# Full wwPDB NMR Structure Validation Report (i)

Jun 18, 2024 – 12:34 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 5UHU |
| Title | : | Solution conformation of cytochrome P450 MycG with mycinamicin IV bound |
| Authors | : | Pochapsky, T.C.; Tietz, D.R. |
| Deposited on | : | 2017-01-12 |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

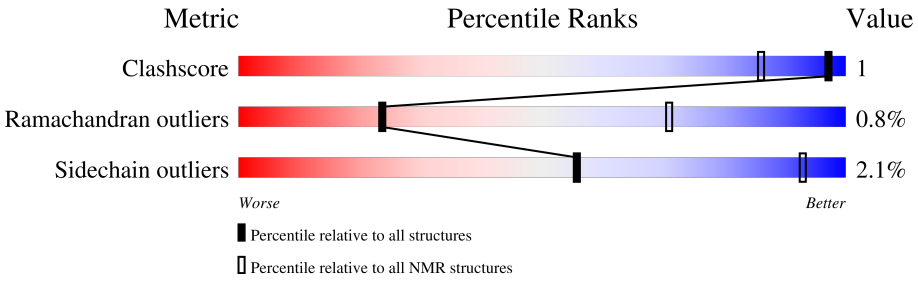
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.37.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 21%.

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) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 397 | 71% 24% • • |

## 2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

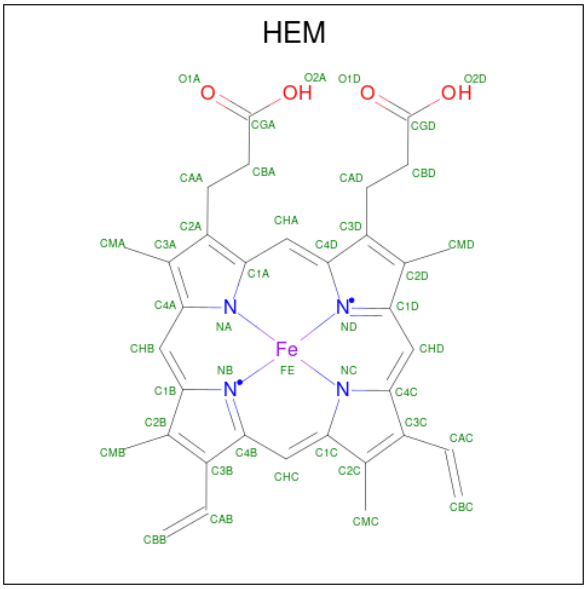
# 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6366 atoms, of which 3179 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mycinamicin IV hydroxylase/epoxidase.

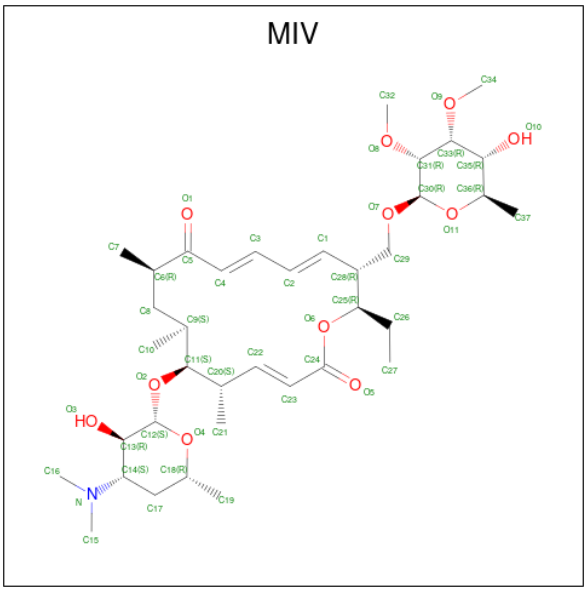
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 393 | 6180 | 1939 | 3086 | 567 | 577 | 11 | 0 |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).




| Mol | Chain | Residues | Atoms | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | H | N | O |
| 2 | A | 1 | 73 | 34 | 1 | 30 | 4 | 4 |

- Molecule 3 is MYCINAMICIN IV (three-letter code: MIV) (formula: $C_{37}H_{61}NO_{11}$).




| Mol | Chain | Residues | Atoms | | | | |
|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | H | N | O |
| | | | 110 | 37 | 61 | 1 | 11 |

- Molecule 4 is water.

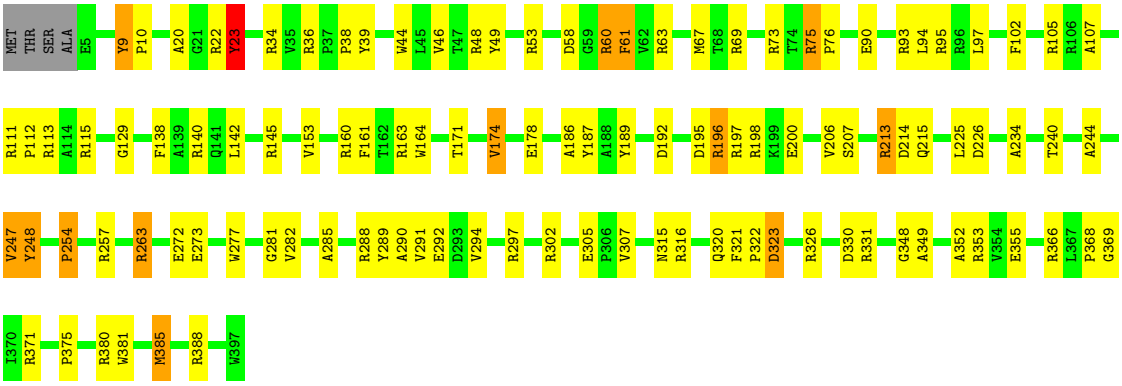
| Mol | Chain | Residues | Atoms | | |
|---|---|---|---|---|---|
| 4 | A | 1 | Total | H | O |
| | | | 3 | 2 | 1 |

# 4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Mycinamicin IV hydroxylase/epoxidase

Chain A:

# 5 Refinement protocol and experimental data overview

Of the 1200 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---|---|---|
| Amber | refinement | 14 |
| Amber | structure calculation | 14 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | working_cs.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 1135 |
| Number of shifts mapped to atoms | 1125 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 10 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 21% |

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.61 | 22/3158 ( 0.7%) | 2.24 | 124/4294 ( 2.9%) |
| All | All | 1.61 | 22/3158 ( 0.7%) | 2.24 | 124/4294 ( 2.9%) |

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

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | A | 0 | 14 |
| All | All | 0 | 14 |

All bond outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 23 | TYR | CE2-CZ | 9.15 | 1.50 | 1.38 |
| 1 | A | 292 | GLU | CD-OE1 | 7.29 | 1.33 | 1.25 |
| 1 | A | 22 | ARG | CZ-NH2 | -6.81 | 1.24 | 1.33 |
| 1 | A | 272 | GLU | CD-OE1 | 6.09 | 1.32 | 1.25 |
| 1 | A | 381 | TRP | CD2-CE3 | 6.05 | 1.49 | 1.40 |
| 1 | A | 129 | GLY | N-CA | 5.85 | 1.54 | 1.46 |
| 1 | A | 138 | PHE | CG-CD1 | 5.77 | 1.47 | 1.38 |
| 1 | A | 102 | PHE | CG-CD1 | 5.75 | 1.47 | 1.38 |
| 1 | A | 353 | ARG | CZ-NH2 | -5.61 | 1.25 | 1.33 |
| 1 | A | 248 | TYR | CD1-CE1 | 5.55 | 1.47 | 1.39 |
| 1 | A | 75 | ARG | CZ-NH1 | -5.46 | 1.25 | 1.33 |
| 1 | A | 111 | ARG | CA-C | 5.40 | 1.67 | 1.52 |
| 1 | A | 207 | SER | CB-OG | 5.34 | 1.49 | 1.42 |
| 1 | A | 60 | ARG | CZ-NH2 | -5.32 | 1.26 | 1.33 |
| 1 | A | 200 | GLU | CG-CD | 5.32 | 1.59 | 1.51 |
| 1 | A | 189 | TYR | CE2-CZ | 5.25 | 1.45 | 1.38 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 9 | TYR | CE2-CZ | 5.19 | 1.45 | 1.38 |
| 1 | A | 192 | ASP | CB-CG | -5.17 | 1.40 | 1.51 |
| 1 | A | 297 | ARG | CZ-NH1 | -5.15 | 1.26 | 1.33 |
| 1 | A | 105 | ARG | CZ-NH1 | -5.14 | 1.26 | 1.33 |
| 1 | A | 200 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | A | 38 | PRO | CA-C | 5.03 | 1.62 | 1.52 |

All angle outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 140 | ARG | NE-CZ-NH1 | 20.39 | 130.50 | 120.30 |
| 1 | A | 326 | ARG | NE-CZ-NH1 | -17.76 | 111.42 | 120.30 |
| 1 | A | 326 | ARG | NE-CZ-NH2 | 17.69 | 129.15 | 120.30 |
| 1 | A | 48 | ARG | NE-CZ-NH1 | 16.03 | 128.32 | 120.30 |
| 1 | A | 198 | ARG | NE-CZ-NH1 | 15.99 | 128.29 | 120.30 |
| 1 | A | 95 | ARG | NE-CZ-NH1 | 15.95 | 128.28 | 120.30 |
| 1 | A | 163 | ARG | NE-CZ-NH1 | 15.67 | 128.14 | 120.30 |
| 1 | A | 95 | ARG | NE-CZ-NH2 | -15.24 | 112.68 | 120.30 |
| 1 | A | 113 | ARG | NE-CZ-NH1 | 14.79 | 127.69 | 120.30 |
| 1 | A | 257 | ARG | NE-CZ-NH1 | 14.43 | 127.52 | 120.30 |
| 1 | A | 160 | ARG | NE-CZ-NH1 | 13.73 | 127.16 | 120.30 |
| 1 | A | 197 | ARG | NE-CZ-NH1 | 13.29 | 126.95 | 120.30 |
| 1 | A | 257 | ARG | NE-CZ-NH2 | -13.24 | 113.68 | 120.30 |
| 1 | A | 111 | ARG | NE-CZ-NH1 | 13.09 | 126.84 | 120.30 |
| 1 | A | 53 | ARG | NE-CZ-NH1 | 13.01 | 126.80 | 120.30 |
| 1 | A | 113 | ARG | NE-CZ-NH2 | -12.14 | 114.23 | 120.30 |
| 1 | A | 69 | ARG | NE-CZ-NH1 | 12.01 | 126.30 | 120.30 |
| 1 | A | 160 | ARG | NE-CZ-NH2 | -11.62 | 114.49 | 120.30 |
| 1 | A | 248 | TYR | CB-CG-CD2 | -11.58 | 114.05 | 121.00 |
| 1 | A | 34 | ARG | NE-CZ-NH1 | 11.27 | 125.94 | 120.30 |
| 1 | A | 145 | ARG | NE-CZ-NH1 | 11.16 | 125.88 | 120.30 |
| 1 | A | 63 | ARG | NE-CZ-NH1 | 11.12 | 125.86 | 120.30 |
| 1 | A | 198 | ARG | NE-CZ-NH2 | -10.98 | 114.81 | 120.30 |
| 1 | A | 366 | ARG | NE-CZ-NH2 | 10.83 | 125.72 | 120.30 |
| 1 | A | 36 | ARG | NE-CZ-NH2 | -10.31 | 115.14 | 120.30 |
| 1 | A | 302 | ARG | NE-CZ-NH1 | 9.96 | 125.28 | 120.30 |
| 1 | A | 331 | ARG | NE-CZ-NH1 | -9.93 | 115.33 | 120.30 |
| 1 | A | 161 | PHE | CB-CG-CD2 | -9.75 | 113.97 | 120.80 |
| 1 | A | 226 | ASP | CB-CG-OD2 | 9.37 | 126.73 | 118.30 |
| 1 | A | 353 | ARG | NE-CZ-NH2 | 9.09 | 124.85 | 120.30 |
| 1 | A | 145 | ARG | NE-CZ-NH2 | -8.80 | 115.90 | 120.30 |
| 1 | A | 115 | ARG | NE-CZ-NH2 | 8.79 | 124.69 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 9 | TYR | CB-CG-CD2 | -8.63 | 115.82 | 121.00 |
| 1 | A | 22 | ARG | NE-CZ-NH2 | 8.38 | 124.49 | 120.30 |
| 1 | A | 107 | ALA | CB-CA-C | 8.24 | 122.46 | 110.10 |
| 1 | A | 90 | GLU | OE1-CD-OE2 | -8.23 | 113.43 | 123.30 |
| 1 | A | 140 | ARG | NE-CZ-NH2 | -8.14 | 116.23 | 120.30 |
| 1 | A | 196 | ARG | NE-CZ-NH1 | 8.12 | 124.36 | 120.30 |
| 1 | A | 213 | ARG | NE-CZ-NH2 | 8.08 | 124.34 | 120.30 |
| 1 | A | 321 | PHE | CB-CG-CD2 | -8.08 | 115.14 | 120.80 |
| 1 | A | 307 | VAL | CA-CB-CG1 | 8.04 | 122.97 | 110.90 |
| 1 | A | 111 | ARG | NE-CZ-NH2 | -7.89 | 116.35 | 120.30 |
| 1 | A | 34 | ARG | NE-CZ-NH2 | -7.85 | 116.37 | 120.30 |
| 1 | A | 49 | TYR | CB-CG-CD2 | -7.83 | 116.31 | 121.00 |
| 1 | A | 206 | VAL | CA-CB-CG1 | 7.66 | 122.39 | 110.90 |
| 1 | A | 105 | ARG | NE-CZ-NH1 | 7.63 | 124.11 | 120.30 |
| 1 | A | 187 | TYR | CB-CG-CD2 | -7.55 | 116.47 | 121.00 |
| 1 | A | 289 | TYR | CB-CG-CD2 | -7.28 | 116.64 | 121.00 |
| 1 | A | 234 | ALA | N-CA-CB | 7.25 | 120.26 | 110.10 |
| 1 | A | 226 | ASP | CB-CG-OD1 | -7.25 | 111.77 | 118.30 |
| 1 | A | 380 | ARG | CD-NE-CZ | 7.17 | 133.64 | 123.60 |
| 1 | A | 61 | PHE | CB-CG-CD2 | -7.06 | 115.86 | 120.80 |
| 1 | A | 305 | GLU | OE1-CD-OE2 | -7.02 | 114.88 | 123.30 |
| 1 | A | 297 | ARG | NE-CZ-NH2 | -6.81 | 116.89 | 120.30 |
| 1 | A | 9 | TYR | CG-CD2-CE2 | -6.67 | 115.96 | 121.30 |
| 1 | A | 49 | TYR | CB-CG-CD1 | 6.64 | 124.99 | 121.00 |
| 1 | A | 225 | LEU | CB-CG-CD2 | -6.62 | 99.75 | 111.00 |
| 1 | A | 282 | VAL | CG1-CB-CG2 | -6.55 | 100.43 | 110.90 |
| 1 | A | 254 | PRO | N-CA-CB | 6.48 | 111.08 | 103.30 |
| 1 | A | 277 | TRP | NE1-CE2-CD2 | -6.43 | 100.87 | 107.30 |
| 1 | A | 355 | GLU | O-C-N | -6.39 | 112.47 | 122.70 |
| 1 | A | 322 | PRO | N-CA-CB | 6.38 | 110.96 | 103.30 |
| 1 | A | 44 | TRP | CZ3-CH2-CZ2 | 6.32 | 129.19 | 121.60 |
| 1 | A | 352 | ALA | N-CA-CB | -6.30 | 101.28 | 110.10 |
| 1 | A | 214 | ASP | CB-CG-OD1 | -6.29 | 112.64 | 118.30 |
| 1 | A | 263 | ARG | NE-CZ-NH2 | -6.26 | 117.17 | 120.30 |
| 1 | A | 288 | ARG | NE-CZ-NH2 | 6.17 | 123.39 | 120.30 |
| 1 | A | 247 | VAL | CG1-CB-CG2 | -6.15 | 101.06 | 110.90 |
| 1 | A | 69 | ARG | NH1-CZ-NH2 | -6.12 | 112.67 | 119.40 |
| 1 | A | 73 | ARG | CD-NE-CZ | 6.10 | 132.14 | 123.60 |
| 1 | A | 39 | TYR | CG-CD1-CE1 | -6.08 | 116.44 | 121.30 |
| 1 | A | 244 | ALA | N-CA-CB | -6.06 | 101.61 | 110.10 |
| 1 | A | 44 | TRP | CE3-CZ3-CH2 | -6.05 | 114.55 | 121.20 |
| 1 | A | 323 | ASP | CB-CG-OD1 | 6.02 | 123.72 | 118.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 248 | TYR | CG-CD1-CE1 | -6.01 | 116.49 | 121.30 |
| 1 | A | 240 | THR | CA-CB-OG1 | 6.01 | 121.62 | 109.00 |
| 1 | A | 142 | LEU | CB-CG-CD1 | 5.99 | 121.19 | 111.00 |
| 1 | A | 349 | ALA | N-CA-CB | -5.94 | 101.79 | 110.10 |
| 1 | A | 330 | ASP | CB-CG-OD1 | -5.84 | 113.04 | 118.30 |
| 1 | A | 197 | ARG | NH1-CZ-NH2 | -5.84 | 112.98 | 119.40 |
| 1 | A | 195 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | A | 186 | ALA | CB-CA-C | 5.82 | 118.83 | 110.10 |
| 1 | A | 76 | PRO | N-CD-CG | 5.79 | 111.89 | 103.20 |
| 1 | A | 213 | ARG | NH1-CZ-NH2 | -5.79 | 113.03 | 119.40 |
| 1 | A | 163 | ARG | NH1-CZ-NH2 | -5.78 | 113.04 | 119.40 |
| 1 | A | 291 | VAL | CA-CB-CG2 | 5.78 | 119.58 | 110.90 |
| 1 | A | 164 | TRP | NE1-CE2-CD2 | -5.78 | 101.52 | 107.30 |
| 1 | A | 368 | PRO | CA-C-N | 5.74 | 127.68 | 116.20 |
| 1 | A | 63 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | A | 315 | ASN | N-CA-CB | -5.66 | 100.42 | 110.60 |
| 1 | A | 140 | ARG | NH1-CZ-NH2 | -5.64 | 113.19 | 119.40 |
| 1 | A | 22 | ARG | CD-NE-CZ | 5.59 | 131.43 | 123.60 |
| 1 | A | 20 | ALA | N-CA-CB | -5.59 | 102.28 | 110.10 |
| 1 | A | 161 | PHE | CB-CG-CD1 | 5.57 | 124.70 | 120.80 |
| 1 | A | 23 | TYR | CB-CG-CD2 | -5.48 | 117.71 | 121.00 |
| 1 | A | 164 | TRP | CE2-CD2-CG | 5.46 | 111.67 | 107.30 |
| 1 | A | 277 | TRP | CE2-CD2-CE3 | -5.44 | 112.17 | 118.70 |
| 1 | A | 248 | TYR | CG-CD2-CE2 | -5.43 | 116.96 | 121.30 |
| 1 | A | 174 | VAL | CG1-CB-CG2 | -5.42 | 102.22 | 110.90 |
| 1 | A | 371 | ARG | CD-NE-CZ | 5.42 | 131.18 | 123.60 |
| 1 | A | 277 | TRP | CE2-CD2-CG | 5.39 | 111.61 | 107.30 |
| 1 | A | 320 | GLN | CA-C-N | 5.38 | 129.04 | 117.20 |
| 1 | A | 48 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 1 | A | 385 | MET | CB-CA-C | 5.36 | 121.12 | 110.40 |
| 1 | A | 153 | VAL | CA-CB-CG1 | 5.35 | 118.93 | 110.90 |
| 1 | A | 39 | TYR | CB-CG-CD2 | -5.31 | 117.81 | 121.00 |
| 1 | A | 323 | ASP | CB-CG-OD2 | -5.31 | 113.52 | 118.30 |
| 1 | A | 273 | GLU | CG-CD-OE1 | 5.30 | 128.90 | 118.30 |
| 1 | A | 34 | ARG | CB-CG-CD | 5.29 | 125.35 | 111.60 |
| 1 | A | 331 | ARG | NH1-CZ-NH2 | 5.26 | 125.19 | 119.40 |
| 1 | A | 39 | TYR | O-C-N | -5.19 | 114.38 | 123.20 |
| 1 | A | 316 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |
| 1 | A | 140 | ARG | CD-NE-CZ | 5.15 | 130.81 | 123.60 |
| 1 | A | 46 | VAL | CG1-CB-CG2 | -5.14 | 102.68 | 110.90 |
| 1 | A | 257 | ARG | CD-NE-CZ | 5.13 | 130.78 | 123.60 |
| 1 | A | 206 | VAL | CG1-CB-CG2 | -5.12 | 102.70 | 110.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 97 | LEU | CB-CA-C | 5.11 | 119.92 | 110.20 |
| 1 | A | 289 | TYR | CB-CG-CD1 | 5.11 | 124.07 | 121.00 |
| 1 | A | 22 | ARG | NH1-CZ-NH2 | -5.09 | 113.80 | 119.40 |
| 1 | A | 277 | TRP | CB-CG-CD2 | 5.08 | 133.20 | 126.60 |
| 1 | A | 53 | ARG | NH1-CZ-NH2 | -5.06 | 113.83 | 119.40 |
| 1 | A | 316 | ARG | NE-CZ-NH2 | 5.06 | 122.83 | 120.30 |
| 1 | A | 285 | ALA | N-CA-CB | -5.04 | 103.05 | 110.10 |
| 1 | A | 58 | ASP | CB-CG-OD1 | -5.03 | 113.77 | 118.30 |

There are no chirality outliers.

All planar outliers are listed below.

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 23 | TYR | Sidechain |
| 1 | A | 60 | ARG | Sidechain |
| 1 | A | 75 | ARG | Sidechain |
| 1 | A | 112 | PRO | Mainchain |
| 1 | A | 196 | ARG | Sidechain |
| 1 | A | 213 | ARG | Sidechain |
| 1 | A | 248 | TYR | Sidechain,Mainchain |
| 1 | A | 263 | ARG | Sidechain |
| 1 | A | 323 | ASP | Peptide |
| 1 | A | 369 | GLY | Mainchain |
| 1 | A | 375 | PRO | Peptide |
| 1 | A | 385 | MET | Peptide |
| 1 | A | 388 | ARG | Sidechain |

## 6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 3094 | 3086 | 3085 | 4 |
| 2 | A | 43 | 30 | 30 | 1 |
| All | All | 3187 | 3179 | 3176 | 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 1.

All clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|---|---|---|---|
| 1:A:9:TYR:CG | 1:A:10:PRO:HA | 0.48 | 2.44 |
| 1:A:61:PHE:CE2 | 1:A:290:ALA:HB2 | 0.44 | 2.47 |
| 1:A:348:GLY:HA3 | 2:A:401:HEM:C2C | 0.43 | 2.48 |
| 1:A:174:VAL:CG1 | 1:A:178:GLU:HG2 | 0.41 | 2.45 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 391/397 (98%) | 357 (91%) | 31 (8%) | 3 (1%) | 24 71 |
| All | All | 391/397 (98%) | 357 (91%) | 31 (8%) | 3 (1%) | 24 71 |

All 3 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 215 | GLN |
| 1 | A | 254 | PRO |
| 1 | A | 281 | GLY |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 326/329 (99%) | 319 (98%) | 7 (2%) | 56 93 |
| All | All | 326/329 (99%) | 319 (98%) | 7 (2%) | 56 93 |

All 7 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 23 | TYR |
| 1 | A | 67 | MET |
| 1 | A | 93 | ARG |
| 1 | A | 94 | LEU |
| 1 | A | 171 | THR |
| 1 | A | 247 | VAL |
| 1 | A | 294 | VAL |

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | HEM | A | 401 | 1,4 | 41,50,50 | 1.67 | 10 (24%) |
| 3 | MIV | A | 402 | - | 51,51,51 | 1.70 | 10 (19%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | HEM | A | 401 | 1,4 | 45,82,82 | 1.85 | 10 (22%) |
| 3 | MIV | A | 402 | - | 62,71,71 | 1.78 | 17 (27%) |

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 | HEM | A | 401 | 1,4 | - | 0,12,54,54 | - |
| 3 | MIV | A | 402 | - | - | 0,55,91,91 | 0,2,3,3 |

All bond outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | A | 402 | MIV | O7-C30 | 5.05 | 1.48 | 1.40 |
| 2 | A | 401 | HEM | CMA-C3A | 4.14 | 1.60 | 1.51 |
| 3 | A | 402 | MIV | O6-C24 | 3.95 | 1.42 | 1.34 |
| 2 | A | 401 | HEM | CAA-C2A | 3.81 | 1.46 | 1.52 |
| 2 | A | 401 | HEM | CBA-CGA | 3.68 | 1.59 | 1.50 |
| 3 | A | 402 | MIV | C30-C31 | 3.37 | 1.61 | 1.52 |
| 3 | A | 402 | MIV | C17-C14 | 2.98 | 1.60 | 1.53 |
| 3 | A | 402 | MIV | C14-N | 2.82 | 1.54 | 1.48 |
| 3 | A | 402 | MIV | O1-C5 | 2.81 | 1.26 | 1.22 |
| 3 | A | 402 | MIV | C35-C36 | 2.75 | 1.58 | 1.52 |
| 3 | A | 402 | MIV | O4-C12 | 2.52 | 1.48 | 1.41 |
| 2 | A | 401 | HEM | C3B-C2B | 2.49 | 1.32 | 1.37 |
| 2 | A | 401 | HEM | CHB-C1B | 2.31 | 1.40 | 1.35 |
| 2 | A | 401 | HEM | C4A-NA | 2.27 | 1.40 | 1.36 |
| 2 | A | 401 | HEM | C2C-C1C | 2.23 | 1.47 | 1.42 |
| 3 | A | 402 | MIV | O3-C13 | 2.23 | 1.48 | 1.43 |
| 2 | A | 401 | HEM | C4B-NB | 2.21 | 1.34 | 1.38 |
| 2 | A | 401 | HEM | CHA-C4D | 2.21 | 1.40 | 1.35 |
| 3 | A | 402 | MIV | C31-C33 | 2.19 | 1.56 | 1.52 |
| 2 | A | 401 | HEM | CHD-C1D | 2.02 | 1.35 | 1.41 |

All angle outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 401 | HEM | C3B-C2B-C1B | 6.77 | 111.51 | 106.49 |
| 3 | A | 402 | MIV | C25-O6-C24 | 4.63 | 110.57 | 117.45 |
| 3 | A | 402 | MIV | C10-C9-C11 | 3.96 | 117.63 | 111.15 |
| 3 | A | 402 | MIV | C30-O11-C36 | 3.91 | 120.39 | 113.67 |
| 2 | A | 401 | HEM | C2B-C1B-NB | 3.90 | 105.22 | 109.84 |
| 2 | A | 401 | HEM | C4B-C3B-C2B | 3.77 | 104.12 | 107.11 |
| 3 | A | 402 | MIV | C19-C18-C17 | 3.48 | 107.94 | 113.40 |
| 3 | A | 402 | MIV | C12-O4-C18 | 2.92 | 117.53 | 112.91 |
| 3 | A | 402 | MIV | C21-C20-C11 | 2.73 | 116.17 | 111.11 |
| 3 | A | 402 | MIV | C20-C22-C23 | 2.73 | 119.00 | 126.44 |
| 3 | A | 402 | MIV | C30-C31-C33 | 2.64 | 105.47 | 110.75 |
| 2 | A | 401 | HEM | C4C-CHD-C1D | 2.62 | 126.01 | 122.56 |
| 2 | A | 401 | HEM | CMA-C3A-C2A | 2.54 | 129.73 | 124.94 |
| 2 | A | 401 | HEM | CHA-C4D-ND | 2.46 | 127.42 | 124.38 |
| 3 | A | 402 | MIV | C27-C26-C25 | 2.44 | 106.55 | 113.27 |
| 3 | A | 402 | MIV | O10-C35-C33 | 2.39 | 116.28 | 109.94 |
| 2 | A | 401 | HEM | CMA-C3A-C4A | 2.39 | 124.79 | 128.46 |
| 3 | A | 402 | MIV | C17-C14-N | 2.38 | 108.95 | 115.67 |
| 3 | A | 402 | MIV | O4-C12-C13 | 2.36 | 105.35 | 110.35 |
| 3 | A | 402 | MIV | O11-C36-C37 | 2.33 | 111.74 | 106.70 |
| 3 | A | 402 | MIV | O2-C11-C20 | 2.29 | 106.15 | 110.89 |
| 3 | A | 402 | MIV | O11-C30-O7 | 2.27 | 104.61 | 109.97 |
| 2 | A | 401 | HEM | CHB-C1B-NB | 2.24 | 127.14 | 124.38 |
| 2 | A | 401 | HEM | O1D-CGD-CBD | 2.23 | 115.92 | 123.08 |
| 2 | A | 401 | HEM | C4A-C3A-C2A | 2.19 | 105.47 | 107.00 |
| 3 | A | 402 | MIV | C17-C14-C13 | 2.11 | 113.00 | 109.97 |
| 3 | A | 402 | MIV | C10-C9-C8 | 2.10 | 113.83 | 110.69 |

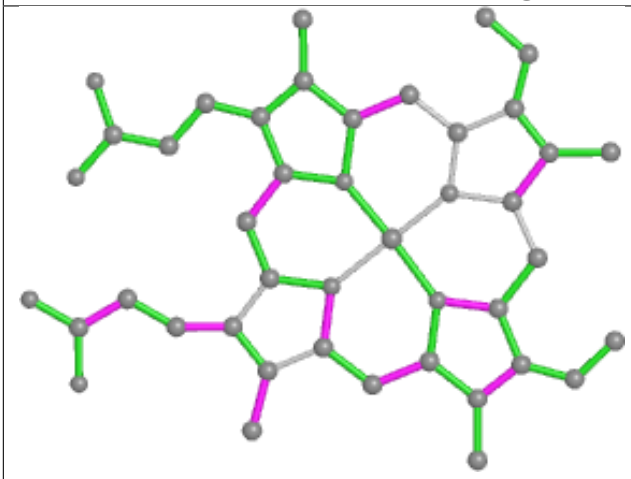
There are no chirality outliers.

There are no torsion outliers.

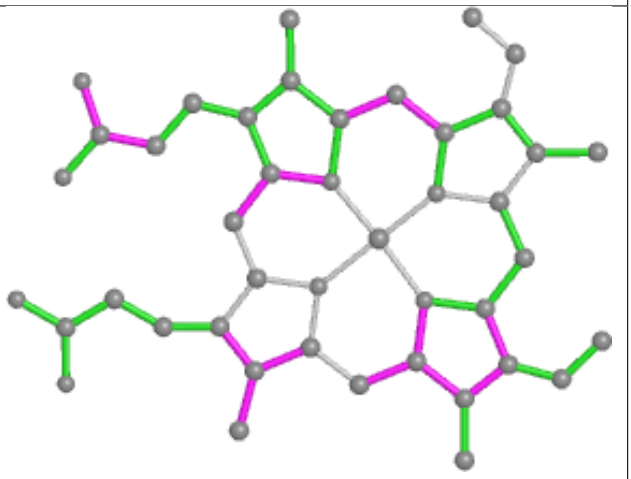
There are no ring outliers.

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

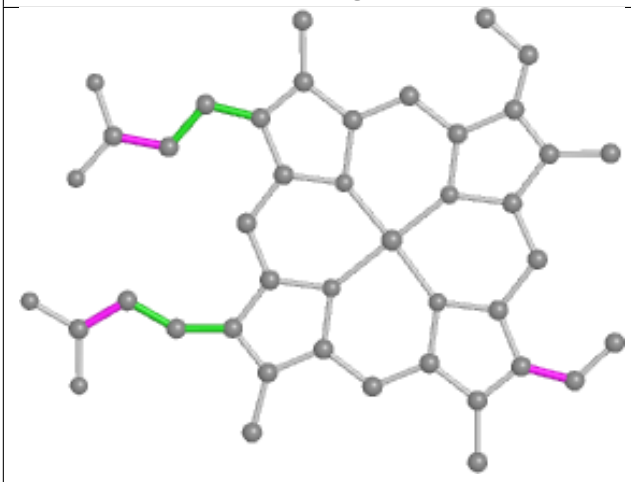
## Ligand HEM A 401



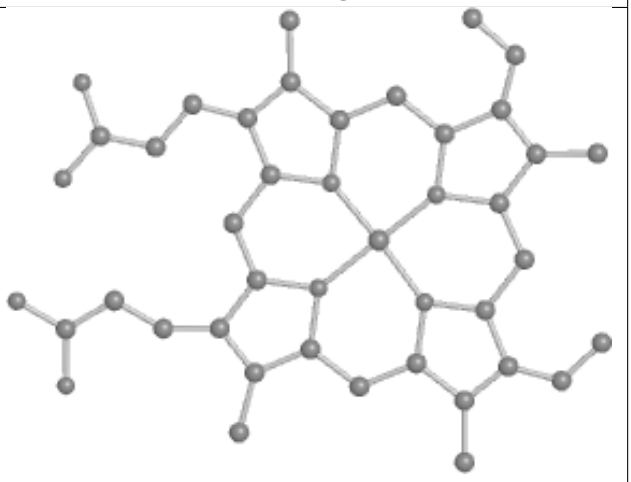
Bond lengths



Bond angles

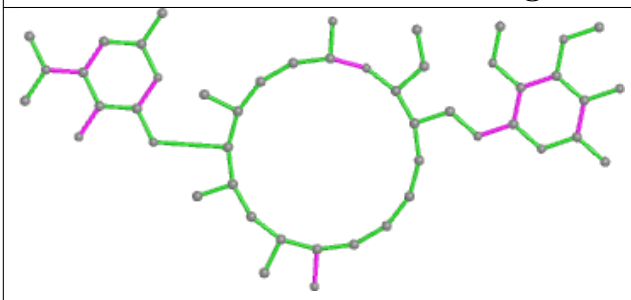


Torsions

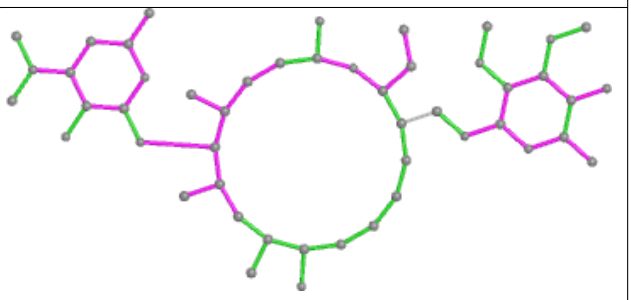


Rings

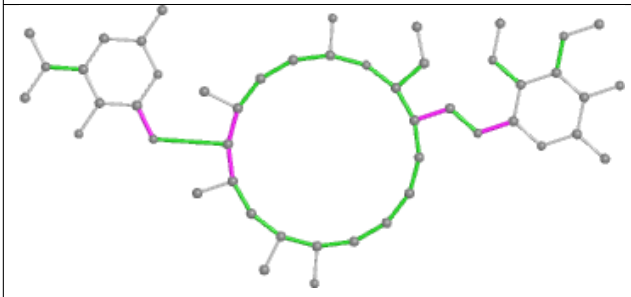
## Ligand MIV A 402



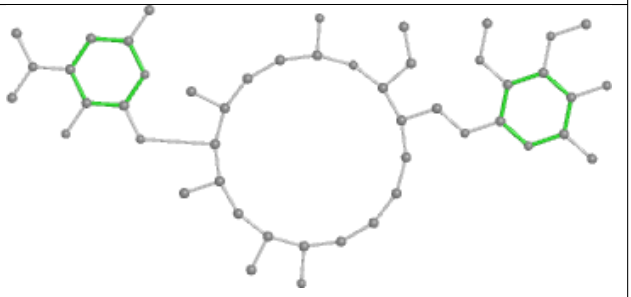
Bond lengths



Bond angles



Torsions



Rings

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 21% for the entire structure.

## 7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *data_ complete.str*

### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 1135 |
| Number of shifts mapped to atoms | 1125 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 10 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 3 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 10 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---|---|---|---|---|---|---|---|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 2 | THR | CA | 63.0 | 0.2 | 1 |
| 1 | A | 2 | THR | CB | 71.6 | 0.2 | 1 |
| 1 | A | 3 | SER | H | 7.91 | 0.05 | 1 |
| 1 | A | 3 | SER | CA | 57.8 | 0.2 | 1 |
| 1 | A | 3 | SER | CB | 64.2 | 0.2 | 1 |
| 1 | A | 3 | SER | N | 122.6 | 0.1 | 1 |
| 1 | A | 4 | ALA | H | 8.29 | 0.05 | 1 |
| 1 | A | 4 | ALA | CA | 51.8 | 0.2 | 1 |
| 1 | A | 4 | ALA | CB | 18.5 | 0.2 | 1 |
| 1 | A | 4 | ALA | N | 126.6 | 0.1 | 1 |

### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 313 | 0.29 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 249 | 1.26 ± 0.11 | Should be checked |
| $^{13}C'$ | 0 | — | None (insufficient data) |
| $^{15}N$ | 280 | 0.30 ± 0.32 | None needed (< 0.5 ppm) |

### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 1125 atoms were assigned a chemical shift out of a possible 5466. 0 out of 83 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 866/1937 (45%) | 278/786 (35%) | 310/786 (39%) | 278/365 (76%) |
| Sidechain | 255/3232 (8%) | 6/2104 (0%) | 246/975 (25%) | 3/153 (2%) |
| Aromatic | 4/297 (1%) | 2/148 (1%) | 0/136 (0%) | 2/13 (15%) |
| Overall | 1125/5466 (21%) | 286/3038 (9%) | 556/1897 (29%) | 283/531 (53%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 1125 atoms were assigned a chemical shift out of a possible 5466. 0 out of 83 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 866/1937 (45%) | 278/786 (35%) | 310/786 (39%) | 278/365 (76%) |
| Sidechain | 255/3232 (8%) | 6/2104 (0%) | 246/975 (25%) | 3/153 (2%) |
| Aromatic | 4/297 (1%) | 2/148 (1%) | 0/136 (0%) | 2/13 (15%) |
| Overall | 1125/5466 (21%) | 286/3038 (9%) | 556/1897 (29%) | 283/531 (53%) |

### 7.1.4 Statistically unusual chemical shifts

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 347 | LEU | H | 2.69 | 5.09 – 11.34 | -8.8 |
| 1 | A | 158 | HIS | CB | 42.20 | 19.76 – 40.75 | 5.7 |
| 1 | A | 235 | GLY | H | 11.60 | 5.23 – 11.42 | 5.3 |

### 7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: