



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 02:24 PM EDT

PDB ID : 5A1U
EMDB ID: : EMD-2985
Title : The structure of the COPI coat triad
Authors : Dodonova, S.O.; Diestelkoetter-Bachert, P.; von Appen, A.; Hagen, W.J.H.;
Beck, R.; Beck, M.; Wieland, F.; Briggs, J.A.G.
Deposited on : unknown
Resolution : 13.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

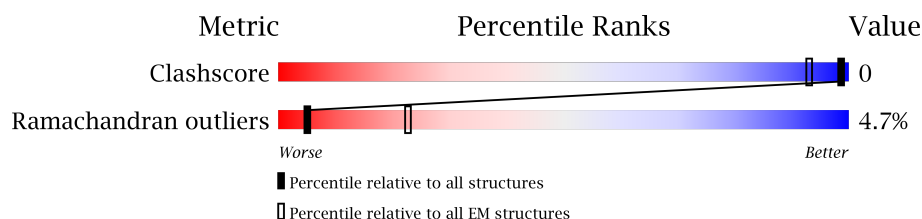
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY








The reported resolution of this entry is 13.00 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 181 |  88% 12% |
| 1 | B | 181 |  88% 12% |
| 2 | C | 1262 |  59% 5% 36% |
| 3 | D | 905 |  80% 9% 11% |
| 4 | E | 874 |  88% 5% • 6% |
| 5 | F | 177 |  75% • 21% |
| 6 | G | 968 |  73% 10% • 16% |
| 7 | H | 511 |  25% • 74% |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ADP-RIBOSYLATION FACTOR 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1 | A | 159 | Total | C | N | O | 0 | 0 |
| | | | 636 | 318 | 159 | 159 | | |
| 1 | B | 159 | Total | C | N | O | 0 | 0 |
| | | | 636 | 318 | 159 | 159 | | |

- Molecule 2 is a protein called COATOMER SUBUNIT ALPHA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 2 | C | 813 | Total | C | N | O | 0 | 0 |
| | | | 3251 | 1626 | 813 | 812 | | |

There are 38 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1225 | LEU | - | expression tag | UNP Q8CIE6 |
| C | 1226 | GLU | - | expression tag | UNP Q8CIE6 |
| C | 1227 | VAL | - | expression tag | UNP Q8CIE6 |
| C | 1228 | LEU | - | expression tag | UNP Q8CIE6 |
| C | 1229 | PHE | - | expression tag | UNP Q8CIE6 |
| C | 1230 | GLN | - | expression tag | UNP Q8CIE6 |
| C | 1231 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1232 | PRO | - | expression tag | UNP Q8CIE6 |
| C | 1233 | SER | - | expression tag | UNP Q8CIE6 |
| C | 1234 | ALA | - | expression tag | UNP Q8CIE6 |
| C | 1235 | TRP | - | expression tag | UNP Q8CIE6 |
| C | 1236 | SER | - | expression tag | UNP Q8CIE6 |
| C | 1237 | HIS | - | expression tag | UNP Q8CIE6 |
| C | 1238 | PRO | - | expression tag | UNP Q8CIE6 |
| C | 1239 | GLN | - | expression tag | UNP Q8CIE6 |
| C | 1240 | PHE | - | expression tag | UNP Q8CIE6 |
| C | 1241 | GLU | - | expression tag | UNP Q8CIE6 |
| C | 1242 | LYS | - | expression tag | UNP Q8CIE6 |
| C | 1243 | GLY | - | expression tag | UNP Q8CIE6 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1244 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1245 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1246 | SER | - | expression tag | UNP Q8CIE6 |
| C | 1247 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1248 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1249 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1250 | SER | - | expression tag | UNP Q8CIE6 |
| C | 1251 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1252 | GLY | - | expression tag | UNP Q8CIE6 |
| C | 1253 | SER | - | expression tag | UNP Q8CIE6 |
| C | 1254 | ALA | - | expression tag | UNP Q8CIE6 |
| C | 1255 | TRP | - | expression tag | UNP Q8CIE6 |
| C | 1256 | SER | - | expression tag | UNP Q8CIE6 |
| C | 1257 | HIS | - | expression tag | UNP Q8CIE6 |
| C | 1258 | PRO | - | expression tag | UNP Q8CIE6 |
| C | 1259 | GLN | - | expression tag | UNP Q8CIE6 |
| C | 1260 | PHE | - | expression tag | UNP Q8CIE6 |
| C | 1261 | GLU | - | expression tag | UNP Q8CIE6 |
| C | 1262 | LYS | - | expression tag | UNP Q8CIE6 |

- Molecule 3 is a protein called COATOMER SUBUNIT BETA'.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 3 | D | 803 | Total | C | N | O | 0 | 0 |
| | | | 3211 | 1606 | 803 | 802 | | |

- Molecule 4 is a protein called COATOMER SUBUNIT GAMMA-1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 4 | E | 824 | Total | C | N | O | 0 | 0 |
| | | | 3294 | 1648 | 824 | 822 | | |

- Molecule 5 is a protein called COATOMER SUBUNIT ZETA-1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5 | F | 139 | Total | C | N | O | 0 | 0 |
| | | | 555 | 278 | 139 | 138 | | |

- Molecule 6 is a protein called COATOMER SUBUNIT BETA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 6 | G | 813 | Total | C | N | O | 0 | 0 |
| | | | 3250 | 1626 | 813 | 811 | | |

There are 15 discrepancies between the modelled and reference sequences:

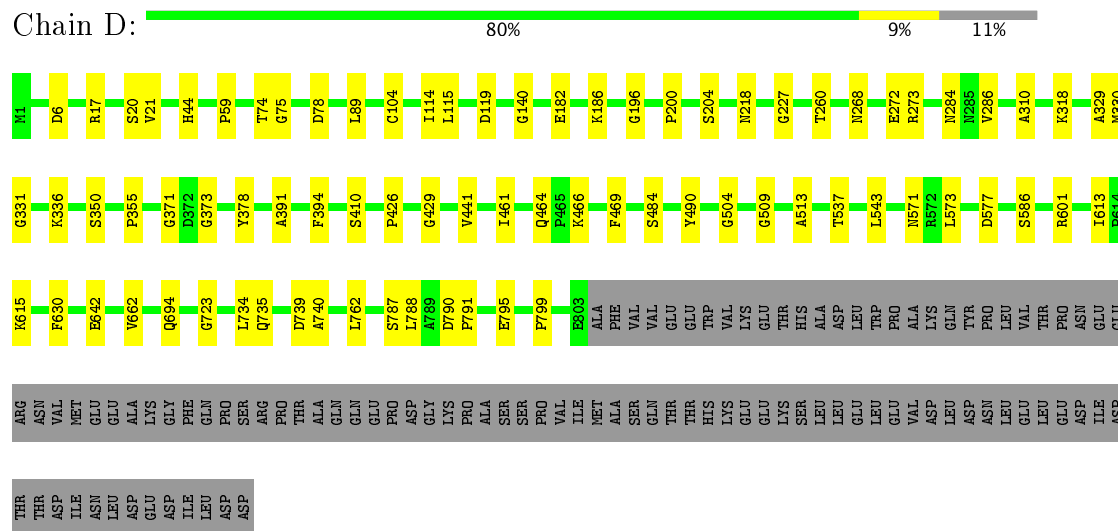
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | -14 | MET | - | expression tag | UNP Q9JIF7 |
| G | -13 | HIS | - | expression tag | UNP Q9JIF7 |
| G | -12 | HIS | - | expression tag | UNP Q9JIF7 |
| G | -11 | HIS | - | expression tag | UNP Q9JIF7 |
| G | -10 | HIS | - | expression tag | UNP Q9JIF7 |
| G | -9 | HIS | - | expression tag | UNP Q9JIF7 |
| G | -8 | HIS | - | expression tag | UNP Q9JIF7 |
| G | -7 | GLU | - | expression tag | UNP Q9JIF7 |
| G | -6 | ASN | - | expression tag | UNP Q9JIF7 |
| G | -5 | LEU | - | expression tag | UNP Q9JIF7 |
| G | -4 | TYR | - | expression tag | UNP Q9JIF7 |
| G | -3 | PHE | - | expression tag | UNP Q9JIF7 |
| G | -2 | GLN | - | expression tag | UNP Q9JIF7 |
| G | -1 | GLY | - | expression tag | UNP Q9JIF7 |
| G | 0 | HIS | - | expression tag | UNP Q9JIF7 |

- Molecule 7 is a protein called COATOMER SUBUNIT DELTA.

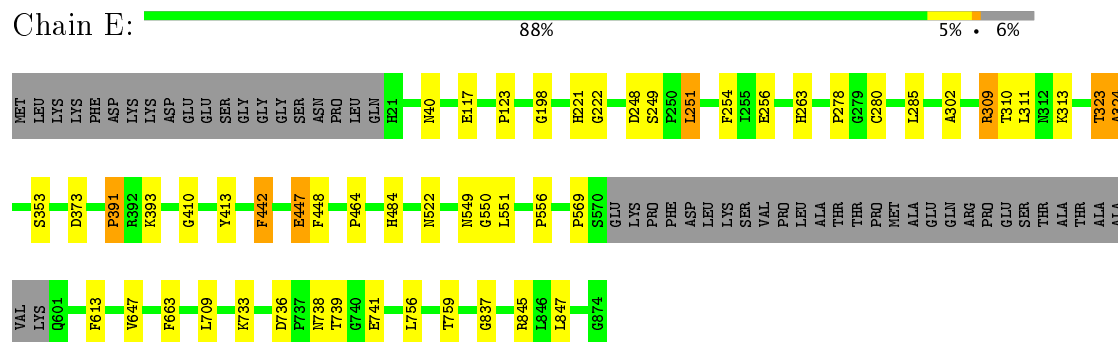
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7 | H | 135 | Total | C | N | O | 0 | 0 |
| | | | 539 | 270 | 135 | 134 | | |

[illegible]

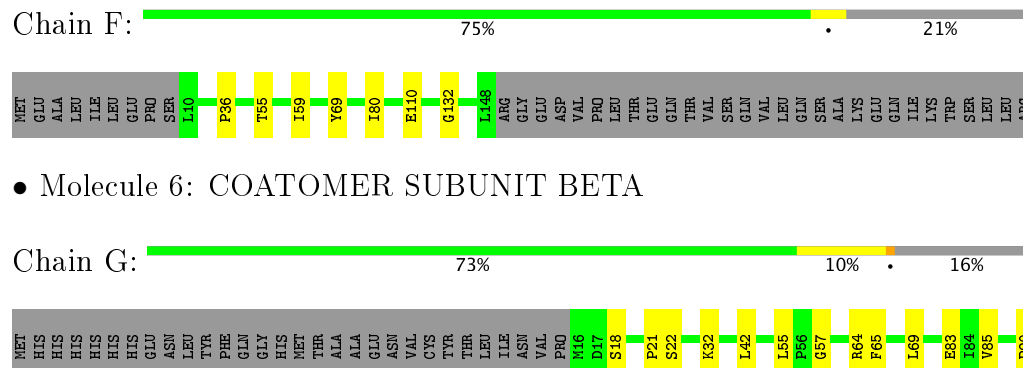
• Molecule 3: COATOMER SUBUNIT BETA'



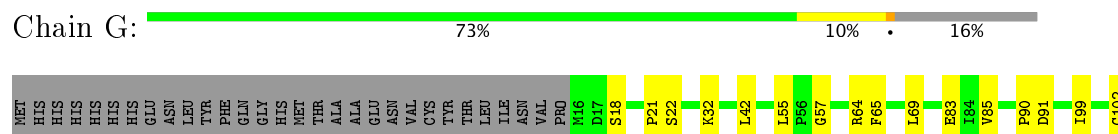
- Molecule 4: COATOMER SUBUNIT GAMMA-1

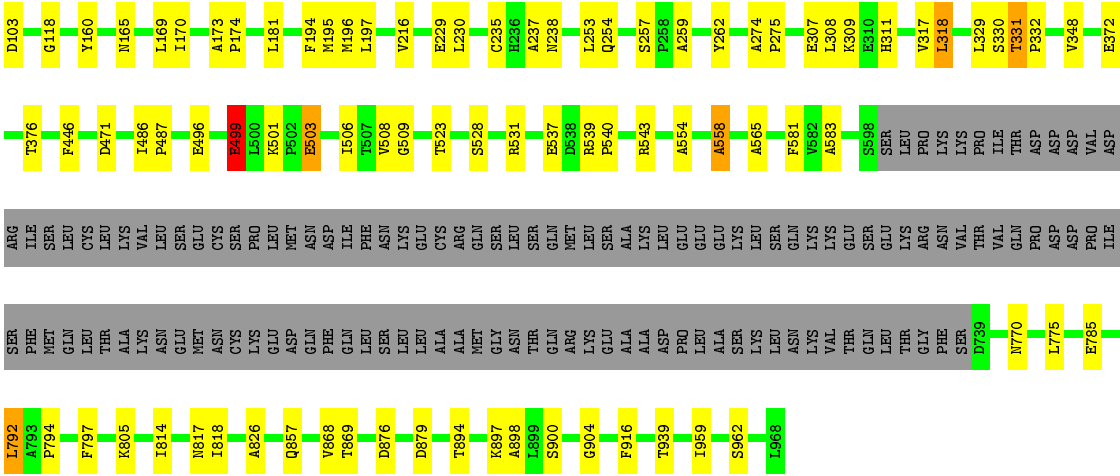


- Molecule 5: COATOMER SUBUNIT ZETA-1

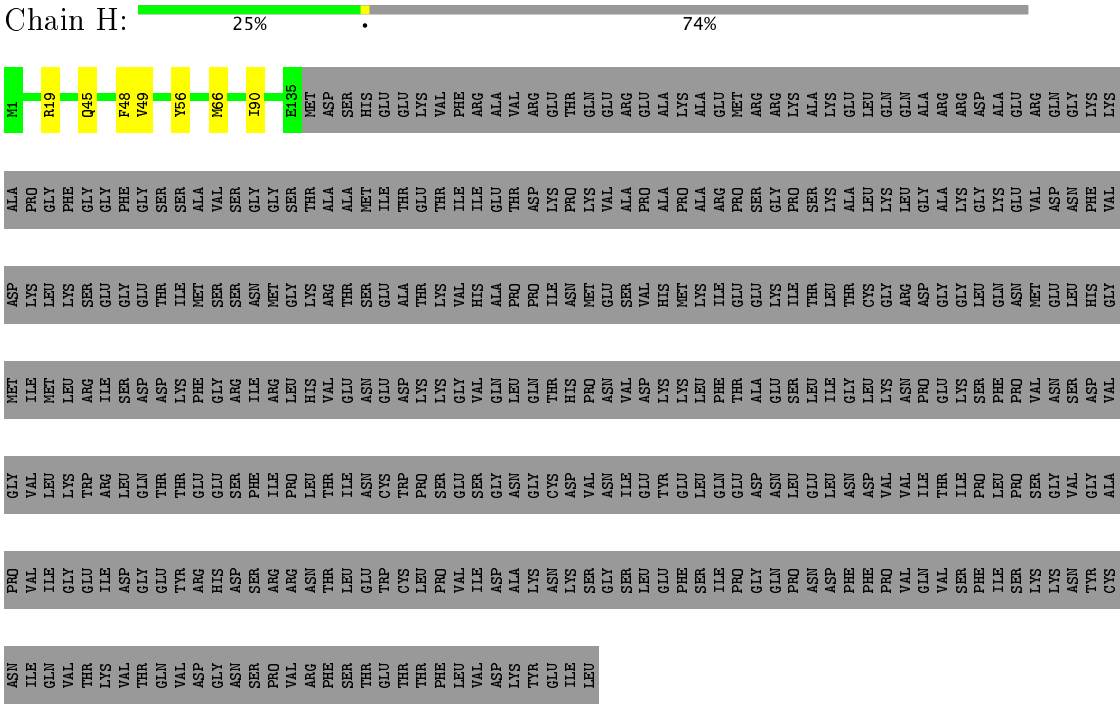


• Molecule 6: COATOMER SUBUNIT BETA





● Molecule 7: COATOMER SUBUNIT DELTA



4 Experimental information

| Property | Value | Source |
|--------------------------------------|------------------------------------|-----------|
| Reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | POINT, C3 | Depositor |
| Number of tilted images used | 13186 | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | PHASE FLIPPING OF INDIVIDUAL TILTS | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 45 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 42000 | Depositor |
| Image detector | GATAN MULTISCAN | Depositor |

5 Model quality

5.1 Standard geometry

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 > 2$ | RMSZ | # $ Z > 2$ |
| 1 | A | 0.43 | 0/635 | 0.69 | 0/792 |
| 1 | B | 0.43 | 0/635 | 0.69 | 0/792 |
| 2 | C | 1.55 | 8/3250 (0.2%) | 1.71 | 14/4061 (0.3%) |
| 3 | D | 1.60 | 17/3210 (0.5%) | 1.72 | 24/4011 (0.6%) |
| 4 | E | 1.52 | 4/3292 (0.1%) | 1.63 | 19/4112 (0.5%) |
| 5 | F | 1.55 | 1/554 (0.2%) | 1.74 | 3/691 (0.4%) |
| 6 | G | 1.50 | 7/3248 (0.2%) | 1.71 | 23/4057 (0.6%) |
| 7 | H | 1.46 | 0/538 | 1.76 | 7/671 (1.0%) |
| All | All | 1.48 | 37/15362 (0.2%) | 1.64 | 90/19187 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | C | 0 | 4 |
| 3 | D | 0 | 2 |
| 4 | E | 0 | 4 |
| 5 | F | 0 | 1 |
| 6 | G | 0 | 14 |
| All | All | 0 | 25 |

All (37) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | C | 621 | VAL | C-N | 6.93 | 1.45 | 1.33 |
| 3 | D | 330 | MET | N-CA | -6.80 | 1.32 | 1.46 |
| 4 | E | 198 | GLY | CA-C | -6.43 | 1.41 | 1.51 |
| 3 | D | 378 | TYR | N-CA | -6.38 | 1.33 | 1.46 |
| 3 | D | 537 | THR | N-CA | -6.33 | 1.33 | 1.46 |
| 3 | D | 723 | GLY | CA-C | -6.28 | 1.41 | 1.51 |
| 6 | G | 118 | GLY | CA-C | -6.28 | 1.41 | 1.51 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | D | 799 | PRO | C-N | 6.20 | 1.44 | 1.33 |
| 3 | D | 464 | GLN | N-CA | -6.09 | 1.34 | 1.46 |
| 4 | E | 123 | PRO | N-CA | -5.96 | 1.37 | 1.47 |
| 3 | D | 186 | LYS | C-N | 5.94 | 1.43 | 1.33 |
| 2 | C | 631 | LYS | N-CA | -5.90 | 1.34 | 1.46 |
| 3 | D | 331 | GLY | CA-C | -5.87 | 1.42 | 1.51 |
| 2 | C | 204 | HIS | N-CA | -5.75 | 1.34 | 1.46 |
| 3 | D | 227 | GLY | CA-C | -5.73 | 1.42 | 1.51 |
| 4 | E | 837 | GLY | N-CA | -5.71 | 1.37 | 1.46 |
| 3 | D | 373 | GLY | N-CA | -5.71 | 1.37 | 1.46 |
| 6 | G | 509 | GLY | CA-C | -5.61 | 1.42 | 1.51 |
| 2 | C | 259 | PRO | CA-C | -5.44 | 1.42 | 1.52 |
| 2 | C | 186 | GLY | N-CA | -5.44 | 1.37 | 1.46 |
| 6 | G | 539 | ARG | C-N | 5.43 | 1.44 | 1.34 |
| 5 | F | 132 | GLY | N-CA | -5.31 | 1.38 | 1.46 |
| 4 | E | 613 | PHE | N-CA | -5.31 | 1.35 | 1.46 |
| 6 | G | 57 | GLY | N-CA | 5.27 | 1.53 | 1.46 |
| 2 | C | 740 | GLY | CA-C | -5.23 | 1.43 | 1.51 |
| 3 | D | 466 | LYS | N-CA | -5.22 | 1.35 | 1.46 |
| 6 | G | 160 | TYR | N-CA | -5.20 | 1.35 | 1.46 |
| 2 | C | 353 | ALA | N-CA | -5.17 | 1.36 | 1.46 |
| 3 | D | 509 | GLY | N-CA | -5.15 | 1.38 | 1.46 |
| 2 | C | 130 | VAL | C-N | 5.15 | 1.45 | 1.34 |
| 3 | D | 504 | GLY | N-CA | 5.13 | 1.53 | 1.46 |
| 3 | D | 310 | ALA | N-CA | -5.13 | 1.36 | 1.46 |
| 3 | D | 586 | SER | N-CA | -5.11 | 1.36 | 1.46 |
| 6 | G | 857 | GLN | N-CA | -5.06 | 1.36 | 1.46 |
| 3 | D | 371 | GLY | CA-C | -5.06 | 1.43 | 1.51 |
| 6 | G | 565 | ALA | N-CA | -5.01 | 1.36 | 1.46 |
| 3 | D | 74 | THR | C-O | -5.00 | 1.13 | 1.23 |

All (90) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6 | G | 496 | GLU | N-CA-C | 7.82 | 132.11 | 111.00 |
| 4 | E | 302 | ALA | C-N-CA | 7.05 | 139.33 | 121.70 |
| 2 | C | 54 | VAL | N-CA-C | -6.91 | 92.35 | 111.00 |
| 6 | G | 486 | ILE | O-C-N | -6.80 | 108.18 | 121.10 |
| 6 | G | 869 | THR | N-CA-C | -6.72 | 92.85 | 111.00 |
| 4 | E | 756 | LEU | N-CA-C | -6.71 | 92.87 | 111.00 |
| 3 | D | 490 | TYR | N-CA-C | -6.64 | 93.08 | 111.00 |
| 6 | G | 486 | ILE | CA-C-N | 6.60 | 135.58 | 117.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | D | 286 | VAL | N-CA-C | -6.52 | 93.40 | 111.00 |
| 6 | G | 792 | LEU | N-CA-C | -6.42 | 93.65 | 111.00 |
| 7 | H | 90 | ILE | CA-C-N | 6.42 | 135.09 | 117.10 |
| 3 | D | 461 | ILE | N-CA-C | -6.41 | 93.69 | 111.00 |
| 4 | E | 254 | PHE | N-CA-C | -6.41 | 93.70 | 111.00 |
| 4 | E | 324 | ALA | N-CA-C | 6.31 | 128.03 | 111.00 |
| 3 | D | 642 | GLU | O-C-N | 6.29 | 132.76 | 122.70 |
| 5 | F | 69 | TYR | O-C-N | 6.28 | 132.75 | 122.70 |
| 3 | D | 204 | SER | N-CA-C | -6.26 | 94.10 | 111.00 |
| 2 | C | 400 | ALA | N-CA-C | -6.24 | 94.16 | 111.00 |
| 7 | H | 66 | MET | N-CA-C | -6.22 | 94.21 | 111.00 |
| 3 | D | 78 | ASP | C-N-CA | 6.20 | 137.19 | 121.70 |
| 3 | D | 196 | GLY | CA-C-O | 6.19 | 131.74 | 120.60 |
| 3 | D | 573 | LEU | N-CA-C | -6.18 | 94.31 | 111.00 |
| 3 | D | 613 | ILE | N-CA-C | -6.18 | 94.33 | 111.00 |
| 3 | D | 469 | PHE | N-CA-C | -6.11 | 94.50 | 111.00 |
| 7 | H | 56 | TYR | N-CA-C | -6.00 | 94.80 | 111.00 |
| 6 | G | 376 | THR | N-CA-C | -5.90 | 95.08 | 111.00 |
| 4 | E | 738 | ASN | N-CA-C | -5.88 | 95.12 | 111.00 |
| 2 | C | 223 | GLY | N-CA-C | -5.87 | 98.42 | 113.10 |
| 4 | E | 709 | LEU | N-CA-C | -5.83 | 95.27 | 111.00 |
| 2 | C | 732 | HIS | C-N-CA | 5.70 | 135.95 | 121.70 |
| 2 | C | 105 | TYR | N-CA-C | -5.68 | 95.65 | 111.00 |
| 4 | E | 759 | THR | N-CA-C | -5.68 | 95.66 | 111.00 |
| 5 | F | 80 | ILE | N-CA-C | -5.68 | 95.67 | 111.00 |
| 4 | E | 550 | GLY | C-N-CA | 5.65 | 135.83 | 121.70 |
| 6 | G | 499 | GLU | N-CA-C | 5.65 | 126.26 | 111.00 |
| 4 | E | 222 | GLY | N-CA-C | -5.64 | 99.00 | 113.10 |
| 3 | D | 75 | GLY | N-CA-C | -5.63 | 99.02 | 113.10 |
| 3 | D | 182 | GLU | N-CA-C | -5.61 | 95.85 | 111.00 |
| 2 | C | 15 | LEU | N-CA-C | -5.60 | 95.88 | 111.00 |
| 6 | G | 818 | ILE | N-CA-C | -5.60 | 95.89 | 111.00 |
| 4 | E | 391 | PRO | N-CA-C | 5.58 | 126.62 | 112.10 |
| 6 | G | 503 | GLU | N-CA-C | -5.57 | 95.97 | 111.00 |
| 6 | G | 196 | MET | N-CA-C | -5.54 | 96.04 | 111.00 |
| 6 | G | 170 | ILE | CA-C-N | 5.51 | 132.53 | 117.10 |
| 3 | D | 429 | GLY | N-CA-C | -5.51 | 99.33 | 113.10 |
| 4 | E | 733 | LYS | N-CA-C | -5.50 | 96.14 | 111.00 |
| 6 | G | 195 | MET | N-CA-C | -5.50 | 96.16 | 111.00 |
| 2 | C | 630 | GLN | N-CA-C | -5.47 | 96.23 | 111.00 |
| 5 | F | 110 | GLU | N-CA-C | -5.47 | 96.24 | 111.00 |
| 4 | E | 847 | LEU | N-CA-C | -5.46 | 96.25 | 111.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | D | 115 | LEU | N-CA-C | -5.43 | 96.34 | 111.00 |
| 6 | G | 558 | ALA | N-CA-C | -5.41 | 96.39 | 111.00 |
| 4 | E | 736 | ASP | CA-C-O | -5.41 | 108.75 | 120.10 |
| 4 | E | 845 | ARG | N-CA-C | -5.40 | 96.43 | 111.00 |
| 2 | C | 273 | ILE | N-CA-C | -5.39 | 96.44 | 111.00 |
| 2 | C | 226 | ASP | N-CA-C | -5.38 | 96.48 | 111.00 |
| 3 | D | 642 | GLU | CA-C-O | -5.38 | 108.81 | 120.10 |
| 4 | E | 285 | LEU | O-C-N | -5.34 | 114.15 | 122.70 |
| 6 | G | 318 | LEU | N-CA-C | 5.34 | 125.42 | 111.00 |
| 7 | H | 90 | ILE | CA-C-O | -5.33 | 108.90 | 120.10 |
| 4 | E | 647 | VAL | N-CA-C | -5.32 | 96.64 | 111.00 |
| 7 | H | 49 | VAL | N-CA-C | -5.30 | 96.70 | 111.00 |
| 3 | D | 441 | VAL | N-CA-C | -5.29 | 96.71 | 111.00 |
| 3 | D | 394 | PHE | N-CA-C | -5.21 | 96.92 | 111.00 |
| 6 | G | 64 | ARG | N-CA-C | 5.20 | 125.05 | 111.00 |
| 7 | H | 19 | ARG | C-N-CA | 5.19 | 134.68 | 121.70 |
| 2 | C | 423 | ARG | C-N-CA | 5.18 | 134.65 | 121.70 |
| 3 | D | 268 | ASN | N-CA-C | -5.16 | 97.06 | 111.00 |
| 7 | H | 48 | PHE | N-CA-C | -5.16 | 97.06 | 111.00 |
| 4 | E | 663 | PHE | N-CA-C | -5.15 | 97.09 | 111.00 |
| 3 | D | 21 | VAL | N-CA-C | -5.15 | 97.10 | 111.00 |
| 2 | C | 200 | VAL | O-C-N | 5.14 | 130.92 | 122.70 |
| 6 | G | 775 | LEU | N-CA-C | -5.13 | 97.15 | 111.00 |
| 6 | G | 169 | LEU | N-CA-C | -5.12 | 97.17 | 111.00 |
| 6 | G | 229 | GLU | C-N-CA | 5.12 | 134.49 | 121.70 |
| 6 | G | 868 | VAL | N-CA-C | -5.11 | 97.19 | 111.00 |
| 3 | D | 104 | CYS | C-N-CA | 5.10 | 134.45 | 121.70 |
| 2 | C | 168 | ARG | N-CA-C | -5.08 | 97.27 | 111.00 |
| 3 | D | 543 | LEU | O-C-N | -5.08 | 114.58 | 122.70 |
| 3 | D | 114 | ILE | N-CA-C | -5.07 | 97.30 | 111.00 |
| 4 | E | 447 | GLU | C-N-CA | 5.07 | 134.37 | 121.70 |
| 4 | E | 248 | ASP | O-C-N | -5.05 | 114.62 | 122.70 |
| 2 | C | 684 | GLN | C-N-CA | 5.04 | 132.88 | 122.30 |
| 6 | G | 165 | ASN | C-N-CA | 5.04 | 134.30 | 121.70 |
| 6 | G | 797 | PHE | N-CA-C | -5.04 | 97.39 | 111.00 |
| 6 | G | 805 | LYS | N-CA-C | -5.03 | 97.41 | 111.00 |
| 3 | D | 20 | SER | C-N-CA | 5.03 | 134.27 | 121.70 |
| 3 | D | 218 | ASN | O-C-N | 5.01 | 130.72 | 122.70 |
| 6 | G | 42 | LEU | O-C-N | -5.01 | 114.68 | 122.70 |
| 2 | C | 709 | ILE | C-N-CA | 5.01 | 134.22 | 121.70 |

There are no chirality outliers.

All (25) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | C | 317 | PHE | Mainchain |
| 2 | C | 380 | CYS | Mainchain |
| 2 | C | 559 | GLY | Mainchain |
| 2 | C | 63 | GLN | Peptide |
| 3 | D | 119 | ASP | Mainchain |
| 3 | D | 44 | HIS | Mainchain |
| 4 | E | 309 | ARG | Peptide |
| 4 | E | 323 | THR | Peptide |
| 4 | E | 442 | PHE | Peptide |
| 4 | E | 447 | GLU | Peptide |
| 5 | F | 59 | ILE | Mainchain |
| 6 | G | 235 | CYS | Peptide |
| 6 | G | 254 | GLN | Peptide |
| 6 | G | 274 | ALA | Peptide |
| 6 | G | 309 | LYS | Peptide |
| 6 | G | 311 | HIS | Peptide |
| 6 | G | 329 | LEU | Peptide |
| 6 | G | 331 | THR | Peptide |
| 6 | G | 348 | VAL | Peptide |
| 6 | G | 471 | ASP | Peptide |
| 6 | G | 499 | GLU | Mainchain |
| 6 | G | 581 | PHE | Peptide |
| 6 | G | 65 | PHE | Mainchain |
| 6 | G | 897 | LYS | Peptide |
| 6 | G | 91 | ASP | Mainchain |

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 | 636 | 0 | 181 | 0 | 0 |
| 1 | B | 636 | 0 | 181 | 0 | 0 |
| 2 | C | 3251 | 0 | 869 | 0 | 0 |
| 3 | D | 3211 | 0 | 880 | 0 | 0 |
| 4 | E | 3294 | 0 | 852 | 1 | 0 |
| 5 | F | 555 | 0 | 148 | 0 | 0 |
| 6 | G | 3250 | 0 | 833 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | H | 539 | 0 | 142 | 0 | 0 |
| All | All | 15372 | 0 | 4086 | 1 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (1) 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) |
|---------------|---------------|--------------------------|-------------------|
| 4:E:249:SER:C | 4:E:251:LEU:H | 2.23 | 0.42 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 157/181 (87%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | B | 157/181 (87%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | C | 811/1262 (64%) | 671 (83%) | 97 (12%) | 43 (5%) | 2 | 26 |
| 3 | D | 801/905 (88%) | 700 (87%) | 64 (8%) | 37 (5%) | 3 | 28 |
| 4 | E | 820/874 (94%) | 749 (91%) | 40 (5%) | 31 (4%) | 4 | 32 |
| 5 | F | 137/177 (77%) | 128 (93%) | 7 (5%) | 2 (2%) | 12 | 53 |
| 6 | G | 809/968 (84%) | 658 (81%) | 84 (10%) | 67 (8%) | 1 | 16 |
| 7 | H | 133/511 (26%) | 116 (87%) | 16 (12%) | 1 (1%) | 22 | 67 |
| All | All | 3825/5059 (76%) | 3328 (87%) | 316 (8%) | 181 (5%) | 5 | 28 |

All (181) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 11 | ARG |
| 2 | C | 227 | ARG |
| 2 | C | 526 | GLU |
| 2 | C | 572 | ARG |
| 2 | C | 686 | ASN |
| 3 | D | 6 | ASP |
| 3 | D | 284 | ASN |
| 3 | D | 329 | ALA |
| 3 | D | 336 | LYS |
| 3 | D | 350 | SER |
| 3 | D | 484 | SER |
| 3 | D | 513 | ALA |
| 3 | D | 615 | LYS |
| 3 | D | 791 | PRO |
| 3 | D | 795 | GLU |
| 4 | E | 117 | GLU |
| 4 | E | 280 | CYS |
| 4 | E | 309 | ARG |
| 4 | E | 323 | THR |
| 4 | E | 324 | ALA |
| 4 | E | 391 | PRO |
| 4 | E | 393 | LYS |
| 4 | E | 413 | TYR |
| 4 | E | 448 | PHE |
| 4 | E | 549 | ASN |
| 5 | F | 36 | PRO |
| 6 | G | 55 | LEU |
| 6 | G | 69 | LEU |
| 6 | G | 85 | VAL |
| 6 | G | 90 | PRO |
| 6 | G | 173 | ALA |
| 6 | G | 181 | LEU |
| 6 | G | 197 | LEU |
| 6 | G | 237 | ALA |
| 6 | G | 253 | LEU |
| 6 | G | 275 | PRO |
| 6 | G | 331 | THR |
| 6 | G | 499 | GLU |
| 6 | G | 506 | ILE |
| 6 | G | 508 | VAL |
| 6 | G | 523 | THR |
| 6 | G | 543 | ARG |
| 6 | G | 770 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | G | 785 | GLU |
| 6 | G | 792 | LEU |
| 6 | G | 814 | ILE |
| 6 | G | 826 | ALA |
| 6 | G | 939 | THR |
| 6 | G | 959 | ILE |
| 2 | C | 137 | TYR |
| 2 | C | 226 | ASP |
| 2 | C | 425 | ARG |
| 2 | C | 441 | LYS |
| 2 | C | 498 | ALA |
| 2 | C | 538 | SER |
| 2 | C | 546 | SER |
| 2 | C | 621 | VAL |
| 2 | C | 630 | GLN |
| 2 | C | 642 | VAL |
| 3 | D | 17 | ARG |
| 3 | D | 59 | PRO |
| 3 | D | 273 | ARG |
| 3 | D | 410 | SER |
| 3 | D | 426 | PRO |
| 3 | D | 630 | PHE |
| 3 | D | 739 | ASP |
| 4 | E | 263 | HIS |
| 4 | E | 310 | THR |
| 4 | E | 313 | LYS |
| 4 | E | 373 | ASP |
| 4 | E | 442 | PHE |
| 4 | E | 484 | HIS |
| 4 | E | 551 | LEU |
| 4 | E | 739 | THR |
| 4 | E | 741 | GLU |
| 6 | G | 83 | GLU |
| 6 | G | 103 | ASP |
| 6 | G | 174 | PRO |
| 6 | G | 307 | GLU |
| 6 | G | 554 | ALA |
| 6 | G | 558 | ALA |
| 6 | G | 879 | ASP |
| 2 | C | 205 | ASP |
| 2 | C | 337 | LYS |
| 2 | C | 345 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 348 | SER |
| 2 | C | 349 | SER |
| 2 | C | 387 | GLU |
| 2 | C | 469 | ALA |
| 2 | C | 594 | PRO |
| 2 | C | 619 | LYS |
| 2 | C | 624 | SER |
| 2 | C | 627 | ALA |
| 2 | C | 790 | PRO |
| 3 | D | 140 | GLY |
| 3 | D | 260 | THR |
| 3 | D | 272 | GLU |
| 3 | D | 571 | ASN |
| 3 | D | 601 | ARG |
| 3 | D | 662 | VAL |
| 3 | D | 694 | GLN |
| 3 | D | 735 | GLN |
| 4 | E | 256 | GLU |
| 4 | E | 353 | SER |
| 4 | E | 522 | ASN |
| 4 | E | 569 | PRO |
| 5 | F | 55 | THR |
| 6 | G | 18 | SER |
| 6 | G | 22 | SER |
| 6 | G | 194 | PHE |
| 6 | G | 257 | SER |
| 6 | G | 259 | ALA |
| 6 | G | 308 | LEU |
| 6 | G | 318 | LEU |
| 6 | G | 487 | PRO |
| 6 | G | 501 | LYS |
| 6 | G | 528 | SER |
| 6 | G | 817 | ASN |
| 6 | G | 904 | GLY |
| 7 | H | 45 | GLN |
| 2 | C | 133 | GLY |
| 2 | C | 193 | THR |
| 2 | C | 271 | LYS |
| 2 | C | 423 | ARG |
| 2 | C | 452 | ASN |
| 2 | C | 731 | GLY |
| 3 | D | 89 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 318 | LYS |
| 3 | D | 577 | ASP |
| 3 | D | 734 | LEU |
| 3 | D | 740 | ALA |
| 3 | D | 787 | SER |
| 3 | D | 788 | LEU |
| 4 | E | 40 | ASN |
| 4 | E | 251 | LEU |
| 4 | E | 464 | PRO |
| 6 | G | 332 | PRO |
| 6 | G | 446 | PHE |
| 6 | G | 537 | GLU |
| 6 | G | 583 | ALA |
| 6 | G | 876 | ASP |
| 6 | G | 916 | PHE |
| 2 | C | 470 | ASP |
| 2 | C | 698 | LYS |
| 2 | C | 793 | LYS |
| 2 | C | 812 | THR |
| 4 | E | 221 | HIS |
| 4 | E | 311 | LEU |
| 4 | E | 410 | GLY |
| 6 | G | 32 | LYS |
| 6 | G | 99 | ILE |
| 6 | G | 262 | TYR |
| 6 | G | 330 | SER |
| 6 | G | 372 | GLU |
| 6 | G | 794 | PRO |
| 6 | G | 894 | THR |
| 6 | G | 898 | ALA |
| 6 | G | 900 | SER |
| 6 | G | 962 | SER |
| 2 | C | 442 | ASN |
| 2 | C | 781 | GLU |
| 3 | D | 391 | ALA |
| 6 | G | 21 | PRO |
| 6 | G | 102 | CYS |
| 6 | G | 230 | LEU |
| 6 | G | 503 | GLU |
| 3 | D | 790 | ASP |
| 6 | G | 216 | VAL |
| 6 | G | 238 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 780 | PRO |
| 2 | C | 799 | ALA |
| 3 | D | 355 | PRO |
| 6 | G | 540 | PRO |
| 3 | D | 762 | LEU |
| 4 | E | 278 | PRO |
| 6 | G | 531 | ARG |
| 4 | E | 556 | PRO |
| 6 | G | 317 | VAL |
| 2 | C | 247 | GLY |
| 2 | C | 488 | ILE |
| 3 | D | 200 | PRO |

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.