# Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:08 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 6LYY / pdb_00006lyy |
| EMDB ID | : | EMD-30019 |
| Title | : | Cryo-EM structure of the human MCT1/Basigin-2 complex in the presence of anti-cancer drug candidate AZD3965 in the outward-open conformation. |
| Authors | : | Wang, N.; Jiang, X.; Zhang, S.; Zhu, A.; Yuan, Y.; Lei, J.; Yan, C. |
| Deposited on | : | 2020-02-16 |
| Resolution | : | 3.20 Å(reported) |

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

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

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

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

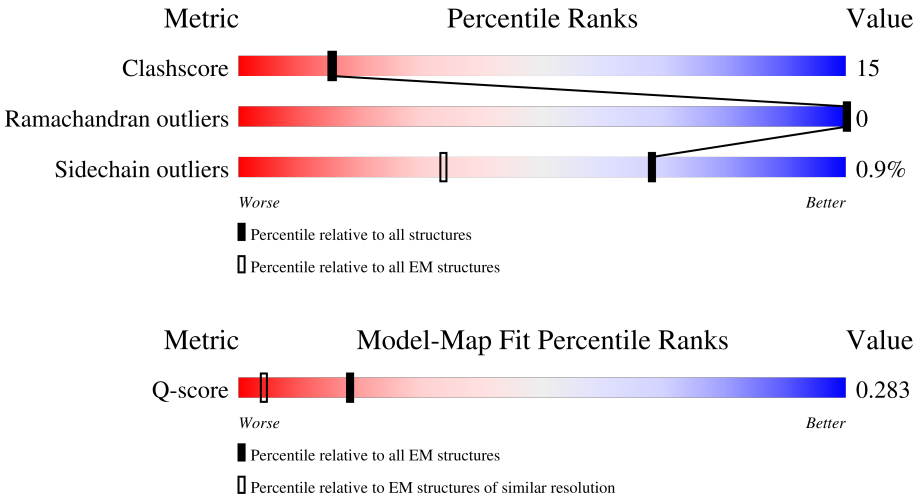
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 15020 ( 2.70 - 3.70 ) |

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 | 500 | 25% 52% 24% 24% |
| 2 | B | 269 | 75% 72% 8% 20% |

# 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4104 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.

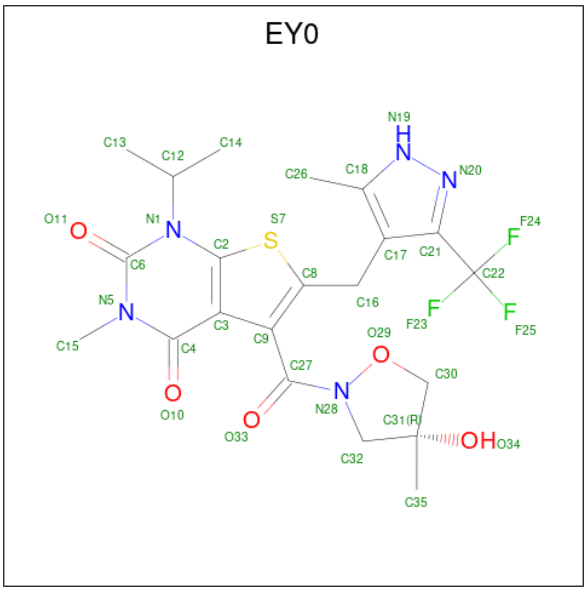
- Molecule 1 is a protein called Monocarboxylate transporter 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 382 | 2902 | 1934 | 459 | 484 | 25 | 0 | 0 |

- Molecule 2 is a protein called Basigin.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 2 | B | 215 | 1167 | 715 | 230 | 222 | 0 | 0 |

- Molecule 3 is 3-methyl-5-[[(4 {R})-4-methyl-4-oxidanyl-1,2-oxazolidin-2-yl]carbonyl]-6-[[5-methyl-3-(trifluoromethyl)-1 {H}-pyrazol-4-yl]methyl]-1-propan-2-yl-thieno[2,3-d]pyrimidine-2,4-dione (CCD ID: EY0) (formula: $C_{21}H_{24}F_3N_5O_5S$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | F | N | O | S | |
| 3 | A | 1 | 35 | 21 | 3 | 5 | 5 | 1 | 0 |

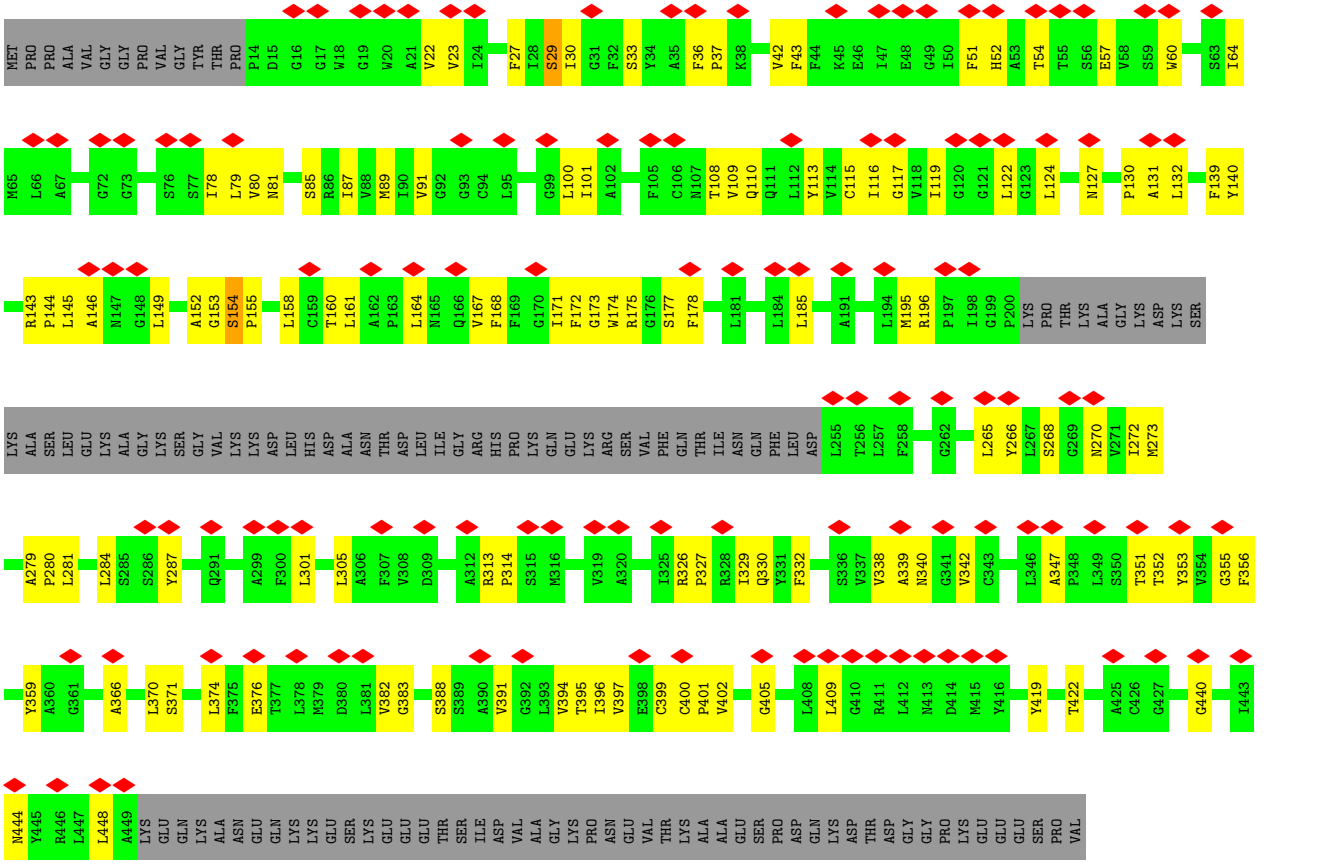
# 3 Residue-property plots (i)

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: Monocarboxylate transporter 1

Chain A:

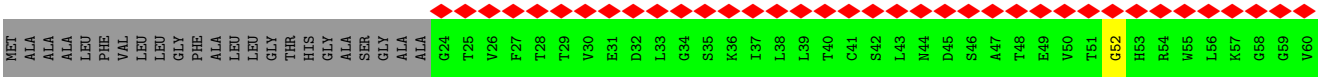


• Molecule 2: Basigin

Chain B:




V61 L62 K63 E64 D65 A66 L67 P68 G69 Q70 K71 T72 E73 F74 K75 V76 D77 S78 D79 D80 Q81 W82 G83 E84 Y85 S86 C87 V88 F89 L90 P91 E92 P93 M94 G95 T96 A97 N98 I99 Q100 L101 H102 G103 P104 P105 R106 V107 K108 A109 V110 K111 S112 S113 E114 H115 I116 N117 E118 G119 E120
T121 A122 M123 L124 V125 C126 K127 S128 E129 S130 V131 P132 P133 V134 T135 D136 W137 A138 W139 Y140 K141 I142 T143 D144 S145 E146 D147 K148 A149 L150 M151 N152 G153 S154 E155 S156 R157 F158 F159 V160 S161 S162 S163 Q164 G165 R166 S167 E168 L169 H170 I171 E172 N173 L174 N175 M176 E177 A178 D179 P180
G181 Q182 Y183 R184 C185 N186 G187 T188 S189 S190 K191 G192 S193 D194 T198 T199 L200 R201 V202 R203 S204 H205 L206 A207 A208 L209 W210 P211 F212 L213 G214 I215 V216 A217 E218 V219 L220 V221 L222 V223 T224 I225 I226 F227 I228 Y229 E230 K231 R232 R233 K234 P235 E236 D237 V238 LEU ASP ASP ASP
ASP ALA GLY SER ALA PRO LEU LYS SER SER GLY GLN HIS GLN ASN ASP LYS GLY LYS ASN VAL ARG GLN ARG ASN SER SER

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 1326285 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 37.6 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 5.126 | Depositor |
| Minimum map value | -3.357 | Depositor |
| Average map value | 0.007 | Depositor |
| Map value standard deviation | 0.120 | Depositor |
| Recommended contour level | 1.14 | Depositor |
| Map size (Å) | 218.2, 218.2, 218.2 | wwPDB |
| Map dimensions | 200, 200, 200 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.091, 1.091, 1.091 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EY0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.27 | 0/2984 | 0.48 | 1/4052 (0.0%) |
| 2 | B | 0.85 | 0/1174 | 1.25 | 1/1623 (0.1%) |
| All | All | 0.51 | 0/4158 | 0.78 | 2/5675 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 108 | THR | OG1-CB-CG2 | 5.17 | 119.64 | 109.30 |
| 2 | B | 142 | ILE | N-CA-C | 5.12 | 114.98 | 108.12 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2902 | 0 | 2958 | 95 | 0 |
| 2 | B | 1167 | 0 | 685 | 22 | 0 |
| 3 | A | 35 | 0 | 0 | 4 | 0 |
| All | All | 4104 | 0 | 3643 | 114 | 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 15.

All (114) 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:284:LEU:HD21 | 1:A:301:LEU:HD22 | 1.36 | 1.04 |
| 2:B:211:PRO:O | 2:B:215:ILE:HG12 | 1.60 | 1.02 |
| 2:B:115:HIS:ND1 | 2:B:203:ARG:NH2 | 2.22 | 0.86 |
| 1:A:313:ARG:NH1 | 1:A:371:SER:HB3 | 1.96 | 0.80 |
| 2:B:212:PHE:O | 2:B:216:VAL:HG23 | 1.82 | 0.77 |
| 1:A:158:LEU:HD22 | 3:A:601:EY0:C35 | 2.15 | 0.76 |
| 1:A:281:LEU:CD2 | 3:A:601:EY0:F24 | 2.27 | 0.72 |
| 1:A:100:LEU:HD22 | 1:A:185:LEU:HD12 | 1.70 | 0.72 |
| 1:A:313:ARG:NH1 | 1:A:371:SER:CB | 2.52 | 0.72 |
| 2:B:102:HIS:CB | 2:B:132:PRO:CB | 2.68 | 0.71 |
| 1:A:167:VAL:O | 1:A:171:ILE:HG22 | 1.91 | 0.70 |
| 2:B:220:LEU:C | 2:B:220:LEU:HD23 | 2.18 | 0.68 |
| 2:B:222:LEU:C | 2:B:222:LEU:HD23 | 2.17 | 0.68 |
| 2:B:102:HIS:CB | 2:B:132:PRO:N | 2.57 | 0.68 |
| 2:B:222:LEU:HD23 | 2:B:222:LEU:O | 1.94 | 0.68 |
| 1:A:89:MET:HG3 | 1:A:127:ASN:HD22 | 1.60 | 0.66 |
| 1:A:401:PRO:O | 1:A:405:GLY:N | 2.28 | 0.66 |
| 1:A:268:SER:O | 1:A:272:ILE:HD13 | 1.96 | 0.65 |
| 1:A:89:MET:CG | 1:A:127:ASN:HD22 | 2.10 | 0.65 |
| 1:A:351:THR:O | 1:A:352:THR:OG1 | 2.15 | 0.63 |
| 1:A:281:LEU:HD22 | 3:A:601:EY0:F24 | 1.89 | 0.61 |
| 1:A:339:ALA:O | 1:A:342:VAL:HG22 | 2.01 | 0.61 |
| 1:A:329:ILE:HD13 | 1:A:376:GLU:OE1 | 2.03 | 0.58 |
| 1:A:444:ASN:O | 1:A:448:LEU:HD13 | 2.05 | 0.57 |
| 1:A:329:ILE:O | 1:A:332:PHE:N | 2.34 | 0.57 |
| 1:A:164:LEU:HD21 | 1:A:168:PHE:CZ | 2.39 | 0.57 |
| 1:A:313:ARG:HH11 | 1:A:371:SER:HB3 | 1.69 | 0.57 |
| 2:B:220:LEU:HD23 | 2:B:220:LEU:O | 2.05 | 0.57 |
| 1:A:391:VAL:HA | 1:A:394:VAL:HG12 | 1.88 | 0.56 |
| 2:B:103:GLY:O | 2:B:191:LYS:CB | 2.54 | 0.55 |
| 1:A:33:SER:HA | 1:A:124:LEU:HD22 | 1.89 | 0.54 |
| 1:A:305:LEU:C | 1:A:305:LEU:HD23 | 2.33 | 0.54 |
| 1:A:158:LEU:CD2 | 3:A:601:EY0:C35 | 2.85 | 0.54 |
| 1:A:399:CYS:SG | 1:A:400:CYS:N | 2.81 | 0.54 |
| 1:A:171:ILE:HG23 | 1:A:172:PHE:N | 2.23 | 0.54 |
| 1:A:347:ALA:HB2 | 1:A:359:TYR:CE1 | 2.44 | 0.52 |
| 2:B:115:HIS:H | 2:B:115:HIS:CD2 | 2.27 | 0.52 |
| 1:A:89:MET:HE1 | 1:A:195:MET:HE3 | 1.92 | 0.52 |
| 1:A:391:VAL:O | 1:A:395:THR:HG22 | 2.10 | 0.51 |
| 1:A:352:THR:O | 1:A:355:GLY:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:352:THR:HG22 | 1:A:353:TYR:H | 1.76 | 0.51 |
| 1:A:89:MET:CG | 1:A:127:ASN:ND2 | 2.74 | 0.50 |
| 1:A:29:SER:OG | 1:A:127:ASN:ND2 | 2.44 | 0.50 |
| 1:A:143:ARG:N | 1:A:144:PRO:HD2 | 2.26 | 0.50 |
| 1:A:196:ARG:NH1 | 2:B:230:GLU:OE1 | 2.45 | 0.49 |
| 1:A:273:MET:CE | 1:A:370:LEU:HD11 | 2.42 | 0.49 |
| 2:B:220:LEU:C | 2:B:220:LEU:CD2 | 2.86 | 0.49 |
| 1:A:23:VAL:HG11 | 1:A:149:LEU:HD12 | 1.94 | 0.48 |
| 1:A:80:VAL:HG23 | 1:A:85:SER:HA | 1.95 | 0.48 |
| 1:A:81:ASN:ND2 | 1:A:388:SER:OG | 2.47 | 0.48 |
| 1:A:140:TYR:HA | 1:A:143:ARG:HB3 | 1.96 | 0.47 |
| 1:A:352:THR:HG22 | 1:A:353:TYR:N | 2.29 | 0.47 |
| 2:B:222:LEU:C | 2:B:222:LEU:CD2 | 2.85 | 0.47 |
| 2:B:115:HIS:H | 2:B:115:HIS:HD2 | 1.63 | 0.47 |
| 1:A:101:ILE:HD11 | 2:B:212:PHE:HZ | 1.78 | 0.47 |
| 2:B:52:GLY:HA3 | 2:B:65:ASP:HA | 1.97 | 0.46 |
| 1:A:287:TYR:HD1 | 1:A:419:TYR:CB | 2.29 | 0.46 |
| 1:A:326:ARG:N | 1:A:327:PRO:CD | 2.79 | 0.46 |
| 1:A:139:PHE:CZ | 1:A:146:ALA:HB2 | 2.51 | 0.46 |
| 1:A:152:ALA:HA | 1:A:313:ARG:HD2 | 1.97 | 0.46 |
| 1:A:30:ILE:HD11 | 1:A:132:LEU:HD21 | 1.97 | 0.46 |
| 1:A:119:ILE:O | 1:A:122:LEU:HD23 | 2.15 | 0.46 |
| 1:A:279:ALA:HB3 | 1:A:280:PRO:HD3 | 1.97 | 0.46 |
| 1:A:270:ASN:O | 1:A:273:MET:HG3 | 2.16 | 0.46 |
| 1:A:171:ILE:HG23 | 1:A:172:PHE:H | 1.81 | 0.46 |
| 1:A:287:TYR:HE2 | 1:A:356:PHE:CE1 | 2.34 | 0.46 |
| 1:A:174:TRP:CE3 | 1:A:175:ARG:HG3 | 2.51 | 0.45 |
| 1:A:338:VAL:O | 1:A:342:VAL:HG13 | 2.16 | 0.45 |
| 1:A:340:ASN:OD1 | 1:A:366:ALA:HB1 | 2.16 | 0.45 |
| 2:B:102:HIS:CB | 2:B:132:PRO:CA | 2.94 | 0.45 |
| 1:A:329:ILE:HG23 | 1:A:330:GLN:N | 2.32 | 0.45 |
| 1:A:397:VAL:HG22 | 1:A:397:VAL:O | 2.17 | 0.45 |
| 1:A:42:VAL:HG13 | 1:A:43:PHE:N | 2.32 | 0.45 |
| 1:A:110:GLN:O | 1:A:113:TYR:HB2 | 2.18 | 0.44 |
| 1:A:130:PRO:O | 1:A:131:ALA:C | 2.59 | 0.44 |
| 1:A:173:GLY:O | 1:A:177:SER:OG | 2.33 | 0.44 |
| 1:A:161:LEU:O | 1:A:164:LEU:N | 2.50 | 0.44 |
| 1:A:173:GLY:O | 1:A:177:SER:N | 2.46 | 0.43 |
| 1:A:174:TRP:NE1 | 1:A:178:PHE:HE2 | 2.16 | 0.43 |
| 2:B:116:ILE:O | 2:B:202:VAL:HA | 2.17 | 0.43 |
| 1:A:27:PHE:CE1 | 1:A:153:GLY:HA2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:284:LEU:CD2 | 1:A:301:LEU:HD22 | 2.28 | 0.43 |
| 1:A:339:ALA:O | 1:A:342:VAL:CG2 | 2.66 | 0.43 |
| 1:A:329:ILE:O | 1:A:330:GLN:C | 2.61 | 0.43 |
| 1:A:347:ALA:HB2 | 1:A:359:TYR:CZ | 2.53 | 0.42 |
| 2:B:206:LEU:HD11 | 2:B:210:TRP:HE1 | 1.84 | 0.42 |
| 1:A:87:ILE:O | 1:A:91:VAL:HG23 | 2.20 | 0.42 |
| 1:A:339:ALA:HA | 1:A:342:VAL:HG22 | 2.01 | 0.42 |
| 1:A:145:LEU:O | 1:A:149:LEU:HG | 2.20 | 0.42 |
| 1:A:265:LEU:HD23 | 1:A:440:GLY:O | 2.20 | 0.42 |
| 1:A:273:MET:HE1 | 1:A:370:LEU:HD11 | 2.02 | 0.42 |
| 1:A:399:CYS:O | 1:A:402:VAL:HG12 | 2.19 | 0.42 |
| 1:A:78:ILE:HG23 | 1:A:79:LEU:N | 2.35 | 0.42 |
| 1:A:51:PHE:O | 1:A:52:HIS:C | 2.63 | 0.41 |
| 1:A:89:MET:HG2 | 1:A:127:ASN:ND2 | 2.35 | 0.41 |
| 1:A:109:VAL:HG13 | 1:A:110:GLN:N | 2.35 | 0.41 |
| 1:A:172:PHE:O | 2:B:203:ARG:HD3 | 2.20 | 0.41 |
| 1:A:60:TRP:O | 1:A:64:ILE:HG12 | 2.19 | 0.41 |
| 1:A:22:VAL:HG13 | 1:A:195:MET:SD | 2.60 | 0.41 |
| 1:A:396:ILE:HG23 | 1:A:397:VAL:N | 2.35 | 0.41 |
| 1:A:115:CYS:O | 1:A:119:ILE:HB | 2.20 | 0.41 |
| 1:A:409:LEU:HB3 | 1:A:422:THR:HG23 | 2.02 | 0.41 |
| 1:A:313:ARG:HB2 | 1:A:314:PRO:HD3 | 2.02 | 0.41 |
| 1:A:351:THR:C | 1:A:352:THR:HG1 | 2.24 | 0.41 |
| 1:A:154:SER:HB2 | 1:A:155:PRO:CD | 2.51 | 0.41 |
| 2:B:83:GLY:N | 2:B:101:LEU:O | 2.54 | 0.41 |
| 1:A:54:THR:N | 1:A:57:GLU:OE1 | 2.48 | 0.41 |
| 1:A:160:THR:HG23 | 1:A:161:LEU:HD12 | 2.03 | 0.41 |
| 1:A:36:PHE:N | 1:A:37:PRO:CD | 2.84 | 0.40 |
| 1:A:382:VAL:HG13 | 1:A:383:GLY:N | 2.36 | 0.40 |
| 1:A:100:LEU:CD2 | 1:A:185:LEU:HD12 | 2.47 | 0.40 |
| 1:A:266:TYR:OH | 1:A:374:LEU:HD12 | 2.21 | 0.40 |
| 1:A:116:ILE:O | 1:A:117:GLY:C | 2.64 | 0.40 |
| 1:A:281:LEU:O | 1:A:281:LEU:HD23 | 2.22 | 0.40 |

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 | 378/500 (76%) | 343 (91%) | 35 (9%) | 0 | 100 | 100 |
| 2 | B | 213/269 (79%) | 199 (93%) | 14 (7%) | 0 | 100 | 100 |
| All | All | 591/769 (77%) | 542 (92%) | 49 (8%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 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 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 | 306/405 (76%) | 304 (99%) | 2 (1%) | 76 | 83 |
| 2 | B | 28/225 (12%) | 27 (96%) | 1 (4%) | 31 | 63 |
| All | All | 334/630 (53%) | 331 (99%) | 3 (1%) | 68 | 81 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 29 | SER |
| 1 | A | 154 | SER |
| 2 | B | 203 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 81 | ASN |
| 1 | A | 127 | ASN |
| 1 | A | 270 | ASN |
| 1 | A | 330 | GLN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | EY0 | A | 601 | - | 35,38,38 | 3.81 | 12 (34%) | 39,61,61 | 3.36 | 15 (38%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | EY0 | A | 601 | - | - | 5/21/33/33 | 0/4/4/4 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | A | 601 | EY0 | C30-C31 | -14.12 | 1.32 | 1.53 |
| 3 | A | 601 | EY0 | C32-N28 | 9.38 | 1.56 | 1.46 |
| 3 | A | 601 | EY0 | O10-C4 | 8.88 | 1.41 | 1.23 |
| 3 | A | 601 | EY0 | O29-C30 | 7.70 | 1.61 | 1.44 |
| 3 | A | 601 | EY0 | C9-C8 | 2.93 | 1.41 | 1.37 |
| 3 | A | 601 | EY0 | O34-C31 | 2.79 | 1.48 | 1.44 |
| 3 | A | 601 | EY0 | C4-N5 | -2.65 | 1.34 | 1.40 |
| 3 | A | 601 | EY0 | C35-C31 | 2.51 | 1.55 | 1.52 |
| 3 | A | 601 | EY0 | C16-C17 | 2.50 | 1.54 | 1.51 |
| 3 | A | 601 | EY0 | C9-C27 | 2.37 | 1.55 | 1.50 |
| 3 | A | 601 | EY0 | C16-C8 | 2.32 | 1.55 | 1.49 |
| 3 | A | 601 | EY0 | O33-C27 | -2.11 | 1.18 | 1.23 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 601 | EY0 | C8-S7-C2 | 14.16 | 98.98 | 90.80 |
| 3 | A | 601 | EY0 | C22-C21-N20 | 7.53 | 126.65 | 118.51 |
| 3 | A | 601 | EY0 | C17-C21-N20 | -7.43 | 106.89 | 111.34 |
| 3 | A | 601 | EY0 | C3-C2-S7 | -6.08 | 106.69 | 112.53 |
| 3 | A | 601 | EY0 | O29-N28-C27 | 3.57 | 127.06 | 116.68 |
| 3 | A | 601 | EY0 | C26-C18-N19 | 2.92 | 126.42 | 121.81 |
| 3 | A | 601 | EY0 | C26-C18-C17 | -2.79 | 126.49 | 131.20 |
| 3 | A | 601 | EY0 | C21-N20-N19 | 2.70 | 110.59 | 104.96 |
| 3 | A | 601 | EY0 | C4-N5-C6 | -2.62 | 121.40 | 125.66 |
| 3 | A | 601 | EY0 | O10-C4-C3 | -2.36 | 120.11 | 125.16 |
| 3 | A | 601 | EY0 | C32-N28-C27 | 2.20 | 127.07 | 118.26 |
| 3 | A | 601 | EY0 | C3-C4-N5 | 2.19 | 119.70 | 116.10 |
| 3 | A | 601 | EY0 | F25-C22-C21 | -2.11 | 109.38 | 112.39 |
| 3 | A | 601 | EY0 | F23-C22-C21 | -2.06 | 109.46 | 112.39 |
| 3 | A | 601 | EY0 | F24-C22-C21 | -2.01 | 109.53 | 112.39 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | A | 601 | EY0 | O33-C27-C9-C3 |
| 3 | A | 601 | EY0 | N28-C27-C9-C3 |
| 3 | A | 601 | EY0 | N20-C21-C22-F24 |
| 3 | A | 601 | EY0 | C17-C21-C22-F24 |
| 3 | A | 601 | EY0 | N20-C21-C22-F23 |

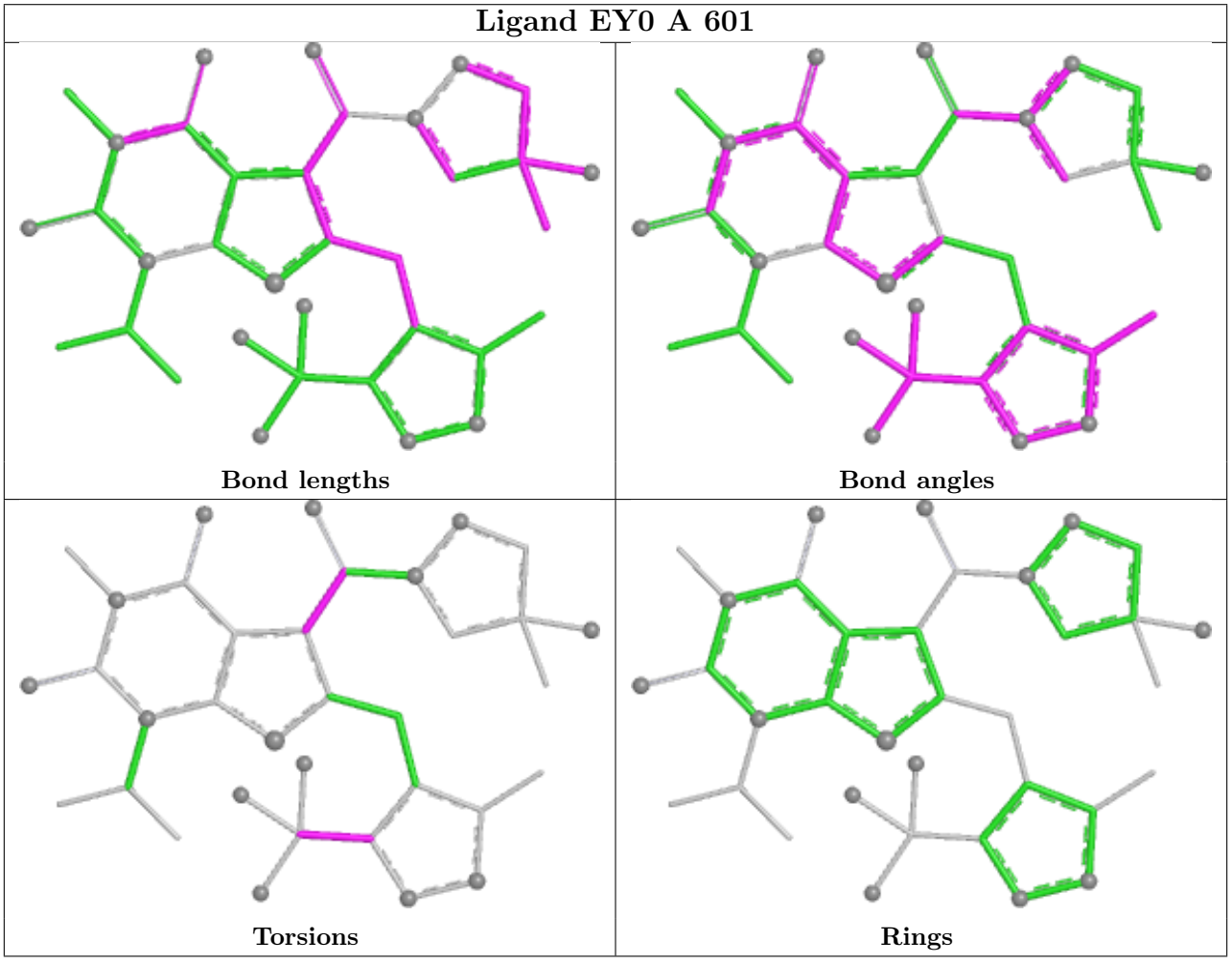
There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 601 | EY0 | 4 | 0 |

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 EY0 A 601**



## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

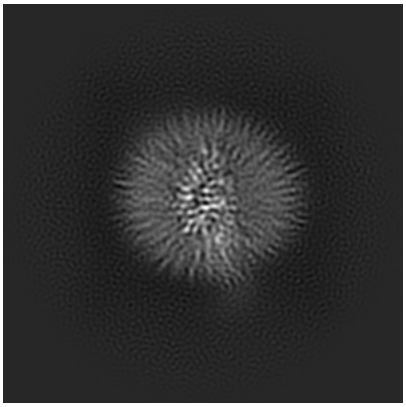
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30019. These allow visual inspection of the internal detail of the map and identification of artifacts.

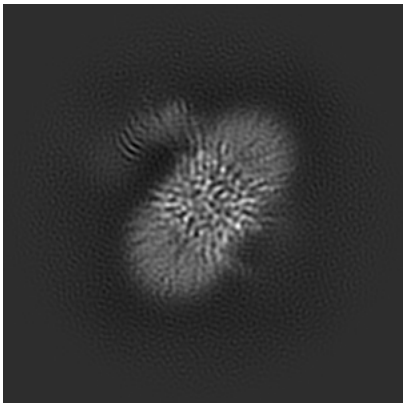
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

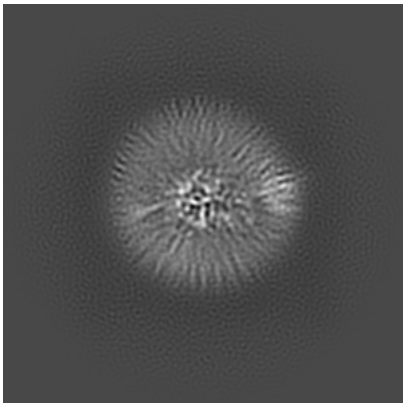
### 6.1.1 Primary map



X



Y

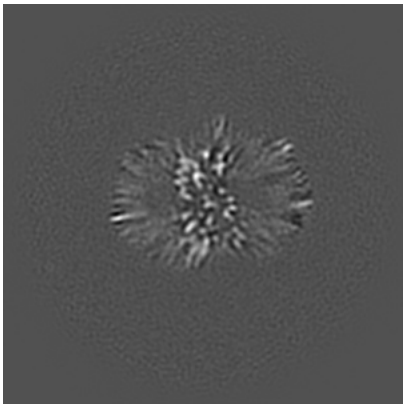


Z

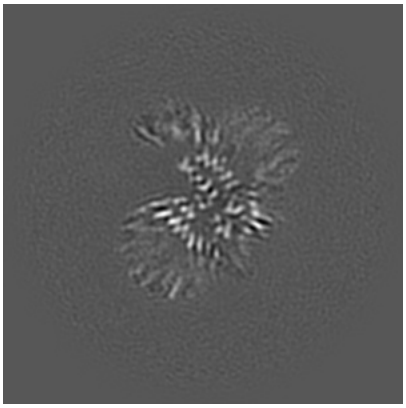
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

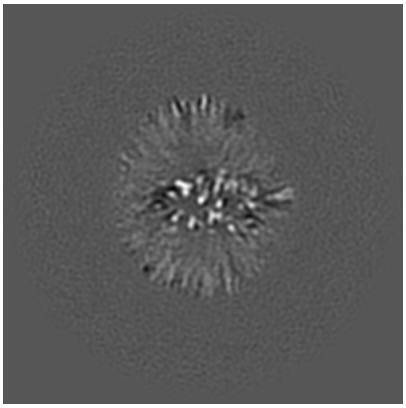
### 6.2.1 Primary map



X Index: 100



Y Index: 100

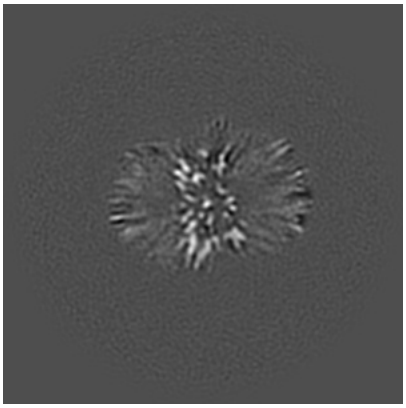


Z Index: 100

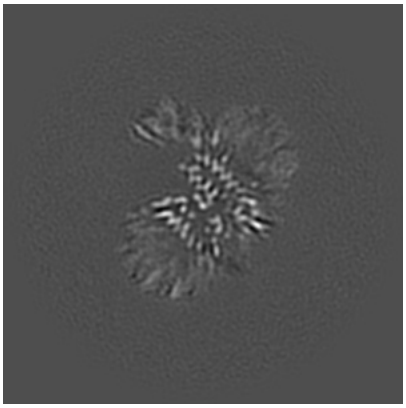
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

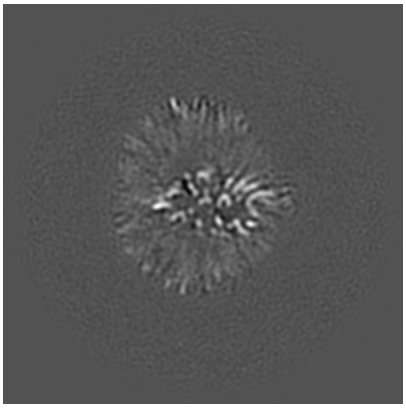
### 6.3.1 Primary map



X Index: 99



Y Index: 101

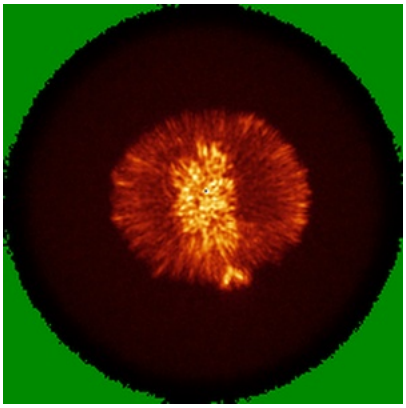


Z Index: 98

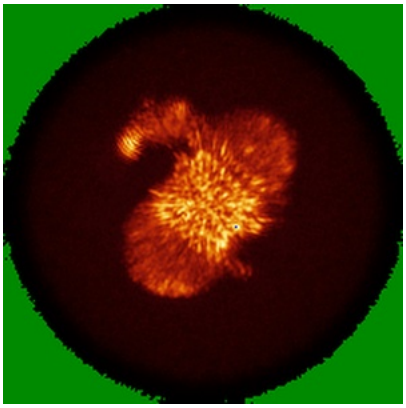
The images above show the largest variance slices of the map in three orthogonal directions.

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

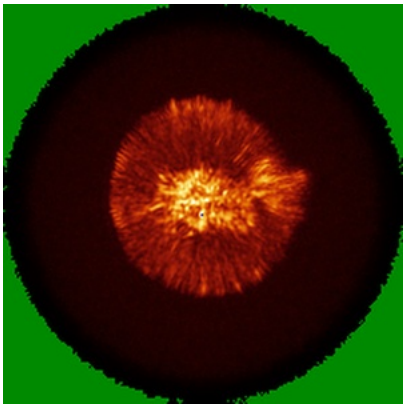
### 6.4.1 Primary map



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 (i)

This section was not generated.

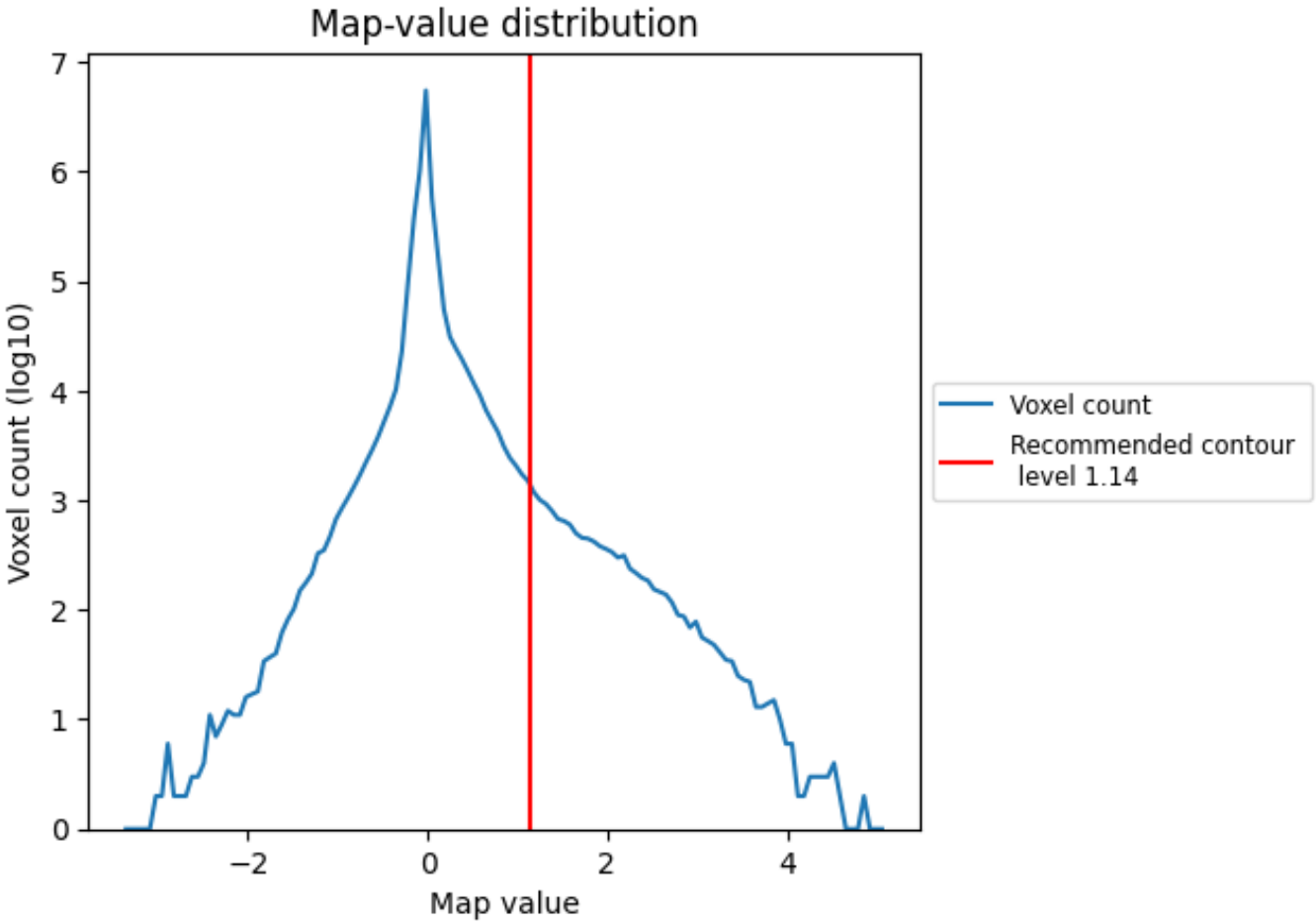
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

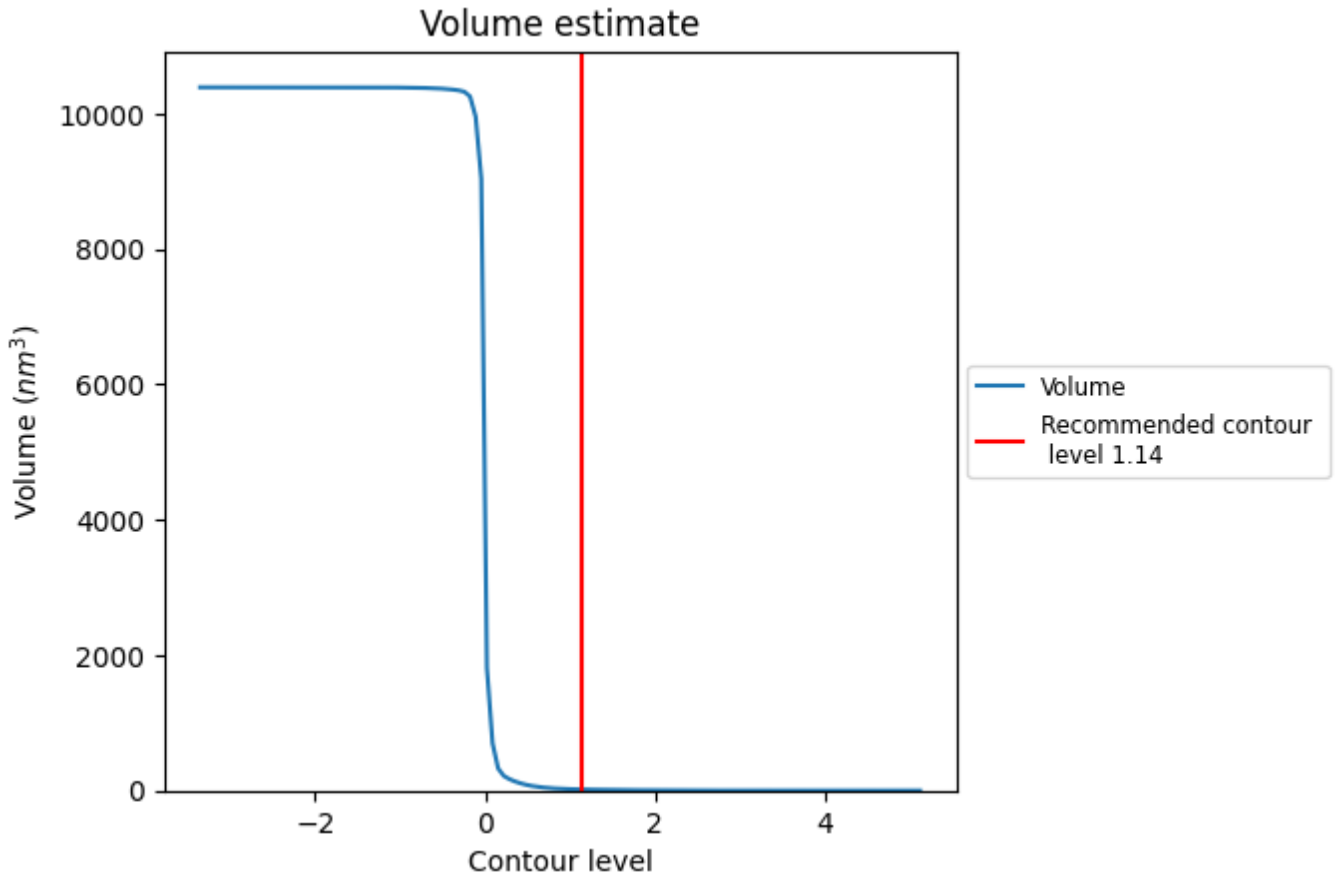
This section contains the results of statistical analysis of the map.

## 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.

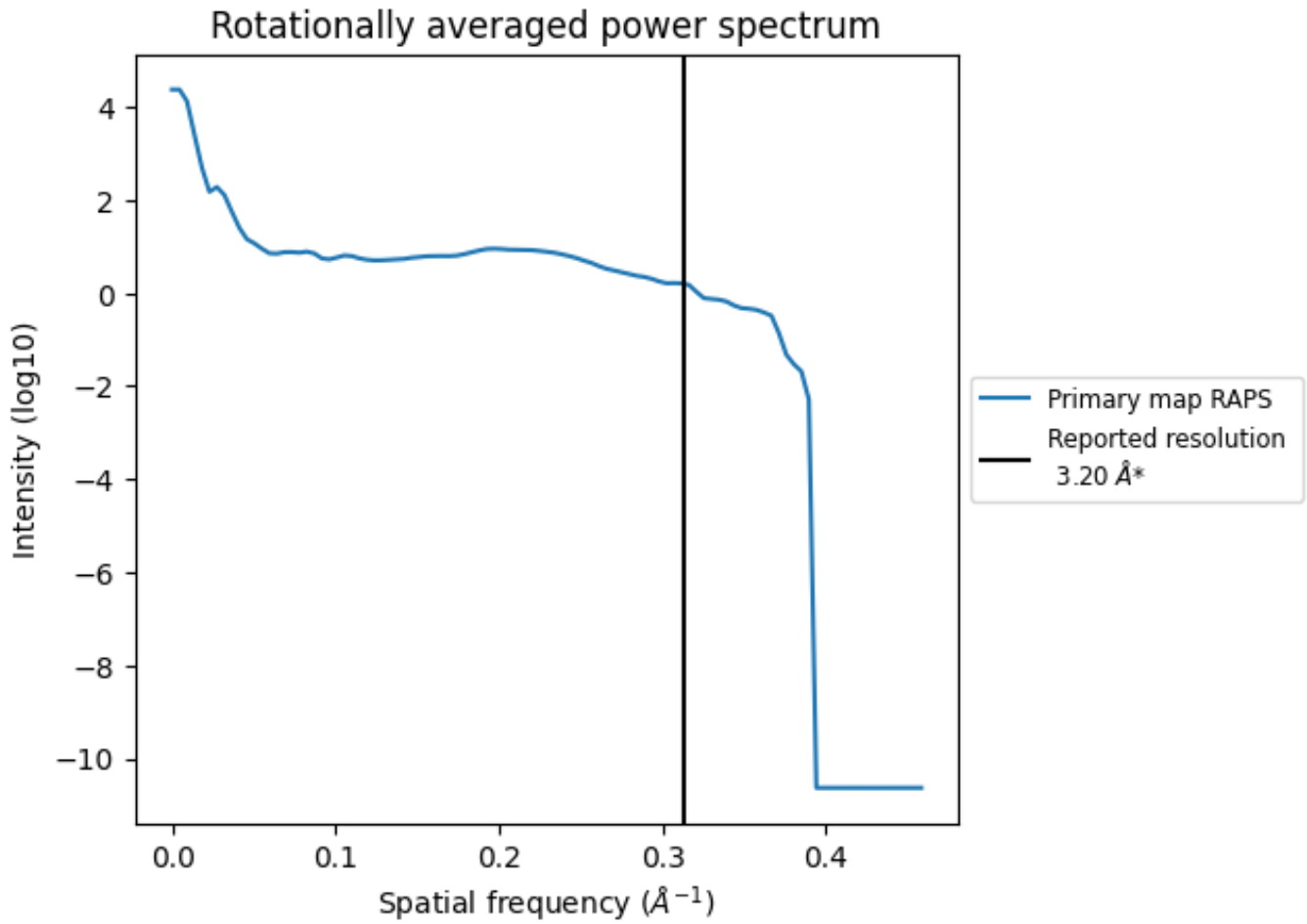
## 7.2 Volume estimate




The volume at the recommended contour level is 16 $nm^3$; this corresponds to an approximate mass of 15 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 (i)




*Reported resolution corresponds to spatial frequency of 0.312 Å$^{-1}$

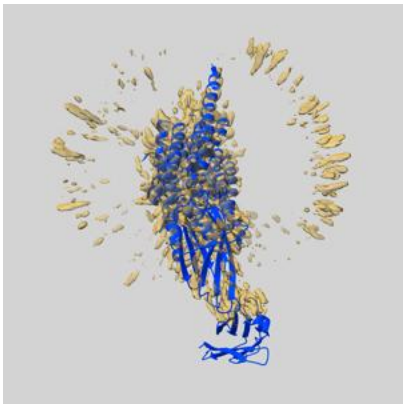
# 8 Fourier-Shell correlation (i)

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

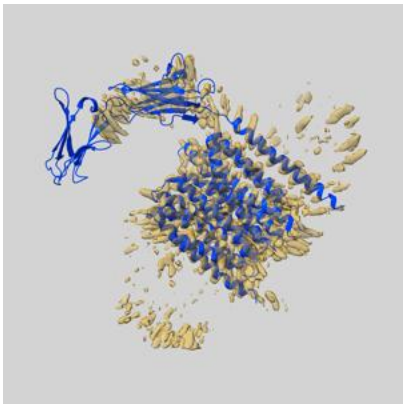
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30019 and PDB model 6LYY. Per-residue inclusion information can be found in section 3 on page 4.

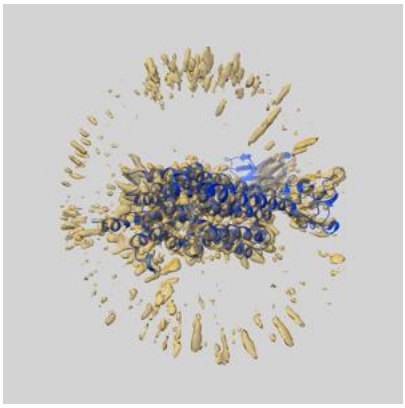
## 9.1 Map-model overlay



X



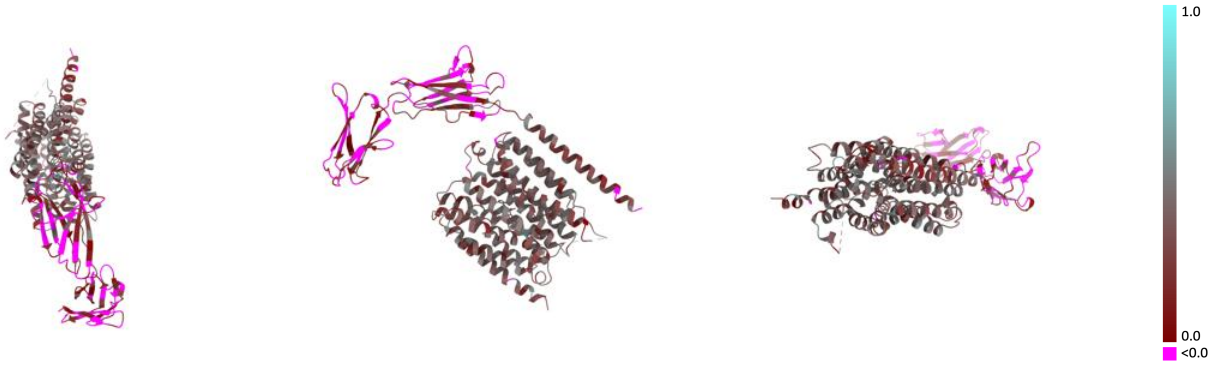
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.14 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.

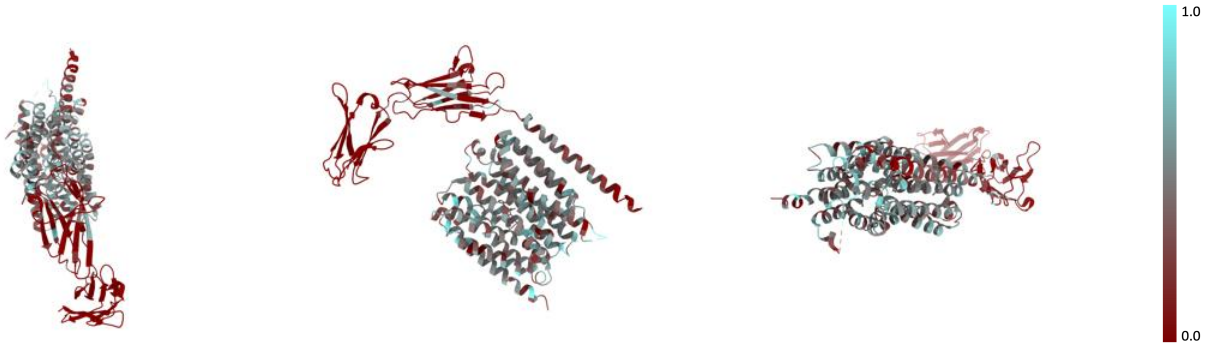
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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.

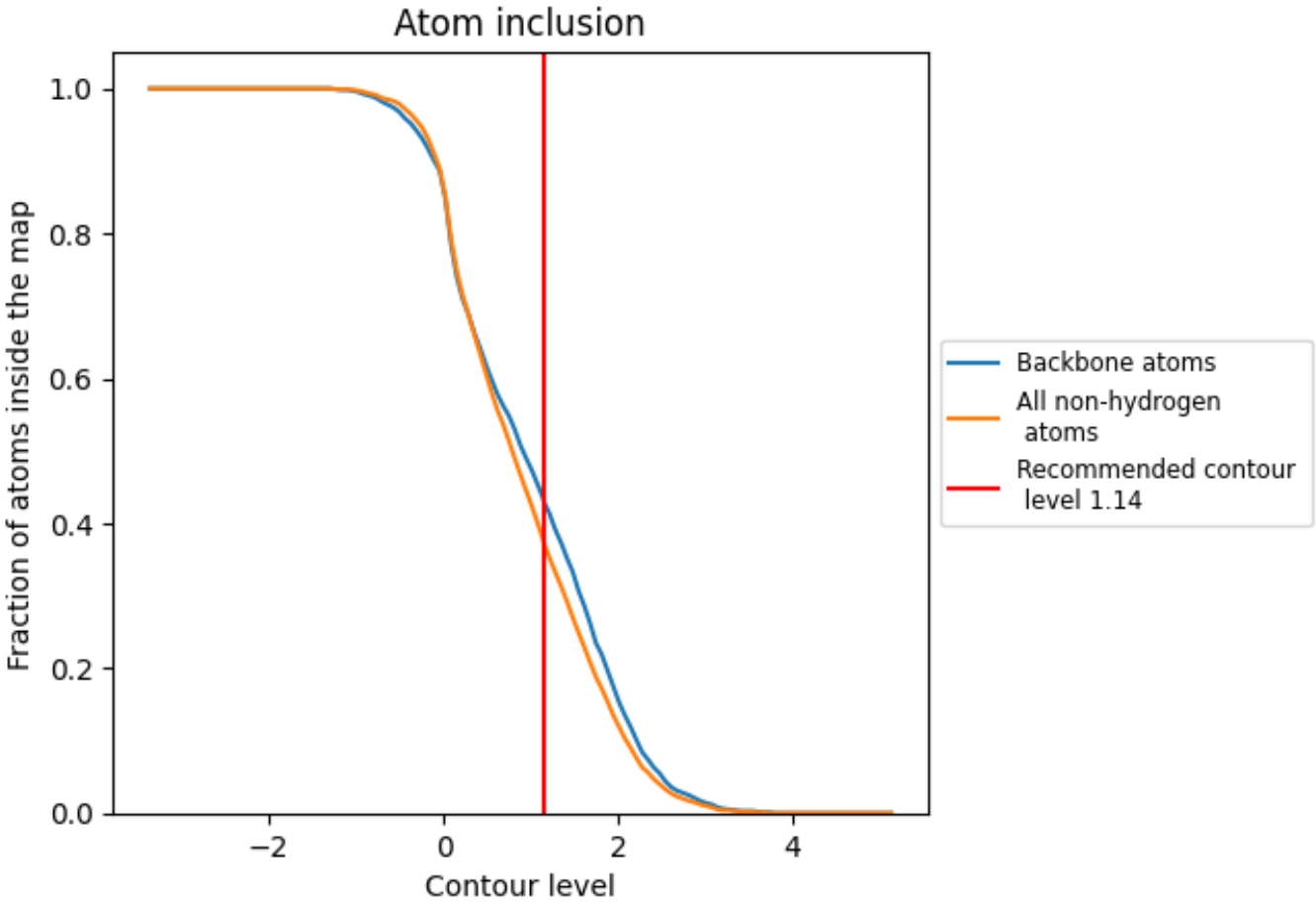
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (1.14).

## 9.4 Atom inclusion (i)




At the recommended contour level, 44% of all backbone atoms, 38% 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 (1.14) and Q-score for the entire model and for each chain.




| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3780 | 0.2830 |
| A | 0.4830 | 0.3620 |
| B | 0.1170 | 0.0850 |