# W O R L D W I D E

# wwPDB

## P R O T E I N   D A T A   B A N K

# wwPDB EM Validation Summary Report (i)

Mar 5, 2024 – 10:23 AM EST

|  |  |  |
|---|---|---|
| PDB ID | : | 6MZV |
| EMDB ID | : | EMD-9308 |
| Title | : | Cryo-EM structure of the HO BMC shell: BMC-TD focused structure, widened inner ring |
| Authors | : | Greber, B.J.; Sutter, M.; Kerfeld, C.A. |
| Deposited on | : | 2018-11-05 |
| Resolution | : | 3.40 Å(reported) |
| Based on initial model | : | 5V74 |

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

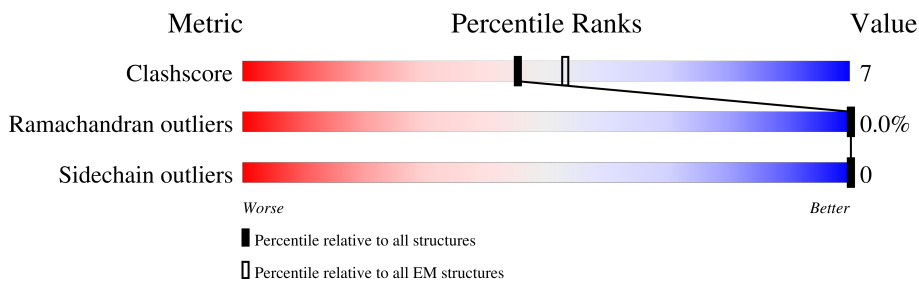|  |  |  |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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 | Percentile Ranks | Value |
|---|---|---|
| Clashscore | | 7 |
| Ramachandran outliers | | 0.0% |
| Sidechain outliers | | 0 |

*Worse* *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
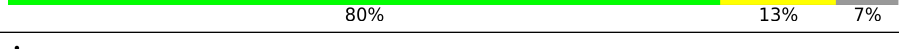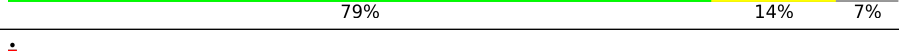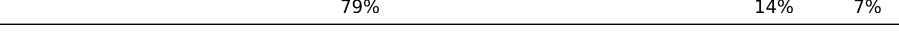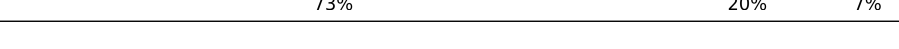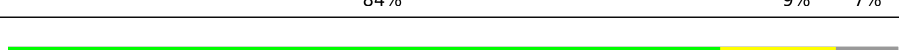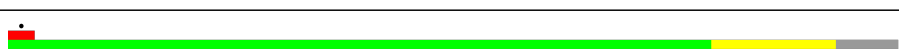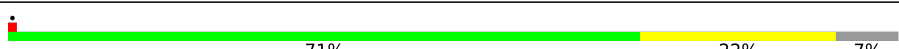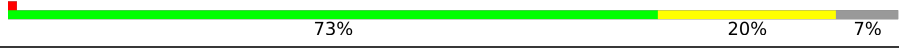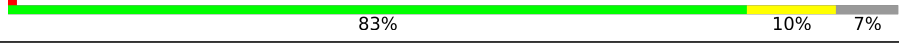
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 212 | 78% 17% 5% |
| 1 | B | 212 | 80% 15% 5% |
| 1 | C | 212 | 82% 13% 5% |
| 1 | D | 212 | 81% 15% 5% |
| 1 | E | 212 | 76% 18% 5% |
| 1 | F | 212 | 80% 15% 5% |
| 2 | GA | 99 | 79% 14% 7% |
| 2 | GB | 99 | 79% 14% 7% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | GC | 99 | 76% 17% 7% |
| 2 | GD | 99 | 74% 19% 7% |
| 2 | GE | 99 | 73% 20% 7% |
| 2 | GF | 99 | 78% 15% 7% |
| 2 | HA | 99 | 76% 17% 7% |
| 2 | HB | 99 | 78% 15% 7% |
| 2 | HC | 99 | 80% 13% 7% |
| 2 | HD | 99 | 79% 14% 7% |
| 2 | HE | 99 | 79% 14% 7% |
| 2 | HF | 99 | 73% 20% 7% |
| 2 | IA | 99 | 84% 9% 7% |
| 2 | IB | 99 | 80% 13% 7% |
| 2 | IC | 99 | 76% 17% 7% |
| 2 | ID | 99 | 79% 14% 7% |
| 2 | IE | 99 | 79% 14% 7% |
| 2 | IF | 99 | 71% 22% 7% |
| 2 | JA | 99 | 76% 17% 7% |
| 2 | JB | 99 | 77% 16% 7% |
| 2 | JC | 99 | 82% 11% 7% |
| 2 | JD | 99 | 80% 13% 7% |
| 2 | JE | 99 | 72% 21% 7% |
| 2 | JF | 99 | 73% 20% 7% |
| 2 | KA | 99 | 83% 10% 7% |
| 2 | KB | 99 | 82% 11% 7% |
| 2 | KC | 99 | 77% 16% 7% |

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | KD | 99 | 73% 20% 7% |
| 2 | KE | 99 | 77% 16% 7% |
| 2 | KF | 99 | 81% 12% 7% |
| 2 | LA | 99 | 73% 20% 7% |
| 2 | LB | 99 | 5% 74% 19% 7% |
| 2 | LC | 99 | 80% 13% 7% |
| 2 | LD | 99 | 79% 14% 7% |
| 2 | LE | 99 | 77% 16% 7% |
| 2 | LF | 99 | 77% 16% 7% |

## 2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 32833 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 Microcompartments protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 1 | A | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 971 | 265 | 286 | 3 | | |
| 1 | B | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 971 | 265 | 286 | 3 | | |
| 1 | C | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 971 | 265 | 286 | 3 | | |
| 1 | D | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 971 | 265 | 286 | 3 | | |
| 1 | E | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 971 | 265 | 286 | 3 | | |
| 1 | F | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1520 | 968 | 264 | 285 | 3 | | |

- Molecule 2 is a protein called Microcompartments protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 2 | GA | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | GB | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | GC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | GD | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | GE | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | GF | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | HA | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | HB | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | HC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | HD | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | HE | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | HF | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | IA | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | IB | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | IC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | ID | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | IE | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | IF | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | JA | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | JB | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | JC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | JD | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | JE | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | JF | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | KA | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | KB | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | KC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | KD | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | KE | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |
| 2 | KF | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 413 | 120 | 122 | 3 | | |

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | LA | 92 | Total<br>658 | C<br>413 | N<br>120 | O<br>122 | S<br>3 | 0 | 0 |
| 2 | LB | 92 | Total<br>658 | C<br>413 | N<br>120 | O<br>122 | S<br>3 | 0 | 0 |
| 2 | LC | 92 | Total<br>658 | C<br>413 | N<br>120 | O<br>122 | S<br>3 | 0 | 0 |
| 2 | LD | 92 | Total<br>658 | C<br>413 | N<br>120 | O<br>122 | S<br>3 | 0 | 0 |
| 2 | LE | 92 | Total<br>658 | C<br>413 | N<br>120 | O<br>122 | S<br>3 | 0 | 0 |
| 2 | LF | 92 | Total<br>658 | C<br>413 | N<br>120 | O<br>122 | S<br>3 | 0 | 0 |

# 3  Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Microcompartments protein
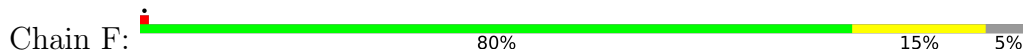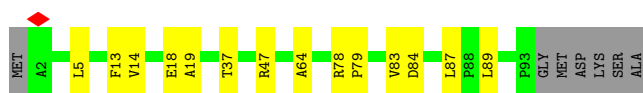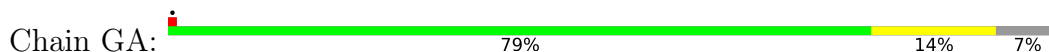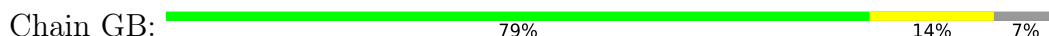
Chain A:



- Molecule 1: Microcompartments protein

Chain B:



- Molecule 1: Microcompartments protein

Chain C:



- Molecule 1: Microcompartments protein

Chain D:

MET SER ILE T4 L5 R6 L11 D12 G23 R27 L30 A36 S37 V40 R50 Q66 Q82 I92 E97 V98 R99 L104 K105 Q112 Q123 I124 I125 N126 M133 I134 F141 I142 L143 E144 V152 L153 A154 A155 N156 P171 R177

L178 Y179 L180 E195 I198 R199 A205 GLN GLU PHE ARG ASP ARG

• Molecule 1: Microcompartments protein

Chain E:　　　76%　　　18%　　5%

MET SER ILE T4 T7 Y8 I9 F10 L11 D12 G23 L30 S37 V40 E41 I42 I48 N49 R50 L56 K57 A58 P63 Q66 E69 T91 I92 E97 V98 R99 R103 L104 K105 Q112 I124 I125 N126 R127 I134 I135 P136 F141 I142

L143 E144 V152 L153 A154 A155 N156 P171 R177 L178 Y179 L180 E195 I198 R199 A205 GLN GLU PHE ARG ASP ARG

• Molecule 1: Microcompartments protein

Chain F:　　　80%　　　15%　　5%

MET SER ILE T4 L5 R6 L11 G23 R27 L30 V40 E41 I42 I48 N49 R50 L56 P63 A64 V65 Q66 R70 H78 I92 E97 V98 R99 L104 Q112 R115 Q123 I124 I125 N126 R127 I134 F141 E144 V152

N156 P171 R177 L180 E195 R199 V204 ALA GLN GLU SER PHE ARG ASP ARG

• Molecule 2: Microcompartments protein

Chain GA:　　　79%　　　14%　　7%

MET A2 L5 F13 V14 E18 A19 T37 R47 A64 R78 P79 V83 D84 L87 P88 L89 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain GB:　　　79%　　　14%　　7%

MET A2 L5 G6 M7 V10 F13 V14 G15 M16 V17 E18 A19 T37 R47 A64 H74 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein
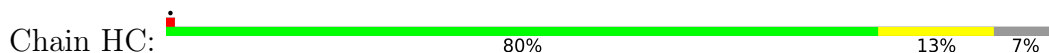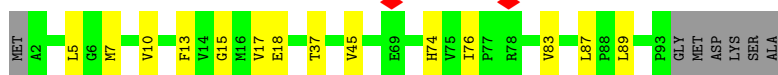
Chain GC:　　　76%　　　17%　　7%

• Molecule 2: Microcompartments protein

Chain GD:





• Molecule 2: Microcompartments protein

Chain GE:





• Molecule 2: Microcompartments protein

Chain GF:





• Molecule 2: Microcompartments protein
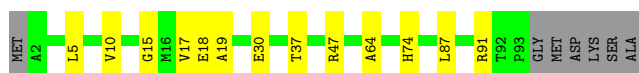
Chain HA:





• Molecule 2: Microcompartments protein
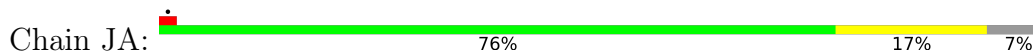
Chain HB:





• Molecule 2: Microcompartments protein

Chain HC:





• Molecule 2: Microcompartments protein

Chain HD:

79%　　14%　7%

MET A2 L5 G6 M7 V10 F13 V14 G15 M16 V17 E18 T37 V45 E69 H74 V75 I76 P77 R78 V83 L87 P88 L89 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain HE:

79%　　14%　7%

MET A2 L5 G6 M7 V10 G15 M16 V17 E18 A19 K36 T37 A64 H74 V75 I76 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain HF:

73%　　20%　7%

MET A2 L5 G6 M7 V10 F13 V14 G15 M16 V17 E18 A19 A27 T37 V45 V46 R47 A52 A64 H74 V75 I76 P79 V83 L87 P88 L89 G90 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain IA:

84%　　9%　7%

MET A2 F13 V17 E18 A19 A20 D21 T37 A64 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain IB:

80%　　13%　7%

MET A2 L5 V10 G15 M16 V17 E18 A19 E30 T37 R47 A64 H74 L87 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain IC:

76%　　17%　7%

MET A2 L5 G6 M7 V10 F13 V14 G15 M16 V17 E18 A19 A44 R47 A64 E69 H74 R78 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain ID:

79%　　14%　7%

MET A2 L5 F13 V17 E18 A19 A27 T37 V45 A52 A64 E65 R66 E69 H74 V75 I76 V83 L87 P88 L89 P93 GLY MET ASP LYS SER ALA
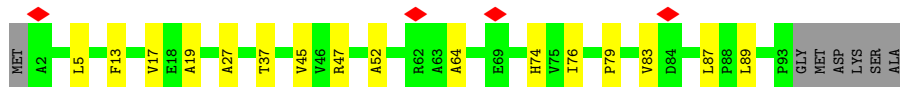
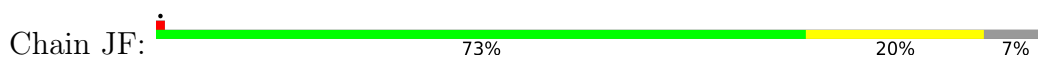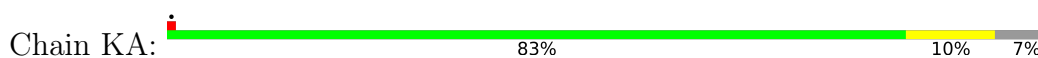• Molecule 2: Microcompartments protein

Chain IE:



• Molecule 2: Microcompartments protein

Chain IF:



• Molecule 2: Microcompartments protein

Chain JA:



• Molecule 2: Microcompartments protein
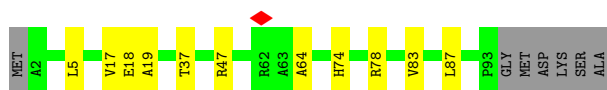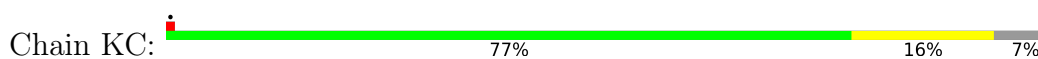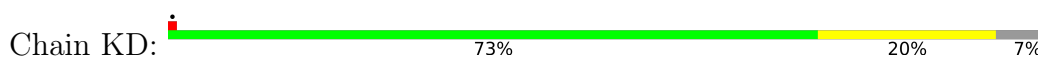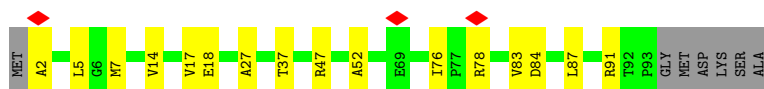
Chain JB:



• Molecule 2: Microcompartments protein

Chain JC:



• Molecule 2: Microcompartments protein

Chain JD:



• Molecule 2: Microcompartments protein

Chain JE:

• Molecule 2: Microcompartments protein

Chain JF:

73%  20%  7%

MET A2 L5 G6 M7 F13 V17 E18 A19 A27 K36 T37 R47 G48 D49 A52 A64 H74 V75 I76 P79 N82 V83 L87 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain KA:

83%  10%  7%

MET A2 L5 F13 E18 A19 K36 R47 A64 R78 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain KB:

82%  11%  7%

MET A2 L5 V17 E18 A19 T37 R47 R62 A63 A64 H74 R78 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain KC:

77%  16%  7%

MET A2 L5 G6 M7 V10 F13 V14 G15 M16 V17 E18 A19 R47 A64 H74 V75 I76 P77 R78 V83 L87 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain KD:

73%  20%  7%

MET A2 L5 G6 M7 V10 F13 V14 G15 M16 V17 E18 A19 A27 T37 V45 V46 R47 A52 A64 H74 V75 I76 P79 V83 D84 L87 P88 L89 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain KE:

77%  16%  7%

MET A2 L5 G6 M7 V14 V17 E18 A27 T37 R47 A52 E69 I76 P77 R78 V83 D84 L87 R91 T92 P93 GLY MET ASP LYS SER ALA

• Molecule 2: Microcompartments protein

Chain KF:

81%  12%  7%

• Molecule 2: Microcompartments protein
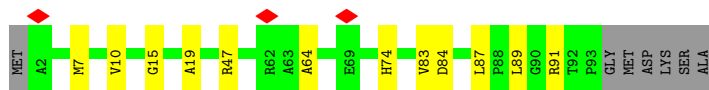
Chain LA:





• Molecule 2: Microcompartments protein

Chain LB:





• Molecule 2: Microcompartments protein

Chain LC:





• Molecule 2: Microcompartments protein

Chain LD:





• Molecule 2: Microcompartments protein

Chain LE:





• Molecule 2: Microcompartments protein
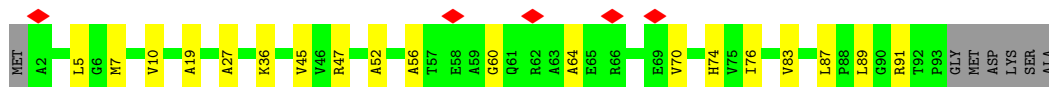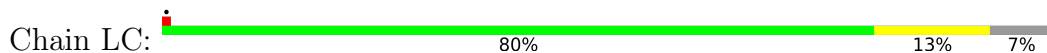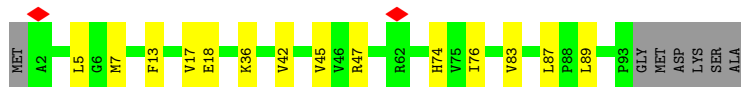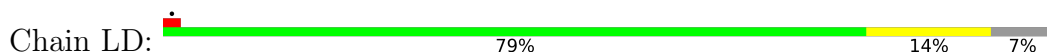
Chain LF:

# 4 Experimental information ⓘ

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 149628 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; Initial CTF fitting using CTFFIND4, CTF correction applied within RELION. | Depositor |
| Microscope | FEI TITAN | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 25 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | 48543 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.148 | Depositor |
| Minimum map value | -0.086 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.03 | Depositor |
| Map size (Å) | 527.36, 527.36, 527.36 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.03, 1.03, 1.03 | 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 RMSZ | Bond lengths $\#|Z|>5$ | Bond angles RMSZ | Bond angles $\#|Z|>5$ |
|-----|-------|------|--------|------|--------|
| 1 | A | 0.34 | 0/1551 | 0.52 | 0/2111 |
| 1 | B | 0.34 | 0/1551 | 0.52 | 0/2111 |
| 1 | C | 0.34 | 0/1551 | 0.51 | 0/2111 |
| 1 | D | 0.32 | 0/1551 | 0.50 | 0/2111 |
| 1 | E | 0.32 | 0/1551 | 0.50 | 0/2111 |
| 1 | F | 0.32 | 0/1546 | 0.49 | 0/2104 |
| 2 | GA | 0.36 | 0/666 | 0.52 | 0/904 |
| 2 | GB | 0.36 | 0/666 | 0.52 | 0/904 |
| 2 | GC | 0.35 | 0/666 | 0.51 | 0/904 |
| 2 | GD | 0.34 | 0/666 | 0.50 | 0/904 |
| 2 | GE | 0.33 | 0/666 | 0.51 | 0/904 |
| 2 | GF | 0.35 | 0/666 | 0.51 | 0/904 |
| 2 | HA | 0.37 | 0/666 | 0.52 | 0/904 |
| 2 | HB | 0.33 | 0/666 | 0.51 | 0/904 |
| 2 | HC | 0.34 | 0/666 | 0.52 | 0/904 |
| 2 | HD | 0.35 | 0/666 | 0.51 | 0/904 |
| 2 | HE | 0.36 | 0/666 | 0.52 | 0/904 |
| 2 | HF | 0.38 | 0/666 | 0.53 | 0/904 |
| 2 | IA | 0.36 | 0/666 | 0.52 | 0/904 |
| 2 | IB | 0.39 | 0/666 | 0.53 | 0/904 |
| 2 | IC | 0.35 | 0/666 | 0.52 | 0/904 |
| 2 | ID | 0.37 | 0/666 | 0.51 | 0/904 |
| 2 | IE | 0.34 | 0/666 | 0.52 | 0/904 |
| 2 | IF | 0.35 | 0/666 | 0.53 | 0/904 |
| 2 | JA | 0.38 | 0/666 | 0.52 | 0/904 |
| 2 | JB | 0.34 | 0/666 | 0.52 | 0/904 |
| 2 | JC | 0.35 | 0/666 | 0.50 | 0/904 |
| 2 | JD | 0.35 | 0/666 | 0.51 | 0/904 |
| 2 | JE | 0.36 | 0/666 | 0.52 | 0/904 |
| 2 | JF | 0.36 | 0/666 | 0.52 | 0/904 |
| 2 | KA | 0.36 | 0/666 | 0.51 | 0/904 |
| 2 | KB | 0.38 | 0/666 | 0.53 | 0/904 |
| 2 | KC | 0.35 | 0/666 | 0.53 | 0/904 |
| 2 | KD | 0.35 | 0/666 | 0.51 | 0/904 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|------|--------|------|--------|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | KE | 0.34 | 0/666 | 0.51 | 0/904 |
| 2 | KF | 0.36 | 0/666 | 0.53 | 0/904 |
| 2 | LA | 0.37 | 0/666 | 0.54 | 0/904 |
| 2 | LB | 0.34 | 0/666 | 0.51 | 0/904 |
| 2 | LC | 0.35 | 0/666 | 0.51 | 0/904 |
| 2 | LD | 0.35 | 0/666 | 0.50 | 0/904 |
| 2 | LE | 0.37 | 0/666 | 0.53 | 0/904 |
| 2 | LF | 0.38 | 0/666 | 0.52 | 0/904 |
| All | All | 0.35 | 0/33277 | 0.51 | 0/45203 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | F | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 70 | ARG | Peptide |
| 1 | E | 126 | ASN | Peptide |
| 1 | F | 126 | ASN | Peptide |

## 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 | 1525 | 0 | 1549 | 23 | 0 |

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | B | 1525 | 0 | 1549 | 21 | 0 |
| 1 | C | 1525 | 0 | 1549 | 21 | 0 |
| 1 | D | 1525 | 0 | 1549 | 21 | 0 |
| 1 | E | 1525 | 0 | 1549 | 26 | 0 |
| 1 | F | 1520 | 0 | 1544 | 23 | 0 |
| 2 | GA | 658 | 0 | 678 | 11 | 0 |
| 2 | GB | 658 | 0 | 678 | 11 | 0 |
| 2 | GC | 658 | 0 | 678 | 15 | 0 |
| 2 | GD | 658 | 0 | 678 | 17 | 0 |
| 2 | GE | 658 | 0 | 678 | 16 | 0 |
| 2 | GF | 658 | 0 | 678 | 10 | 0 |
| 2 | HA | 658 | 0 | 678 | 13 | 0 |
| 2 | HB | 658 | 0 | 678 | 13 | 0 |
| 2 | HC | 658 | 0 | 678 | 10 | 0 |
| 2 | HD | 658 | 0 | 678 | 11 | 0 |
| 2 | HE | 658 | 0 | 678 | 13 | 0 |
| 2 | HF | 658 | 0 | 678 | 16 | 0 |
| 2 | IA | 658 | 0 | 678 | 8 | 0 |
| 2 | IB | 658 | 0 | 678 | 10 | 0 |
| 2 | IC | 658 | 0 | 678 | 12 | 0 |
| 2 | ID | 658 | 0 | 678 | 12 | 0 |
| 2 | IE | 658 | 0 | 678 | 12 | 0 |
| 2 | IF | 658 | 0 | 678 | 17 | 0 |
| 2 | JA | 658 | 0 | 678 | 13 | 0 |
| 2 | JB | 658 | 0 | 678 | 11 | 0 |
| 2 | JC | 658 | 0 | 678 | 11 | 0 |
| 2 | JD | 658 | 0 | 678 | 10 | 0 |
| 2 | JE | 658 | 0 | 678 | 17 | 0 |
| 2 | JF | 658 | 0 | 678 | 19 | 0 |
| 2 | KA | 658 | 0 | 678 | 7 | 0 |
| 2 | KB | 658 | 0 | 678 | 9 | 0 |
| 2 | KC | 658 | 0 | 678 | 13 | 0 |
| 2 | KD | 658 | 0 | 678 | 16 | 0 |
| 2 | KE | 658 | 0 | 678 | 15 | 0 |
| 2 | KF | 658 | 0 | 678 | 10 | 0 |
| 2 | LA | 658 | 0 | 678 | 15 | 0 |
| 2 | LB | 658 | 0 | 678 | 11 | 0 |
| 2 | LC | 658 | 0 | 678 | 9 | 0 |
| 2 | LD | 658 | 0 | 678 | 12 | 0 |
| 2 | LE | 658 | 0 | 678 | 12 | 0 |
| 2 | LF | 658 | 0 | 678 | 14 | 0 |
| All | All | 32833 | 0 | 33697 | 446 | 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 7.

The worst 5 of 446 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) |
|---|---|---|---|
| 1:A:22:ILE:O | 1:A:26:ALA:HB2 | 1.94 | 0.67 |
| 2:HF:5:LEU:HD23 | 2:HF:76:ILE:HD12 | 1.80 | 0.63 |
| 1:A:124:ILE:HG21 | 1:C:66:GLN:HB3 | 1.80 | 0.63 |
| 1:B:11:LEU:HD22 | 1:B:156:ASN:HD22 | 1.65 | 0.62 |
| 2:HE:5:LEU:HD23 | 2:HE:76:ILE:HD12 | 1.82 | 0.62 |

There are no symmetry-related clashes.

## 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 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 | 200/212 (94%) | 188 (94%) | 11 (6%) | 1 (0%) | 29 | 61 |
| 1 | B | 200/212 (94%) | 190 (95%) | 10 (5%) | 0 | 100 | 100 |
| 1 | C | 200/212 (94%) | 188 (94%) | 12 (6%) | 0 | 100 | 100 |
| 1 | D | 200/212 (94%) | 194 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | E | 200/212 (94%) | 192 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | F | 199/212 (94%) | 189 (95%) | 10 (5%) | 0 | 100 | 100 |
| 2 | GA | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | GB | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | GC | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | GD | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | GE | 90/99 (91%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | GF | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-----|-----|
| 2 | HA | 90/99 (91%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | HB | 90/99 (91%) | 85 (94%) | 5 (6%) | 0 | 100 | 100 |
| 2 | HC | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | HD | 90/99 (91%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | HE | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | HF | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | IA | 90/99 (91%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | IB | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | IC | 90/99 (91%) | 85 (94%) | 5 (6%) | 0 | 100 | 100 |
| 2 | ID | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | IE | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | IF | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | JA | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | JB | 90/99 (91%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | JC | 90/99 (91%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | JD | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | JE | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | JF | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | KA | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | KB | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | KC | 90/99 (91%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | KD | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | KE | 90/99 (91%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | KF | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | LA | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | LB | 90/99 (91%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | LC | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | LD | 90/99 (91%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | LE | 90/99 (91%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | LF | 90/99 (91%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| All | All | 4439/4836 (92%) | 4287 (97%) | 151 (3%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 71 | ALA |

### 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 PDB entries followed by that with respect to all EM 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 | 154/164 (94%) | 154 (100%) | 0 | 100 | 100 |
| 1 | B | 154/164 (94%) | 154 (100%) | 0 | 100 | 100 |
| 1 | C | 154/164 (94%) | 154 (100%) | 0 | 100 | 100 |
| 1 | D | 154/164 (94%) | 154 (100%) | 0 | 100 | 100 |
| 1 | E | 154/164 (94%) | 154 (100%) | 0 | 100 | 100 |
| 1 | F | 154/164 (94%) | 154 (100%) | 0 | 100 | 100 |
| 2 | GA | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | GB | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | GC | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | GD | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | GE | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | GF | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | HA | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | HB | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | HC | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | HD | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | HE | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | HF | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | IA | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | IB | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | IC | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | ID | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | IE | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | IF | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | JA | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | JB | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | JC | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | JD | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | JE | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | JF | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | KA | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | KB | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | KC | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | KD | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | KE | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | KF | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | LA | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | LB | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | LC | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | LD | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | LE | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| 2 | LF | 63/68 (93%) | 63 (100%) | 0 | 100 | 100 |
| All | All | 3192/3432 (93%) | 3192 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 79 | HIS |
| 2 | JF | 82 | ASN |
| 1 | D | 156 | ASN |
| 2 | KB | 82 | ASN |
| 1 | F | 123 | GLN |

### 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 monosaccharides 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.

# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9308. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

### 6.1.1 Primary map



| X | Y | Z |
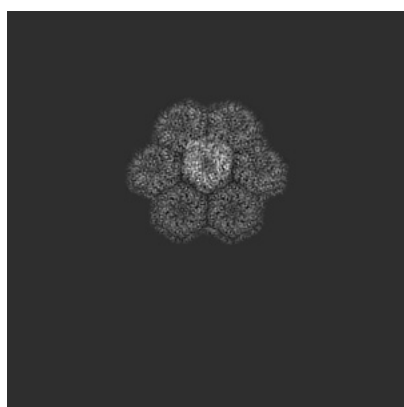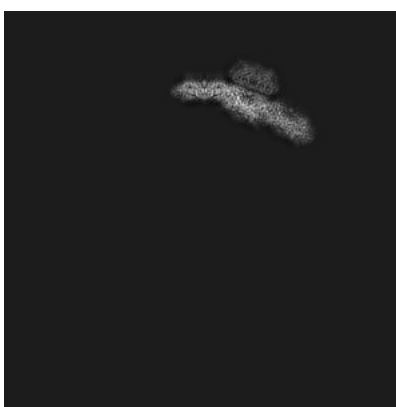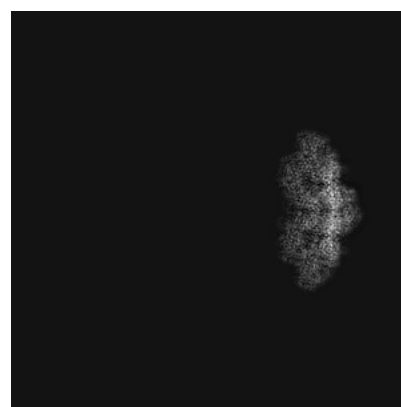
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

### 6.2.1 Primary map
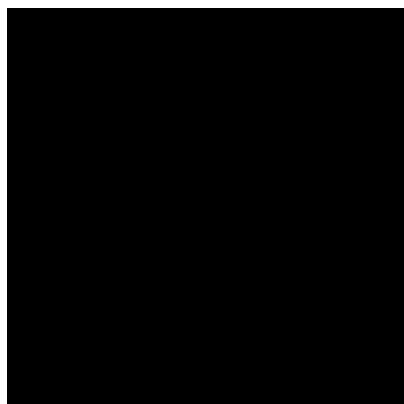


| X Index: 256 | Y Index: 256 | Z Index: 256 |

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices ⓘ
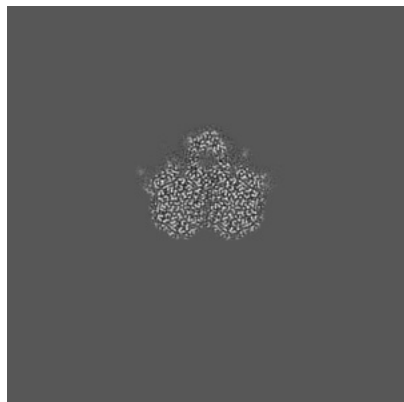
### 6.3.1 Primary map
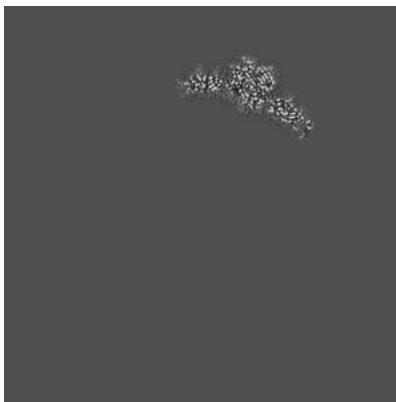


| X Index: 410 | Y Index: 242 | Z Index: 297 |

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

### 6.4.1 Primary map



| X | Y | Z |
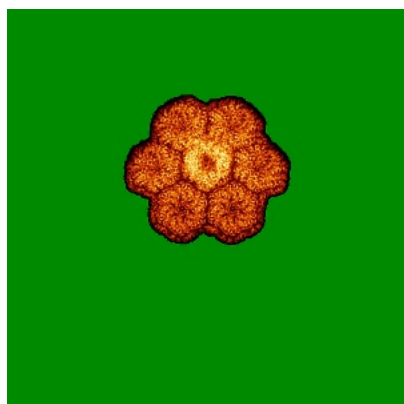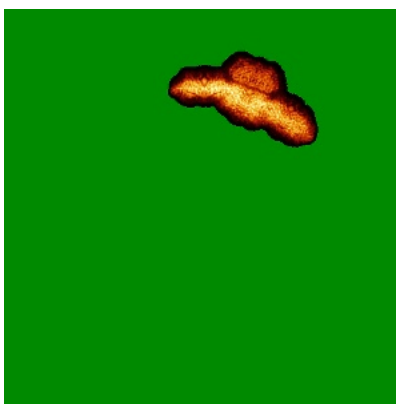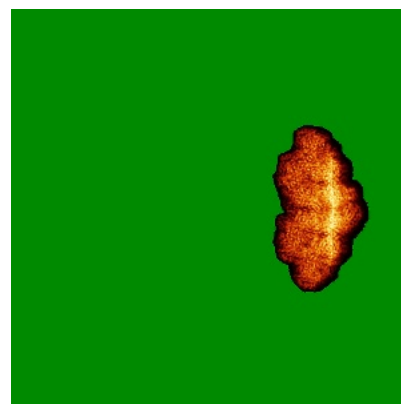
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5  Orthogonal surface views ⓘ
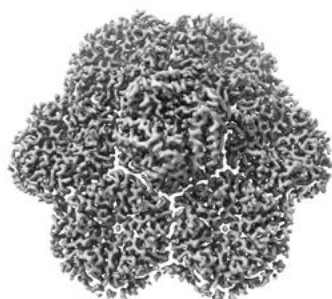
### 6.5.1  Primary map



X                              Y                              Z
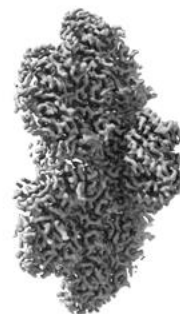
The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6  Mask visualisation ⓘ

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

# 7    Map analysis ⓘ

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

## 7.1    Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2   Volume estimate ⓘ
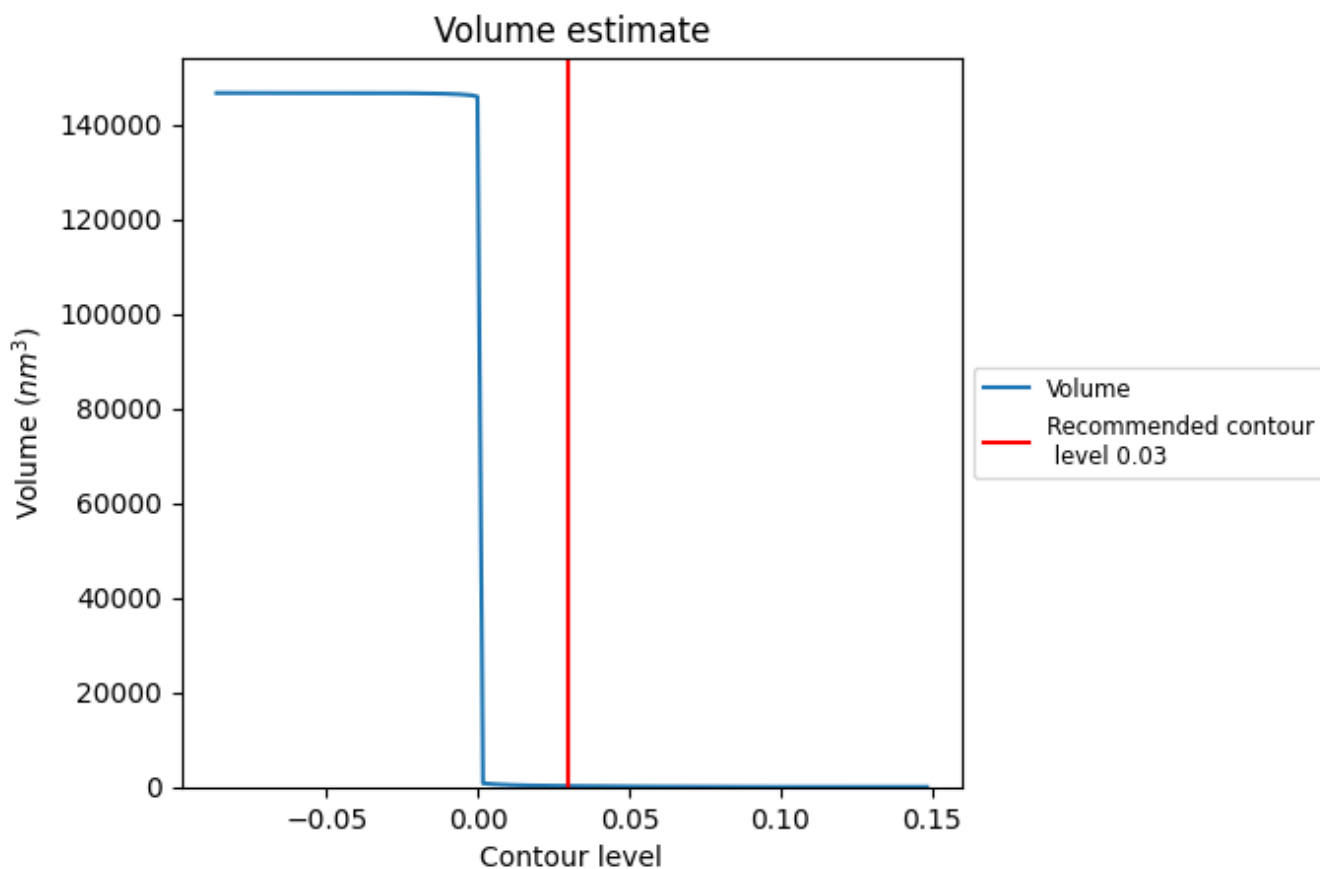


The volume at the recommended contour level is 200 nm$^3$; this corresponds to an approximate mass of 181 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3　Rotationally averaged power spectrum ⓘ
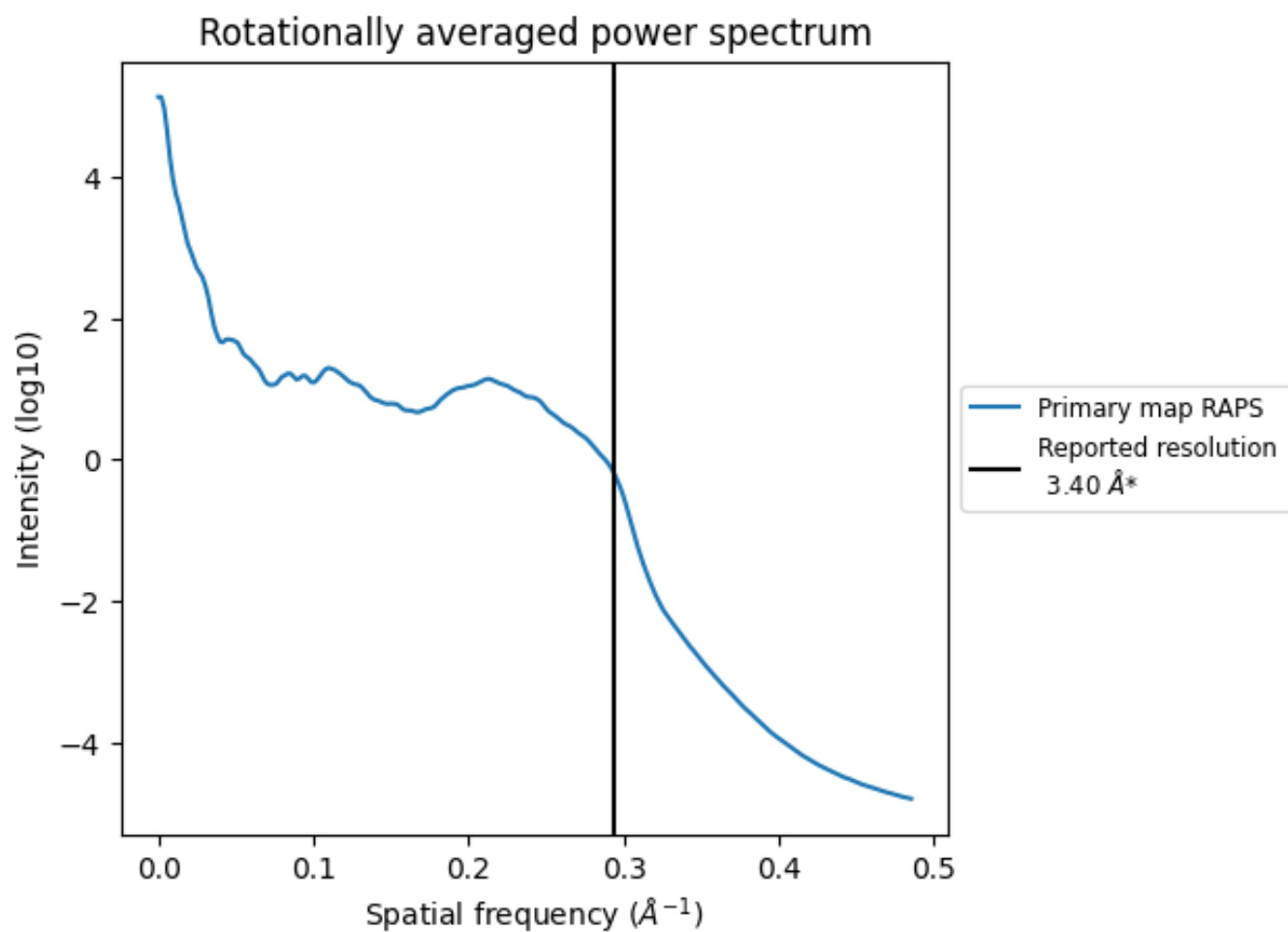


*Reported resolution corresponds to spatial frequency of 0.294 $\text{Å}^{-1}$

# 8 Fourier-Shell correlation ⓘ

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

# 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9308 and PDB model 6MZV. Per-residue inclusion information can be found in section 3 on page 8.

## 9.1 Map-model overlay ⓘ



X                Y                Z
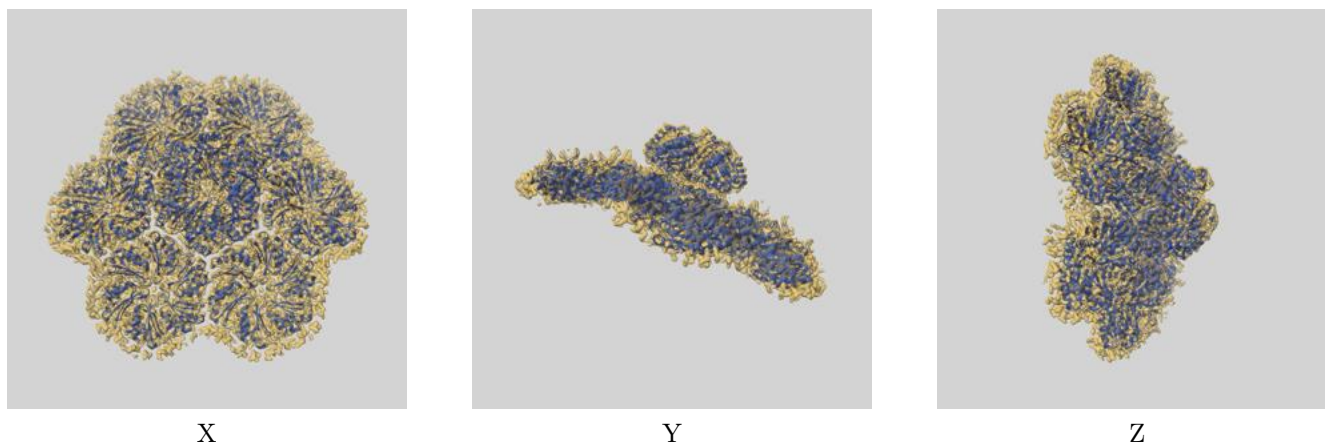
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2　Q-score mapped to coordinate model　ⓘ



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3　Atom inclusion mapped to coordinate model　ⓘ
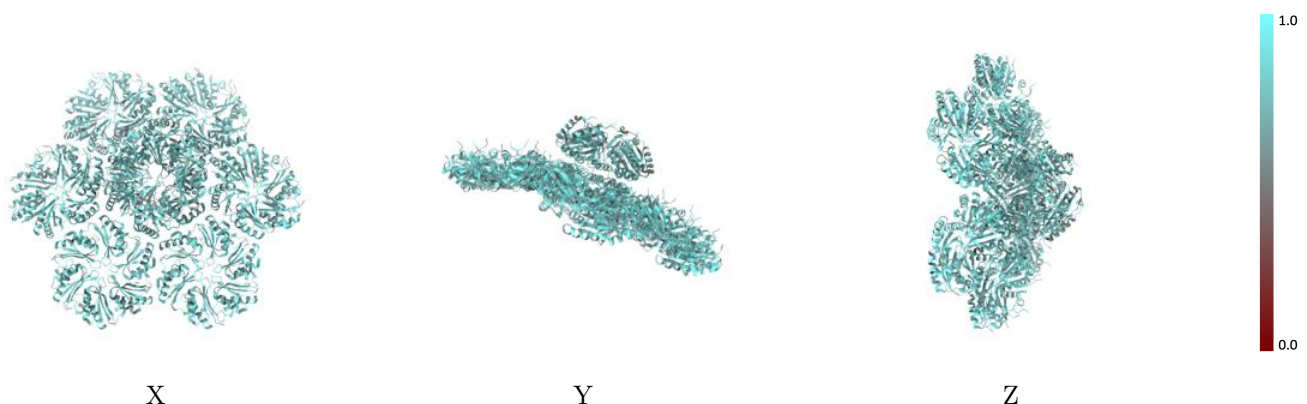


The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4    Atom inclusion ⓘ
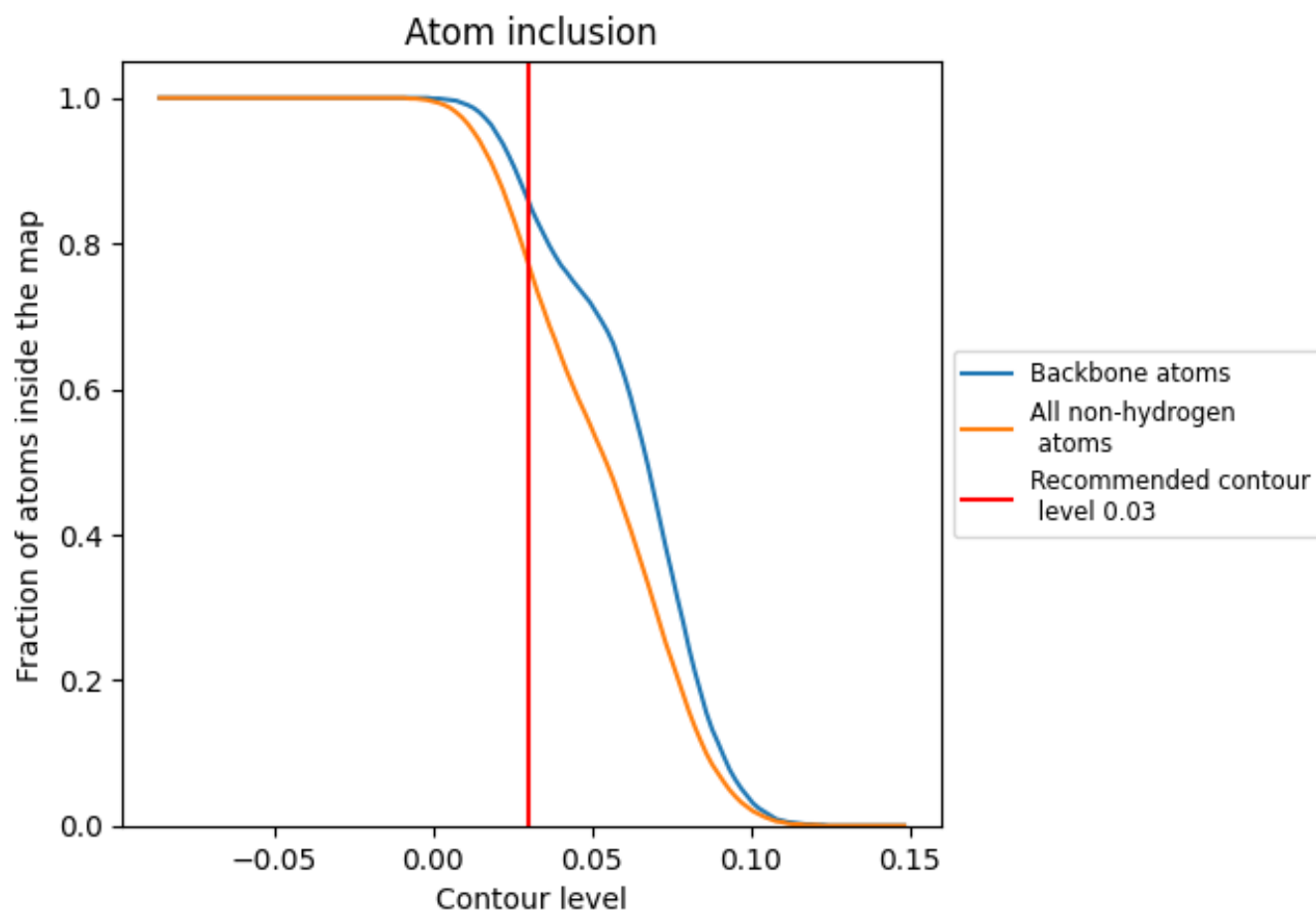


At the recommended contour level, 86% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.7720 | 0.5240 |
| A | 0.7560 | 0.5140 |
| B | 0.7470 | 0.5110 |
| C | 0.7620 | 0.5150 |
| D | 0.7430 | 0.5040 |
| E | 0.7430 | 0.5040 |
| F | 0.7460 | 0.5040 |
| GA | 0.8120 | 0.5350 |
| GB | 0.7900 | 0.5350 |
| GC | 0.7690 | 0.5370 |
| GD | 0.7760 | 0.5300 |
| GE | 0.7780 | 0.5240 |
| GF | 0.7720 | 0.5180 |
| HA | 0.7890 | 0.5270 |
| HB | 0.7410 | 0.5200 |
| HC | 0.7650 | 0.5330 |
| HD | 0.7790 | 0.5330 |
| HE | 0.7810 | 0.5330 |
| HF | 0.8000 | 0.5330 |
| IA | 0.7970 | 0.5380 |
| IB | 0.8040 | 0.5410 |
| IC | 0.7860 | 0.5340 |
| ID | 0.7550 | 0.5300 |
| IE | 0.7700 | 0.5230 |
| IF | 0.7810 | 0.5180 |
| JA | 0.7920 | 0.5300 |
| JB | 0.7590 | 0.5250 |
| JC | 0.7700 | 0.5330 |
| JD | 0.8000 | 0.5330 |
| JE | 0.7830 | 0.5300 |
| JF | 0.7980 | 0.5270 |
| KA | 0.8040 | 0.5370 |
| KB | 0.7970 | 0.5340 |
| KC | 0.7860 | 0.5340 |
| KD | 0.7810 | 0.5280 |

1.0

0.0
<0.0

*Continued on next page...*

W O R L D W I D E
**PDB**
PROTEIN DATA BANK

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| KE | 0.7750 | 0.5260 |
| KF | 0.7810 | 0.5280 |
| LA | 0.7900 | 0.5260 |
| LB | 0.7550 | 0.5210 |
| LC | 0.7590 | 0.5220 |
| LD | 0.7810 | 0.5360 |
| LE | 0.7900 | 0.5350 |
| LF | 0.7810 | 0.5280 |