O | 2.12 | 0.48 |
| 2:S:75:ARG:NH2 | 9:S:312:HOH:O | 2.45 | 0.48 |
| 1:E:114:ARG:HG3 | 9:E:450:HOH:O | 2.14 | 0.48 |
| 1:F:156:LEU:HB3 | 9:F:347:HOH:O | 2.14 | 0.48 |
| 1:E:1[A]:MET:HG3 | 1:E:103:GLY:HA3 | 1.95 | 0.48 |
| 2:R:148:ARG:NH1 | 3:R:188:PEB:HND | 2.11 | 0.48 |
| 2:M:27:GLN:HE21 | 2:M:31[A]:GLU:HG3 | 1.79 | 0.48 |
| 2:P:89:ARG:NH2 | 9:P:306:HOH:O | 2.45 | 0.48 |
| 2:Q:29:ILE:HD13 | 7:Q:204:MPD:C5 | 2.44 | 0.47 |
| 2:U:133:LYS:HE3 | 2:U:173:SER:HB3 | 1.96 | 0.47 |
| 3:X:186:PEB:HMB2 | 3:X:186:PEB:HNA | 1.79 | 0.47 |
| 2:N:148:ARG:NH1 | 3:N:188:PEB:HND | 2.13 | 0.47 |
| 2:T:122[B]:THR:HG22 | 9:T:477:HOH:O | 2.14 | 0.47 |
| 2:W:148:ARG:NH1 | 3:W:188:PEB:HND | 2.13 | 0.47 |
| 3:R:187:PEB:HHA1 | 3:R:187:PEB:HBA3 | 1.96 | 0.47 |
| 1:K:1[A]:MET:HE1 | 1:K:104:PRO:HG3 | 1.95 | 0.47 |
| 1:J:43[B]:LYS:NZ | 9:J:307:HOH:O | 2.47 | 0.47 |
| 3:H:167:PEB:NA | 3:H:167:PEB:HMB2 | 2.29 | 0.47 |
| 2:X:101[A]:SER:HB2 | 9:X:318:HOH:O | 2.13 | 0.47 |
| 2:T:28[B]:PHE:HA | 2:T:31[B]:GLU:HG2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:G:28:GLN:HG3 | 1:J:32[B]:GLN:HG2 | 1.97 | 0.46 |
| 3:N:188:PEB:HNA | 3:N:188:PEB:HMB3 | 1.81 | 0.46 |
| 2:S:148:ARG:NH1 | 3:S:188:PEB:HND | 2.12 | 0.46 |
| 1:D:51:VAL:HG21 | 9:D:413:HOH:O | 2.15 | 0.46 |
| 1:F:115[B]:GLU:HG3 | 9:F:303:HOH:O | 2.15 | 0.46 |
| 2:U:144:PRO:HG2 | 2:U:153[B]:LEU:HD21 | 1.97 | 0.46 |
| 2:M:67:ALA:HB2 | 2:N:16[A]:THR:HG23 | 1.97 | 0.46 |
| 2:O:148:ARG:NH1 | 3:O:188:PEB:HND | 2.14 | 0.46 |
| 2:W:129:VAL:HG13 | 9:W:307:HOH:O | 2.15 | 0.46 |
| 1:A:124[A]:THR:OG1 | 1:F:118[A]:ARG:NH1 | 2.49 | 0.45 |
| 1:G:124[A]:THR:OG1 | 1:L:118[A]:ARG:NH1 | 2.50 | 0.45 |
| 2:P:146:GLU:OE1 | 2:P:153:LEU:HD22 | 2.17 | 0.45 |
| 2:T:28[A]:PHE:HE1 | 8:T:204:MRD:C5 | 2.26 | 0.45 |
| 1:H:43[A]:LYS:HD3 | 9:H:492:HOH:O | 2.16 | 0.45 |
| 2:P:22[A]:MET:HA | 2:P:22[A]:MET:HE2 | 1.99 | 0.45 |
| 1:F:92:LEU:HD23 | 9:F:350:HOH:O | 2.16 | 0.45 |
| 2:W:16[A]:THR:HG23 | 2:X:67:ALA:HB2 | 1.97 | 0.45 |
| 1:F:160:ILE:CD1 | 9:F:347:HOH:O | 2.64 | 0.45 |
| 1:G:28:GLN:CG | 1:J:32[B]:GLN:HG2 | 2.47 | 0.45 |
| 2:T:28[A]:PHE:CE1 | 8:T:204:MRD:C5 | 2.99 | 0.45 |
| 2:Q:135:GLN:HG2 | 3:Q:188:PEB:C1B | 2.46 | 0.45 |
| 1:F:160:ILE:HD11 | 9:F:347:HOH:O | 2.17 | 0.45 |
| 1:H:42[A]:GLU:HG2 | 9:H:492:HOH:O | 2.15 | 0.45 |
| 2:M:5:PHE:HE1 | 2:M:28[A]:PHE:CD1 | 2.35 | 0.45 |
| 2:Q:148:ARG:NH1 | 3:Q:188:PEB:HND | 2.14 | 0.45 |
| 3:W:188:PEB:HMB3 | 3:W:188:PEB:HNA | 1.82 | 0.45 |
| 1:K:62[B]:LYS:HG2 | 1:K:63:TYR:CE2 | 2.52 | 0.45 |
| 2:V:178[B]:ARG:HH21 | 2:V:178[B]:ARG:HG3 | 1.81 | 0.45 |
| 2:U:130[A]:GLN:CD | 9:U:303:HOH:O | 2.05 | 0.45 |
| 3:U:188:PEB:HMB3 | 3:U:188:PEB:HNA | 1.81 | 0.45 |
| 2:V:148:ARG:NH1 | 3:V:188:PEB:HND | 2.15 | 0.45 |
| 2:N:82[B]:ARG:HB2 | 2:N:82[B]:ARG:NH1 | 2.32 | 0.44 |
| 2:O:27:GLN:NE2 | 2:O:31:GLU:OE2 | 2.44 | 0.44 |
| 1:A:121:GLY:HA2 | 9:A:394:HOH:O | 2.16 | 0.44 |
| 1:G:163:LEU:O | 1:L:118[A]:ARG:HD2 | 2.18 | 0.44 |
| 1:D:113:GLN:NE2 | 1:D:114[B]:ARG:HH12 | 2.03 | 0.44 |
| 2:X:10:VAL:CG2 | 9:X:302:HOH:O | 2.66 | 0.44 |
| 3:T:187:PEB:HHA1 | 3:T:187:PEB:HBA3 | 2.00 | 0.44 |
| 9:G:321:HOH:O | 1:L:118[B]:ARG:CD | 2.45 | 0.44 |
| 2:U:31[B]:GLU:HG3 | 9:U:349:HOH:O | 2.18 | 0.44 |
| 1:J:118[A]:ARG:CD | 9:J:333:HOH:O | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:T:125:THR:HG21 | 2:T:183:LEU:HD13 | 1.99 | 0.44 |
| 2:T:24:ALA:HB3 | 9:T:402:HOH:O | 2.17 | 0.44 |
| 1:E:61[A]:GLN:NE2 | 9:E:313:HOH:O | 2.50 | 0.43 |
| 1:L:1[A]:MET:HG3 | 1:L:103:GLY:HA3 | 2.00 | 0.43 |
| 2:O:130[B]:GLN:NE2 | 9:O:305:HOH:O | 2.31 | 0.43 |
| 2:U:31[B]:GLU:HG3 | 9:U:458:HOH:O | 2.18 | 0.43 |
| 2:V:183:LEU:HD22 | 9:V:481:HOH:O | 2.18 | 0.43 |
| 3:M:187:PEB:NA | 3:M:187:PEB:HMB2 | 2.31 | 0.43 |
| 3:O:188:PEB:HMB3 | 3:O:188:PEB:HNA | 1.83 | 0.43 |
| 9:C:342:HOH:O | 7:O:204:MPD:CM | 2.66 | 0.43 |
| 2:Q:24:ALA:HB3 | 9:Q:364:HOH:O | 2.19 | 0.43 |
| 3:T:188:PEB:HNA | 3:T:188:PEB:HMB3 | 1.83 | 0.43 |
| 2:U:31[B]:GLU:CG | 9:U:458:HOH:O | 2.67 | 0.43 |
| 1:E:118[A]:ARG:NH1 | 9:E:314:HOH:O | 2.51 | 0.43 |
| 3:X:188:PEB:HMC1 | 9:X:316:HOH:O | 2.19 | 0.43 |
| 3:P:187:PEB:HBA3 | 3:P:187:PEB:HHA1 | 2.00 | 0.43 |
| 3:V:188:PEB:HNA | 3:V:188:PEB:HMB3 | 1.83 | 0.43 |
| 1:A:114[B]:ARG:CG | 5:A:204:PI:O4 | 2.45 | 0.43 |
| 4:I:203:NO3:O2 | 1:K:118[A]:ARG:NH2 | 2.51 | 0.43 |
| 1:C:2:LYS:HB3 | 9:C:307:HOH:O | 2.18 | 0.43 |
| 3:E:167:PEB:HMB2 | 3:E:167:PEB:NA | 2.32 | 0.43 |
| 2:O:31:GLU:HB3 | 9:O:358:HOH:O | 2.18 | 0.42 |
| 2:R:159:PRO:HB3 | 9:R:574:HOH:O | 2.18 | 0.42 |
| 1:C:1[B]:MET:HG3 | 1:C:103:GLY:HA3 | 2.01 | 0.42 |
| 2:N:146:GLU:OE2 | 2:N:153:LEU:HD22 | 2.19 | 0.42 |
| 1:L:87:LYS:HE2 | 9:X:366:HOH:O | 2.20 | 0.42 |
| 2:P:66:GLN:HA | 9:P:302:HOH:O | 2.19 | 0.42 |
| 1:G:118[A]:ARG:HA | 1:G:118[A]:ARG:HD3 | 1.90 | 0.42 |
| 1:K:42[A]:GLU:CD | 2:W:22[A]:MET:HG3 | 2.39 | 0.42 |
| 3:L:167:PEB:HMB2 | 3:L:167:PEB:NA | 2.34 | 0.42 |
| 3:G:167:PEB:NA | 3:G:167:PEB:HMB2 | 2.34 | 0.42 |
| 1:I:1[A]:MET:HG3 | 1:I:103:GLY:HA3 | 2.02 | 0.42 |
| 1:F:118[A]:ARG:HD3 | 1:F:118[A]:ARG:HH11 | 1.71 | 0.41 |
| 2:S:22[B]:MET:HA | 2:S:22[B]:MET:HE3 | 1.95 | 0.41 |
| 9:S:418:HOH:O | 2:T:16:THR:HG21 | 2.19 | 0.41 |
| 3:C:166:PEB:HMC2 | 2:N:77:MET:HG2 | 2.01 | 0.41 |
| 2:Q:82[A]:ARG:NH1 | 3:Q:186:PEB:O2C | 2.53 | 0.41 |
| 2:R:155[B]:LYS:CE | 2:R:155[B]:LYS:HA | 2.49 | 0.41 |
| 3:T:187:PEB:NA | 3:T:187:PEB:HMB2 | 2.29 | 0.41 |
| 1:I:118[A]:ARG:NH1 | 1:K:124[A]:THR:OG1 | 2.53 | 0.41 |
| 3:M:188:PEB:HNA | 3:M:188:PEB:HMB3 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:H:19:PRO:CD | 2:T:92[B]:THR:HG23 | 2.50 | 0.41 |
| 3:P:188:PEB:HNA | 3:P:188:PEB:HMB3 | 1.85 | 0.41 |
| 2:T:16:THR:O | 2:T:16:THR:OG1 | 2.35 | 0.41 |
| 1:F:62[A]:LYS:HE2 | 1:F:63:TYR:OH | 2.20 | 0.41 |
| 3:N:187:PEB:HMB2 | 3:N:187:PEB:NA | 2.29 | 0.41 |
| 2:O:135:GLN:HG2 | 3:O:188:PEB:C1B | 2.51 | 0.41 |
| 2:Q:27:GLN:NE2 | 2:Q:31[A]:GLU:OE2 | 2.53 | 0.41 |
| 1:I:27:VAL:O | 1:I:30[B]:SER:HB3 | 2.21 | 0.41 |
| 2:T:135:GLN:HG2 | 3:T:188:PEB:C1B | 2.50 | 0.41 |
| 3:X:187:PEB:HMB2 | 3:X:187:PEB:NA | 2.30 | 0.41 |
| 1:J:2:LYS:HB3 | 9:J:305:HOH:O | 2.19 | 0.41 |
| 2:X:27:GLN:NE2 | 2:X:31[A]:GLU:OE1 | 2.54 | 0.41 |
| 1:D:114[A]:ARG:HG2 | 9:D:459:HOH:O | 2.21 | 0.41 |
| 3:F:167:PEB:HMB2 | 3:F:167:PEB:NA | 2.36 | 0.41 |
| 2:W:122[A]:THR:HG21 | 9:W:491:HOH:O | 2.06 | 0.41 |
| 9:C:342:HOH:O | 7:O:204:MPD:HM3 | 2.20 | 0.40 |
| 1:G:35:ALA:HB1 | 9:G:580:HOH:O | 2.22 | 0.40 |
| 3:Q:187:PEB:NA | 3:Q:187:PEB:HMB2 | 2.27 | 0.40 |
| 2:S:132:MET:HA | 2:S:135:GLN:OE1 | 2.21 | 0.40 |
| 1:A:43[A]:LYS:HG3 | 3:A:167:PEB:CBD | 2.51 | 0.40 |
| 1:F:139:CYS:SG | 3:F:167:PEB:HHA1 | 2.61 | 0.40 |
| 2:R:144:PRO:HG2 | 2:R:153:LEU:HD11 | 2.03 | 0.40 |
| 2:S:28[A]:PHE:CZ | 2:S:35:ARG:NH2 | 2.89 | 0.40 |
| 3:U:187:PEB:HBA3 | 3:U:187:PEB:HHA1 | 2.03 | 0.40 |
| 1:H:19:PRO:HD2 | 2:T:92[B]:THR:HG21 | 2.04 | 0.40 |
| 1:L:118[A]:ARG:NH2 | 9:L:305:HOH:O | 2.23 | 0.40 |
| 2:M:155[A]:LYS:CA | 2:M:155[A]:LYS:HE2 | 2.44 | 0.40 |
| 2:W:22[B]:MET:CE | 2:W:25:LEU:HD12 | 2.51 | 0.40 |

All (4) 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) |
|---------------|----------------------|--------------------------|-------------------|
| 9:M:484:HOH:O | 9:W:355:HOH:O[1_654] | 2.12 | 0.08 |
| 9:R:491:HOH:O | 9:T:570:HOH:O[1_565] | 2.17 | 0.03 |
| 9:N:329:HOH:O | 9:X:463:HOH:O[1_564] | 2.18 | 0.02 |
| 9:D:636:HOH:O | 9:O:484:HOH:O[1_645] | 2.19 | 0.01 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 171/164 (104%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | B | 169/164 (103%) | 167 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | C | 170/164 (104%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | D | 173/164 (106%) | 171 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | E | 169/164 (103%) | 166 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | F | 172/164 (105%) | 170 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | G | 170/164 (104%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | H | 172/164 (105%) | 169 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | I | 174/164 (106%) | 172 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | J | 171/164 (104%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | K | 171/164 (104%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | L | 170/164 (104%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | M | 194/184 (105%) | 188 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | N | 192/184 (104%) | 185 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | O | 190/184 (103%) | 185 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | P | 192/184 (104%) | 188 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | Q | 191/184 (104%) | 187 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | R | 191/184 (104%) | 187 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | S | 193/184 (105%) | 189 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | T | 192/184 (104%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | U | 197/184 (107%) | 194 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | V | 196/184 (106%) | 192 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | W | 195/184 (106%) | 190 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | X | 192/184 (104%) | 189 (98%) | 3 (2%) | 0 | 100 | 100 |
| All | All | 4367/4176 (105%) | 4286 (98%) | 81 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 137/127 (108%) | 137 (100%) | 0 | 100 | 100 |
| 1 | B | 135/127 (106%) | 133 (98%) | 2 (2%) | 70 | 29 |
| 1 | C | 136/127 (107%) | 136 (100%) | 0 | 100 | 100 |
| 1 | D | 139/127 (109%) | 139 (100%) | 0 | 100 | 100 |
| 1 | E | 135/127 (106%) | 135 (100%) | 0 | 100 | 100 |
| 1 | F | 138/127 (109%) | 132 (96%) | 6 (4%) | 33 | 4 |
| 1 | G | 136/127 (107%) | 136 (100%) | 0 | 100 | 100 |
| 1 | H | 138/127 (109%) | 138 (100%) | 0 | 100 | 100 |
| 1 | I | 140/127 (110%) | 140 (100%) | 0 | 100 | 100 |
| 1 | J | 137/127 (108%) | 137 (100%) | 0 | 100 | 100 |
| 1 | K | 137/127 (108%) | 135 (98%) | 2 (2%) | 70 | 29 |
| 1 | L | 136/127 (107%) | 136 (100%) | 0 | 100 | 100 |
| 2 | M | 151/138 (109%) | 149 (99%) | 2 (1%) | 73 | 34 |
| 2 | N | 150/138 (109%) | 147 (98%) | 3 (2%) | 60 | 18 |
| 2 | O | 147/138 (106%) | 146 (99%) | 1 (1%) | 87 | 57 |
| 2 | P | 149/138 (108%) | 145 (97%) | 4 (3%) | 50 | 10 |
| 2 | Q | 148/138 (107%) | 148 (100%) | 0 | 100 | 100 |
| 2 | R | 148/138 (107%) | 146 (99%) | 2 (1%) | 71 | 32 |
| 2 | S | 150/138 (109%) | 148 (99%) | 2 (1%) | 73 | 34 |
| 2 | T | 150/138 (109%) | 145 (97%) | 5 (3%) | 43 | 7 |
| 2 | U | 155/138 (112%) | 152 (98%) | 3 (2%) | 62 | 20 |
| 2 | V | 154/138 (112%) | 148 (96%) | 6 (4%) | 37 | 5 |
| 2 | W | 153/138 (111%) | 152 (99%) | 1 (1%) | 87 | 57 |
| 2 | X | 149/138 (108%) | 147 (99%) | 2 (1%) | 73 | 34 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| All | All | 3448/3180 (108%) | 3407 (99%) | 41 (1%) | 85 | 38 |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | B | 1[A] | MET |
| 1 | B | 1[B] | MET |
| 1 | F | 1[A] | MET |
| 1 | F | 1[B] | MET |
| 1 | F | 42[A] | GLU |
| 1 | F | 42[B] | GLU |
| 1 | F | 118[A] | ARG |
| 1 | F | 118[B] | ARG |
| 1 | K | 118[A] | ARG |
| 1 | K | 118[B] | ARG |
| 2 | M | 155[A] | LYS |
| 2 | M | 155[B] | LYS |
| 2 | N | 73 | PRO |
| 2 | N | 92[A] | THR |
| 2 | N | 92[B] | THR |
| 2 | O | 178 | ARG |
| 2 | P | 26 | LYS |
| 2 | P | 27 | GLN |
| 2 | P | 109[A] | ASN |
| 2 | P | 109[B] | ASN |
| 2 | R | 28[A] | PHE |
| 2 | R | 28[B] | PHE |
| 2 | S | 28[A] | PHE |
| 2 | S | 28[B] | PHE |
| 2 | T | 16 | THR |
| 2 | T | 123 | THR |
| 2 | T | 155 | LYS |
| 2 | T | 184[A] | SER |
| 2 | T | 184[B] | SER |
| 2 | U | 25 | LEU |
| 2 | U | 26[A] | LYS |
| 2 | U | 26[B] | LYS |
| 2 | V | 109[A] | ASN |
| 2 | V | 109[B] | ASN |
| 2 | V | 155 | LYS |
| 2 | V | 162 | GLU |
| 2 | V | 178[A] | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | V | 178[B] | ARG |
| 2 | W | 178 | ARG |
| 2 | X | 28[A] | PHE |
| 2 | X | 28[B] | PHE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 68 | ASN |
| 1 | D | 61 | GLN |
| 1 | D | 113 | GLN |
| 1 | I | 61 | GLN |
| 2 | M | 27 | GLN |
| 2 | P | 27 | GLN |
| 2 | R | 11 | GLN |
| 2 | R | 62 | GLN |
| 2 | X | 11 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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 | MEN | M | 70 | 2 | 8,8,9 | 0.74 | 0 | 8,9,11 | 0.81 | 0 |
| 2 | MEN | N | 70 | 2 | 8,8,9 | 1.39 | 1 (12%) | 8,9,11 | 0.96 | 0 |
| 2 | MEN | O | 70 | 2 | 8,8,9 | 0.91 | 1 (12%) | 8,9,11 | 1.28 | 1 (12%) |
| 2 | MEN | P | 70 | 2 | 8,8,9 | 0.58 | 0 | 8,9,11 | 1.11 | 1 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | MEN | Q | 70 | 2 | 8,8,9 | 0.74 | 0 | 8,9,11 | 1.23 | 1 (12%) |
| 2 | MEN | R | 70 | 2 | 8,8,9 | 0.69 | 0 | 8,9,11 | 1.76 | 3 (37%) |
| 2 | MEN | S | 70 | 2 | 8,8,9 | 0.75 | 0 | 8,9,11 | 1.69 | 2 (25%) |
| 2 | MEN | T | 70 | 2 | 8,8,9 | 0.73 | 0 | 8,9,11 | 0.96 | 1 (12%) |
| 2 | MEN | U | 70 | 2 | 8,8,9 | 0.72 | 0 | 8,9,11 | 1.56 | 2 (25%) |
| 2 | MEN | V | 70 | 2 | 8,8,9 | 0.77 | 0 | 8,9,11 | 0.93 | 0 |
| 2 | MEN | W | 70 | 2 | 8,8,9 | 1.15 | 1 (12%) | 8,9,11 | 0.85 | 1 (12%) |
| 2 | MEN | X | 70 | 2 | 8,8,9 | 0.70 | 0 | 8,9,11 | 0.90 | 1 (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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | MEN | M | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | N | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | O | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | P | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | Q | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | R | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | S | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | T | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | U | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | V | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | W | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |
| 2 | MEN | X | 70 | 2 | - | 0/6/8/10 | 0/0/0/0 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | O | 70 | MEN | CA-C | 2.28 | 1.53 | 1.50 |
| 2 | W | 70 | MEN | CA-C | 2.78 | 1.53 | 1.50 |
| 2 | N | 70 | MEN | CA-C | 3.54 | 1.54 | 1.50 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | S | 70 | MEN | OD1-CG-CB | -3.20 | 116.59 | 121.42 |
| 2 | R | 70 | MEN | OD1-CG-CB | -3.04 | 116.83 | 121.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | S | 70 | MEN | O-C-CA | -2.83 | 117.19 | 125.02 |
| 2 | R | 70 | MEN | O-C-CA | -2.73 | 117.48 | 125.02 |
| 2 | U | 70 | MEN | O-C-CA | -2.72 | 117.52 | 125.02 |
| 2 | Q | 70 | MEN | O-C-CA | -2.61 | 117.81 | 125.02 |
| 2 | P | 70 | MEN | O-C-CA | -2.60 | 117.83 | 125.02 |
| 2 | O | 70 | MEN | O-C-CA | -2.32 | 118.60 | 125.02 |
| 2 | T | 70 | MEN | O-C-CA | -2.14 | 119.11 | 125.02 |
| 2 | X | 70 | MEN | O-C-CA | -2.13 | 119.13 | 125.02 |
| 2 | W | 70 | MEN | O-C-CA | -2.08 | 119.27 | 125.02 |
| 2 | R | 70 | MEN | CB-CG-ND2 | 2.43 | 118.89 | 115.36 |
| 2 | U | 70 | MEN | CB-CA-C | 2.68 | 116.58 | 111.41 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 16 are monoatomic - leaving 103 for Mogul analysis.

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 | $\# Z > 2$ |
| 3 | PEB | A | 166 | 1 | 37,46,46 | 1.86 | 4 (10%) | 39,67,67 | 1.73 | 5 (12%) |
| 3 | PEB | A | 167 | 1 | 37,46,46 | 1.94 | 7 (18%) | 39,67,67 | 1.65 | 10 (25%) |
| 4 | NO3 | A | 203 | - | 1,3,3 | 2.25 | 1 (100%) | 0,3,3 | 0.00 | - |
| 5 | PI | A | 204 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.83 | 0 |
| 3 | PEB | B | 166 | 1 | 37,46,46 | 2.42 | 7 (18%) | 39,67,67 | 1.77 | 7 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | PEB | B | 167 | 1 | 37,46,46 | 2.23 | 8 (21%) | 39,67,67 | 1.73 | 11 (28%) |
| 7 | MPD | B | 203 | - | 7,7,7 | 0.61 | 0 | 9,10,10 | 1.57 | 2 (22%) |
| 5 | PI | B | 204 | - | 4,4,4 | 1.02 | 0 | 6,6,6 | 1.62 | 2 (33%) |
| 3 | PEB | C | 166 | 1 | 37,46,46 | 2.99 | 9 (24%) | 39,67,67 | 2.04 | 13 (33%) |
| 3 | PEB | C | 167 | 1 | 37,46,46 | 2.22 | 9 (24%) | 39,67,67 | 2.20 | 13 (33%) |
| 4 | NO3 | C | 203 | - | 1,3,3 | 1.74 | 0 | 0,3,3 | 0.00 | - |
| 5 | PI | C | 204 | - | 4,4,4 | 0.94 | 0 | 6,6,6 | 1.25 | 1 (16%) |
| 3 | PEB | D | 166 | 1 | 37,46,46 | 2.47 | 9 (24%) | 39,67,67 | 1.71 | 8 (20%) |
| 3 | PEB | D | 167 | 1 | 37,46,46 | 2.05 | 10 (27%) | 39,67,67 | 1.56 | 7 (17%) |
| 4 | NO3 | D | 203 | - | 1,3,3 | 2.77 | 1 (100%) | 0,3,3 | 0.00 | - |
| 5 | PI | D | 204 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.38 | 0 |
| 3 | PEB | E | 166 | 1 | 37,46,46 | 3.29 | 11 (29%) | 39,67,67 | 2.06 | 11 (28%) |
| 3 | PEB | E | 167 | 1 | 37,46,46 | 2.56 | 9 (24%) | 39,67,67 | 1.46 | 6 (15%) |
| 5 | PI | E | 203 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.59 | 0 |
| 3 | PEB | F | 166 | 1 | 37,46,46 | 2.11 | 6 (16%) | 39,67,67 | 1.74 | 8 (20%) |
| 3 | PEB | F | 167 | 1 | 37,46,46 | 2.44 | 11 (29%) | 39,67,67 | 1.76 | 10 (25%) |
| 5 | PI | F | 203 | - | 4,4,4 | 0.86 | 0 | 6,6,6 | 0.43 | 0 |
| 3 | PEB | G | 166 | 1 | 37,46,46 | 2.01 | 8 (21%) | 39,67,67 | 1.70 | 8 (20%) |
| 3 | PEB | G | 167 | 1 | 37,46,46 | 2.61 | 13 (35%) | 39,67,67 | 1.57 | 7 (17%) |
| 5 | PI | G | 203 | - | 4,4,4 | 0.78 | 0 | 6,6,6 | 0.74 | 0 |
| 3 | PEB | H | 166 | 1 | 37,46,46 | 2.71 | 7 (18%) | 39,67,67 | 2.11 | 11 (28%) |
| 3 | PEB | H | 167 | 1 | 37,46,46 | 2.31 | 8 (21%) | 39,67,67 | 1.64 | 6 (15%) |
| 5 | PI | H | 203 | - | 4,4,4 | 1.15 | 0 | 6,6,6 | 1.00 | 0 |
| 3 | PEB | I | 166 | 1 | 37,46,46 | 2.87 | 9 (24%) | 39,67,67 | 1.80 | 10 (25%) |
| 3 | PEB | I | 167 | 1 | 37,46,46 | 2.20 | 11 (29%) | 39,67,67 | 1.69 | 13 (33%) |
| 4 | NO3 | I | 203 | - | 1,3,3 | 2.34 | 1 (100%) | 0,3,3 | 0.00 | - |
| 5 | PI | I | 204 | - | 4,4,4 | 0.92 | 0 | 6,6,6 | 0.94 | 0 |
| 3 | PEB | J | 166 | 1 | 37,46,46 | 2.14 | 5 (13%) | 39,67,67 | 1.69 | 6 (15%) |
| 3 | PEB | J | 167 | 1 | 37,46,46 | 2.31 | 7 (18%) | 39,67,67 | 2.00 | 12 (30%) |
| 4 | NO3 | J | 203 | - | 1,3,3 | 2.07 | 1 (100%) | 0,3,3 | 0.00 | - |
| 5 | PI | J | 204 | - | 4,4,4 | 0.97 | 0 | 6,6,6 | 0.61 | 0 |
| 3 | PEB | K | 166 | 1 | 37,46,46 | 2.48 | 9 (24%) | 39,67,67 | 1.81 | 7 (17%) |
| 3 | PEB | K | 167 | 1 | 37,46,46 | 2.60 | 9 (24%) | 39,67,67 | 1.71 | 8 (20%) |
| 5 | PI | K | 203 | - | 4,4,4 | 0.81 | 0 | 6,6,6 | 0.78 | 0 |
| 3 | PEB | L | 166 | 1 | 37,46,46 | 2.17 | 7 (18%) | 39,67,67 | 1.82 | 11 (28%) |
| 3 | PEB | L | 167 | 1 | 37,46,46 | 1.98 | 9 (24%) | 39,67,67 | 1.68 | 7 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NO3 | L | 203 | - | 1,3,3 | 2.37 | 1 (100%) | 0,3,3 | 0.00 | - |
| 5 | PI | L | 204 | - | 4,4,4 | 0.91 | 0 | 6,6,6 | 0.78 | 0 |
| 3 | PEB | M | 186 | 2 | 37,46,46 | 2.78 | 9 (24%) | 39,67,67 | 1.93 | 11 (28%) |
| 3 | PEB | M | 187 | 2 | 37,46,46 | 2.23 | 9 (24%) | 39,67,67 | 1.47 | 6 (15%) |
| 3 | PEB | M | 188 | 2 | 37,46,46 | 2.33 | 8 (21%) | 39,67,67 | 1.63 | 7 (17%) |
| 7 | MPD | M | 204 | 2 | 7,7,7 | 0.18 | 0 | 9,10,10 | 1.09 | 1 (11%) |
| 5 | PI | M | 205 | - | 4,4,4 | 1.16 | 1 (25%) | 6,6,6 | 0.99 | 0 |
| 3 | PEB | N | 186 | 2 | 37,46,46 | 2.57 | 7 (18%) | 39,67,67 | 1.88 | 12 (30%) |
| 3 | PEB | N | 187 | 2 | 37,46,46 | 2.11 | 6 (16%) | 39,67,67 | 1.52 | 7 (17%) |
| 3 | PEB | N | 188 | 2 | 37,46,46 | 2.56 | 6 (16%) | 39,67,67 | 1.62 | 9 (23%) |
| 5 | PI | N | 204 | - | 4,4,4 | 0.73 | 0 | 6,6,6 | 1.11 | 0 |
| 3 | PEB | O | 186 | 2 | 37,46,46 | 2.44 | 6 (16%) | 39,67,67 | 1.69 | 9 (23%) |
| 3 | PEB | O | 187 | 2 | 37,46,46 | 2.61 | 8 (21%) | 39,67,67 | 1.32 | 6 (15%) |
| 3 | PEB | O | 188 | 2 | 37,46,46 | 2.43 | 11 (29%) | 39,67,67 | 1.44 | 5 (12%) |
| 7 | MPD | O | 204 | 2 | 7,7,7 | 0.90 | 0 | 9,10,10 | 1.26 | 1 (11%) |
| 5 | PI | O | 205 | - | 4,4,4 | 0.85 | 0 | 6,6,6 | 0.89 | 0 |
| 3 | PEB | P | 186 | 2 | 37,46,46 | 3.11 | 10 (27%) | 39,67,67 | 1.81 | 12 (30%) |
| 3 | PEB | P | 187 | 2 | 37,46,46 | 2.21 | 8 (21%) | 39,67,67 | 1.65 | 10 (25%) |
| 3 | PEB | P | 188 | 2 | 37,46,46 | 2.26 | 7 (18%) | 39,67,67 | 1.59 | 9 (23%) |
| 7 | MPD | P | 204 | 2 | 7,7,7 | 0.27 | 0 | 9,10,10 | 0.84 | 0 |
| 5 | PI | P | 205 | - | 4,4,4 | 0.48 | 0 | 6,6,6 | 1.18 | 1 (16%) |
| 3 | PEB | Q | 186 | 2 | 37,46,46 | 2.76 | 8 (21%) | 39,67,67 | 1.74 | 12 (30%) |
| 3 | PEB | Q | 187 | 2 | 37,46,46 | 2.49 | 7 (18%) | 39,67,67 | 1.62 | 7 (17%) |
| 3 | PEB | Q | 188 | 2 | 37,46,46 | 2.06 | 7 (18%) | 39,67,67 | 1.58 | 8 (20%) |
| 7 | MPD | Q | 204 | 2 | 7,7,7 | 0.59 | 0 | 9,10,10 | 0.92 | 0 |
| 5 | PI | Q | 205 | - | 4,4,4 | 0.84 | 0 | 6,6,6 | 1.02 | 0 |
| 3 | PEB | R | 186 | 2 | 37,46,46 | 2.89 | 10 (27%) | 39,67,67 | 2.10 | 13 (33%) |
| 3 | PEB | R | 187 | 2 | 37,46,46 | 2.86 | 8 (21%) | 39,67,67 | 1.80 | 11 (28%) |
| 3 | PEB | R | 188 | 2 | 37,46,46 | 2.50 | 9 (24%) | 39,67,67 | 1.50 | 7 (17%) |
| 7 | MPD | R | 204 | - | 7,7,7 | 0.16 | 0 | 9,10,10 | 1.54 | 2 (22%) |
| 5 | PI | R | 205 | - | 4,4,4 | 0.65 | 0 | 6,6,6 | 0.56 | 0 |
| 3 | PEB | S | 186[A] | - | 37,46,46 | 2.75 | 8 (21%) | 39,67,67 | 2.16 | 13 (33%) |
| 3 | PEB | S | 186[B] | - | 37,46,46 | 2.73 | 8 (21%) | 39,67,67 | 2.16 | 14 (35%) |
| 3 | PEB | S | 187 | 2 | 37,46,46 | 2.52 | 8 (21%) | 39,67,67 | 1.64 | 8 (20%) |
| 3 | PEB | S | 188 | 2 | 37,46,46 | 2.59 | 9 (24%) | 39,67,67 | 1.53 | 8 (20%) |
| 7 | MPD | S | 204 | - | 7,7,7 | 0.22 | 0 | 9,10,10 | 0.68 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | PI | S | 205 | - | 4,4,4 | 0.87 | 0 | 6,6,6 | 0.35 | 0 |
| 3 | PEB | T | 186 | 2 | 37,46,46 | 2.84 | 8 (21%) | 39,67,67 | 2.13 | 15 (38%) |
| 3 | PEB | T | 187 | 2 | 37,46,46 | 2.38 | 9 (24%) | 39,67,67 | 1.82 | 11 (28%) |
| 3 | PEB | T | 188 | 2 | 37,46,46 | 2.36 | 8 (21%) | 39,67,67 | 2.01 | 15 (38%) |
| 8 | MRD | T | 204 | 2 | 7,7,7 | 0.46 | 0 | 9,10,10 | 0.51 | 0 |
| 5 | PI | T | 205 | - | 4,4,4 | 0.81 | 0 | 6,6,6 | 1.17 | 0 |
| 3 | PEB | U | 186 | 2 | 37,46,46 | 2.53 | 9 (24%) | 39,67,67 | 2.11 | 11 (28%) |
| 3 | PEB | U | 187 | 2 | 37,46,46 | 2.61 | 7 (18%) | 39,67,67 | 1.60 | 10 (25%) |
| 3 | PEB | U | 188 | 2 | 37,46,46 | 2.38 | 7 (18%) | 39,67,67 | 1.62 | 9 (23%) |
| 7 | MPD | U | 204 | 2 | 7,7,7 | 0.33 | 0 | 9,10,10 | 0.89 | 0 |
| 5 | PI | U | 205 | - | 4,4,4 | 1.44 | 1 (25%) | 6,6,6 | 0.50 | 0 |
| 3 | PEB | V | 186 | 2 | 37,46,46 | 2.27 | 6 (16%) | 39,67,67 | 1.66 | 8 (20%) |
| 3 | PEB | V | 187 | 2 | 37,46,46 | 2.57 | 5 (13%) | 39,67,67 | 1.58 | 7 (17%) |
| 3 | PEB | V | 188 | 2 | 37,46,46 | 2.41 | 10 (27%) | 39,67,67 | 1.53 | 8 (20%) |
| 8 | MRD | V | 204 | 2 | 7,7,7 | 0.26 | 0 | 9,10,10 | 1.08 | 0 |
| 5 | PI | V | 205 | - | 4,4,4 | 0.81 | 0 | 6,6,6 | 0.75 | 0 |
| 3 | PEB | W | 186 | 2 | 37,46,46 | 2.80 | 9 (24%) | 39,67,67 | 1.90 | 13 (33%) |
| 3 | PEB | W | 187 | 2 | 37,46,46 | 2.36 | 6 (16%) | 39,67,67 | 1.48 | 8 (20%) |
| 3 | PEB | W | 188 | 2 | 37,46,46 | 2.83 | 6 (16%) | 39,67,67 | 1.71 | 10 (25%) |
| 7 | MPD | W | 204 | 2 | 7,7,7 | 0.21 | 0 | 9,10,10 | 0.99 | 0 |
| 5 | PI | W | 205 | - | 4,4,4 | 1.09 | 1 (25%) | 6,6,6 | 0.99 | 0 |
| 3 | PEB | X | 186 | 2 | 37,46,46 | 2.47 | 7 (18%) | 39,67,67 | 1.67 | 8 (20%) |
| 3 | PEB | X | 187 | 2 | 37,46,46 | 2.24 | 7 (18%) | 39,67,67 | 1.46 | 6 (15%) |
| 3 | PEB | X | 188 | 2 | 37,46,46 | 2.45 | 8 (21%) | 39,67,67 | 1.79 | 12 (30%) |
| 7 | MPD | X | 204 | - | 7,7,7 | 0.35 | 0 | 9,10,10 | 0.79 | 0 |
| 5 | PI | X | 205 | - | 4,4,4 | 0.85 | 0 | 6,6,6 | 0.70 | 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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | PEB | A | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | A | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 4 | NO3 | A | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | PI | A | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | B | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | PEB | B | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | B | 203 | - | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | B | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | C | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | C | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 4 | NO3 | C | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | PI | C | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | D | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | D | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 4 | NO3 | D | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | PI | D | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | E | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | E | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 5 | PI | E | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | F | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | F | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 5 | PI | F | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | G | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | G | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 5 | PI | G | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | H | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | H | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 5 | PI | H | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | I | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | I | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 4 | NO3 | I | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | PI | I | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | J | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | J | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 4 | NO3 | J | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | PI | J | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | K | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | K | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 5 | PI | K | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | L | 166 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | L | 167 | 1 | - | 2/19/74/74 | 0/4/4/4 |
| 4 | NO3 | L | 203 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|---------|------------|---------|
| 5 | PI | L | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | M | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | M | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | M | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | M | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | M | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | N | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | N | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | N | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 5 | PI | N | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | O | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | O | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | O | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | O | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | O | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | P | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | P | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | P | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | P | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | P | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | Q | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | Q | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | Q | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | Q | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | Q | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | R | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | R | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | R | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | R | 204 | - | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | R | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | S | 186[A] | - | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | S | 186[B] | - | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | S | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | S | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | S | 204 | - | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | S | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | T | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | PEB | T | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | T | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 8 | MRD | T | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | T | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | U | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | U | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | U | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | U | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | U | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | V | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | V | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | V | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 8 | MRD | V | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | V | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | W | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | W | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | W | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | W | 204 | 2 | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | W | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | PEB | X | 186 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | X | 187 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 3 | PEB | X | 188 | 2 | - | 2/19/74/74 | 0/4/4/4 |
| 7 | MPD | X | 204 | - | - | 0/5/5/5 | 0/0/0/0 |
| 5 | PI | X | 205 | - | - | 0/0/0/0 | 0/0/0/0 |

All (499) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | K | 167 | PEB | C1A-NA | -5.92 | 1.30 | 1.37 |
| 3 | B | 167 | PEB | C1A-NA | -4.83 | 1.31 | 1.37 |
| 3 | K | 166 | PEB | C2A-C1A | -4.77 | 1.47 | 1.52 |
| 3 | X | 188 | PEB | C1A-NA | -4.42 | 1.32 | 1.37 |
| 3 | B | 167 | PEB | C2A-C1A | -4.26 | 1.48 | 1.52 |
| 3 | W | 187 | PEB | C1A-NA | -4.20 | 1.32 | 1.37 |
| 3 | D | 166 | PEB | C2A-C1A | -4.20 | 1.48 | 1.52 |
| 3 | E | 167 | PEB | C1A-NA | -4.17 | 1.32 | 1.37 |
| 3 | C | 167 | PEB | C1A-NA | -4.15 | 1.32 | 1.37 |
| 3 | K | 167 | PEB | C2A-C1A | -4.13 | 1.48 | 1.52 |
| 3 | G | 167 | PEB | C1A-NA | -4.08 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3 | O | 187 | PEB | C1A-NA | -3.98 | 1.32 | 1.37 |
| 3 | A | 167 | PEB | C1A-NA | -3.91 | 1.32 | 1.37 |
| 3 | J | 167 | PEB | C1A-NA | -3.87 | 1.32 | 1.37 |
| 3 | L | 167 | PEB | C1A-NA | -3.84 | 1.32 | 1.37 |
| 3 | M | 188 | PEB | C1A-NA | -3.71 | 1.32 | 1.37 |
| 3 | U | 188 | PEB | C1A-NA | -3.67 | 1.33 | 1.37 |
| 3 | L | 166 | PEB | C4D-ND | -3.58 | 1.29 | 1.35 |
| 3 | U | 187 | PEB | C1A-NA | -3.57 | 1.33 | 1.37 |
| 3 | D | 167 | PEB | C1A-NA | -3.57 | 1.33 | 1.37 |
| 3 | L | 166 | PEB | C4B-C3B | -3.56 | 1.39 | 1.45 |
| 3 | R | 188 | PEB | C1A-NA | -3.56 | 1.33 | 1.37 |
| 3 | I | 167 | PEB | CAC-C2C | -3.56 | 1.46 | 1.52 |
| 3 | E | 166 | PEB | C1A-NA | -3.48 | 1.33 | 1.37 |
| 3 | D | 166 | PEB | C1A-NA | -3.45 | 1.33 | 1.37 |
| 3 | B | 166 | PEB | C1A-NA | -3.42 | 1.33 | 1.37 |
| 3 | I | 167 | PEB | C1A-NA | -3.40 | 1.33 | 1.37 |
| 3 | O | 186 | PEB | C2A-C1A | -3.39 | 1.48 | 1.52 |
| 3 | Q | 188 | PEB | C1A-NA | -3.31 | 1.33 | 1.37 |
| 3 | Q | 187 | PEB | C2A-C1A | -3.29 | 1.49 | 1.52 |
| 3 | O | 187 | PEB | C2A-C1A | -3.25 | 1.49 | 1.52 |
| 3 | S | 188 | PEB | C2A-C1A | -3.25 | 1.49 | 1.52 |
| 3 | H | 167 | PEB | C2A-C1A | -3.20 | 1.49 | 1.52 |
| 3 | V | 188 | PEB | C1A-NA | -3.06 | 1.33 | 1.37 |
| 3 | O | 188 | PEB | C1A-NA | -3.03 | 1.33 | 1.37 |
| 3 | P | 186 | PEB | CMB-C2B | -3.02 | 1.44 | 1.50 |
| 3 | C | 166 | PEB | C1A-NA | -3.00 | 1.33 | 1.37 |
| 3 | C | 166 | PEB | C2A-C1A | -2.99 | 1.49 | 1.52 |
| 3 | C | 167 | PEB | C4A-NA | -2.98 | 1.31 | 1.37 |
| 3 | O | 188 | PEB | C4D-ND | -2.87 | 1.30 | 1.35 |
| 3 | J | 166 | PEB | C2A-C1A | -2.84 | 1.49 | 1.52 |
| 3 | F | 167 | PEB | C2A-C1A | -2.82 | 1.49 | 1.52 |
| 3 | P | 186 | PEB | C1A-NA | -2.77 | 1.34 | 1.37 |
| 3 | P | 186 | PEB | C2A-C1A | -2.76 | 1.49 | 1.52 |
| 3 | R | 186 | PEB | C2A-C1A | -2.74 | 1.49 | 1.52 |
| 3 | H | 167 | PEB | C1A-NA | -2.73 | 1.34 | 1.37 |
| 3 | Q | 187 | PEB | C1A-NA | -2.68 | 1.34 | 1.37 |
| 3 | W | 187 | PEB | C2A-C1A | -2.66 | 1.49 | 1.52 |
| 3 | C | 167 | PEB | C4B-NB | -2.65 | 1.32 | 1.38 |
| 3 | G | 167 | PEB | C4D-ND | -2.63 | 1.31 | 1.35 |
| 3 | L | 166 | PEB | C2A-C1A | -2.61 | 1.49 | 1.52 |
| 3 | S | 186[A] | PEB | C1A-NA | -2.59 | 1.34 | 1.37 |
| 3 | S | 186[B] | PEB | C1A-NA | -2.59 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3 | X | 187 | PEB | C1A-NA | -2.59 | 1.34 | 1.37 |
| 3 | F | 167 | PEB | C1A-NA | -2.58 | 1.34 | 1.37 |
| 3 | U | 187 | PEB | CAC-C2C | -2.57 | 1.47 | 1.52 |
| 3 | D | 167 | PEB | C2A-C1A | -2.56 | 1.49 | 1.52 |
| 3 | D | 166 | PEB | C4B-C3B | -2.54 | 1.41 | 1.45 |
| 3 | K | 166 | PEB | C1A-NA | -2.54 | 1.34 | 1.37 |
| 3 | G | 167 | PEB | C4A-NA | -2.53 | 1.31 | 1.37 |
| 3 | E | 166 | PEB | C4D-ND | -2.51 | 1.31 | 1.35 |
| 3 | R | 187 | PEB | C1A-NA | -2.50 | 1.34 | 1.37 |
| 3 | L | 167 | PEB | C4D-ND | -2.49 | 1.31 | 1.35 |
| 3 | S | 188 | PEB | CAC-C2C | -2.49 | 1.47 | 1.52 |
| 3 | S | 186[A] | PEB | C2A-C1A | -2.49 | 1.49 | 1.52 |
| 3 | S | 186[B] | PEB | C2A-C1A | -2.49 | 1.49 | 1.52 |
| 3 | I | 167 | PEB | C1D-ND | -2.46 | 1.42 | 1.45 |
| 3 | E | 167 | PEB | C2A-C1A | -2.46 | 1.49 | 1.52 |
| 3 | P | 187 | PEB | CAC-C2C | -2.46 | 1.47 | 1.52 |
| 3 | S | 187 | PEB | C1A-NA | -2.45 | 1.34 | 1.37 |
| 3 | C | 166 | PEB | C4D-ND | -2.45 | 1.31 | 1.35 |
| 3 | N | 188 | PEB | C4A-NA | -2.44 | 1.32 | 1.37 |
| 3 | G | 166 | PEB | CAC-C2C | -2.43 | 1.47 | 1.52 |
| 3 | D | 167 | PEB | CAC-C2C | -2.38 | 1.48 | 1.52 |
| 3 | T | 186 | PEB | C1A-NA | -2.38 | 1.34 | 1.37 |
| 3 | W | 186 | PEB | C1A-NA | -2.37 | 1.34 | 1.37 |
| 3 | N | 186 | PEB | C1A-NA | -2.36 | 1.34 | 1.37 |
| 3 | V | 188 | PEB | C4D-ND | -2.35 | 1.31 | 1.35 |
| 3 | J | 167 | PEB | C2A-C1A | -2.34 | 1.49 | 1.52 |
| 3 | D | 166 | PEB | CMC-C3C | -2.34 | 1.46 | 1.51 |
| 3 | M | 187 | PEB | C1A-NA | -2.32 | 1.34 | 1.37 |
| 3 | U | 186 | PEB | C1A-NA | -2.32 | 1.34 | 1.37 |
| 3 | R | 186 | PEB | C1A-NA | -2.31 | 1.34 | 1.37 |
| 3 | M | 186 | PEB | C1A-NA | -2.30 | 1.34 | 1.37 |
| 3 | K | 167 | PEB | C1B-NB | -2.30 | 1.31 | 1.36 |
| 3 | T | 187 | PEB | CAC-C2C | -2.28 | 1.48 | 1.52 |
| 3 | G | 167 | PEB | C4B-NB | -2.28 | 1.33 | 1.38 |
| 3 | F | 167 | PEB | C4A-NA | -2.26 | 1.32 | 1.37 |
| 3 | W | 186 | PEB | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 3 | U | 186 | PEB | CHA-C4A | -2.24 | 1.32 | 1.36 |
| 3 | G | 166 | PEB | C4B-C3B | -2.23 | 1.41 | 1.45 |
| 3 | E | 166 | PEB | C2A-C1A | -2.23 | 1.49 | 1.52 |
| 3 | T | 187 | PEB | C2A-C1A | -2.23 | 1.50 | 1.52 |
| 3 | Q | 186 | PEB | C2A-C1A | -2.22 | 1.50 | 1.52 |
| 3 | T | 188 | PEB | C4B-NB | -2.22 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | F | 166 | PEB | CAC-C2C | -2.22 | 1.48 | 1.52 |
| 3 | V | 188 | PEB | CHA-C4A | -2.18 | 1.32 | 1.36 |
| 3 | V | 187 | PEB | C4B-C3B | -2.18 | 1.42 | 1.45 |
| 3 | R | 188 | PEB | C4B-NB | -2.16 | 1.33 | 1.38 |
| 3 | M | 187 | PEB | C2A-C1A | -2.15 | 1.50 | 1.52 |
| 3 | M | 188 | PEB | C4D-ND | -2.14 | 1.31 | 1.35 |
| 3 | I | 167 | PEB | C4D-ND | -2.13 | 1.31 | 1.35 |
| 3 | V | 186 | PEB | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 3 | B | 166 | PEB | C2A-C1A | -2.11 | 1.50 | 1.52 |
| 3 | M | 187 | PEB | CMC-C3C | -2.10 | 1.47 | 1.51 |
| 3 | G | 167 | PEB | CMC-C3C | -2.09 | 1.47 | 1.51 |
| 3 | H | 166 | PEB | CAC-C2C | -2.08 | 1.48 | 1.52 |
| 3 | I | 166 | PEB | C1A-NA | -2.08 | 1.35 | 1.37 |
| 3 | I | 166 | PEB | C2A-C1A | -2.07 | 1.50 | 1.52 |
| 3 | I | 167 | PEB | C2A-C1A | -2.07 | 1.50 | 1.52 |
| 3 | M | 186 | PEB | CMC-C3C | -2.07 | 1.47 | 1.51 |
| 3 | S | 188 | PEB | C1A-NA | -2.06 | 1.35 | 1.37 |
| 3 | G | 167 | PEB | CAC-C2C | -2.06 | 1.48 | 1.52 |
| 3 | R | 186 | PEB | C4B-NB | -2.06 | 1.33 | 1.38 |
| 3 | T | 187 | PEB | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 3 | V | 186 | PEB | C2A-C1A | -2.05 | 1.50 | 1.52 |
| 3 | L | 166 | PEB | C1A-NA | -2.02 | 1.35 | 1.37 |
| 3 | X | 187 | PEB | CAC-C2C | -2.02 | 1.48 | 1.52 |
| 3 | G | 167 | PEB | C4B-C3B | -2.02 | 1.42 | 1.45 |
| 3 | G | 166 | PEB | C1A-NA | -2.02 | 1.35 | 1.37 |
| 3 | K | 166 | PEB | C3C-C4C | 2.02 | 1.45 | 1.42 |
| 3 | R | 188 | PEB | C1D-ND | 2.02 | 1.48 | 1.45 |
| 3 | P | 186 | PEB | C2C-C3C | 2.03 | 1.43 | 1.37 |
| 3 | U | 186 | PEB | OD-C4D | 2.03 | 1.27 | 1.23 |
| 3 | F | 167 | PEB | C1B-C2B | 2.03 | 1.50 | 1.45 |
| 3 | P | 187 | PEB | C3A-C4A | 2.04 | 1.54 | 1.50 |
| 3 | V | 188 | PEB | CMD-C2D | 2.04 | 1.54 | 1.50 |
| 3 | P | 187 | PEB | C1D-ND | 2.06 | 1.49 | 1.45 |
| 4 | J | 203 | NO3 | O1-N | 2.07 | 1.31 | 1.23 |
| 3 | M | 186 | PEB | C2C-C3C | 2.07 | 1.43 | 1.37 |
| 3 | N | 186 | PEB | C2C-C3C | 2.08 | 1.43 | 1.37 |
| 3 | P | 188 | PEB | C2C-C3C | 2.08 | 1.43 | 1.37 |
| 5 | W | 205 | PI | P-O1 | 2.08 | 1.54 | 1.50 |
| 3 | I | 167 | PEB | C2C-C3C | 2.08 | 1.43 | 1.37 |
| 3 | D | 167 | PEB | C2C-C3C | 2.08 | 1.43 | 1.37 |
| 5 | M | 205 | PI | P-O1 | 2.09 | 1.54 | 1.50 |
| 3 | O | 188 | PEB | CMD-C2D | 2.09 | 1.54 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | V | 188 | PEB | C3A-C4A | 2.10 | 1.54 | 1.50 |
| 3 | O | 186 | PEB | CHA-C1B | 2.12 | 1.45 | 1.40 |
| 3 | A | 167 | PEB | C3B-C2B | 2.12 | 1.41 | 1.36 |
| 3 | R | 188 | PEB | OD-C4D | 2.13 | 1.27 | 1.23 |
| 3 | A | 166 | PEB | OD-C4D | 2.15 | 1.27 | 1.23 |
| 3 | C | 166 | PEB | CHA-C1B | 2.17 | 1.45 | 1.40 |
| 3 | N | 187 | PEB | C2C-C3C | 2.17 | 1.44 | 1.37 |
| 3 | M | 188 | PEB | OD-C4D | 2.17 | 1.27 | 1.23 |
| 3 | N | 186 | PEB | C3C-C4C | 2.18 | 1.45 | 1.42 |
| 3 | B | 167 | PEB | OD-C4D | 2.18 | 1.27 | 1.23 |
| 3 | O | 187 | PEB | OD-C4D | 2.19 | 1.27 | 1.23 |
| 3 | Q | 187 | PEB | C2C-C3C | 2.19 | 1.44 | 1.37 |
| 3 | X | 188 | PEB | C3C-C4C | 2.20 | 1.45 | 1.42 |
| 3 | C | 166 | PEB | C2C-C3C | 2.21 | 1.44 | 1.37 |
| 3 | T | 187 | PEB | C3C-C4C | 2.21 | 1.45 | 1.42 |
| 3 | H | 166 | PEB | C2C-C3C | 2.23 | 1.44 | 1.37 |
| 3 | M | 188 | PEB | C3C-C4C | 2.23 | 1.45 | 1.42 |
| 3 | O | 188 | PEB | C3C-C4C | 2.23 | 1.45 | 1.42 |
| 3 | S | 187 | PEB | C2C-C3C | 2.23 | 1.44 | 1.37 |
| 3 | T | 188 | PEB | OD-C4D | 2.24 | 1.27 | 1.23 |
| 3 | U | 188 | PEB | C2C-C3C | 2.24 | 1.44 | 1.37 |
| 3 | E | 166 | PEB | C1C-CHB | 2.25 | 1.48 | 1.40 |
| 3 | F | 167 | PEB | OD-C4D | 2.25 | 1.27 | 1.23 |
| 4 | A | 203 | NO3 | O1-N | 2.25 | 1.32 | 1.23 |
| 3 | M | 187 | PEB | OD-C4D | 2.25 | 1.27 | 1.23 |
| 3 | E | 167 | PEB | C1D-ND | 2.25 | 1.49 | 1.45 |
| 3 | X | 186 | PEB | C3C-C4C | 2.26 | 1.45 | 1.42 |
| 3 | X | 188 | PEB | OD-C4D | 2.26 | 1.27 | 1.23 |
| 3 | J | 167 | PEB | C2C-C3C | 2.28 | 1.44 | 1.37 |
| 3 | K | 167 | PEB | CHA-C1B | 2.29 | 1.45 | 1.40 |
| 3 | P | 187 | PEB | C2C-C3C | 2.30 | 1.44 | 1.37 |
| 3 | I | 166 | PEB | C2C-C3C | 2.30 | 1.44 | 1.37 |
| 3 | G | 166 | PEB | CHA-C1B | 2.32 | 1.46 | 1.40 |
| 3 | P | 188 | PEB | C3C-C4C | 2.32 | 1.45 | 1.42 |
| 3 | D | 167 | PEB | C2D-C3D | 2.33 | 1.37 | 1.34 |
| 4 | I | 203 | NO3 | O1-N | 2.34 | 1.32 | 1.23 |
| 3 | S | 188 | PEB | C3C-C4C | 2.34 | 1.45 | 1.42 |
| 3 | H | 167 | PEB | C3C-C4C | 2.34 | 1.45 | 1.42 |
| 3 | U | 188 | PEB | C3C-C4C | 2.35 | 1.45 | 1.42 |
| 3 | T | 188 | PEB | C3C-C4C | 2.37 | 1.45 | 1.42 |
| 3 | X | 186 | PEB | OD-C4D | 2.37 | 1.28 | 1.23 |
| 4 | L | 203 | NO3 | O1-N | 2.37 | 1.32 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 3 | N | 188 | PEB | CHA-C1B | 2.39 | 1.46 | 1.40 |
| 3 | A | 167 | PEB | C2C-C3C | 2.41 | 1.44 | 1.37 |
| 3 | O | 187 | PEB | C3C-C4C | 2.41 | 1.45 | 1.42 |
| 3 | X | 187 | PEB | OD-C4D | 2.43 | 1.28 | 1.23 |
| 3 | V | 188 | PEB | C2C-C3C | 2.44 | 1.44 | 1.37 |
| 3 | M | 186 | PEB | C1B-NB | 2.46 | 1.42 | 1.36 |
| 3 | L | 167 | PEB | C1D-ND | 2.47 | 1.49 | 1.45 |
| 3 | A | 167 | PEB | C3C-C4C | 2.48 | 1.45 | 1.42 |
| 3 | F | 167 | PEB | C2C-C3C | 2.50 | 1.45 | 1.37 |
| 3 | W | 186 | PEB | C2C-C3C | 2.50 | 1.45 | 1.37 |
| 3 | G | 166 | PEB | C3C-C4C | 2.50 | 1.45 | 1.42 |
| 3 | E | 167 | PEB | C2C-C3C | 2.51 | 1.45 | 1.37 |
| 3 | R | 187 | PEB | C3C-C4C | 2.51 | 1.45 | 1.42 |
| 3 | M | 187 | PEB | C3C-C4C | 2.53 | 1.45 | 1.42 |
| 3 | M | 186 | PEB | OD-C4D | 2.53 | 1.28 | 1.23 |
| 3 | O | 186 | PEB | C3C-C4C | 2.53 | 1.45 | 1.42 |
| 3 | Q | 186 | PEB | OD-C4D | 2.54 | 1.28 | 1.23 |
| 3 | S | 188 | PEB | OD-C4D | 2.54 | 1.28 | 1.23 |
| 3 | N | 187 | PEB | CAA-C3A | 2.54 | 1.59 | 1.54 |
| 3 | D | 167 | PEB | OD-C4D | 2.54 | 1.28 | 1.23 |
| 3 | I | 166 | PEB | C1D-ND | 2.56 | 1.49 | 1.45 |
| 3 | S | 187 | PEB | C1D-ND | 2.56 | 1.49 | 1.45 |
| 3 | R | 188 | PEB | C3C-C4C | 2.57 | 1.45 | 1.42 |
| 3 | F | 166 | PEB | CHA-C1B | 2.58 | 1.46 | 1.40 |
| 3 | W | 188 | PEB | OD-C4D | 2.58 | 1.28 | 1.23 |
| 3 | S | 186[B] | PEB | C2C-C3C | 2.59 | 1.45 | 1.37 |
| 3 | S | 187 | PEB | OD-C4D | 2.60 | 1.28 | 1.23 |
| 3 | B | 167 | PEB | C2C-C3C | 2.60 | 1.45 | 1.37 |
| 3 | M | 188 | PEB | CHA-C1B | 2.60 | 1.46 | 1.40 |
| 3 | X | 186 | PEB | C2C-C3C | 2.60 | 1.45 | 1.37 |
| 3 | X | 187 | PEB | CHA-C1B | 2.61 | 1.46 | 1.40 |
| 3 | T | 186 | PEB | C2C-C3C | 2.63 | 1.45 | 1.37 |
| 3 | L | 167 | PEB | C3C-C4C | 2.63 | 1.45 | 1.42 |
| 3 | D | 166 | PEB | C3C-C4C | 2.63 | 1.45 | 1.42 |
| 3 | T | 186 | PEB | OD-C4D | 2.63 | 1.28 | 1.23 |
| 3 | B | 167 | PEB | C3C-C4C | 2.64 | 1.45 | 1.42 |
| 3 | S | 187 | PEB | C3B-C2B | 2.64 | 1.42 | 1.36 |
| 3 | Q | 188 | PEB | CHA-C1B | 2.64 | 1.46 | 1.40 |
| 3 | X | 188 | PEB | C2C-C3C | 2.64 | 1.45 | 1.37 |
| 3 | W | 186 | PEB | C3C-C4C | 2.64 | 1.45 | 1.42 |
| 3 | E | 167 | PEB | C3B-C2B | 2.64 | 1.42 | 1.36 |
| 3 | U | 186 | PEB | C2C-C3C | 2.65 | 1.45 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 3 | L | 167 | PEB | C2D-C3D | 2.66 | 1.38 | 1.34 |
| 3 | T | 187 | PEB | C2C-C3C | 2.68 | 1.45 | 1.37 |
| 3 | P | 186 | PEB | C1D-ND | 2.69 | 1.50 | 1.45 |
| 3 | J | 166 | PEB | CHA-C1B | 2.71 | 1.46 | 1.40 |
| 3 | E | 166 | PEB | C2C-C3C | 2.71 | 1.45 | 1.37 |
| 3 | K | 166 | PEB | C3A-C4A | 2.72 | 1.55 | 1.50 |
| 3 | T | 187 | PEB | C3B-C2B | 2.72 | 1.42 | 1.36 |
| 3 | L | 167 | PEB | OD-C4D | 2.72 | 1.28 | 1.23 |
| 3 | I | 167 | PEB | C3C-C4C | 2.73 | 1.46 | 1.42 |
| 3 | F | 167 | PEB | CHA-C1B | 2.73 | 1.47 | 1.40 |
| 3 | L | 167 | PEB | C3B-C2B | 2.74 | 1.42 | 1.36 |
| 3 | H | 167 | PEB | C3B-C2B | 2.74 | 1.42 | 1.36 |
| 3 | T | 188 | PEB | C2C-C3C | 2.76 | 1.45 | 1.37 |
| 5 | U | 205 | PI | P-O1 | 2.76 | 1.56 | 1.50 |
| 4 | D | 203 | NO3 | O1-N | 2.77 | 1.34 | 1.23 |
| 3 | G | 167 | PEB | C3C-C4C | 2.77 | 1.46 | 1.42 |
| 3 | J | 167 | PEB | CHA-C1B | 2.78 | 1.47 | 1.40 |
| 3 | U | 186 | PEB | C3C-C4C | 2.78 | 1.46 | 1.42 |
| 3 | A | 166 | PEB | CHA-C1B | 2.78 | 1.47 | 1.40 |
| 3 | E | 167 | PEB | CHA-C1B | 2.78 | 1.47 | 1.40 |
| 3 | I | 166 | PEB | C3C-C4C | 2.79 | 1.46 | 1.42 |
| 3 | R | 187 | PEB | C2C-C3C | 2.80 | 1.46 | 1.37 |
| 3 | G | 167 | PEB | OD-C4D | 2.81 | 1.28 | 1.23 |
| 3 | Q | 186 | PEB | C2C-C3C | 2.81 | 1.46 | 1.37 |
| 3 | S | 188 | PEB | CHA-C1B | 2.81 | 1.47 | 1.40 |
| 3 | P | 188 | PEB | OD-C4D | 2.83 | 1.28 | 1.23 |
| 3 | M | 187 | PEB | CHA-C1B | 2.84 | 1.47 | 1.40 |
| 3 | O | 188 | PEB | C2C-C3C | 2.85 | 1.46 | 1.37 |
| 3 | X | 186 | PEB | C3B-C2B | 2.86 | 1.42 | 1.36 |
| 3 | S | 186[A] | PEB | OD-C4D | 2.87 | 1.29 | 1.23 |
| 3 | S | 186[B] | PEB | OD-C4D | 2.87 | 1.29 | 1.23 |
| 3 | P | 186 | PEB | OD-C4D | 2.88 | 1.29 | 1.23 |
| 3 | N | 188 | PEB | C2C-C3C | 2.88 | 1.46 | 1.37 |
| 3 | R | 186 | PEB | OD-C4D | 2.89 | 1.29 | 1.23 |
| 3 | L | 167 | PEB | CHA-C1B | 2.89 | 1.47 | 1.40 |
| 3 | R | 187 | PEB | OD-C4D | 2.89 | 1.29 | 1.23 |
| 3 | Q | 186 | PEB | C3C-C4C | 2.90 | 1.46 | 1.42 |
| 3 | V | 187 | PEB | CHA-C1B | 2.90 | 1.47 | 1.40 |
| 3 | K | 166 | PEB | CHA-C1B | 2.91 | 1.47 | 1.40 |
| 3 | Q | 188 | PEB | OD-C4D | 2.92 | 1.29 | 1.23 |
| 3 | W | 186 | PEB | OD-C4D | 2.92 | 1.29 | 1.23 |
| 3 | I | 167 | PEB | C3B-C2B | 2.93 | 1.43 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 3 | Q | 188 | PEB | C3A-C4A | 2.94 | 1.55 | 1.50 |
| 3 | C | 166 | PEB | C3C-C4C | 2.94 | 1.46 | 1.42 |
| 3 | K | 167 | PEB | C3B-C2B | 2.94 | 1.43 | 1.36 |
| 3 | P | 186 | PEB | CHA-C1B | 2.94 | 1.47 | 1.40 |
| 3 | V | 188 | PEB | CHA-C1B | 2.95 | 1.47 | 1.40 |
| 3 | M | 188 | PEB | C3B-C2B | 2.95 | 1.43 | 1.36 |
| 3 | G | 167 | PEB | CHA-C1B | 2.95 | 1.47 | 1.40 |
| 3 | I | 166 | PEB | CHA-C1B | 2.98 | 1.47 | 1.40 |
| 3 | D | 167 | PEB | CHA-C1B | 2.98 | 1.47 | 1.40 |
| 3 | W | 186 | PEB | CHA-C1B | 2.98 | 1.47 | 1.40 |
| 3 | I | 167 | PEB | CHA-C1B | 3.02 | 1.47 | 1.40 |
| 3 | H | 167 | PEB | C2C-C3C | 3.02 | 1.46 | 1.37 |
| 3 | Q | 188 | PEB | C3B-C2B | 3.03 | 1.43 | 1.36 |
| 3 | S | 186[A] | PEB | CHA-C1B | 3.04 | 1.47 | 1.40 |
| 3 | S | 186[B] | PEB | CHA-C1B | 3.04 | 1.47 | 1.40 |
| 3 | V | 187 | PEB | C3B-C2B | 3.04 | 1.43 | 1.36 |
| 3 | S | 187 | PEB | CHA-C1B | 3.05 | 1.47 | 1.40 |
| 3 | X | 188 | PEB | CHA-C1B | 3.07 | 1.47 | 1.40 |
| 3 | E | 166 | PEB | CHA-C1B | 3.08 | 1.47 | 1.40 |
| 3 | F | 166 | PEB | C3B-C2B | 3.10 | 1.43 | 1.36 |
| 3 | D | 166 | PEB | CHA-C1B | 3.11 | 1.47 | 1.40 |
| 3 | N | 186 | PEB | C3B-C2B | 3.12 | 1.43 | 1.36 |
| 3 | P | 188 | PEB | CHA-C1B | 3.13 | 1.47 | 1.40 |
| 3 | U | 186 | PEB | CHA-C1B | 3.13 | 1.48 | 1.40 |
| 3 | V | 186 | PEB | C3B-C2B | 3.14 | 1.43 | 1.36 |
| 3 | V | 186 | PEB | CHA-C1B | 3.15 | 1.48 | 1.40 |
| 3 | O | 187 | PEB | CHA-C1B | 3.16 | 1.48 | 1.40 |
| 3 | K | 167 | PEB | C2C-C3C | 3.16 | 1.47 | 1.37 |
| 3 | B | 166 | PEB | CHA-C1B | 3.17 | 1.48 | 1.40 |
| 3 | B | 167 | PEB | C3B-C2B | 3.18 | 1.43 | 1.36 |
| 3 | R | 186 | PEB | C2C-C3C | 3.18 | 1.47 | 1.37 |
| 3 | F | 166 | PEB | C3C-C4C | 3.20 | 1.46 | 1.42 |
| 3 | H | 166 | PEB | CHA-C1B | 3.21 | 1.48 | 1.40 |
| 3 | A | 167 | PEB | CHA-C1B | 3.21 | 1.48 | 1.40 |
| 3 | V | 188 | PEB | C3B-C2B | 3.21 | 1.43 | 1.36 |
| 3 | S | 186[A] | PEB | C2C-C3C | 3.22 | 1.47 | 1.37 |
| 3 | E | 167 | PEB | C3C-C4C | 3.22 | 1.46 | 1.42 |
| 3 | N | 187 | PEB | C3B-C2B | 3.25 | 1.43 | 1.36 |
| 3 | K | 167 | PEB | C3C-C4C | 3.25 | 1.46 | 1.42 |
| 3 | O | 188 | PEB | OD-C4D | 3.25 | 1.29 | 1.23 |
| 3 | U | 188 | PEB | C3B-C2B | 3.25 | 1.43 | 1.36 |
| 3 | U | 187 | PEB | C3B-C2B | 3.25 | 1.43 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | C | 167 | PEB | C2C-C3C | 3.26 | 1.47 | 1.37 |
| 3 | O | 188 | PEB | C1D-ND | 3.27 | 1.50 | 1.45 |
| 3 | K | 166 | PEB | OD-C4D | 3.28 | 1.29 | 1.23 |
| 3 | D | 167 | PEB | C3C-C4C | 3.31 | 1.46 | 1.42 |
| 3 | M | 187 | PEB | C3B-C2B | 3.32 | 1.43 | 1.36 |
| 3 | C | 167 | PEB | C3B-C2B | 3.32 | 1.43 | 1.36 |
| 3 | Q | 187 | PEB | C3B-C2B | 3.32 | 1.43 | 1.36 |
| 3 | M | 186 | PEB | CHA-C1B | 3.35 | 1.48 | 1.40 |
| 3 | P | 187 | PEB | C3B-C2B | 3.36 | 1.43 | 1.36 |
| 3 | D | 166 | PEB | C3B-C2B | 3.36 | 1.43 | 1.36 |
| 3 | G | 167 | PEB | C3B-C2B | 3.37 | 1.43 | 1.36 |
| 3 | T | 187 | PEB | CHA-C1B | 3.38 | 1.48 | 1.40 |
| 3 | J | 166 | PEB | C2D-C3D | 3.38 | 1.39 | 1.34 |
| 3 | E | 166 | PEB | OD-C4D | 3.39 | 1.29 | 1.23 |
| 3 | W | 188 | PEB | CHA-C1B | 3.39 | 1.48 | 1.40 |
| 3 | C | 167 | PEB | CHA-C1B | 3.40 | 1.48 | 1.40 |
| 3 | Q | 187 | PEB | CHA-C1B | 3.41 | 1.48 | 1.40 |
| 3 | R | 186 | PEB | CHA-C1B | 3.41 | 1.48 | 1.40 |
| 3 | D | 167 | PEB | C3B-C2B | 3.41 | 1.44 | 1.36 |
| 3 | O | 188 | PEB | C3B-C2B | 3.43 | 1.44 | 1.36 |
| 3 | R | 187 | PEB | CHA-C1B | 3.44 | 1.48 | 1.40 |
| 3 | W | 188 | PEB | C2C-C3C | 3.44 | 1.47 | 1.37 |
| 3 | P | 186 | PEB | C3B-C2B | 3.48 | 1.44 | 1.36 |
| 3 | X | 186 | PEB | CHA-C1B | 3.48 | 1.48 | 1.40 |
| 3 | B | 166 | PEB | C3C-C4C | 3.49 | 1.47 | 1.42 |
| 3 | U | 188 | PEB | CHA-C1B | 3.53 | 1.48 | 1.40 |
| 3 | F | 167 | PEB | C3C-C4C | 3.53 | 1.47 | 1.42 |
| 3 | P | 187 | PEB | CHA-C1B | 3.54 | 1.48 | 1.40 |
| 3 | M | 186 | PEB | C3B-C2B | 3.56 | 1.44 | 1.36 |
| 3 | F | 167 | PEB | C3B-C2B | 3.56 | 1.44 | 1.36 |
| 3 | N | 187 | PEB | CHA-C1B | 3.57 | 1.49 | 1.40 |
| 3 | W | 186 | PEB | C3B-C2B | 3.57 | 1.44 | 1.36 |
| 3 | C | 167 | PEB | C3C-C4C | 3.58 | 1.47 | 1.42 |
| 3 | X | 188 | PEB | C3B-C2B | 3.60 | 1.44 | 1.36 |
| 3 | T | 188 | PEB | C3B-C2B | 3.61 | 1.44 | 1.36 |
| 3 | S | 188 | PEB | C3B-C2B | 3.62 | 1.44 | 1.36 |
| 3 | O | 187 | PEB | C3B-C2B | 3.63 | 1.44 | 1.36 |
| 3 | B | 167 | PEB | C2D-C3D | 3.65 | 1.39 | 1.34 |
| 3 | O | 186 | PEB | C3B-C2B | 3.66 | 1.44 | 1.36 |
| 3 | X | 187 | PEB | C3B-C2B | 3.68 | 1.44 | 1.36 |
| 3 | A | 167 | PEB | C2D-C3D | 3.68 | 1.39 | 1.34 |
| 3 | U | 187 | PEB | CHA-C1B | 3.68 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 3 | R | 186 | PEB | C3B-C2B | 3.71 | 1.44 | 1.36 |
| 3 | K | 166 | PEB | C3B-C2B | 3.71 | 1.44 | 1.36 |
| 3 | Q | 186 | PEB | CHA-C1B | 3.73 | 1.49 | 1.40 |
| 3 | S | 186[A] | PEB | C3B-C2B | 3.74 | 1.44 | 1.36 |
| 3 | S | 186[B] | PEB | C3B-C2B | 3.74 | 1.44 | 1.36 |
| 3 | Q | 186 | PEB | C3B-C2B | 3.76 | 1.44 | 1.36 |
| 3 | H | 167 | PEB | CHA-C1B | 3.80 | 1.49 | 1.40 |
| 3 | W | 187 | PEB | C3B-C2B | 3.81 | 1.44 | 1.36 |
| 3 | I | 166 | PEB | C3B-C2B | 3.82 | 1.44 | 1.36 |
| 3 | P | 188 | PEB | C3B-C2B | 3.83 | 1.44 | 1.36 |
| 3 | O | 188 | PEB | CHA-C1B | 3.89 | 1.49 | 1.40 |
| 3 | L | 166 | PEB | CHA-C1B | 3.90 | 1.49 | 1.40 |
| 3 | T | 186 | PEB | CHA-C1B | 3.95 | 1.49 | 1.40 |
| 3 | V | 186 | PEB | C2D-C3D | 3.95 | 1.39 | 1.34 |
| 3 | B | 166 | PEB | C3B-C2B | 3.99 | 1.45 | 1.36 |
| 3 | W | 187 | PEB | C3C-C4C | 4.05 | 1.48 | 1.42 |
| 3 | G | 166 | PEB | C3B-C2B | 4.05 | 1.45 | 1.36 |
| 3 | N | 186 | PEB | CHA-C1B | 4.06 | 1.50 | 1.40 |
| 3 | R | 188 | PEB | C3B-C2B | 4.09 | 1.45 | 1.36 |
| 3 | U | 186 | PEB | C3B-C2B | 4.11 | 1.45 | 1.36 |
| 3 | H | 166 | PEB | C3B-C2B | 4.12 | 1.45 | 1.36 |
| 3 | U | 187 | PEB | C3A-C4A | 4.13 | 1.57 | 1.50 |
| 3 | T | 188 | PEB | CHA-C1B | 4.15 | 1.50 | 1.40 |
| 3 | N | 188 | PEB | C3B-C2B | 4.24 | 1.45 | 1.36 |
| 3 | W | 188 | PEB | C3B-C2B | 4.30 | 1.46 | 1.36 |
| 3 | B | 166 | PEB | C2D-C3D | 4.32 | 1.40 | 1.34 |
| 3 | A | 166 | PEB | C2D-C3D | 4.32 | 1.40 | 1.34 |
| 3 | C | 167 | PEB | C2D-C3D | 4.37 | 1.40 | 1.34 |
| 3 | J | 167 | PEB | C3B-C2B | 4.39 | 1.46 | 1.36 |
| 3 | T | 187 | PEB | C2D-C3D | 4.40 | 1.40 | 1.34 |
| 3 | R | 187 | PEB | C3B-C2B | 4.44 | 1.46 | 1.36 |
| 3 | R | 186 | PEB | C3C-C4C | 4.51 | 1.48 | 1.42 |
| 3 | J | 167 | PEB | C2D-C3D | 4.62 | 1.40 | 1.34 |
| 3 | J | 166 | PEB | C3B-C2B | 4.65 | 1.46 | 1.36 |
| 3 | R | 188 | PEB | CHA-C1B | 4.67 | 1.51 | 1.40 |
| 3 | T | 186 | PEB | C3B-C2B | 4.74 | 1.46 | 1.36 |
| 3 | C | 166 | PEB | C3B-C2B | 4.78 | 1.47 | 1.36 |
| 3 | G | 167 | PEB | C2D-C3D | 4.82 | 1.40 | 1.34 |
| 3 | T | 186 | PEB | C3C-C4C | 4.93 | 1.49 | 1.42 |
| 3 | M | 187 | PEB | C2D-C3D | 4.97 | 1.41 | 1.34 |
| 3 | E | 166 | PEB | C3C-C4C | 4.97 | 1.49 | 1.42 |
| 3 | L | 166 | PEB | C2D-C3D | 5.02 | 1.41 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 3 | G | 166 | PEB | C2D-C3D | 5.06 | 1.41 | 1.34 |
| 3 | H | 166 | PEB | C3C-C4C | 5.06 | 1.49 | 1.42 |
| 3 | W | 187 | PEB | C2D-C3D | 5.11 | 1.41 | 1.34 |
| 3 | S | 186[A] | PEB | C2D-C3D | 5.22 | 1.41 | 1.34 |
| 3 | S | 186[B] | PEB | C2D-C3D | 5.22 | 1.41 | 1.34 |
| 3 | O | 186 | PEB | C2D-C3D | 5.26 | 1.41 | 1.34 |
| 3 | Q | 187 | PEB | C2D-C3D | 5.29 | 1.41 | 1.34 |
| 3 | E | 166 | PEB | C3B-C2B | 5.33 | 1.48 | 1.36 |
| 3 | P | 187 | PEB | C2D-C3D | 5.42 | 1.41 | 1.34 |
| 3 | K | 166 | PEB | C2D-C3D | 5.50 | 1.41 | 1.34 |
| 3 | N | 187 | PEB | C2D-C3D | 5.52 | 1.41 | 1.34 |
| 3 | E | 167 | PEB | C2D-C3D | 5.55 | 1.41 | 1.34 |
| 3 | N | 186 | PEB | C2D-C3D | 5.57 | 1.41 | 1.34 |
| 3 | F | 167 | PEB | C2D-C3D | 5.61 | 1.41 | 1.34 |
| 3 | R | 188 | PEB | C2D-C3D | 5.73 | 1.41 | 1.34 |
| 3 | S | 188 | PEB | C2D-C3D | 5.86 | 1.42 | 1.34 |
| 3 | R | 186 | PEB | C2D-C3D | 5.91 | 1.42 | 1.34 |
| 3 | U | 187 | PEB | C2D-C3D | 6.02 | 1.42 | 1.34 |
| 3 | H | 167 | PEB | C2D-C3D | 6.06 | 1.42 | 1.34 |
| 3 | E | 166 | PEB | C2D-C3D | 6.15 | 1.42 | 1.34 |
| 3 | F | 166 | PEB | C2D-C3D | 6.16 | 1.42 | 1.34 |
| 3 | X | 187 | PEB | C2D-C3D | 6.24 | 1.42 | 1.34 |
| 3 | W | 186 | PEB | C2D-C3D | 6.28 | 1.42 | 1.34 |
| 3 | Q | 188 | PEB | C2D-C3D | 6.28 | 1.42 | 1.34 |
| 3 | I | 167 | PEB | C2D-C3D | 6.33 | 1.42 | 1.34 |
| 3 | M | 186 | PEB | C2D-C3D | 6.37 | 1.42 | 1.34 |
| 3 | C | 166 | PEB | C2D-C3D | 6.54 | 1.43 | 1.34 |
| 3 | T | 188 | PEB | C2D-C3D | 6.54 | 1.43 | 1.34 |
| 3 | T | 186 | PEB | C2D-C3D | 6.54 | 1.43 | 1.34 |
| 3 | U | 186 | PEB | C2D-C3D | 6.67 | 1.43 | 1.34 |
| 3 | S | 187 | PEB | C2D-C3D | 6.68 | 1.43 | 1.34 |
| 3 | D | 166 | PEB | C2D-C3D | 6.76 | 1.43 | 1.34 |
| 3 | X | 186 | PEB | C2D-C3D | 6.88 | 1.43 | 1.34 |
| 3 | K | 167 | PEB | C2D-C3D | 6.94 | 1.43 | 1.34 |
| 3 | I | 167 | PEB | CHB-C4B | 7.03 | 1.41 | 1.35 |
| 3 | H | 166 | PEB | C2D-C3D | 7.09 | 1.43 | 1.34 |
| 3 | O | 188 | PEB | CHB-C4B | 7.16 | 1.41 | 1.35 |
| 3 | R | 187 | PEB | C2D-C3D | 7.17 | 1.43 | 1.34 |
| 3 | L | 167 | PEB | CHB-C4B | 7.21 | 1.41 | 1.35 |
| 3 | I | 166 | PEB | C2D-C3D | 7.27 | 1.43 | 1.34 |
| 3 | U | 188 | PEB | C2D-C3D | 7.28 | 1.43 | 1.34 |
| 3 | A | 167 | PEB | CHB-C4B | 7.35 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | M | 188 | PEB | C2D-C3D | 7.41 | 1.44 | 1.34 |
| 3 | X | 188 | PEB | CHB-C4B | 7.45 | 1.41 | 1.35 |
| 3 | Q | 188 | PEB | CHB-C4B | 7.48 | 1.41 | 1.35 |
| 3 | N | 188 | PEB | C2D-C3D | 7.53 | 1.44 | 1.34 |
| 3 | Q | 186 | PEB | C2D-C3D | 7.71 | 1.44 | 1.34 |
| 3 | O | 188 | PEB | C2D-C3D | 7.72 | 1.44 | 1.34 |
| 3 | V | 188 | PEB | C2D-C3D | 7.74 | 1.44 | 1.34 |
| 3 | C | 167 | PEB | CHB-C4B | 7.96 | 1.42 | 1.35 |
| 3 | W | 188 | PEB | C2D-C3D | 8.00 | 1.44 | 1.34 |
| 3 | D | 167 | PEB | CHB-C4B | 8.03 | 1.42 | 1.35 |
| 3 | G | 166 | PEB | CHB-C4B | 8.05 | 1.42 | 1.35 |
| 3 | P | 188 | PEB | C2D-C3D | 8.07 | 1.44 | 1.34 |
| 3 | V | 187 | PEB | C2D-C3D | 8.25 | 1.45 | 1.34 |
| 3 | P | 188 | PEB | CHB-C4B | 8.29 | 1.42 | 1.35 |
| 3 | O | 187 | PEB | C2D-C3D | 8.31 | 1.45 | 1.34 |
| 3 | F | 166 | PEB | CHB-C4B | 8.33 | 1.42 | 1.35 |
| 3 | A | 166 | PEB | CHB-C4B | 8.51 | 1.42 | 1.35 |
| 3 | L | 166 | PEB | CHB-C4B | 8.63 | 1.42 | 1.35 |
| 3 | N | 187 | PEB | CHB-C4B | 8.75 | 1.42 | 1.35 |
| 3 | M | 188 | PEB | CHB-C4B | 8.76 | 1.42 | 1.35 |
| 3 | B | 167 | PEB | CHB-C4B | 8.79 | 1.42 | 1.35 |
| 3 | P | 186 | PEB | C2D-C3D | 8.88 | 1.46 | 1.34 |
| 3 | T | 188 | PEB | CHB-C4B | 9.06 | 1.43 | 1.35 |
| 3 | X | 187 | PEB | CHB-C4B | 9.13 | 1.43 | 1.35 |
| 3 | U | 188 | PEB | CHB-C4B | 9.22 | 1.43 | 1.35 |
| 3 | K | 167 | PEB | CHB-C4B | 9.27 | 1.43 | 1.35 |
| 3 | P | 187 | PEB | CHB-C4B | 9.36 | 1.43 | 1.35 |
| 3 | V | 188 | PEB | CHB-C4B | 9.36 | 1.43 | 1.35 |
| 3 | M | 187 | PEB | CHB-C4B | 9.36 | 1.43 | 1.35 |
| 3 | X | 188 | PEB | C2D-C3D | 9.37 | 1.46 | 1.34 |
| 3 | H | 167 | PEB | CHB-C4B | 9.41 | 1.43 | 1.35 |
| 3 | J | 166 | PEB | CHB-C4B | 9.55 | 1.43 | 1.35 |
| 3 | W | 187 | PEB | CHB-C4B | 9.68 | 1.43 | 1.35 |
| 3 | D | 166 | PEB | CHB-C4B | 9.70 | 1.43 | 1.35 |
| 3 | K | 166 | PEB | CHB-C4B | 9.86 | 1.43 | 1.35 |
| 3 | J | 167 | PEB | CHB-C4B | 9.96 | 1.44 | 1.35 |
| 3 | F | 167 | PEB | CHB-C4B | 10.01 | 1.44 | 1.35 |
| 3 | O | 187 | PEB | CHB-C4B | 10.09 | 1.44 | 1.35 |
| 3 | R | 188 | PEB | CHB-C4B | 10.33 | 1.44 | 1.35 |
| 3 | B | 166 | PEB | CHB-C4B | 10.36 | 1.44 | 1.35 |
| 3 | V | 186 | PEB | CHB-C4B | 10.47 | 1.44 | 1.35 |
| 3 | U | 186 | PEB | CHB-C4B | 10.68 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3 | T | 187 | PEB | CHB-C4B | 10.92 | 1.44 | 1.35 |
| 3 | X | 186 | PEB | CHB-C4B | 10.93 | 1.44 | 1.35 |
| 3 | N | 188 | PEB | CHB-C4B | 11.25 | 1.45 | 1.35 |
| 3 | G | 167 | PEB | CHB-C4B | 11.29 | 1.45 | 1.35 |
| 3 | E | 167 | PEB | CHB-C4B | 11.39 | 1.45 | 1.35 |
| 3 | S | 187 | PEB | CHB-C4B | 11.43 | 1.45 | 1.35 |
| 3 | V | 187 | PEB | CHB-C4B | 11.44 | 1.45 | 1.35 |
| 3 | O | 186 | PEB | CHB-C4B | 11.44 | 1.45 | 1.35 |
| 3 | U | 187 | PEB | CHB-C4B | 11.60 | 1.45 | 1.35 |
| 3 | Q | 187 | PEB | CHB-C4B | 11.76 | 1.45 | 1.35 |
| 3 | H | 166 | PEB | CHB-C4B | 11.86 | 1.45 | 1.35 |
| 3 | S | 188 | PEB | CHB-C4B | 11.93 | 1.45 | 1.35 |
| 3 | W | 188 | PEB | CHB-C4B | 12.41 | 1.46 | 1.35 |
| 3 | N | 186 | PEB | CHB-C4B | 12.43 | 1.46 | 1.35 |
| 3 | Q | 186 | PEB | CHB-C4B | 12.45 | 1.46 | 1.35 |
| 3 | T | 186 | PEB | CHB-C4B | 12.66 | 1.46 | 1.35 |
| 3 | M | 186 | PEB | CHB-C4B | 13.24 | 1.46 | 1.35 |
| 3 | R | 187 | PEB | CHB-C4B | 13.30 | 1.46 | 1.35 |
| 3 | R | 186 | PEB | CHB-C4B | 13.33 | 1.46 | 1.35 |
| 3 | I | 166 | PEB | CHB-C4B | 13.36 | 1.47 | 1.35 |
| 3 | S | 186[A] | PEB | CHB-C4B | 13.36 | 1.47 | 1.35 |
| 3 | S | 186[B] | PEB | CHB-C4B | 13.36 | 1.47 | 1.35 |
| 3 | W | 186 | PEB | CHB-C4B | 13.51 | 1.47 | 1.35 |
| 3 | P | 186 | PEB | CHB-C4B | 13.90 | 1.47 | 1.35 |
| 3 | C | 166 | PEB | CHB-C4B | 14.55 | 1.48 | 1.35 |
| 3 | E | 166 | PEB | CHB-C4B | 15.60 | 1.49 | 1.35 |

All (580) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3 | J | 166 | PEB | CHA-C1B-NB | -6.18 | 113.09 | 124.97 |
| 3 | H | 166 | PEB | CHA-C1B-NB | -5.96 | 113.52 | 124.97 |
| 3 | C | 166 | PEB | CHA-C1B-NB | -5.76 | 113.91 | 124.97 |
| 3 | E | 166 | PEB | CHA-C1B-NB | -5.49 | 114.43 | 124.97 |
| 3 | S | 186[A] | PEB | OA-C1A-C2A | -5.26 | 122.00 | 126.25 |
| 3 | S | 186[B] | PEB | OA-C1A-C2A | -5.26 | 122.00 | 126.25 |
| 3 | A | 166 | PEB | CHA-C1B-NB | -5.20 | 114.98 | 124.97 |
| 3 | U | 186 | PEB | OA-C1A-C2A | -5.04 | 122.18 | 126.25 |
| 3 | K | 166 | PEB | CHA-C1B-NB | -4.98 | 115.41 | 124.97 |
| 3 | E | 166 | PEB | CHC-C4C-C3C | -4.95 | 122.05 | 130.41 |
| 3 | C | 167 | PEB | CHC-C1D-ND | -4.94 | 108.08 | 114.03 |
| 3 | F | 166 | PEB | CHA-C1B-NB | -4.92 | 115.52 | 124.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3 | I | 166 | PEB | CHA-C1B-NB | -4.87 | 115.61 | 124.97 |
| 3 | E | 166 | PEB | C1B-C2B-C3B | -4.87 | 100.87 | 106.51 |
| 3 | W | 188 | PEB | CHC-C4C-C3C | -4.81 | 122.29 | 130.41 |
| 3 | G | 166 | PEB | CHA-C1B-NB | -4.73 | 115.89 | 124.97 |
| 3 | W | 186 | PEB | CHA-C1B-NB | -4.72 | 115.91 | 124.97 |
| 3 | M | 186 | PEB | CHA-C1B-NB | -4.69 | 115.96 | 124.97 |
| 3 | D | 166 | PEB | CHA-C1B-NB | -4.61 | 116.12 | 124.97 |
| 3 | B | 166 | PEB | CHA-C1B-NB | -4.53 | 116.27 | 124.97 |
| 3 | T | 187 | PEB | CHC-C1D-ND | -4.49 | 108.62 | 114.03 |
| 3 | L | 166 | PEB | CHA-C1B-NB | -4.48 | 116.36 | 124.97 |
| 3 | O | 188 | PEB | CHC-C1D-ND | -4.44 | 108.68 | 114.03 |
| 3 | Q | 187 | PEB | CHC-C1D-ND | -4.43 | 108.70 | 114.03 |
| 3 | R | 186 | PEB | C1D-ND-C4D | -4.35 | 108.12 | 113.78 |
| 3 | N | 186 | PEB | CHA-C1B-NB | -4.33 | 116.66 | 124.97 |
| 3 | R | 186 | PEB | OA-C1A-C2A | -4.29 | 122.78 | 126.25 |
| 3 | X | 187 | PEB | CHC-C1D-ND | -4.28 | 108.87 | 114.03 |
| 3 | S | 186[A] | PEB | C1D-ND-C4D | -4.28 | 108.22 | 113.78 |
| 3 | S | 186[B] | PEB | C1D-ND-C4D | -4.28 | 108.22 | 113.78 |
| 3 | U | 186 | PEB | CHA-C1B-NB | -4.24 | 116.82 | 124.97 |
| 3 | X | 188 | PEB | OA-C1A-C2A | -4.22 | 122.84 | 126.25 |
| 3 | S | 186[A] | PEB | CHC-C1D-ND | -4.20 | 108.97 | 114.03 |
| 3 | S | 186[B] | PEB | CHC-C1D-ND | -4.20 | 108.97 | 114.03 |
| 3 | T | 186 | PEB | OA-C1A-C2A | -4.15 | 122.90 | 126.25 |
| 3 | A | 167 | PEB | C1D-ND-C4D | -4.11 | 108.44 | 113.78 |
| 3 | D | 167 | PEB | OA-C1A-C2A | -4.10 | 122.94 | 126.25 |
| 3 | R | 188 | PEB | CHC-C4C-C3C | -4.09 | 123.50 | 130.41 |
| 3 | B | 166 | PEB | CHC-C1D-ND | -4.02 | 109.19 | 114.03 |
| 3 | P | 188 | PEB | CHC-C1D-ND | -3.92 | 109.30 | 114.03 |
| 3 | S | 187 | PEB | C4B-C3B-C2B | -3.91 | 102.42 | 106.81 |
| 3 | A | 166 | PEB | CHC-C1D-ND | -3.91 | 109.32 | 114.03 |
| 3 | K | 167 | PEB | C4B-C3B-C2B | -3.80 | 102.54 | 106.81 |
| 3 | Q | 186 | PEB | CHA-C1B-NB | -3.79 | 117.68 | 124.97 |
| 3 | T | 186 | PEB | CHA-C1B-NB | -3.79 | 117.70 | 124.97 |
| 3 | C | 167 | PEB | CHC-C4C-C3C | -3.77 | 124.05 | 130.41 |
| 3 | N | 186 | PEB | CHC-C1D-ND | -3.76 | 109.50 | 114.03 |
| 3 | C | 166 | PEB | C4B-C3B-C2B | -3.74 | 102.61 | 106.81 |
| 3 | V | 186 | PEB | CHA-C1B-NB | -3.74 | 117.79 | 124.97 |
| 3 | P | 186 | PEB | CHA-C1B-NB | -3.74 | 117.80 | 124.97 |
| 3 | U | 186 | PEB | CHC-C1D-ND | -3.71 | 109.56 | 114.03 |
| 3 | B | 166 | PEB | OA-C1A-C2A | -3.70 | 123.27 | 126.25 |
| 3 | R | 186 | PEB | CHA-C1B-NB | -3.68 | 117.90 | 124.97 |
| 3 | Q | 188 | PEB | CHC-C1D-ND | -3.66 | 109.62 | 114.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3 | T | 187 | PEB | CHC-C4C-C3C | -3.63 | 124.28 | 130.41 |
| 3 | T | 186 | PEB | CHC-C4C-C3C | -3.62 | 124.29 | 130.41 |
| 3 | H | 166 | PEB | OD-C4D-C3D | -3.62 | 121.39 | 129.77 |
| 3 | M | 188 | PEB | OD-C4D-C3D | -3.61 | 121.41 | 129.77 |
| 3 | O | 186 | PEB | C1D-ND-C4D | -3.56 | 109.16 | 113.78 |
| 3 | F | 167 | PEB | CHC-C1D-ND | -3.56 | 109.75 | 114.03 |
| 3 | E | 166 | PEB | CHC-C1D-ND | -3.54 | 109.76 | 114.03 |
| 3 | J | 167 | PEB | OA-C1A-C2A | -3.54 | 123.39 | 126.25 |
| 3 | H | 167 | PEB | CAB-CBB-CGB | -3.54 | 106.61 | 112.66 |
| 3 | W | 186 | PEB | CHC-C1D-ND | -3.53 | 109.78 | 114.03 |
| 3 | R | 186 | PEB | CHC-C1D-ND | -3.52 | 109.79 | 114.03 |
| 3 | L | 167 | PEB | C1D-ND-C4D | -3.51 | 109.21 | 113.78 |
| 3 | J | 167 | PEB | C1B-C2B-C3B | -3.42 | 102.54 | 106.51 |
| 3 | H | 167 | PEB | C1B-C2B-C3B | -3.42 | 102.54 | 106.51 |
| 3 | Q | 186 | PEB | CHC-C1D-ND | -3.41 | 109.92 | 114.03 |
| 3 | F | 167 | PEB | C4B-C3B-C2B | -3.41 | 102.98 | 106.81 |
| 3 | C | 167 | PEB | C1B-C2B-C3B | -3.41 | 102.56 | 106.51 |
| 3 | Q | 187 | PEB | CHC-C4C-C3C | -3.37 | 124.72 | 130.41 |
| 3 | H | 166 | PEB | C1B-C2B-C3B | -3.36 | 102.61 | 106.51 |
| 3 | J | 167 | PEB | CHC-C1D-ND | -3.36 | 109.98 | 114.03 |
| 3 | N | 188 | PEB | CBC-CAC-C2C | -3.31 | 106.16 | 112.48 |
| 3 | G | 167 | PEB | CHC-C1D-ND | -3.29 | 110.06 | 114.03 |
| 3 | V | 188 | PEB | OD-C4D-C3D | -3.27 | 122.20 | 129.77 |
| 3 | K | 166 | PEB | OA-C1A-C2A | -3.26 | 123.62 | 126.25 |
| 3 | U | 186 | PEB | C3A-C4A-NA | -3.25 | 104.90 | 107.97 |
| 3 | S | 186[A] | PEB | CHA-C1B-NB | -3.24 | 118.75 | 124.97 |
| 3 | S | 186[B] | PEB | CHA-C1B-NB | -3.24 | 118.75 | 124.97 |
| 3 | B | 166 | PEB | CAC-CBC-CGC | -3.23 | 107.14 | 112.66 |
| 3 | H | 167 | PEB | CHC-C1D-ND | -3.22 | 110.16 | 114.03 |
| 3 | J | 167 | PEB | C1D-ND-C4D | -3.22 | 109.60 | 113.78 |
| 3 | M | 186 | PEB | OA-C1A-C2A | -3.21 | 123.66 | 126.25 |
| 3 | X | 188 | PEB | CHC-C4C-C3C | -3.17 | 125.06 | 130.41 |
| 3 | L | 166 | PEB | CMA-C2A-C1A | -3.17 | 105.77 | 112.43 |
| 3 | N | 188 | PEB | OA-C1A-C2A | -3.16 | 123.70 | 126.25 |
| 3 | S | 188 | PEB | CHC-C4C-C3C | -3.15 | 125.09 | 130.41 |
| 3 | L | 167 | PEB | OD-C4D-ND | -3.14 | 120.74 | 125.83 |
| 3 | O | 186 | PEB | CHC-C1D-ND | -3.13 | 110.26 | 114.03 |
| 3 | I | 167 | PEB | CHC-C4C-C3C | -3.12 | 125.14 | 130.41 |
| 3 | H | 166 | PEB | CHC-C4C-C3C | -3.11 | 125.16 | 130.41 |
| 3 | T | 186 | PEB | OD-C4D-C3D | -3.09 | 122.61 | 129.77 |
| 3 | P | 188 | PEB | C4B-C3B-C2B | -3.09 | 103.34 | 106.81 |
| 3 | N | 186 | PEB | CHB-C4B-C3B | -3.08 | 118.09 | 125.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3 | H | 166 | PEB | C1D-ND-C4D | -3.07 | 109.79 | 113.78 |
| 3 | M | 188 | PEB | OA-C1A-C2A | -3.07 | 123.78 | 126.25 |
| 3 | K | 167 | PEB | OD-C4D-ND | -3.06 | 120.87 | 125.83 |
| 3 | C | 166 | PEB | CAC-CBC-CGC | -3.06 | 107.44 | 112.66 |
| 3 | K | 167 | PEB | C1D-ND-C4D | -3.05 | 109.81 | 113.78 |
| 3 | M | 187 | PEB | CHC-C1D-ND | -3.05 | 110.36 | 114.03 |
| 3 | C | 167 | PEB | CHB-C4B-NB | -3.04 | 124.18 | 128.79 |
| 3 | T | 188 | PEB | CHC-C4C-C3C | -3.04 | 125.28 | 130.41 |
| 3 | S | 188 | PEB | OD-C4D-C3D | -3.01 | 122.81 | 129.77 |
| 3 | H | 166 | PEB | CHB-C4B-NB | -3.00 | 124.24 | 128.79 |
| 3 | K | 166 | PEB | CAC-CBC-CGC | -3.00 | 107.53 | 112.66 |
| 7 | R | 204 | MPD | C5-C4-C3 | -2.99 | 97.27 | 112.11 |
| 3 | N | 188 | PEB | OD-C4D-C3D | -2.98 | 122.86 | 129.77 |
| 3 | S | 186[A] | PEB | OD-C4D-C3D | -2.98 | 122.86 | 129.77 |
| 3 | S | 186[B] | PEB | OD-C4D-C3D | -2.98 | 122.86 | 129.77 |
| 3 | V | 186 | PEB | C1D-ND-C4D | -2.97 | 109.92 | 113.78 |
| 3 | T | 188 | PEB | OA-C1A-NA | -2.96 | 121.34 | 124.87 |
| 3 | T | 186 | PEB | CAB-CBB-CGB | -2.96 | 107.60 | 112.66 |
| 3 | C | 167 | PEB | C1D-ND-C4D | -2.96 | 109.94 | 113.78 |
| 3 | J | 167 | PEB | CHC-C4C-C3C | -2.95 | 125.42 | 130.41 |
| 3 | R | 186 | PEB | CHC-C4C-C3C | -2.92 | 125.47 | 130.41 |
| 3 | W | 188 | PEB | C4B-C3B-C2B | -2.92 | 103.53 | 106.81 |
| 3 | W | 186 | PEB | C1D-ND-C4D | -2.91 | 109.99 | 113.78 |
| 3 | A | 166 | PEB | CMA-C2A-C1A | -2.91 | 106.31 | 112.43 |
| 3 | V | 187 | PEB | CHC-C4C-C3C | -2.90 | 125.51 | 130.41 |
| 3 | S | 187 | PEB | OA-C1A-C2A | -2.89 | 123.92 | 126.25 |
| 3 | P | 187 | PEB | OD-C4D-C3D | -2.88 | 123.09 | 129.77 |
| 3 | E | 167 | PEB | CHC-C1D-ND | -2.88 | 110.56 | 114.03 |
| 3 | W | 187 | PEB | CHC-C4C-C3C | -2.87 | 125.55 | 130.41 |
| 3 | X | 186 | PEB | OD-C4D-C3D | -2.87 | 123.12 | 129.77 |
| 3 | D | 166 | PEB | CHB-C4B-NB | -2.86 | 124.46 | 128.79 |
| 3 | K | 166 | PEB | CMA-C2A-C1A | -2.85 | 106.45 | 112.43 |
| 3 | W | 186 | PEB | C4B-C3B-C2B | -2.84 | 103.62 | 106.81 |
| 3 | N | 186 | PEB | C1D-ND-C4D | -2.84 | 110.09 | 113.78 |
| 3 | P | 188 | PEB | CHC-C4C-C3C | -2.84 | 125.61 | 130.41 |
| 3 | E | 166 | PEB | OD-C4D-C3D | -2.83 | 123.21 | 129.77 |
| 3 | I | 166 | PEB | CAC-CBC-CGC | -2.83 | 107.82 | 112.66 |
| 3 | U | 186 | PEB | C1B-C2B-C3B | -2.82 | 103.24 | 106.51 |
| 3 | M | 188 | PEB | CHC-C4C-C3C | -2.82 | 125.65 | 130.41 |
| 3 | F | 167 | PEB | OD-C4D-C3D | -2.81 | 123.26 | 129.77 |
| 3 | I | 166 | PEB | C3A-C4A-NA | -2.80 | 105.33 | 107.97 |
| 3 | T | 188 | PEB | OD-C4D-ND | -2.80 | 121.30 | 125.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | R | 186 | PEB | OD-C4D-C3D | -2.79 | 123.30 | 129.77 |
| 3 | S | 187 | PEB | CHC-C1D-ND | -2.79 | 110.67 | 114.03 |
| 3 | P | 187 | PEB | CHC-C4C-C3C | -2.79 | 125.70 | 130.41 |
| 3 | T | 186 | PEB | CHC-C1D-ND | -2.76 | 110.70 | 114.03 |
| 3 | N | 186 | PEB | OA-C1A-C2A | -2.76 | 124.02 | 126.25 |
| 3 | D | 166 | PEB | CMA-C2A-C1A | -2.76 | 106.63 | 112.43 |
| 3 | J | 166 | PEB | CMA-C2A-C1A | -2.76 | 106.63 | 112.43 |
| 3 | A | 167 | PEB | OD-C4D-ND | -2.75 | 121.37 | 125.83 |
| 3 | Q | 186 | PEB | OA-C1A-C2A | -2.73 | 124.05 | 126.25 |
| 3 | N | 187 | PEB | CHC-C1D-ND | -2.72 | 110.75 | 114.03 |
| 3 | D | 167 | PEB | C4B-C3B-C2B | -2.72 | 103.75 | 106.81 |
| 3 | I | 167 | PEB | CAB-C3B-C2B | -2.72 | 122.83 | 127.88 |
| 5 | B | 204 | PI | O2-P-O1 | -2.72 | 99.41 | 110.97 |
| 3 | J | 167 | PEB | OD-C4D-ND | -2.72 | 121.42 | 125.83 |
| 3 | C | 166 | PEB | OD-C4D-C3D | -2.71 | 123.50 | 129.77 |
| 3 | X | 188 | PEB | OD-C4D-C3D | -2.68 | 123.56 | 129.77 |
| 3 | F | 166 | PEB | CHB-C4B-NB | -2.68 | 124.73 | 128.79 |
| 3 | Q | 186 | PEB | C1D-ND-C4D | -2.67 | 110.31 | 113.78 |
| 3 | A | 167 | PEB | OA-C1A-C2A | -2.67 | 124.10 | 126.25 |
| 3 | K | 167 | PEB | CBC-CAC-C2C | -2.67 | 107.38 | 112.48 |
| 3 | B | 167 | PEB | CHC-C4C-C3C | -2.67 | 125.91 | 130.41 |
| 3 | W | 188 | PEB | CBC-CAC-C2C | -2.66 | 107.39 | 112.48 |
| 3 | R | 187 | PEB | OD-C4D-C3D | -2.66 | 123.61 | 129.77 |
| 3 | O | 188 | PEB | OD-C4D-C3D | -2.65 | 123.63 | 129.77 |
| 3 | X | 188 | PEB | CHC-C1D-ND | -2.65 | 110.84 | 114.03 |
| 3 | W | 188 | PEB | CBD-CAD-C3D | -2.64 | 114.15 | 127.39 |
| 3 | N | 187 | PEB | C2A-C1A-NA | -2.64 | 105.89 | 108.28 |
| 3 | P | 186 | PEB | C1D-ND-C4D | -2.63 | 110.36 | 113.78 |
| 3 | P | 186 | PEB | CHC-C1D-ND | -2.62 | 110.88 | 114.03 |
| 3 | P | 187 | PEB | C1D-ND-C4D | -2.62 | 110.38 | 113.78 |
| 3 | R | 187 | PEB | OA-C1A-C2A | -2.62 | 124.14 | 126.25 |
| 3 | B | 167 | PEB | C1D-ND-C4D | -2.61 | 110.39 | 113.78 |
| 3 | R | 188 | PEB | C1B-C2B-C3B | -2.61 | 103.48 | 106.51 |
| 3 | D | 167 | PEB | CHC-C4C-C3C | -2.61 | 126.00 | 130.41 |
| 3 | C | 167 | PEB | OA-C1A-NA | -2.60 | 121.77 | 124.87 |
| 3 | M | 187 | PEB | C1D-ND-C4D | -2.60 | 110.40 | 113.78 |
| 3 | I | 166 | PEB | C1D-ND-C4D | -2.60 | 110.40 | 113.78 |
| 3 | P | 186 | PEB | OA-C1A-C2A | -2.58 | 124.17 | 126.25 |
| 7 | B | 203 | MPD | C1-C2-C3 | -2.58 | 97.24 | 110.08 |
| 3 | R | 187 | PEB | C1D-ND-C4D | -2.58 | 110.43 | 113.78 |
| 3 | X | 186 | PEB | CHA-C1B-NB | -2.57 | 120.03 | 124.97 |
| 3 | G | 166 | PEB | CAC-CBC-CGC | -2.57 | 108.27 | 112.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3 | V | 188 | PEB | CHC-C4C-C3C | -2.57 | 126.07 | 130.41 |
| 3 | F | 166 | PEB | C1D-ND-C4D | -2.57 | 110.44 | 113.78 |
| 3 | S | 186[A] | PEB | C4B-C3B-C2B | -2.56 | 103.93 | 106.81 |
| 3 | S | 186[B] | PEB | C4B-C3B-C2B | -2.56 | 103.93 | 106.81 |
| 3 | W | 186 | PEB | OD-C4D-C3D | -2.56 | 123.84 | 129.77 |
| 3 | B | 167 | PEB | CHB-C4B-C3B | -2.56 | 119.32 | 125.39 |
| 3 | I | 166 | PEB | OD-C4D-C3D | -2.56 | 123.84 | 129.77 |
| 3 | E | 166 | PEB | CAC-CBC-CGC | -2.56 | 108.29 | 112.66 |
| 3 | S | 187 | PEB | CHB-C4B-C3B | -2.55 | 119.33 | 125.39 |
| 3 | W | 187 | PEB | OD-C4D-ND | -2.55 | 121.69 | 125.83 |
| 3 | O | 186 | PEB | CHA-C1B-NB | -2.55 | 120.07 | 124.97 |
| 3 | V | 188 | PEB | OA-C1A-C2A | -2.55 | 124.19 | 126.25 |
| 3 | U | 187 | PEB | C1B-C2B-C3B | -2.55 | 103.56 | 106.51 |
| 3 | L | 166 | PEB | CHC-C4C-C3C | -2.55 | 126.11 | 130.41 |
| 3 | R | 186 | PEB | OD-C4D-ND | -2.54 | 121.70 | 125.83 |
| 3 | H | 166 | PEB | CHC-C1D-ND | -2.54 | 110.97 | 114.03 |
| 3 | N | 188 | PEB | CHC-C4C-C3C | -2.53 | 126.14 | 130.41 |
| 3 | R | 187 | PEB | CHA-C1B-NB | -2.52 | 120.12 | 124.97 |
| 3 | F | 167 | PEB | C1D-ND-C4D | -2.52 | 110.51 | 113.78 |
| 3 | V | 186 | PEB | OD-C4D-ND | -2.52 | 121.75 | 125.83 |
| 3 | K | 167 | PEB | CHB-C4B-C3B | -2.51 | 119.43 | 125.39 |
| 3 | F | 166 | PEB | CMA-C2A-C1A | -2.51 | 107.16 | 112.43 |
| 3 | N | 188 | PEB | CBD-CAD-C3D | -2.50 | 114.87 | 127.39 |
| 3 | H | 167 | PEB | CHC-C4C-C3C | -2.49 | 126.20 | 130.41 |
| 3 | T | 188 | PEB | C3A-C4A-NA | -2.49 | 105.61 | 107.97 |
| 3 | T | 186 | PEB | CHB-C4B-C3B | -2.49 | 119.49 | 125.39 |
| 3 | T | 186 | PEB | C1D-ND-C4D | -2.48 | 110.55 | 113.78 |
| 3 | R | 186 | PEB | CAB-CBB-CGB | -2.48 | 108.42 | 112.66 |
| 3 | B | 166 | PEB | CHC-C4C-C3C | -2.47 | 126.24 | 130.41 |
| 3 | O | 186 | PEB | OD-C4D-C3D | -2.46 | 124.07 | 129.77 |
| 3 | M | 186 | PEB | OD-C4D-C3D | -2.44 | 124.12 | 129.77 |
| 3 | Q | 187 | PEB | CHA-C1B-NB | -2.44 | 120.28 | 124.97 |
| 3 | B | 167 | PEB | C1C-CHB-C4B | -2.43 | 125.83 | 128.77 |
| 3 | D | 166 | PEB | CHC-C4C-C3C | -2.43 | 126.31 | 130.41 |
| 3 | P | 187 | PEB | CAB-CBB-CGB | -2.42 | 108.52 | 112.66 |
| 3 | T | 188 | PEB | C1D-ND-C4D | -2.42 | 110.63 | 113.78 |
| 7 | B | 203 | MPD | O4-C4-C3 | -2.42 | 100.19 | 111.28 |
| 3 | N | 187 | PEB | C4B-C3B-C2B | -2.42 | 104.09 | 106.81 |
| 3 | J | 166 | PEB | CHC-C4C-C3C | -2.42 | 126.32 | 130.41 |
| 3 | U | 188 | PEB | CHC-C4C-C3C | -2.41 | 126.35 | 130.41 |
| 3 | I | 167 | PEB | CBC-CAC-C2C | -2.40 | 107.89 | 112.48 |
| 3 | T | 188 | PEB | CBC-CAC-C2C | -2.39 | 107.91 | 112.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | G | 167 | PEB | C1B-C2B-C3B | -2.39 | 103.74 | 106.51 |
| 3 | U | 187 | PEB | CHA-C1B-NB | -2.38 | 120.39 | 124.97 |
| 3 | I | 167 | PEB | C1B-C2B-C3B | -2.38 | 103.75 | 106.51 |
| 3 | Q | 188 | PEB | C1D-ND-C4D | -2.38 | 110.69 | 113.78 |
| 3 | U | 188 | PEB | OD-C4D-C3D | -2.38 | 124.27 | 129.77 |
| 3 | R | 187 | PEB | CHC-C1D-ND | -2.36 | 111.19 | 114.03 |
| 3 | W | 186 | PEB | CHC-C4C-C3C | -2.36 | 126.42 | 130.41 |
| 3 | B | 167 | PEB | C4B-C3B-C2B | -2.33 | 104.19 | 106.81 |
| 3 | O | 188 | PEB | CHC-C4C-C3C | -2.33 | 126.47 | 130.41 |
| 3 | I | 167 | PEB | OD-C4D-C3D | -2.33 | 124.38 | 129.77 |
| 3 | L | 166 | PEB | OD-C4D-C3D | -2.32 | 124.39 | 129.77 |
| 3 | L | 166 | PEB | CHB-C4B-NB | -2.32 | 125.27 | 128.79 |
| 3 | W | 186 | PEB | CHB-C4B-C3B | -2.31 | 119.90 | 125.39 |
| 3 | A | 167 | PEB | CHA-C1B-NB | -2.30 | 120.54 | 124.97 |
| 3 | A | 166 | PEB | C1D-ND-C4D | -2.30 | 110.79 | 113.78 |
| 3 | C | 167 | PEB | OD-C4D-C3D | -2.30 | 124.44 | 129.77 |
| 3 | G | 166 | PEB | CHB-C4B-NB | -2.29 | 125.31 | 128.79 |
| 3 | J | 166 | PEB | C1D-ND-C4D | -2.29 | 110.81 | 113.78 |
| 3 | W | 187 | PEB | CAB-CBB-CGB | -2.29 | 108.75 | 112.66 |
| 3 | Q | 188 | PEB | CBD-CAD-C3D | -2.28 | 115.93 | 127.39 |
| 3 | O | 187 | PEB | C1B-C2B-C3B | -2.28 | 103.86 | 106.51 |
| 3 | H | 166 | PEB | C2C-C3C-C4C | -2.28 | 102.23 | 111.33 |
| 3 | P | 188 | PEB | CAC-CBC-CGC | -2.28 | 108.77 | 112.66 |
| 5 | C | 204 | PI | O3-P-O1 | -2.27 | 101.32 | 110.97 |
| 3 | V | 187 | PEB | CHC-C1D-ND | -2.27 | 111.30 | 114.03 |
| 3 | U | 187 | PEB | OD-C4D-C3D | -2.25 | 124.56 | 129.77 |
| 3 | U | 188 | PEB | CBC-CAC-C2C | -2.24 | 108.20 | 112.48 |
| 3 | V | 186 | PEB | OA-C1A-C2A | -2.23 | 124.45 | 126.25 |
| 3 | E | 166 | PEB | C2C-C3C-C4C | -2.23 | 102.43 | 111.33 |
| 3 | P | 186 | PEB | CHB-C4B-C3B | -2.23 | 120.11 | 125.39 |
| 3 | T | 187 | PEB | C1B-C2B-C3B | -2.22 | 103.93 | 106.51 |
| 3 | F | 167 | PEB | C2A-C1A-NA | -2.22 | 106.27 | 108.28 |
| 3 | P | 187 | PEB | OA-C1A-C2A | -2.22 | 124.46 | 126.25 |
| 3 | U | 187 | PEB | OA-C1A-C2A | -2.22 | 124.46 | 126.25 |
| 3 | I | 166 | PEB | CMA-C2A-C1A | -2.22 | 107.77 | 112.43 |
| 3 | S | 187 | PEB | CHA-C1B-NB | -2.21 | 120.72 | 124.97 |
| 3 | X | 188 | PEB | C2C-C3C-C4C | -2.21 | 102.53 | 111.33 |
| 3 | S | 188 | PEB | C1D-ND-C4D | -2.20 | 110.92 | 113.78 |
| 3 | X | 188 | PEB | CHB-C4B-C3B | -2.20 | 120.17 | 125.39 |
| 3 | C | 166 | PEB | CMA-C2A-C1A | -2.19 | 107.83 | 112.43 |
| 3 | X | 187 | PEB | OD-C4D-C3D | -2.19 | 124.70 | 129.77 |
| 3 | E | 167 | PEB | CHA-C1B-NB | -2.18 | 120.77 | 124.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | T | 187 | PEB | C3A-C4A-NA | -2.18 | 105.91 | 107.97 |
| 3 | P | 188 | PEB | CHB-C4B-C3B | -2.17 | 120.23 | 125.39 |
| 3 | T | 187 | PEB | CAB-CBB-CGB | -2.17 | 108.95 | 112.66 |
| 3 | G | 167 | PEB | C1D-ND-C4D | -2.17 | 110.96 | 113.78 |
| 3 | W | 186 | PEB | OA-C1A-C2A | -2.17 | 124.50 | 126.25 |
| 3 | T | 188 | PEB | CHB-C4B-C3B | -2.16 | 120.26 | 125.39 |
| 3 | T | 186 | PEB | C4B-C3B-C2B | -2.16 | 104.38 | 106.81 |
| 3 | C | 166 | PEB | CHB-C4B-C3B | -2.16 | 120.26 | 125.39 |
| 3 | I | 167 | PEB | OA-C1A-C2A | -2.16 | 124.51 | 126.25 |
| 3 | A | 167 | PEB | OD-C4D-C3D | -2.16 | 124.77 | 129.77 |
| 3 | T | 188 | PEB | CBD-CAD-C3D | -2.16 | 116.56 | 127.39 |
| 3 | T | 187 | PEB | CAA-C3A-C2A | -2.15 | 108.84 | 114.24 |
| 3 | U | 187 | PEB | CHC-C4C-C3C | -2.15 | 126.78 | 130.41 |
| 3 | E | 167 | PEB | C4B-C3B-C2B | -2.15 | 104.40 | 106.81 |
| 3 | M | 188 | PEB | CAB-C3B-C2B | -2.15 | 123.89 | 127.88 |
| 3 | L | 167 | PEB | CAB-C3B-C2B | -2.14 | 123.89 | 127.88 |
| 3 | O | 188 | PEB | CBD-CAD-C3D | -2.14 | 116.63 | 127.39 |
| 3 | W | 187 | PEB | OA-C1A-NA | -2.14 | 122.32 | 124.87 |
| 7 | M | 204 | MPD | CM-C2-C1 | -2.14 | 105.65 | 110.42 |
| 3 | O | 186 | PEB | CHB-C4B-NB | -2.13 | 125.56 | 128.79 |
| 3 | P | 186 | PEB | C4B-C3B-C2B | -2.13 | 104.42 | 106.81 |
| 3 | B | 167 | PEB | CHC-C1D-ND | -2.13 | 111.47 | 114.03 |
| 3 | W | 187 | PEB | C1D-ND-C4D | -2.12 | 111.02 | 113.78 |
| 3 | F | 167 | PEB | CBC-CAC-C2C | -2.12 | 108.43 | 112.48 |
| 3 | G | 166 | PEB | CHC-C4C-C3C | -2.12 | 126.83 | 130.41 |
| 3 | Q | 186 | PEB | CAC-CBC-CGC | -2.11 | 109.05 | 112.66 |
| 3 | W | 187 | PEB | CHB-C4B-C3B | -2.11 | 120.39 | 125.39 |
| 3 | U | 187 | PEB | CBC-CAC-C2C | -2.10 | 108.47 | 112.48 |
| 3 | R | 188 | PEB | CHC-C1D-ND | -2.10 | 111.50 | 114.03 |
| 3 | W | 188 | PEB | CHC-C1D-ND | -2.10 | 111.51 | 114.03 |
| 3 | M | 186 | PEB | C1D-ND-C4D | -2.09 | 111.06 | 113.78 |
| 3 | Q | 186 | PEB | OD-C4D-ND | -2.09 | 122.44 | 125.83 |
| 3 | B | 167 | PEB | OD-C4D-ND | -2.09 | 122.45 | 125.83 |
| 3 | N | 187 | PEB | C1D-ND-C4D | -2.09 | 111.07 | 113.78 |
| 3 | O | 187 | PEB | OD-C4D-C3D | -2.08 | 124.94 | 129.77 |
| 3 | N | 186 | PEB | C4B-C3B-C2B | -2.08 | 104.47 | 106.81 |
| 3 | K | 166 | PEB | OD-C4D-ND | -2.08 | 122.46 | 125.83 |
| 3 | L | 166 | PEB | CAB-C3B-C2B | -2.07 | 124.03 | 127.88 |
| 3 | N | 187 | PEB | CHA-C1B-NB | -2.06 | 121.01 | 124.97 |
| 3 | C | 166 | PEB | CHC-C4C-C3C | -2.06 | 126.94 | 130.41 |
| 3 | V | 186 | PEB | CHB-C4B-C3B | -2.05 | 120.53 | 125.39 |
| 3 | N | 186 | PEB | OD-C4D-C3D | -2.05 | 125.03 | 129.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | V | 188 | PEB | CHC-C1D-ND | -2.05 | 111.56 | 114.03 |
| 3 | R | 188 | PEB | OD-C4D-C3D | -2.05 | 125.03 | 129.77 |
| 3 | T | 187 | PEB | OA-C1A-C2A | -2.03 | 124.61 | 126.25 |
| 3 | Q | 188 | PEB | OD-C4D-ND | -2.03 | 122.53 | 125.83 |
| 3 | L | 166 | PEB | CHC-C1D-ND | -2.03 | 111.58 | 114.03 |
| 3 | X | 188 | PEB | C1B-C2B-C3B | -2.03 | 104.16 | 106.51 |
| 3 | V | 187 | PEB | OD-C4D-C3D | -2.02 | 125.09 | 129.77 |
| 3 | F | 167 | PEB | CHC-C4C-C3C | -2.02 | 127.00 | 130.41 |
| 3 | X | 187 | PEB | CMA-C2A-C1A | -2.02 | 108.19 | 112.43 |
| 3 | Q | 188 | PEB | OD-C4D-C3D | -2.02 | 125.10 | 129.77 |
| 3 | H | 167 | PEB | OD-C4D-C3D | -2.02 | 125.10 | 129.77 |
| 3 | A | 167 | PEB | CHB-C4B-NB | -2.02 | 125.73 | 128.79 |
| 3 | W | 188 | PEB | OD-C4D-C3D | -2.01 | 125.11 | 129.77 |
| 3 | O | 187 | PEB | CAA-C3A-C2A | -2.01 | 109.19 | 114.24 |
| 3 | B | 167 | PEB | CHA-C1B-NB | -2.01 | 121.12 | 124.97 |
| 3 | U | 188 | PEB | CBD-CAD-C3D | -2.00 | 117.35 | 127.39 |
| 3 | M | 187 | PEB | C3D-C4D-ND | 2.00 | 111.17 | 107.30 |
| 3 | X | 187 | PEB | C1C-CHB-C4B | 2.01 | 131.21 | 128.77 |
| 3 | W | 188 | PEB | CAD-C3D-C4D | 2.01 | 129.46 | 123.40 |
| 3 | S | 187 | PEB | CMB-C2B-C1B | 2.02 | 128.19 | 125.04 |
| 3 | F | 166 | PEB | CAB-C3B-C4B | 2.02 | 128.61 | 125.00 |
| 3 | X | 188 | PEB | C3D-C4D-ND | 2.02 | 111.20 | 107.30 |
| 3 | P | 188 | PEB | C3D-C4D-ND | 2.03 | 111.21 | 107.30 |
| 7 | R | 204 | MPD | O2-C2-CM | 2.03 | 115.03 | 108.00 |
| 3 | I | 167 | PEB | CAC-CBC-CGC | 2.03 | 116.13 | 112.66 |
| 3 | S | 188 | PEB | C2A-C1A-NA | 2.03 | 110.11 | 108.28 |
| 3 | M | 186 | PEB | OA-C1A-NA | 2.04 | 127.30 | 124.87 |
| 3 | U | 187 | PEB | C3D-C4D-ND | 2.04 | 111.24 | 107.30 |
| 3 | B | 167 | PEB | C2A-C3A-C4A | 2.04 | 104.40 | 101.34 |
| 3 | X | 186 | PEB | CAB-C3B-C4B | 2.05 | 128.65 | 125.00 |
| 3 | R | 188 | PEB | C3A-C4A-NA | 2.05 | 109.90 | 107.97 |
| 7 | O | 204 | MPD | O2-C2-C1 | 2.05 | 115.11 | 108.00 |
| 3 | J | 167 | PEB | CMA-C2A-C1A | 2.05 | 116.74 | 112.43 |
| 3 | Q | 186 | PEB | CAB-C3B-C4B | 2.06 | 128.67 | 125.00 |
| 3 | D | 167 | PEB | OA-C1A-NA | 2.06 | 127.33 | 124.87 |
| 3 | I | 167 | PEB | CAD-C3D-C4D | 2.07 | 129.63 | 123.40 |
| 3 | C | 166 | PEB | CAD-C3D-C4D | 2.07 | 129.65 | 123.40 |
| 3 | E | 167 | PEB | CMB-C2B-C1B | 2.07 | 128.27 | 125.04 |
| 3 | C | 166 | PEB | OA-C1A-NA | 2.08 | 127.35 | 124.87 |
| 3 | I | 166 | PEB | C3D-C4D-ND | 2.09 | 111.33 | 107.30 |
| 3 | T | 188 | PEB | CMB-C2B-C1B | 2.09 | 128.30 | 125.04 |
| 3 | G | 167 | PEB | C3A-C4A-NA | 2.10 | 109.95 | 107.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|------|-------------|----------|
| 3 | X | 188 | PEB | CMC-C3C-C2C | 2.11 | 128.92 | 124.94 |
| 5 | P | 205 | PI | O3-P-O2 | 2.12 | 115.68 | 107.90 |
| 3 | I | 167 | PEB | CMB-C2B-C1B | 2.12 | 128.34 | 125.04 |
| 3 | N | 186 | PEB | C2A-C3A-C4A | 2.14 | 104.55 | 101.34 |
| 3 | P | 187 | PEB | OA-C1A-NA | 2.15 | 127.43 | 124.87 |
| 3 | S | 186[A] | PEB | CAD-C3D-C4D | 2.15 | 129.88 | 123.40 |
| 3 | S | 186[B] | PEB | CAD-C3D-C4D | 2.15 | 129.88 | 123.40 |
| 3 | A | 167 | PEB | C2A-C1A-NA | 2.15 | 110.22 | 108.28 |
| 3 | M | 187 | PEB | CAB-C3B-C4B | 2.15 | 128.84 | 125.00 |
| 3 | L | 166 | PEB | C4B-NB-C1B | 2.16 | 110.80 | 106.52 |
| 3 | S | 186[B] | PEB | CAC-CBC-CGC | 2.16 | 116.36 | 112.66 |
| 3 | T | 186 | PEB | C3D-C4D-ND | 2.16 | 111.48 | 107.30 |
| 3 | J | 167 | PEB | C2A-C3A-C4A | 2.17 | 104.58 | 101.34 |
| 3 | D | 167 | PEB | C3B-C4B-NB | 2.17 | 113.25 | 109.93 |
| 3 | R | 187 | PEB | C3D-C4D-ND | 2.17 | 111.49 | 107.30 |
| 3 | O | 186 | PEB | C1C-CHB-C4B | 2.18 | 131.42 | 128.77 |
| 3 | U | 188 | PEB | C1C-CHB-C4B | 2.20 | 131.44 | 128.77 |
| 3 | Q | 187 | PEB | CAC-CBC-CGC | 2.20 | 116.42 | 112.66 |
| 3 | P | 186 | PEB | C3D-C4D-ND | 2.20 | 111.55 | 107.30 |
| 3 | P | 188 | PEB | CAD-C3D-C4D | 2.21 | 130.06 | 123.40 |
| 3 | E | 166 | PEB | C3A-C4A-NA | 2.21 | 110.05 | 107.97 |
| 3 | X | 187 | PEB | OA-C1A-NA | 2.22 | 127.53 | 124.87 |
| 3 | O | 188 | PEB | CAB-C3B-C4B | 2.23 | 128.98 | 125.00 |
| 3 | Q | 187 | PEB | C2A-C3A-C4A | 2.23 | 104.68 | 101.34 |
| 3 | T | 186 | PEB | CAC-CBC-CGC | 2.23 | 116.47 | 112.66 |
| 3 | K | 167 | PEB | C3D-C4D-ND | 2.23 | 111.61 | 107.30 |
| 3 | N | 188 | PEB | CAB-C3B-C4B | 2.23 | 128.99 | 125.00 |
| 3 | F | 167 | PEB | CAD-C3D-C4D | 2.24 | 130.16 | 123.40 |
| 3 | Q | 186 | PEB | CAD-C3D-C4D | 2.24 | 130.16 | 123.40 |
| 3 | G | 166 | PEB | C1C-CHB-C4B | 2.24 | 131.49 | 128.77 |
| 3 | V | 187 | PEB | CAC-CBC-CGC | 2.25 | 116.50 | 112.66 |
| 3 | S | 188 | PEB | CAB-C3B-C4B | 2.25 | 129.02 | 125.00 |
| 3 | R | 188 | PEB | C3D-C4D-ND | 2.25 | 111.65 | 107.30 |
| 5 | B | 204 | PI | O4-P-O3 | 2.25 | 116.19 | 107.90 |
| 3 | S | 186[A] | PEB | C2A-C3A-C4A | 2.26 | 104.72 | 101.34 |
| 3 | S | 186[B] | PEB | C2A-C3A-C4A | 2.26 | 104.72 | 101.34 |
| 3 | M | 186 | PEB | C2A-C3A-C4A | 2.28 | 104.75 | 101.34 |
| 3 | N | 188 | PEB | CAD-C3D-C4D | 2.29 | 130.33 | 123.40 |
| 3 | W | 188 | PEB | C3D-C4D-ND | 2.30 | 111.73 | 107.30 |
| 3 | U | 188 | PEB | CMB-C2B-C1B | 2.30 | 128.62 | 125.04 |
| 3 | U | 186 | PEB | C3D-C4D-ND | 2.30 | 111.74 | 107.30 |
| 3 | N | 188 | PEB | C2A-C3A-C4A | 2.30 | 104.78 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | T | 187 | PEB | CAC-CBC-CGC | 2.31 | 116.61 | 112.66 |
| 3 | D | 167 | PEB | CAB-C3B-C4B | 2.32 | 129.13 | 125.00 |
| 3 | L | 167 | PEB | C2A-C1A-NA | 2.32 | 110.37 | 108.28 |
| 3 | I | 167 | PEB | C4B-NB-C1B | 2.32 | 111.12 | 106.52 |
| 3 | X | 188 | PEB | CAB-C3B-C4B | 2.32 | 129.15 | 125.00 |
| 3 | V | 188 | PEB | C3D-C4D-ND | 2.33 | 111.79 | 107.30 |
| 3 | W | 186 | PEB | CAD-C3D-C4D | 2.33 | 130.43 | 123.40 |
| 3 | N | 186 | PEB | CAD-C3D-C4D | 2.33 | 130.43 | 123.40 |
| 3 | J | 167 | PEB | C2A-C1A-NA | 2.34 | 110.39 | 108.28 |
| 3 | U | 188 | PEB | C3D-C4D-ND | 2.34 | 111.82 | 107.30 |
| 3 | A | 167 | PEB | CAB-C3B-C4B | 2.34 | 129.18 | 125.00 |
| 3 | F | 166 | PEB | CMB-C2B-C1B | 2.35 | 128.70 | 125.04 |
| 3 | N | 187 | PEB | CMB-C2B-C1B | 2.35 | 128.70 | 125.04 |
| 3 | U | 187 | PEB | CMB-C2B-C1B | 2.35 | 128.71 | 125.04 |
| 3 | R | 187 | PEB | C2A-C3A-C4A | 2.36 | 104.87 | 101.34 |
| 3 | X | 186 | PEB | CHA-C1B-C2B | 2.37 | 130.52 | 124.81 |
| 3 | C | 167 | PEB | C1C-CHB-C4B | 2.38 | 131.66 | 128.77 |
| 3 | W | 188 | PEB | C2A-C3A-C4A | 2.39 | 104.91 | 101.34 |
| 3 | M | 186 | PEB | CAD-C3D-C4D | 2.40 | 130.66 | 123.40 |
| 3 | I | 167 | PEB | CAB-C3B-C4B | 2.41 | 129.30 | 125.00 |
| 3 | W | 186 | PEB | C3D-C4D-ND | 2.41 | 111.95 | 107.30 |
| 3 | O | 186 | PEB | C3D-C4D-ND | 2.42 | 111.98 | 107.30 |
| 3 | P | 188 | PEB | C2A-C3A-C4A | 2.43 | 104.98 | 101.34 |
| 3 | T | 186 | PEB | CHA-C1B-C2B | 2.44 | 130.68 | 124.81 |
| 3 | R | 188 | PEB | CMB-C2B-C1B | 2.44 | 128.85 | 125.04 |
| 3 | Q | 186 | PEB | C2A-C1A-NA | 2.44 | 110.48 | 108.28 |
| 3 | D | 166 | PEB | CAB-C3B-C4B | 2.45 | 129.37 | 125.00 |
| 3 | Q | 188 | PEB | C3D-C4D-ND | 2.46 | 112.04 | 107.30 |
| 3 | A | 167 | PEB | CAD-C3D-C4D | 2.46 | 130.81 | 123.40 |
| 3 | G | 166 | PEB | CMC-C3C-C2C | 2.46 | 129.58 | 124.94 |
| 3 | Q | 186 | PEB | CMB-C2B-C1B | 2.47 | 128.88 | 125.04 |
| 3 | N | 188 | PEB | CMB-C2B-C1B | 2.47 | 128.89 | 125.04 |
| 3 | J | 167 | PEB | CAD-C3D-C4D | 2.48 | 130.88 | 123.40 |
| 3 | E | 167 | PEB | CAD-C3D-C4D | 2.48 | 130.90 | 123.40 |
| 3 | E | 166 | PEB | CHA-C1B-C2B | 2.50 | 130.83 | 124.81 |
| 3 | V | 186 | PEB | CMB-C2B-C1B | 2.50 | 128.94 | 125.04 |
| 3 | T | 188 | PEB | C3B-C4B-NB | 2.51 | 113.76 | 109.93 |
| 3 | G | 167 | PEB | CAD-C3D-C4D | 2.52 | 131.00 | 123.40 |
| 3 | X | 186 | PEB | CAD-C3D-C4D | 2.52 | 131.01 | 123.40 |
| 3 | D | 166 | PEB | C1C-CHB-C4B | 2.52 | 131.83 | 128.77 |
| 3 | Q | 186 | PEB | C3D-C4D-ND | 2.52 | 112.17 | 107.30 |
| 3 | G | 166 | PEB | CMB-C2B-C1B | 2.52 | 128.97 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|------|-------------|----------|
| 3 | V | 186 | PEB | C3D-C4D-ND | 2.52 | 112.17 | 107.30 |
| 3 | S | 188 | PEB | C3A-C4A-NA | 2.55 | 110.37 | 107.97 |
| 3 | C | 166 | PEB | C3D-C4D-ND | 2.55 | 112.23 | 107.30 |
| 3 | P | 187 | PEB | C3D-C4D-ND | 2.57 | 112.26 | 107.30 |
| 3 | R | 186 | PEB | OA-C1A-NA | 2.57 | 127.94 | 124.87 |
| 3 | P | 186 | PEB | C3A-C4A-NA | 2.58 | 110.40 | 107.97 |
| 3 | P | 186 | PEB | CAD-C3D-C4D | 2.58 | 131.19 | 123.40 |
| 3 | P | 188 | PEB | CAB-C3B-C4B | 2.60 | 129.65 | 125.00 |
| 3 | X | 186 | PEB | C3D-C4D-ND | 2.61 | 112.33 | 107.30 |
| 3 | V | 188 | PEB | CAB-CBB-CGB | 2.62 | 117.13 | 112.66 |
| 3 | E | 166 | PEB | CAD-C3D-C4D | 2.62 | 131.31 | 123.40 |
| 3 | C | 167 | PEB | C3D-C4D-ND | 2.62 | 112.36 | 107.30 |
| 3 | M | 187 | PEB | CMB-C2B-C1B | 2.62 | 129.12 | 125.04 |
| 3 | C | 167 | PEB | C2A-C3A-C4A | 2.62 | 105.27 | 101.34 |
| 3 | J | 167 | PEB | C3D-C4D-ND | 2.63 | 112.37 | 107.30 |
| 3 | F | 167 | PEB | CAB-C3B-C4B | 2.63 | 129.69 | 125.00 |
| 3 | W | 186 | PEB | CAB-C3B-C4B | 2.64 | 129.71 | 125.00 |
| 3 | C | 166 | PEB | CMB-C2B-C1B | 2.65 | 129.17 | 125.04 |
| 3 | S | 186[A] | PEB | CHA-C1B-C2B | 2.66 | 131.22 | 124.81 |
| 3 | S | 186[B] | PEB | CHA-C1B-C2B | 2.66 | 131.22 | 124.81 |
| 3 | M | 187 | PEB | C1C-CHB-C4B | 2.67 | 132.01 | 128.77 |
| 3 | I | 166 | PEB | C2A-C3A-C4A | 2.67 | 105.34 | 101.34 |
| 3 | X | 187 | PEB | CMB-C2B-C1B | 2.68 | 129.21 | 125.04 |
| 3 | G | 167 | PEB | CAB-C3B-C4B | 2.70 | 129.82 | 125.00 |
| 3 | Q | 187 | PEB | C1C-CHB-C4B | 2.71 | 132.05 | 128.77 |
| 3 | F | 166 | PEB | CMC-C3C-C2C | 2.71 | 130.05 | 124.94 |
| 3 | V | 188 | PEB | CMB-C2B-C1B | 2.71 | 129.27 | 125.04 |
| 3 | P | 187 | PEB | C1C-CHB-C4B | 2.71 | 132.06 | 128.77 |
| 3 | S | 187 | PEB | C3B-C4B-NB | 2.72 | 114.08 | 109.93 |
| 3 | L | 166 | PEB | C4B-C3B-C2B | 2.72 | 109.85 | 106.81 |
| 3 | Q | 188 | PEB | CMB-C2B-C1B | 2.72 | 129.28 | 125.04 |
| 3 | V | 188 | PEB | C2A-C1A-NA | 2.73 | 110.74 | 108.28 |
| 3 | U | 186 | PEB | CHA-C1B-C2B | 2.73 | 131.39 | 124.81 |
| 3 | U | 186 | PEB | OA-C1A-NA | 2.74 | 128.14 | 124.87 |
| 3 | E | 167 | PEB | CAB-C3B-C4B | 2.75 | 129.91 | 125.00 |
| 3 | Q | 187 | PEB | CMB-C2B-C1B | 2.76 | 129.34 | 125.04 |
| 3 | I | 167 | PEB | C2A-C1A-NA | 2.77 | 110.78 | 108.28 |
| 3 | C | 167 | PEB | CAD-C3D-C4D | 2.77 | 131.76 | 123.40 |
| 3 | O | 187 | PEB | CAC-CBC-CGC | 2.77 | 117.39 | 112.66 |
| 3 | Q | 186 | PEB | CHA-C1B-C2B | 2.78 | 131.50 | 124.81 |
| 3 | O | 186 | PEB | CHA-C1B-C2B | 2.79 | 131.53 | 124.81 |
| 3 | R | 186 | PEB | CAD-C3D-C4D | 2.79 | 131.82 | 123.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|------|-------------|----------|
| 3 | U | 186 | PEB | CAD-C3D-C4D | 2.80 | 131.86 | 123.40 |
| 3 | N | 186 | PEB | CMB-C2B-C1B | 2.82 | 129.43 | 125.04 |
| 3 | T | 187 | PEB | C1C-CHB-C4B | 2.83 | 132.21 | 128.77 |
| 3 | S | 186[A] | PEB | OA-C1A-NA | 2.84 | 128.26 | 124.87 |
| 3 | S | 186[B] | PEB | OA-C1A-NA | 2.84 | 128.26 | 124.87 |
| 3 | M | 188 | PEB | C3D-C4D-ND | 2.84 | 112.79 | 107.30 |
| 3 | R | 187 | PEB | OA-C1A-NA | 2.86 | 128.28 | 124.87 |
| 3 | S | 188 | PEB | C3D-C4D-ND | 2.90 | 112.91 | 107.30 |
| 3 | N | 187 | PEB | C1C-CHB-C4B | 2.92 | 132.31 | 128.77 |
| 3 | M | 188 | PEB | CAB-C3B-C4B | 2.92 | 130.21 | 125.00 |
| 3 | V | 187 | PEB | OA-C1A-C2A | 2.92 | 128.62 | 126.25 |
| 3 | T | 186 | PEB | CAD-C3D-C4D | 2.93 | 132.24 | 123.40 |
| 3 | R | 186 | PEB | CHA-C1B-C2B | 2.93 | 131.87 | 124.81 |
| 3 | J | 166 | PEB | CAB-C3B-C4B | 2.94 | 130.25 | 125.00 |
| 3 | W | 187 | PEB | C2A-C1A-NA | 2.94 | 110.94 | 108.28 |
| 3 | R | 187 | PEB | CAB-C3B-C4B | 2.97 | 130.31 | 125.00 |
| 3 | K | 167 | PEB | CMB-C2B-C1B | 2.98 | 129.68 | 125.04 |
| 3 | L | 166 | PEB | C1C-CHB-C4B | 2.98 | 132.39 | 128.77 |
| 3 | M | 186 | PEB | C3D-C4D-ND | 3.00 | 113.09 | 107.30 |
| 3 | D | 167 | PEB | CMB-C2B-C1B | 3.00 | 129.72 | 125.04 |
| 3 | X | 186 | PEB | CAC-CBC-CGC | 3.00 | 117.79 | 112.66 |
| 3 | T | 188 | PEB | CAB-C3B-C4B | 3.02 | 130.39 | 125.00 |
| 3 | Q | 188 | PEB | C2A-C1A-NA | 3.03 | 111.02 | 108.28 |
| 3 | L | 167 | PEB | C3D-C4D-ND | 3.04 | 113.17 | 107.30 |
| 3 | P | 187 | PEB | CAC-CBC-CGC | 3.05 | 117.87 | 112.66 |
| 3 | W | 187 | PEB | CMB-C2B-C1B | 3.06 | 129.81 | 125.04 |
| 3 | T | 188 | PEB | CAD-C3D-C4D | 3.07 | 132.66 | 123.40 |
| 3 | D | 166 | PEB | CMB-C2B-C1B | 3.08 | 129.84 | 125.04 |
| 3 | H | 166 | PEB | CHA-C1B-C2B | 3.08 | 132.23 | 124.81 |
| 3 | S | 186[A] | PEB | CAB-C3B-C4B | 3.12 | 130.58 | 125.00 |
| 3 | S | 186[B] | PEB | CAB-C3B-C4B | 3.12 | 130.58 | 125.00 |
| 3 | X | 188 | PEB | C2A-C1A-NA | 3.13 | 111.10 | 108.28 |
| 3 | T | 188 | PEB | C3D-C4D-ND | 3.15 | 113.38 | 107.30 |
| 3 | L | 167 | PEB | CAB-C3B-C4B | 3.19 | 130.70 | 125.00 |
| 3 | U | 188 | PEB | C3A-C4A-NA | 3.23 | 111.01 | 107.97 |
| 3 | X | 188 | PEB | CMB-C2B-C1B | 3.25 | 130.10 | 125.04 |
| 3 | I | 166 | PEB | CHA-C1B-C2B | 3.26 | 132.65 | 124.81 |
| 3 | W | 188 | PEB | CAB-C3B-C4B | 3.26 | 130.82 | 125.00 |
| 3 | W | 186 | PEB | CMB-C2B-C1B | 3.27 | 130.13 | 125.04 |
| 3 | S | 188 | PEB | CMB-C2B-C1B | 3.27 | 130.13 | 125.04 |
| 3 | L | 167 | PEB | CMB-C2B-C1B | 3.29 | 130.16 | 125.04 |
| 3 | F | 166 | PEB | CHA-C1B-C2B | 3.29 | 132.72 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|------|-------------|----------|
| 3 | B | 166 | PEB | C2A-C1A-NA | 3.29 | 111.25 | 108.28 |
| 3 | M | 188 | PEB | C2A-C1A-NA | 3.31 | 111.27 | 108.28 |
| 3 | I | 166 | PEB | CMB-C2B-C1B | 3.32 | 130.21 | 125.04 |
| 3 | N | 186 | PEB | CHA-C1B-C2B | 3.33 | 132.83 | 124.81 |
| 3 | B | 166 | PEB | CHA-C1B-C2B | 3.33 | 132.83 | 124.81 |
| 3 | P | 186 | PEB | CHA-C1B-C2B | 3.34 | 132.85 | 124.81 |
| 3 | P | 186 | PEB | C2A-C1A-NA | 3.36 | 111.31 | 108.28 |
| 3 | A | 167 | PEB | C3D-C4D-ND | 3.38 | 113.83 | 107.30 |
| 3 | N | 186 | PEB | CAB-C3B-C4B | 3.38 | 131.04 | 125.00 |
| 3 | S | 187 | PEB | CAB-C3B-C4B | 3.42 | 131.11 | 125.00 |
| 3 | P | 187 | PEB | CMB-C2B-C1B | 3.43 | 130.39 | 125.04 |
| 3 | O | 187 | PEB | CMB-C2B-C1B | 3.44 | 130.40 | 125.04 |
| 3 | H | 166 | PEB | C3D-C4D-ND | 3.45 | 113.96 | 107.30 |
| 3 | W | 186 | PEB | CHA-C1B-C2B | 3.46 | 133.15 | 124.81 |
| 3 | I | 167 | PEB | C3A-C4A-NA | 3.48 | 111.25 | 107.97 |
| 3 | K | 166 | PEB | CHA-C1B-C2B | 3.53 | 133.31 | 124.81 |
| 3 | D | 166 | PEB | CHA-C1B-C2B | 3.54 | 133.34 | 124.81 |
| 3 | S | 186[A] | PEB | CMB-C2B-C1B | 3.59 | 130.64 | 125.04 |
| 3 | S | 186[B] | PEB | CMB-C2B-C1B | 3.59 | 130.64 | 125.04 |
| 3 | T | 186 | PEB | C2A-C1A-NA | 3.61 | 111.54 | 108.28 |
| 3 | M | 186 | PEB | CHA-C1B-C2B | 3.61 | 133.51 | 124.81 |
| 3 | U | 186 | PEB | C2A-C3A-C4A | 3.64 | 106.79 | 101.34 |
| 3 | S | 186[A] | PEB | C3D-C4D-ND | 3.65 | 114.34 | 107.30 |
| 3 | S | 186[B] | PEB | C3D-C4D-ND | 3.65 | 114.34 | 107.30 |
| 3 | R | 186 | PEB | CMB-C2B-C1B | 3.65 | 130.73 | 125.04 |
| 3 | B | 167 | PEB | CAB-C3B-C4B | 3.66 | 131.53 | 125.00 |
| 3 | U | 187 | PEB | CAC-CBC-CGC | 3.66 | 118.92 | 112.66 |
| 3 | J | 166 | PEB | CHA-C1B-C2B | 3.72 | 133.78 | 124.81 |
| 3 | T | 187 | PEB | C2A-C3A-C4A | 3.74 | 106.94 | 101.34 |
| 3 | M | 186 | PEB | CMB-C2B-C1B | 3.76 | 130.90 | 125.04 |
| 3 | R | 186 | PEB | C3D-C4D-ND | 3.80 | 114.65 | 107.30 |
| 3 | U | 187 | PEB | C1C-CHB-C4B | 3.83 | 133.42 | 128.77 |
| 3 | O | 187 | PEB | C1C-CHB-C4B | 3.86 | 133.46 | 128.77 |
| 3 | E | 166 | PEB | CMB-C2B-C1B | 3.92 | 131.14 | 125.04 |
| 3 | R | 187 | PEB | CMB-C2B-C1B | 3.99 | 131.26 | 125.04 |
| 3 | C | 166 | PEB | CHA-C1B-C2B | 4.01 | 134.46 | 124.81 |
| 3 | G | 166 | PEB | CHA-C1B-C2B | 4.02 | 134.48 | 124.81 |
| 3 | V | 187 | PEB | C1C-CHB-C4B | 4.07 | 133.71 | 128.77 |
| 3 | V | 187 | PEB | CMB-C2B-C1B | 4.09 | 131.41 | 125.04 |
| 3 | B | 167 | PEB | CMB-C2B-C1B | 4.09 | 131.41 | 125.04 |
| 3 | P | 186 | PEB | CMB-C2B-C1B | 4.11 | 131.44 | 125.04 |
| 3 | T | 188 | PEB | C2A-C1A-NA | 4.11 | 111.99 | 108.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | L | 166 | PEB | CHA-C1B-C2B | 4.12 | 134.73 | 124.81 |
| 3 | R | 187 | PEB | C1C-CHB-C4B | 4.13 | 133.78 | 128.77 |
| 3 | T | 188 | PEB | C2A-C3A-C4A | 4.13 | 107.53 | 101.34 |
| 3 | G | 167 | PEB | CMB-C2B-C1B | 4.13 | 131.48 | 125.04 |
| 3 | K | 166 | PEB | C2A-C1A-NA | 4.13 | 112.01 | 108.28 |
| 3 | K | 167 | PEB | CAB-C3B-C4B | 4.14 | 132.40 | 125.00 |
| 3 | V | 186 | PEB | CHA-C1B-C2B | 4.16 | 134.82 | 124.81 |
| 3 | H | 166 | PEB | CMB-C2B-C1B | 4.16 | 131.52 | 125.04 |
| 3 | T | 187 | PEB | CMB-C2B-C1B | 4.19 | 131.57 | 125.04 |
| 3 | C | 166 | PEB | CAB-C3B-C4B | 4.25 | 132.59 | 125.00 |
| 3 | O | 186 | PEB | CMB-C2B-C1B | 4.27 | 131.70 | 125.04 |
| 3 | M | 186 | PEB | CAC-CBC-CGC | 4.35 | 120.09 | 112.66 |
| 3 | F | 167 | PEB | CMB-C2B-C1B | 4.37 | 131.84 | 125.04 |
| 3 | X | 186 | PEB | CMB-C2B-C1B | 4.55 | 132.12 | 125.04 |
| 3 | A | 166 | PEB | CHA-C1B-C2B | 4.57 | 135.82 | 124.81 |
| 3 | H | 167 | PEB | CMB-C2B-C1B | 4.59 | 132.19 | 125.04 |
| 3 | U | 188 | PEB | CAC-CBC-CGC | 4.60 | 120.52 | 112.66 |
| 3 | T | 186 | PEB | CMB-C2B-C1B | 4.70 | 132.37 | 125.04 |
| 3 | U | 186 | PEB | CMB-C2B-C1B | 4.81 | 132.54 | 125.04 |
| 3 | C | 167 | PEB | C2A-C1A-NA | 4.99 | 112.79 | 108.28 |
| 3 | C | 167 | PEB | CMB-C2B-C1B | 5.27 | 133.24 | 125.04 |
| 3 | J | 167 | PEB | CMB-C2B-C1B | 5.68 | 133.89 | 125.04 |

There are no chirality outliers.

All (122) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | D | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | B | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | O | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | N | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | R | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | U | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | P | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | K | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | I | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | M | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | W | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | V | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | S | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | T | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | C | 167 | PEB | C4A-CHA-C1B-C2B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | J | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | X | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | L | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | E | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | Q | 188 | PEB | C4A-CHA-C1B-C2B |
| 3 | A | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | G | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | R | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | P | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | V | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | X | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | M | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | H | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | U | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | T | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | W | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | K | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | F | 167 | PEB | C4A-CHA-C1B-C2B |
| 3 | D | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | N | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | S | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | Q | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | O | 187 | PEB | C4A-CHA-C1B-C2B |
| 3 | I | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | B | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | O | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | R | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | C | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | L | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | H | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | A | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | V | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | F | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | E | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | G | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | R | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | U | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | J | 167 | PEB | C4A-CHA-C1B-NB |
| 3 | M | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | X | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | T | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | O | 186 | PEB | C4A-CHA-C1B-C2B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 3 | S | 186[A] | PEB | C4A-CHA-C1B-C2B |
| 3 | S | 186[B] | PEB | C4A-CHA-C1B-C2B |
| 3 | W | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | R | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | P | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | W | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | U | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | S | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | N | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | Q | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | Q | 188 | PEB | C4A-CHA-C1B-NB |
| 3 | P | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | M | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | P | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | Q | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | V | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | U | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | T | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | X | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | V | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | X | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | O | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | N | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | S | 187 | PEB | C4A-CHA-C1B-NB |
| 3 | T | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | N | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | W | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | S | 186[A] | PEB | C4A-CHA-C1B-NB |
| 3 | S | 186[B] | PEB | C4A-CHA-C1B-NB |
| 3 | M | 186 | PEB | C4A-CHA-C1B-C2B |
| 3 | O | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | R | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | Q | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | U | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | J | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | T | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | P | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | N | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | E | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | C | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | F | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | W | 186 | PEB | C4A-CHA-C1B-NB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | X | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | M | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | G | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | F | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | H | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | K | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | B | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | I | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | K | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | V | 186 | PEB | C4A-CHA-C1B-NB |
| 3 | D | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | G | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | H | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | E | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | C | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | L | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | D | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | L | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | B | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | I | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | A | 166 | PEB | C4A-CHA-C1B-NB |
| 3 | J | 166 | PEB | C4A-CHA-C1B-C2B |
| 3 | A | 166 | PEB | C4A-CHA-C1B-C2B |

There are no ring outliers.

69 monomers are involved in 218 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | A | 167 | PEB | 2 | 0 |
| 4 | A | 203 | NO3 | 1 | 0 |
| 5 | A | 204 | PI | 11 | 0 |
| 3 | B | 167 | PEB | 1 | 0 |
| 7 | B | 203 | MPD | 5 | 0 |
| 3 | C | 166 | PEB | 1 | 0 |
| 3 | C | 167 | PEB | 1 | 0 |
| 5 | C | 204 | PI | 1 | 0 |
| 3 | D | 167 | PEB | 1 | 0 |
| 5 | D | 204 | PI | 1 | 0 |
| 3 | E | 167 | PEB | 2 | 0 |
| 3 | F | 167 | PEB | 3 | 0 |
| 5 | F | 203 | PI | 1 | 0 |
| 3 | G | 167 | PEB | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | H | 167 | PEB | 2 | 0 |
| 5 | H | 203 | PI | 2 | 0 |
| 3 | I | 167 | PEB | 1 | 0 |
| 4 | I | 203 | NO3 | 1 | 0 |
| 3 | J | 167 | PEB | 1 | 0 |
| 3 | K | 167 | PEB | 1 | 0 |
| 5 | K | 203 | PI | 1 | 0 |
| 3 | L | 167 | PEB | 2 | 0 |
| 4 | L | 203 | NO3 | 1 | 0 |
| 3 | M | 186 | PEB | 2 | 0 |
| 3 | M | 187 | PEB | 2 | 0 |
| 3 | M | 188 | PEB | 1 | 0 |
| 7 | M | 204 | MPD | 4 | 0 |
| 3 | N | 186 | PEB | 2 | 0 |
| 3 | N | 187 | PEB | 2 | 0 |
| 3 | N | 188 | PEB | 2 | 0 |
| 3 | O | 186 | PEB | 2 | 0 |
| 3 | O | 187 | PEB | 1 | 0 |
| 3 | O | 188 | PEB | 3 | 0 |
| 7 | O | 204 | MPD | 9 | 0 |
| 3 | P | 186 | PEB | 2 | 0 |
| 3 | P | 187 | PEB | 2 | 0 |
| 3 | P | 188 | PEB | 2 | 0 |
| 7 | P | 204 | MPD | 6 | 0 |
| 3 | Q | 186 | PEB | 3 | 0 |
| 3 | Q | 187 | PEB | 2 | 0 |
| 3 | Q | 188 | PEB | 3 | 0 |
| 7 | Q | 204 | MPD | 11 | 0 |
| 3 | R | 186 | PEB | 2 | 0 |
| 3 | R | 187 | PEB | 3 | 0 |
| 3 | R | 188 | PEB | 5 | 0 |
| 7 | R | 204 | MPD | 15 | 0 |
| 3 | S | 187 | PEB | 1 | 0 |
| 3 | S | 188 | PEB | 2 | 0 |
| 7 | S | 204 | MPD | 8 | 0 |
| 3 | T | 186 | PEB | 2 | 0 |
| 3 | T | 187 | PEB | 3 | 0 |
| 3 | T | 188 | PEB | 3 | 0 |
| 8 | T | 204 | MRD | 10 | 0 |
| 3 | U | 186 | PEB | 2 | 0 |
| 3 | U | 187 | PEB | 2 | 0 |
| 3 | U | 188 | PEB | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7 | U | 204 | MPD | 8 | 0 |
| 3 | V | 186 | PEB | 2 | 0 |
| 3 | V | 187 | PEB | 1 | 0 |
| 3 | V | 188 | PEB | 2 | 0 |
| 8 | V | 204 | MRD | 10 | 0 |
| 3 | W | 186 | PEB | 2 | 0 |
| 3 | W | 187 | PEB | 2 | 0 |
| 3 | W | 188 | PEB | 2 | 0 |
| 7 | W | 204 | MPD | 7 | 0 |
| 3 | X | 186 | PEB | 2 | 0 |
| 3 | X | 187 | PEB | 4 | 0 |
| 3 | X | 188 | PEB | 2 | 0 |
| 7 | X | 204 | MPD | 8 | 0 |

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 | 164/164 (100%) | -0.23 | 0 100 100 | 7, 9, 15, 23 | 0 |
| 1 | B | 164/164 (100%) | -0.30 | 1 (0%) 89 87 | 8, 10, 18, 24 | 0 |
| 1 | C | 164/164 (100%) | -0.27 | 0 100 100 | 10, 13, 18, 25 | 0 |
| 1 | D | 164/164 (100%) | -0.26 | 0 100 100 | 7, 10, 18, 28 | 0 |
| 1 | E | 164/164 (100%) | -0.17 | 2 (1%) 79 76 | 8, 13, 28, 38 | 0 |
| 1 | F | 164/164 (100%) | -0.23 | 0 100 100 | 9, 12, 17, 23 | 0 |
| 1 | G | 164/164 (100%) | -0.28 | 0 100 100 | 8, 11, 17, 22 | 0 |
| 1 | H | 164/164 (100%) | -0.18 | 1 (0%) 89 87 | 9, 13, 25, 45 | 0 |
| 1 | I | 164/164 (100%) | -0.18 | 0 100 100 | 8, 12, 20, 31 | 0 |
| 1 | J | 164/164 (100%) | -0.29 | 0 100 100 | 8, 11, 17, 25 | 0 |
| 1 | K | 164/164 (100%) | -0.22 | 0 100 100 | 9, 12, 18, 26 | 0 |
| 1 | L | 164/164 (100%) | -0.24 | 0 100 100 | 8, 10, 16, 23 | 0 |
| 2 | M | 183/184 (99%) | -0.18 | 0 100 100 | 7, 11, 21, 34 | 0 |
| 2 | N | 183/184 (99%) | -0.22 | 0 100 100 | 9, 13, 20, 34 | 0 |
| 2 | O | 183/184 (99%) | -0.19 | 2 (1%) 80 77 | 9, 12, 24, 42 | 0 |
| 2 | P | 183/184 (99%) | -0.17 | 2 (1%) 80 77 | 7, 12, 24, 45 | 0 |
| 2 | Q | 183/184 (99%) | -0.20 | 0 100 100 | 8, 13, 24, 62 | 0 |
| 2 | R | 183/184 (99%) | 0.09 | 4 (2%) 62 60 | 11, 17, 31, 44 | 0 |
| 2 | S | 183/184 (99%) | -0.15 | 3 (1%) 72 69 | 9, 13, 29, 38 | 0 |
| 2 | T | 183/184 (99%) | 0.16 | 6 (3%) 47 46 | 10, 16, 32, 100 | 0 |
| 2 | U | 183/184 (99%) | -0.07 | 7 (3%) 41 40 | 8, 13, 24, 41 | 0 |
| 2 | V | 183/184 (99%) | -0.17 | 1 (0%) 90 88 | 8, 11, 20, 39 | 0 |
| 2 | W | 183/184 (99%) | -0.21 | 1 (0%) 90 88 | 9, 12, 21, 36 | 0 |
| 2 | X | 183/184 (99%) | -0.20 | 1 (0%) 90 88 | 8, 12, 22, 34 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| All | All | 4164/4176 (99%) | -0.18 | 31 (0%) 87 84 | 7, 12, 23, 100 | 0 |

All (31) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 2 | T | 184[A] | SER | 5.2 |
| 2 | T | 24 | ALA | 4.0 |
| 2 | R | 150 | GLY | 3.7 |
| 2 | S | 150 | GLY | 3.4 |
| 2 | U | 28[A] | PHE | 3.2 |
| 2 | U | 22 | MET | 3.2 |
| 2 | T | 28[A] | PHE | 3.2 |
| 2 | X | 150 | GLY | 3.1 |
| 2 | S | 22[A] | MET | 2.9 |
| 1 | E | 69 | SER | 2.8 |
| 2 | O | 150 | GLY | 2.6 |
| 2 | T | 150 | GLY | 2.5 |
| 2 | P | 21 | ASP | 2.5 |
| 2 | U | 184[A] | SER | 2.5 |
| 2 | R | 184 | SER | 2.5 |
| 1 | B | 61[A] | GLN | 2.4 |
| 2 | O | 184 | SER | 2.4 |
| 2 | T | 183 | LEU | 2.4 |
| 2 | W | 28[A] | PHE | 2.4 |
| 2 | V | 184[A] | SER | 2.3 |
| 2 | T | 23 | GLY | 2.3 |
| 2 | P | 22[A] | MET | 2.3 |
| 2 | U | 26[A] | LYS | 2.3 |
| 2 | R | 22 | MET | 2.3 |
| 2 | S | 28[A] | PHE | 2.2 |
| 1 | H | 70 | GLY | 2.2 |
| 2 | U | 24 | ALA | 2.2 |
| 2 | U | 21 | ASP | 2.2 |
| 2 | U | 25 | LEU | 2.0 |
| 2 | R | 27 | GLN | 2.0 |
| 1 | E | 118[A] | ARG | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 2 | MEN | N | 70 | 9/10 | 0.98 | 0.05 | - | 11,11,12,15 | 0 |
| 2 | MEN | M | 70 | 9/10 | 0.98 | 0.06 | - | 9,9,11,13 | 0 |
| 2 | MEN | X | 70 | 9/10 | 0.98 | 0.05 | - | 10,11,12,14 | 0 |
| 2 | MEN | W | 70 | 9/10 | 0.98 | 0.05 | - | 10,11,13,14 | 0 |
| 2 | MEN | R | 70 | 9/10 | 0.97 | 0.08 | - | 17,20,22,26 | 0 |
| 2 | MEN | Q | 70 | 9/10 | 0.99 | 0.05 | - | 11,12,14,16 | 0 |
| 2 | MEN | P | 70 | 9/10 | 0.97 | 0.05 | - | 11,13,15,16 | 0 |
| 2 | MEN | O | 70 | 9/10 | 0.99 | 0.06 | - | 10,10,14,15 | 0 |
| 2 | MEN | V | 70 | 9/10 | 0.98 | 0.06 | - | 9,10,14,15 | 0 |
| 2 | MEN | U | 70 | 9/10 | 0.96 | 0.06 | - | 11,11,14,15 | 0 |
| 2 | MEN | T | 70 | 9/10 | 0.97 | 0.05 | - | 14,15,18,20 | 0 |
| 2 | MEN | S | 70 | 9/10 | 0.96 | 0.07 | - | 14,14,17,20 | 0 |

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 6 | NA | S | 206 | 1/1 | 0.99 | 0.22 | 22.67 | 29,29,29,29 | 0 |
| 7 | MPD | B | 203 | 8/8 | 0.83 | 0.23 | 13.70 | 13,13,18,23 | 8 |
| 5 | PI | W | 205 | 5/5 | 0.83 | 0.16 | 10.52 | 19,22,26,29 | 5 |
| 5 | PI | N | 204 | 5/5 | 0.89 | 0.11 | 7.20 | 18,20,21,27 | 5 |
| 5 | PI | U | 205 | 5/5 | 0.88 | 0.12 | 6.88 | 17,19,20,25 | 5 |
| 7 | MPD | R | 204 | 8/8 | 0.81 | 0.23 | 6.22 | 10,18,21,21 | 8 |
| 6 | NA | N | 205 | 1/1 | 0.99 | 0.17 | 5.49 | 28,28,28,28 | 0 |
| 5 | PI | P | 205 | 5/5 | 0.91 | 0.11 | 5.28 | 18,18,21,22 | 5 |
| 5 | PI | X | 205 | 5/5 | 0.92 | 0.10 | 5.08 | 20,23,26,28 | 5 |
| 6 | NA | W | 206 | 1/1 | 0.99 | 0.16 | 5.05 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|------|-----------------------------|-------|
| 7 | MPD | M | 204 | 8/8 | 0.88 | 0.19 | 5.02 | 12,14,16,17 | 8 |
| 7 | MPD | W | 204 | 8/8 | 0.83 | 0.24 | 4.74 | 12,14,16,16 | 8 |
| 5 | PI | S | 205 | 5/5 | 0.96 | 0.08 | 4.67 | 18,18,21,22 | 5 |
| 7 | MPD | O | 204 | 8/8 | 0.74 | 0.21 | 4.46 | 9,20,24,27 | 8 |
| 7 | MPD | P | 204 | 8/8 | 0.84 | 0.18 | 4.38 | 12,15,16,17 | 8 |
| 8 | MRD | V | 204 | 8/8 | 0.77 | 0.17 | 3.92 | 12,16,19,20 | 8 |
| 5 | PI | M | 205 | 5/5 | 0.92 | 0.10 | 3.16 | 20,22,23,25 | 5 |
| 7 | MPD | Q | 204 | 8/8 | 0.84 | 0.16 | 3.02 | 12,15,16,17 | 8 |
| 5 | PI | V | 205 | 5/5 | 0.94 | 0.11 | 2.71 | 17,17,20,23 | 5 |
| 7 | MPD | S | 204 | 8/8 | 0.85 | 0.16 | 2.58 | 15,17,19,20 | 8 |
| 5 | PI | Q | 205 | 5/5 | 0.95 | 0.09 | 2.19 | 22,23,24,25 | 5 |
| 7 | MPD | U | 204 | 8/8 | 0.85 | 0.15 | 2.11 | 16,18,27,28 | 8 |
| 8 | MRD | T | 204 | 8/8 | 0.88 | 0.17 | 2.02 | 12,14,18,23 | 8 |
| 5 | PI | I | 204 | 5/5 | 0.94 | 0.11 | 1.68 | 14,16,17,18 | 5 |
| 5 | PI | T | 205 | 5/5 | 0.95 | 0.09 | 1.62 | 26,27,29,30 | 5 |
| 7 | MPD | X | 204 | 8/8 | 0.92 | 0.12 | 1.59 | 13,15,18,18 | 8 |
| 5 | PI | C | 204 | 5/5 | 0.94 | 0.12 | 1.05 | 18,18,23,26 | 5 |
| 3 | PEB | Q | 187 | 43/43 | 0.95 | 0.08 | 1.03 | 10,12,20,38 | 0 |
| 3 | PEB | M | 188 | 43/43 | 0.96 | 0.07 | 1.03 | 8,10,14,18 | 0 |
| 5 | PI | L | 204 | 5/5 | 0.96 | 0.13 | 0.97 | 16,18,19,22 | 5 |
| 5 | PI | K | 203 | 5/5 | 0.95 | 0.10 | 0.89 | 15,17,18,21 | 5 |
| 5 | PI | J | 204 | 5/5 | 0.95 | 0.11 | 0.82 | 16,19,21,25 | 5 |
| 5 | PI | F | 203 | 5/5 | 0.97 | 0.10 | 0.81 | 17,18,22,24 | 5 |
| 3 | PEB | U | 187 | 43/43 | 0.94 | 0.09 | 0.72 | 8,12,17,33 | 0 |
| 3 | PEB | K | 166 | 43/43 | 0.96 | 0.07 | 0.70 | 10,12,14,25 | 0 |
| 3 | PEB | T | 186 | 43/43 | 0.94 | 0.08 | 0.66 | 14,17,27,44 | 0 |
| 5 | PI | A | 204 | 5/5 | 0.95 | 0.13 | 0.64 | 15,16,19,23 | 5 |
| 3 | PEB | G | 166 | 43/43 | 0.97 | 0.07 | 0.64 | 8,11,13,18 | 0 |
| 3 | PEB | T | 187 | 43/43 | 0.94 | 0.09 | 0.63 | 10,14,23,39 | 0 |
| 3 | PEB | S | 187 | 43/43 | 0.95 | 0.07 | 0.58 | 11,13,20,33 | 0 |
| 4 | NO3 | L | 203 | 4/4 | 0.94 | 0.10 | 0.58 | 13,15,22,24 | 0 |
| 3 | PEB | C | 167 | 43/43 | 0.95 | 0.08 | 0.57 | 12,18,26,32 | 0 |
| 3 | PEB | B | 166 | 43/43 | 0.97 | 0.07 | 0.56 | 9,10,12,21 | 0 |
| 5 | PI | B | 204 | 5/5 | 0.95 | 0.08 | 0.54 | 14,14,15,19 | 5 |
| 3 | PEB | S | 186[A] | 43/43 | 0.94 | 0.08 | 0.48 | 12,14,26,32 | 6 |
| 3 | PEB | J | 166 | 43/43 | 0.96 | 0.07 | 0.48 | 10,11,14,19 | 0 |
| 3 | PEB | S | 186[B] | 43/43 | 0.94 | 0.08 | 0.48 | 12,14,20,33 | 6 |
| 4 | NO3 | I | 203 | 4/4 | 0.94 | 0.09 | 0.48 | 13,20,22,22 | 0 |
| 5 | PI | G | 203 | 5/5 | 0.95 | 0.10 | 0.43 | 18,20,23,24 | 5 |
| 3 | PEB | F | 166 | 43/43 | 0.97 | 0.07 | 0.39 | 9,11,14,21 | 0 |
| 3 | PEB | J | 167 | 43/43 | 0.95 | 0.08 | 0.38 | 11,16,22,31 | 0 |
| 3 | PEB | X | 188 | 43/43 | 0.95 | 0.08 | 0.38 | 9,11,16,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3 | PEB | C | 166 | 43/43 | 0.96 | 0.07 | 0.32 | 10,12,14,18 | 0 |
| 3 | PEB | U | 188 | 43/43 | 0.96 | 0.07 | 0.28 | 9,11,18,34 | 0 |
| 3 | PEB | T | 188 | 43/43 | 0.94 | 0.09 | 0.26 | 12,15,23,26 | 0 |
| 3 | PEB | W | 186 | 43/43 | 0.96 | 0.07 | 0.23 | 9,13,21,34 | 0 |
| 3 | PEB | R | 186 | 43/43 | 0.94 | 0.07 | 0.22 | 15,18,31,46 | 0 |
| 3 | PEB | Q | 186 | 43/43 | 0.96 | 0.07 | 0.21 | 10,13,25,45 | 0 |
| 5 | PI | H | 203 | 5/5 | 0.94 | 0.10 | 0.20 | 17,18,20,21 | 5 |
| 3 | PEB | R | 188 | 43/43 | 0.93 | 0.09 | 0.18 | 12,16,31,43 | 0 |
| 4 | NO3 | J | 203 | 4/4 | 0.94 | 0.08 | 0.14 | 12,20,20,23 | 0 |
| 3 | PEB | A | 166 | 43/43 | 0.97 | 0.07 | 0.14 | 8,9,13,19 | 0 |
| 3 | PEB | P | 187 | 43/43 | 0.95 | 0.07 | 0.13 | 9,11,18,31 | 0 |
| 3 | PEB | I | 166 | 43/43 | 0.96 | 0.07 | 0.12 | 10,12,17,24 | 0 |
| 5 | PI | E | 203 | 5/5 | 0.93 | 0.10 | 0.12 | 20,20,22,23 | 5 |
| 3 | PEB | O | 186 | 43/43 | 0.97 | 0.07 | 0.11 | 8,12,20,33 | 0 |
| 3 | PEB | L | 166 | 43/43 | 0.98 | 0.07 | 0.08 | 8,9,12,18 | 0 |
| 3 | PEB | H | 166 | 43/43 | 0.97 | 0.06 | 0.06 | 13,16,22,29 | 0 |
| 4 | NO3 | A | 203 | 4/4 | 0.94 | 0.08 | 0.04 | 11,15,19,21 | 0 |
| 3 | PEB | P | 186 | 43/43 | 0.96 | 0.07 | 0.04 | 9,13,24,40 | 0 |
| 3 | PEB | W | 188 | 43/43 | 0.96 | 0.07 | 0.03 | 10,12,16,23 | 0 |
| 3 | PEB | M | 186 | 43/43 | 0.95 | 0.07 | 0.02 | 8,11,20,37 | 0 |
| 3 | PEB | E | 166 | 43/43 | 0.96 | 0.07 | 0.01 | 14,18,26,35 | 0 |
| 3 | PEB | P | 188 | 43/43 | 0.97 | 0.07 | -0.01 | 8,10,17,22 | 0 |
| 3 | PEB | N | 186 | 43/43 | 0.96 | 0.07 | -0.01 | 9,13,23,32 | 0 |
| 3 | PEB | V | 187 | 43/43 | 0.97 | 0.06 | -0.04 | 10,11,17,26 | 0 |
| 3 | PEB | X | 186 | 43/43 | 0.96 | 0.06 | -0.09 | 9,12,24,36 | 0 |
| 3 | PEB | V | 186 | 43/43 | 0.97 | 0.07 | -0.09 | 8,11,21,32 | 0 |
| 3 | PEB | U | 186 | 43/43 | 0.96 | 0.07 | -0.10 | 9,13,21,41 | 0 |
| 3 | PEB | A | 167 | 43/43 | 0.97 | 0.07 | -0.13 | 9,11,17,27 | 0 |
| 3 | PEB | S | 188 | 43/43 | 0.96 | 0.06 | -0.13 | 11,12,17,21 | 0 |
| 3 | PEB | G | 167 | 43/43 | 0.97 | 0.06 | -0.15 | 9,12,16,22 | 0 |
| 3 | PEB | K | 167 | 43/43 | 0.94 | 0.08 | -0.16 | 11,14,21,27 | 0 |
| 3 | PEB | N | 188 | 43/43 | 0.96 | 0.06 | -0.17 | 10,12,17,22 | 0 |
| 3 | PEB | R | 187 | 43/43 | 0.95 | 0.08 | -0.18 | 13,15,23,32 | 0 |
| 3 | PEB | L | 167 | 43/43 | 0.96 | 0.07 | -0.18 | 9,12,17,28 | 0 |
| 4 | NO3 | C | 203 | 4/4 | 0.96 | 0.08 | -0.21 | 16,21,22,23 | 0 |
| 3 | PEB | I | 167 | 43/43 | 0.95 | 0.08 | -0.22 | 9,12,18,25 | 0 |
| 3 | PEB | Q | 188 | 43/43 | 0.97 | 0.06 | -0.24 | 10,13,17,19 | 0 |
| 4 | NO3 | D | 203 | 4/4 | 0.97 | 0.07 | -0.24 | 12,16,19,23 | 0 |
| 3 | PEB | M | 187 | 43/43 | 0.97 | 0.06 | -0.25 | 9,10,16,26 | 0 |
| 3 | PEB | D | 167 | 43/43 | 0.96 | 0.07 | -0.26 | 9,13,17,24 | 0 |
| 3 | PEB | O | 187 | 43/43 | 0.96 | 0.07 | -0.28 | 10,13,20,25 | 0 |
| 3 | PEB | H | 167 | 43/43 | 0.97 | 0.06 | -0.31 | 11,12,16,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 3 | PEB | X | 187 | 43/43 | 0.97 | 0.06 | -0.34 | 9,11,19,29 | 0 |
| 3 | PEB | W | 187 | 43/43 | 0.96 | 0.06 | -0.35 | 9,11,19,28 | 0 |
| 3 | PEB | O | 188 | 43/43 | 0.97 | 0.06 | -0.36 | 9,11,15,16 | 0 |
| 3 | PEB | B | 167 | 43/43 | 0.96 | 0.06 | -0.44 | 9,13,19,26 | 0 |
| 3 | PEB | D | 166 | 43/43 | 0.97 | 0.06 | -0.44 | 9,11,15,20 | 0 |
| 3 | PEB | N | 187 | 43/43 | 0.97 | 0.06 | -0.52 | 9,11,17,27 | 0 |
| 3 | PEB | E | 167 | 43/43 | 0.97 | 0.05 | -0.53 | 11,13,16,20 | 0 |
| 3 | PEB | V | 188 | 43/43 | 0.98 | 0.06 | -0.67 | 8,10,14,16 | 0 |
| 3 | PEB | F | 167 | 43/43 | 0.97 | 0.06 | -0.71 | 10,12,16,21 | 0 |
| 5 | PI | D | 204 | 5/5 | 0.96 | 0.07 | -0.99 | 13,13,16,16 | 5 |
| 6 | NA | B | 205 | 1/1 | 0.99 | 0.12 | - | 21,21,21,21 | 0 |
| 6 | NA | L | 205 | 1/1 | 1.00 | 0.16 | - | 17,17,17,17 | 0 |
| 6 | NA | G | 204 | 1/1 | 1.00 | 0.07 | - | 16,16,16,16 | 0 |
| 6 | NA | H | 204 | 1/1 | 0.99 | 0.14 | - | 21,21,21,21 | 0 |
| 6 | NA | V | 206 | 1/1 | 0.98 | 0.28 | - | 25,25,25,25 | 1 |
| 5 | PI | R | 205 | 5/5 | 0.89 | 0.15 | - | 21,23,24,25 | 5 |
| 5 | PI | O | 205 | 5/5 | 0.94 | 0.11 | - | 19,20,22,22 | 5 |
| 6 | NA | C | 205 | 1/1 | 1.00 | 0.11 | - | 19,19,19,19 | 0 |
| 6 | NA | I | 205 | 1/1 | 0.99 | 0.10 | - | 20,20,20,20 | 0 |
| 6 | NA | F | 204 | 1/1 | 1.00 | 0.10 | - | 17,17,17,17 | 0 |
| 6 | NA | K | 204 | 1/1 | 1.00 | 0.10 | - | 22,22,22,22 | 0 |
| 6 | NA | D | 205 | 1/1 | 0.99 | 0.07 | - | 18,18,18,18 | 0 |
| 6 | NA | J | 205 | 1/1 | 1.00 | 0.09 | - | 17,17,17,17 | 0 |
| 6 | NA | E | 204 | 1/1 | 0.99 | 0.08 | - | 19,19,19,19 | 0 |
| 6 | NA | A | 205 | 1/1 | 1.00 | 0.14 | - | 18,18,18,18 | 0 |

6.5 Other polymers

There are no such residues in this entry.