# wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 09:44 PM EST

| | | |
|---|---|---|
| PDB ID | : | 7N8I |
| EMDB ID | : | EMD-24237 |
| Title | : | SARS-CoV-2 S (B.1.429 / epsilon variant) + S2M11 + S2L20 (Local Refinement of the NTD/S2L20) |
| Authors | : | McCallum, M.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Veesler, D. |
| Deposited on | : | 2021-06-14 |
| Resolution | : | 3.00 Å(reported) |

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

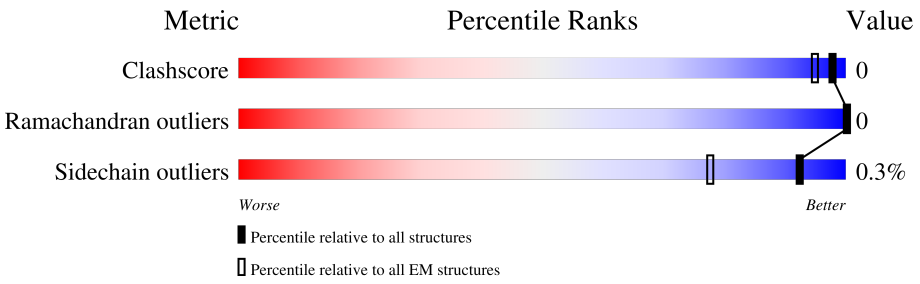
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 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 3.00 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 | 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 | L | 106 | 100% |
| 2 | H | 121 | 100% |
| 3 | A | 1277 | 17% 83% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3600 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 S2L20 Fab Light Chain Variable Region.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | L | 106 | 823 | 523 | 132 | 164 | 4 | 0 | 0 |

- Molecule 2 is a protein called S2L20 Fab Heavy Chain Variable Region.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | H | 121 | 948 | 600 | 163 | 181 | 4 | 0 | 0 |

- Molecule 3 is a protein called Spike glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | A | 218 | 1759 | 1152 | 281 | 321 | 5 | 0 | 0 |

There are 81 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 13 | ILE | SER | conflict | UNP P0DTC2 |
| A | 152 | CYS | TRP | conflict | UNP P0DTC2 |
| A | 452 | ARG | LEU | conflict | UNP P0DTC2 |
| A | 682 | GLY | ARG | conflict | UNP P0DTC2 |
| A | 683 | SER | ARG | conflict | UNP P0DTC2 |
| A | 685 | SER | ARG | conflict | UNP P0DTC2 |
| A | 817 | PRO | PHE | conflict | UNP P0DTC2 |
| A | 892 | PRO | ALA | conflict | UNP P0DTC2 |
| A | 899 | PRO | ALA | conflict | UNP P0DTC2 |
| A | 942 | PRO | ALA | conflict | UNP P0DTC2 |
| A | 986 | PRO | LYS | conflict | UNP P0DTC2 |
| A | 987 | PRO | VAL | conflict | UNP P0DTC2 |
| A | 1209 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1210 | SER | - | expression tag | UNP P0DTC2 |
| A | 1211 | GLY | - | expression tag | UNP P0DTC2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1212 | TYR | - | expression tag | UNP P0DTC2 |
| A | 1213 | ILE | - | expression tag | UNP P0DTC2 |
| A | 1214 | PRO | - | expression tag | UNP P0DTC2 |
| A | 1215 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1216 | ALA | - | expression tag | UNP P0DTC2 |
| A | 1217 | PRO | - | expression tag | UNP P0DTC2 |
| A | 1218 | ARG | - | expression tag | UNP P0DTC2 |
| A | 1219 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1220 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1221 | GLN | - | expression tag | UNP P0DTC2 |
| A | 1222 | ALA | - | expression tag | UNP P0DTC2 |
| A | 1223 | TYR | - | expression tag | UNP P0DTC2 |
| A | 1224 | VAL | - | expression tag | UNP P0DTC2 |
| A | 1225 | ARG | - | expression tag | UNP P0DTC2 |
| A | 1226 | LYS | - | expression tag | UNP P0DTC2 |
| A | 1227 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1228 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1229 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1230 | TRP | - | expression tag | UNP P0DTC2 |
| A | 1231 | VAL | - | expression tag | UNP P0DTC2 |
| A | 1232 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1233 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1234 | SER | - | expression tag | UNP P0DTC2 |
| A | 1235 | THR | - | expression tag | UNP P0DTC2 |
| A | 1236 | PHE | - | expression tag | UNP P0DTC2 |
| A | 1237 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1238 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1239 | ARG | - | expression tag | UNP P0DTC2 |
| A | 1240 | SER | - | expression tag | UNP P0DTC2 |
| A | 1241 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1242 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1243 | VAL | - | expression tag | UNP P0DTC2 |
| A | 1244 | LEU | - | expression tag | UNP P0DTC2 |
| A | 1245 | PHE | - | expression tag | UNP P0DTC2 |
| A | 1246 | GLN | - | expression tag | UNP P0DTC2 |
| A | 1247 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1248 | PRO | - | expression tag | UNP P0DTC2 |
| A | 1249 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1250 | SER | - | expression tag | UNP P0DTC2 |
| A | 1251 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1252 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1253 | LEU | - | expression tag | UNP P0DTC2 |

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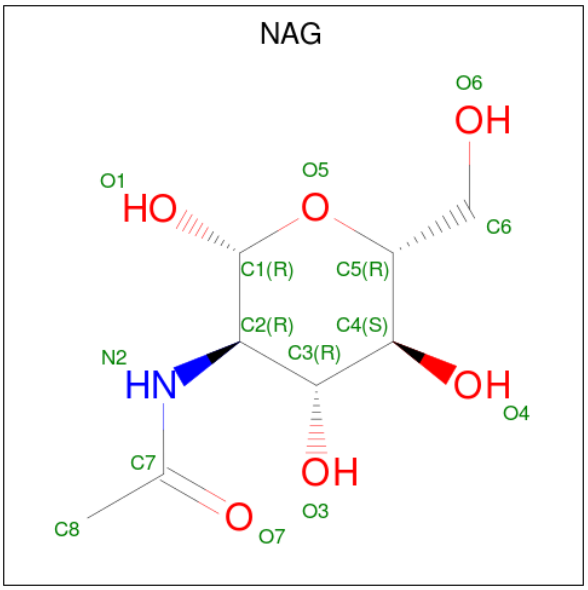
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1254 | ASN | - | expression tag | UNP P0DTC2 |
| A | 1255 | ASP | - | expression tag | UNP P0DTC2 |
| A | 1256 | ILE | - | expression tag | UNP P0DTC2 |
| A | 1257 | PHE | - | expression tag | UNP P0DTC2 |
| A | 1258 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1259 | ALA | - | expression tag | UNP P0DTC2 |
| A | 1260 | GLN | - | expression tag | UNP P0DTC2 |
| A | 1261 | LYS | - | expression tag | UNP P0DTC2 |
| A | 1262 | ILE | - | expression tag | UNP P0DTC2 |
| A | 1263 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1264 | TRP | - | expression tag | UNP P0DTC2 |
| A | 1265 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1266 | GLU | - | expression tag | UNP P0DTC2 |
| A | 1267 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1268 | SER | - | expression tag | UNP P0DTC2 |
| A | 1269 | GLY | - | expression tag | UNP P0DTC2 |
| A | 1270 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1271 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1272 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1273 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1274 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1275 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1276 | HIS | - | expression tag | UNP P0DTC2 |
| A | 1277 | HIS | - | expression tag | UNP P0DTC2 |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | |
| 4 | A | 1 | 70 | 40 | 5 | 25 | 0 |
| | | | Total | C | N | O | |
| 4 | A | 1 | 70 | 40 | 5 | 25 | 0 |
| | | | Total | C | N | O | |
| 4 | A | 1 | 70 | 40 | 5 | 25 | 0 |
| | | | Total | C | N | O | |
| 4 | A | 1 | 70 | 40 | 5 | 25 | 0 |
| | | | Total | C | N | O | |
| 4 | A | 1 | 70 | 40 | 5 | 25 | 0 |

# 3 Residue-property plots (i)

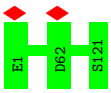
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: S2L20 Fab Light Chain Variable Region

Chain L: 100%

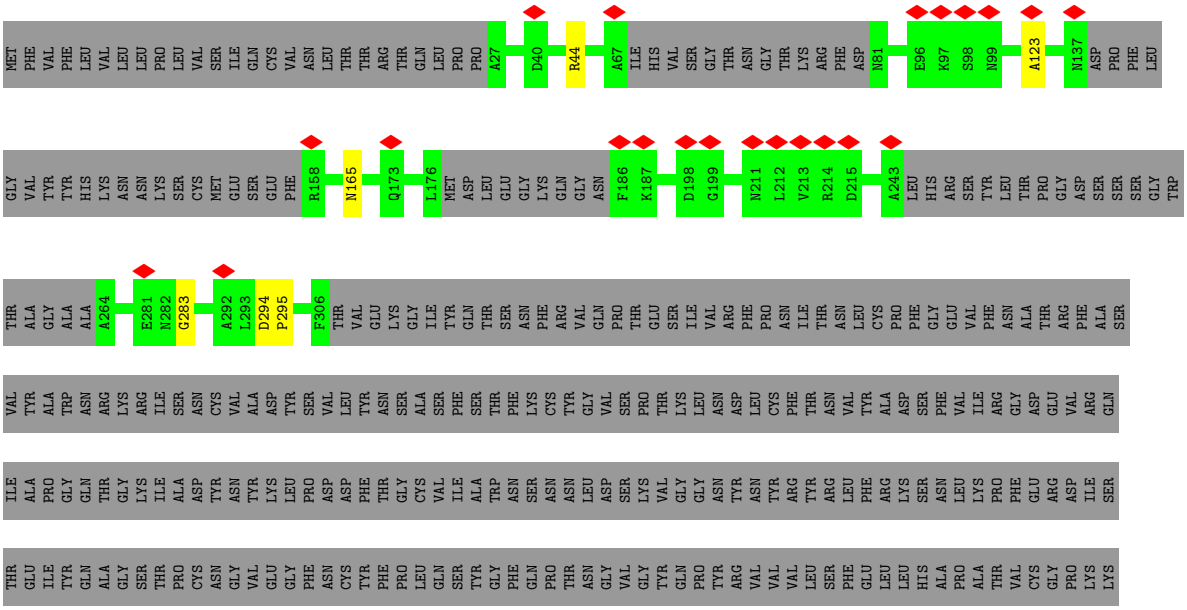
• Molecule 2: S2L20 Fab Heavy Chain Variable Region

Chain H: 100%




• Molecule 3: Spike glycoprotein

Chain A: 17% 83%



SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE ASN PHE ASN GLY LEU THR GLY THR GLY VAL LEU THR GLU SER ASN LYS LYS PHE LEU PRO PHE GLN GLN PHE GLY ARG ASP ILE ALA ASP THR THR ASP ALA VAL ARG ASP PRO GLN THR LEU GLU ILE LEU ASP ILE THR PRO

CYS SER PHE GLY GLY VAL SER VAL ILE THR PRO GLY THR ASN THR SER ASN GLN VAL ALA VAL LEU TYR GLN ASP VAL ASN CYS THR GLU VAL PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY SER ASN VAL PHE GLN THR ARG ALA GLY CYS

LEU ILE GLY ALA GLU HIS VAL ASN ASN SER TYR GLU CYS ASP ILE PRO ILE GLY ALA GLY ILE CYS ALA SER TYR GLN THR GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA SER GLN SER ILE ILE ALA TYR THR MET SER LEU GLY ALA GLU ASN SER VAL ALA TYR SER ASN

ASN SER ILE ALA ILE PRO THR ASN PHE THR ILE SER VAL THR THR GLU ILE LEU PRO VAL SER MET THR LYS THR SER VAL ASP CYS THR MET TYR ILE CYS GLY ASP SER THR GLU CYS SER ASN LEU LEU LEU GLN TYR GLY SER PHE CYS THR GLN LEU ASN ARG ALA LEU THR GLY

ILE ALA VAL GLU GLN ASP LYS ASN THR GLN GLU VAL PHE ALA GLN VAL LYS GLN ILE TYR LYS THR PRO PRO ILE LYS ASP PHE GLY GLY PHE ASN PHE SER GLN ILE LEU PRO ASP PRO SER LYS PRO SER LYS ARG SER PRO ILE GLU ASP LEU LEU PHE ASN LYS VAL THR LEU ALA

ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN LYS PHE ASN GLY LEU THR VAL LEU PRO PRO LEU LEU THR ASP GLU MET ILE ALA GLN TYR THR SER ALA LEU LEU ALA GLY THR ILE THR SER GLY TRP THR PHE GLY

ALA GLY PRO ALA LEU GLN ILE PRO PHE PRO MET GLN MET ALA TYR ARG PHE ASN GLY ILE GLY VAL THR GLN ASN VAL LEU TYR GLU ASN GLN LYS LEU ILE ALA ASN GLN PHE ASN SER ALA ILE GLY LYS ILE GLN ASP SER LEU SER SER THR PRO SER ALA LEU GLY LYS LEU GLN

ASP VAL VAL ASN GLN ASN ALA GLN ALA LEU ASN THR LEU VAL LYS GLN LEU SER SER ASN PHE GLY ALA ILE SER SER VAL LEU ASN ASP ILE LEU SER ARG LEU ASP PRO PRO GLU ALA GLU VAL GLN ILE ASP ARG LEU ILE THR GLY ARG LEU GLN SER LEU GLN THR TYR VAL THR

GLN GLN LEU ILE ARG ALA ALA GLU ILE ARG ALA SER ALA ASN LEU ALA ALA THR LYS MET SER GLU CYS VAL LEU GLY GLN SER LYS ARG VAL ASP PHE CYS GLY LYS GLY TYR HIS LEU MET SER PHE PRO GLN SER ALA PRO HIS GLY VAL VAL PHE LEU HIS VAL THR TYR VAL PRO

ALA GLN GLU LYS ASN PHE THR THR ALA PRO ALA ILE CYS HIS ASP GLY LYS ALA HIS PHE PRO ARG GLU GLY VAL PHE VAL SER ASN GLY THR HIS TRP PHE VAL THR GLN ARG ASN PHE TYR GLU PRO GLN ILE ILE THR THR ASP ASN THR PHE VAL SER GLY ASN CYS ASP VAL VAL

ILE GLY ILE VAL ASN ASN THR VAL TYR ASP PRO LEU GLN PRO GLU LEU ASP SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL

ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY

SER GLY GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU GLY SER GLY HIS HIS HIS HIS HIS HIS HIS HIS

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 254593 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 63 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 8.174 | Depositor |
| Minimum map value | -5.609 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.053 | Depositor |
| Recommended contour level | 1.5 | Depositor |
| Map size (Å) | 431.616, 431.616, 431.616 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.843, 0.843, 0.843 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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 | L | 0.59 | 0/845 | 0.55 | 0/1150 |
| 2 | H | 0.64 | 0/971 | 0.60 | 0/1312 |
| 3 | A | 0.60 | 0/1805 | 0.57 | 0/2454 |
| All | All | 0.61 | 0/3621 | 0.58 | 0/4916 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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 | L | 823 | 0 | 784 | 0 | 0 |
| 2 | H | 948 | 0 | 904 | 0 | 0 |
| 3 | A | 1759 | 0 | 1708 | 3 | 0 |
| 4 | A | 70 | 0 | 65 | 1 | 0 |
| All | All | 3600 | 0 | 3461 | 3 | 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 (3) 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) |
|---|---|---|---|
| 3:A:123:ALA:HB3 | 4:A:1301:NAG:H82 | 2.01 | 0.42 |
| 3:A:44:ARG:O | 3:A:283:GLY:HA2 | 2.20 | 0.41 |
| 3:A:294:ASP:HB2 | 3:A:295:PRO:HD2 | 2.02 | 0.41 |

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 | L | 104/106 (98%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | H | 119/121 (98%) | 119 (100%) | 0 | 0 | 100 | 100 |
| 3 | A | 208/1277 (16%) | 203 (98%) | 5 (2%) | 0 | 100 | 100 |
| All | All | 431/1504 (29%) | 424 (98%) | 7 (2%) | 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 | L | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 2 | H | 98/98 (100%) | 98 (100%) | 0 | 100 | 100 |
| 3 | A | 197/1111 (18%) | 196 (100%) | 1 (0%) | 88 | 96 |
| All | All | 388/1302 (30%) | 387 (100%) | 1 (0%) | 92 | 97 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 165 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | NAG | A | 1305 | 3 | 14,14,15 | 1.09 | 1 (7%) | 17,19,21 | 1.01 | 1 (5%) |
| 4 | NAG | A | 1302 | 3 | 14,14,15 | 1.07 | 1 (7%) | 17,19,21 | 1.05 | 1 (5%) |
| 4 | NAG | A | 1301 | 3 | 14,14,15 | 1.14 | 1 (7%) | 17,19,21 | 1.10 | 1 (5%) |
| 4 | NAG | A | 1303 | 3 | 14,14,15 | 1.16 | 1 (7%) | 17,19,21 | 1.03 | 1 (5%) |
| 4 | NAG | A | 1304 | 3 | 14,14,15 | 1.18 | 1 (7%) | 17,19,21 | 1.10 | 1 (5%) |

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 |
|---|---|---|---|---|---|---|---|
| 4 | NAG | A | 1305 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1302 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1301 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1303 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1304 | 3 | - | 0/6/23/26 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | A | 1303 | NAG | C1-C2 | 3.35 | 1.57 | 1.52 |
| 4 | A | 1301 | NAG | C1-C2 | 3.30 | 1.57 | 1.52 |
| 4 | A | 1304 | NAG | C1-C2 | 3.25 | 1.57 | 1.52 |
| 4 | A | 1305 | NAG | C1-C2 | 3.12 | 1.57 | 1.52 |
| 4 | A | 1302 | NAG | C1-C2 | 3.02 | 1.56 | 1.52 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 1301 | NAG | C8-C7-N2 | 2.60 | 120.50 | 116.10 |
| 4 | A | 1302 | NAG | C8-C7-N2 | 2.57 | 120.44 | 116.10 |
| 4 | A | 1303 | NAG | C8-C7-N2 | 2.50 | 120.34 | 116.10 |
| 4 | A | 1304 | NAG | C8-C7-N2 | 2.39 | 120.14 | 116.10 |
| 4 | A | 1305 | NAG | C8-C7-N2 | 2.27 | 119.94 | 116.10 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 1303 | NAG | O5-C5-C6-O6 |
| 4 | A | 1303 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | A | 1301 | NAG | 1 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

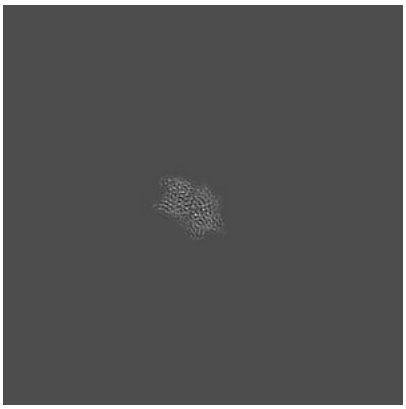
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24237. These allow visual inspection of the internal detail of the map and identification of artifacts.

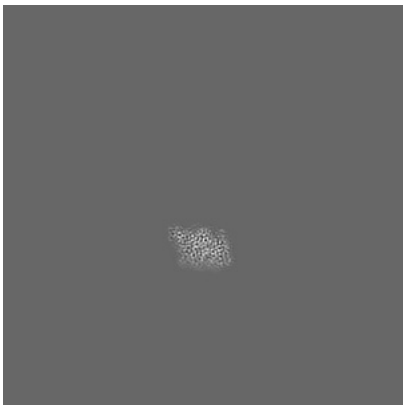
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

### 6.1.1 Primary map



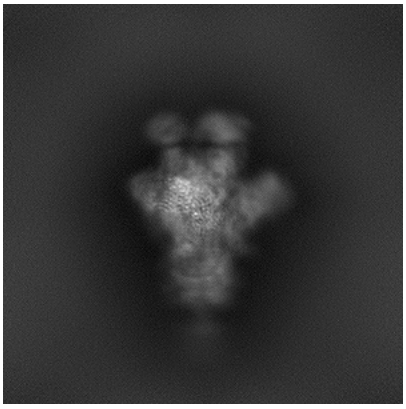
X



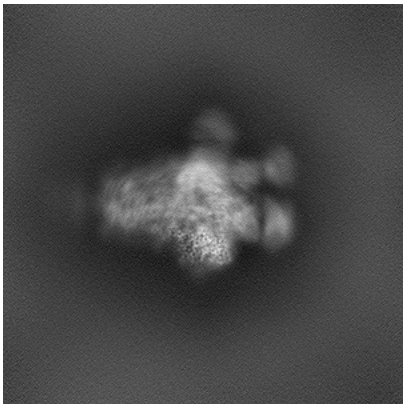
Y

Z

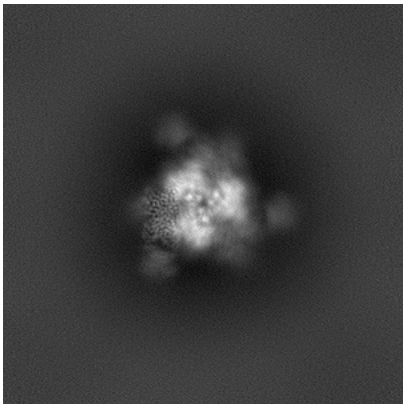
### 6.1.2 Raw map



X



Y

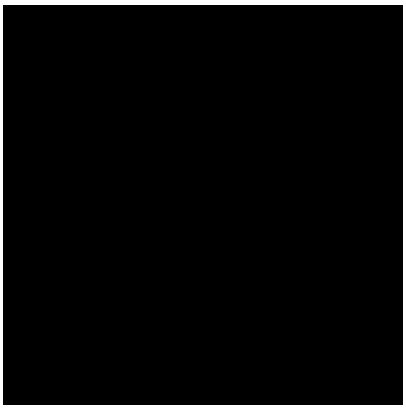


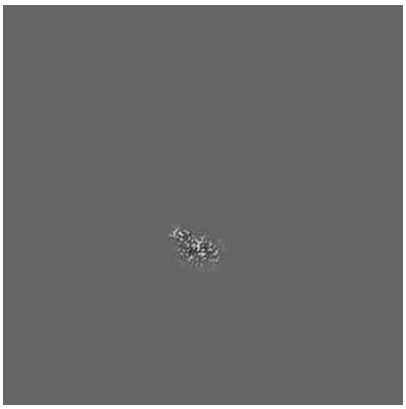
Z

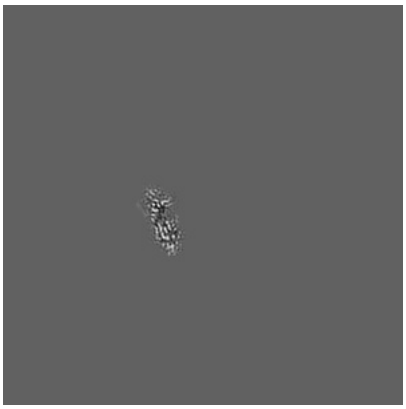
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

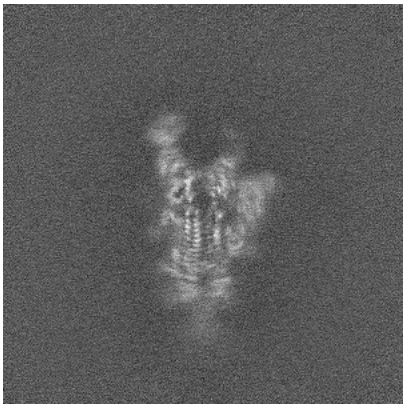
### 6.2.1 Primary map

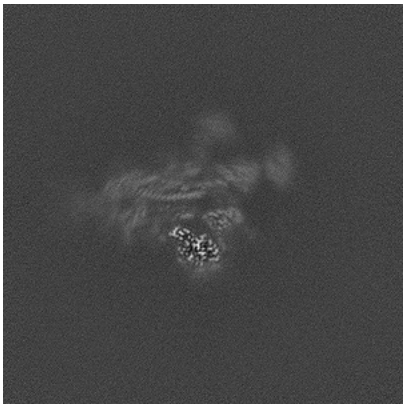

X Index: 256

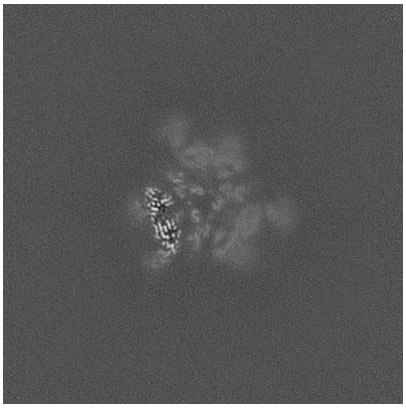

Y Index: 256


Z Index: 256

### 6.2.2 Raw map


X Index: 256

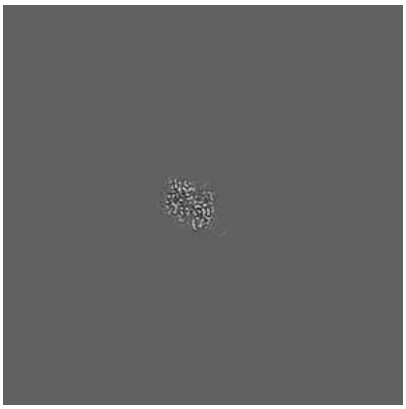

Y Index: 256


Z Index: 256

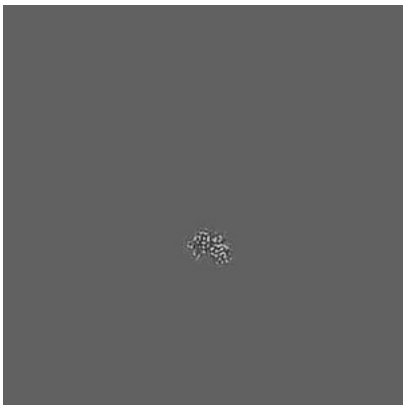
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

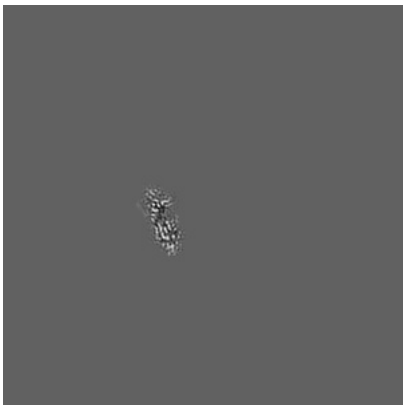
### 6.3.1 Primary map



X Index: 203

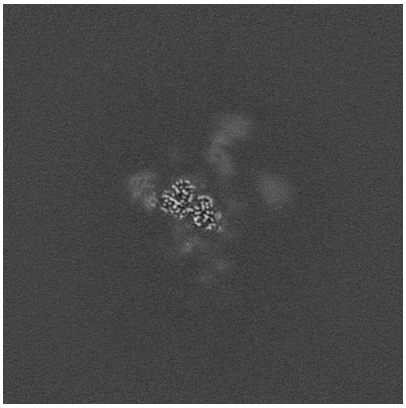


Y Index: 226



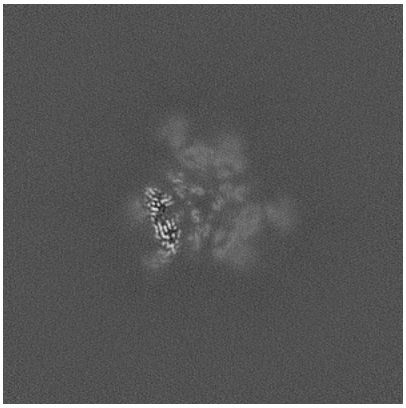
Z Index: 256

### 6.3.2 Raw map



X Index: 208

Y Index: 246

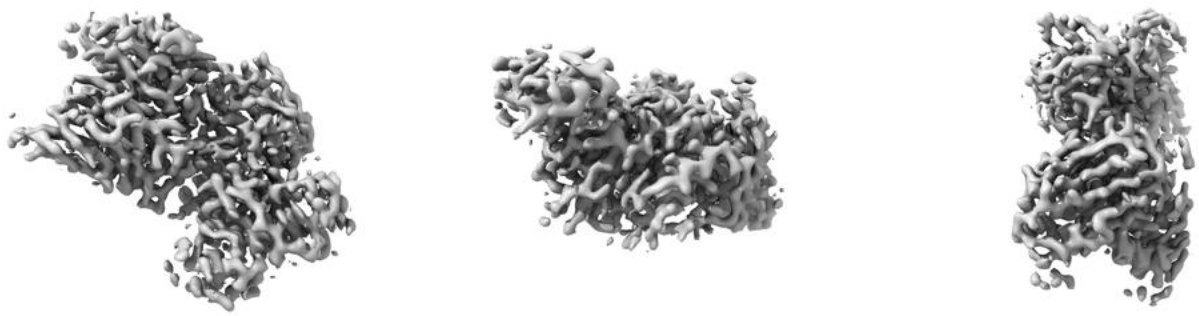


Z Index: 256

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

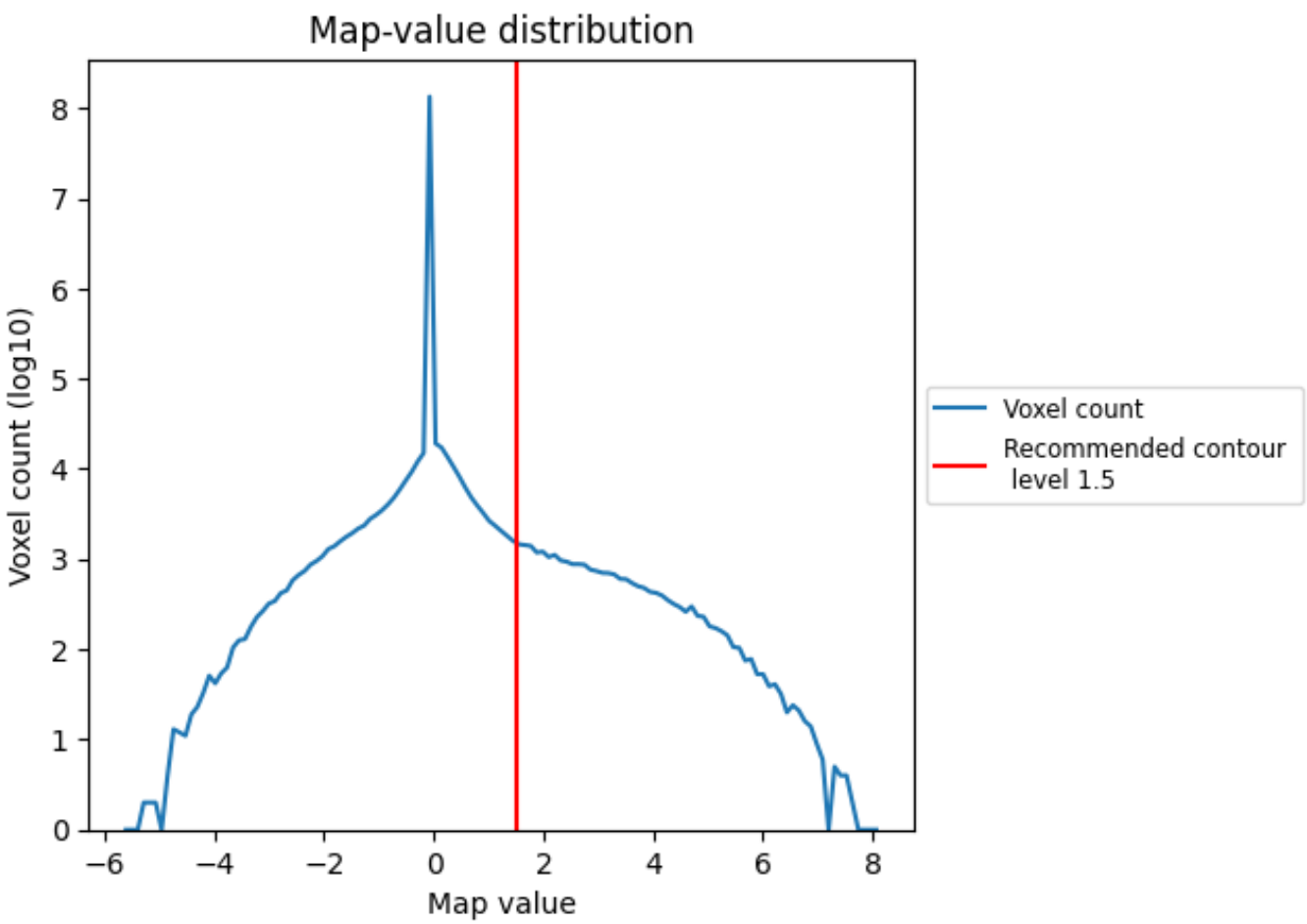
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

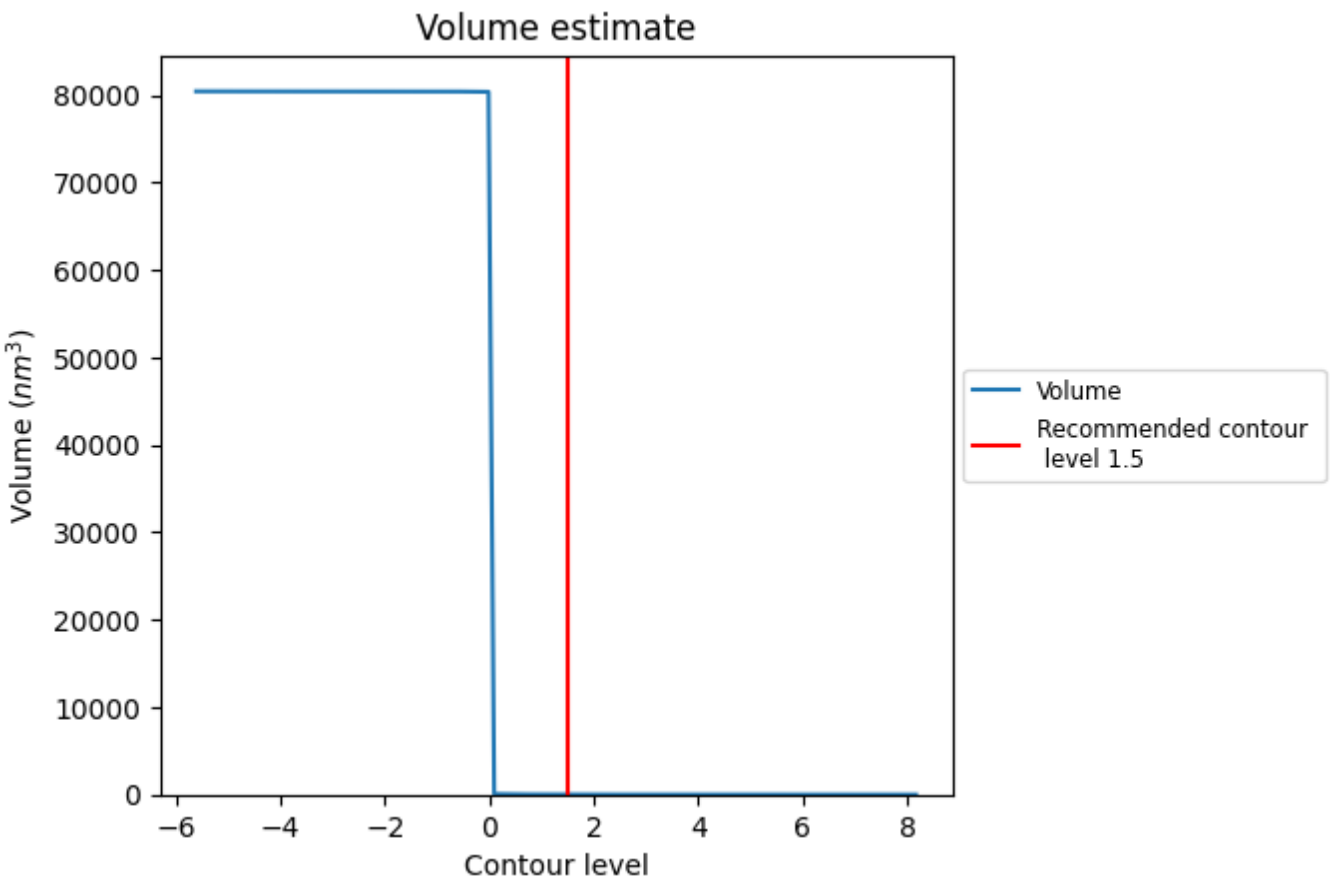
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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.

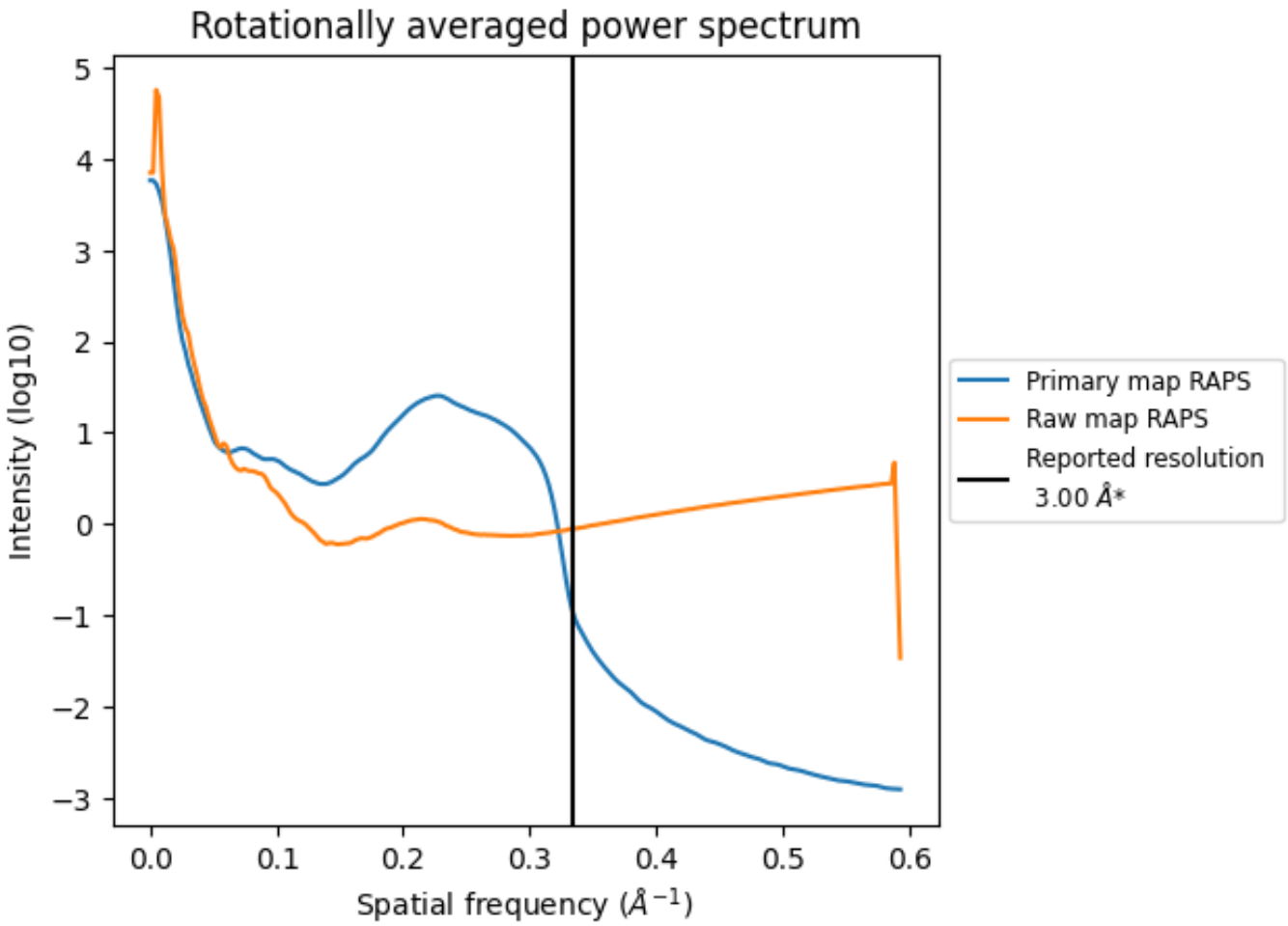
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 15 $nm^3$; this corresponds to an approximate mass of 14 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)

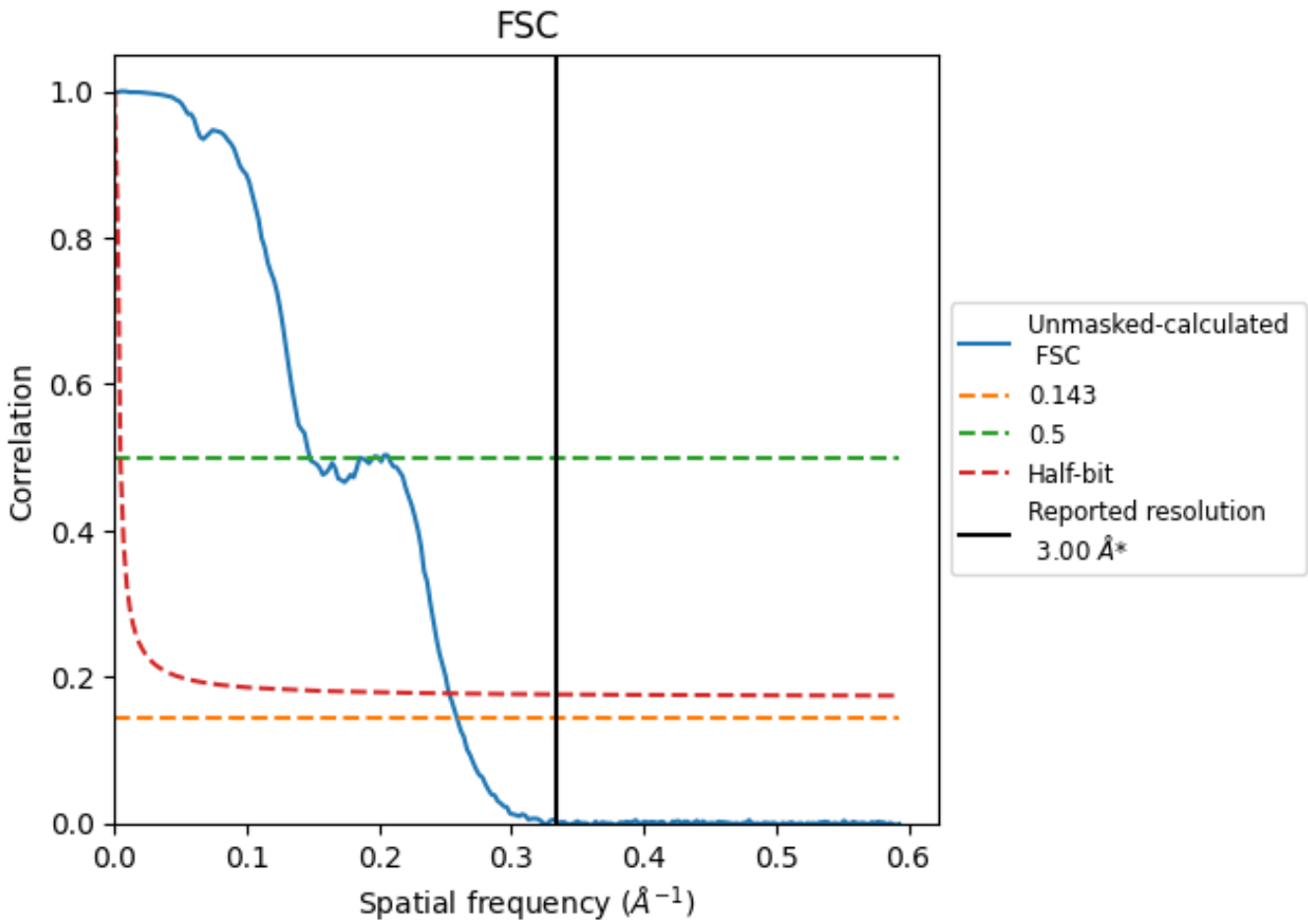



*Reported resolution corresponds to spatial frequency of 0.333 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.333 Å$^{-1}$

## 8.2 Resolution estimates (i)

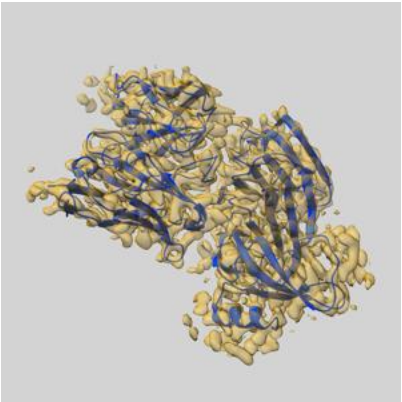
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.00 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.86 | 6.78 | 3.95 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.0 by more than 10 %

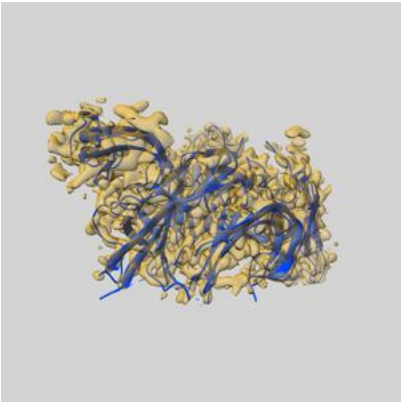
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24237 and PDB model 7N8I. Per-residue inclusion information can be found in section 3 on page 7.

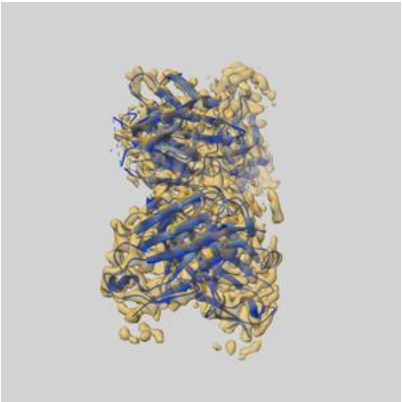
## 9.1 Map-model overlay (i)



X



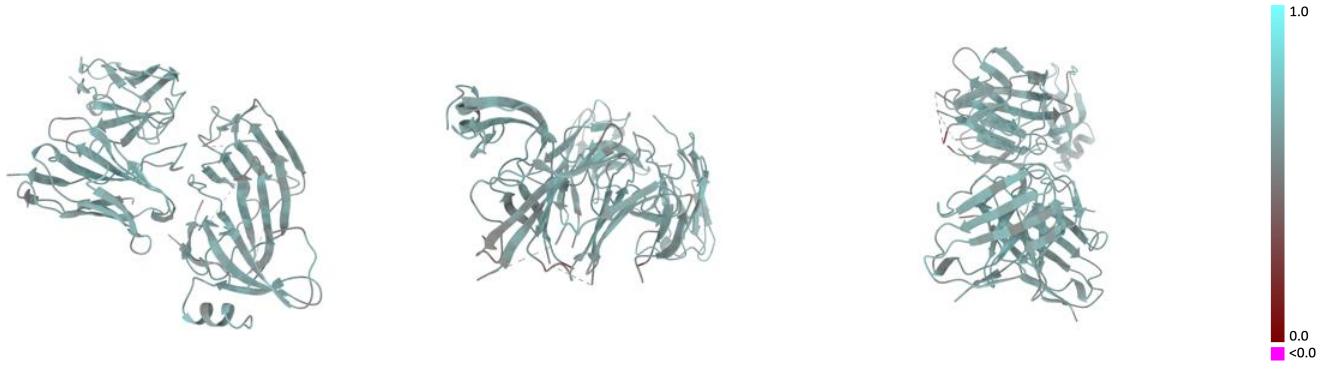
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 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.

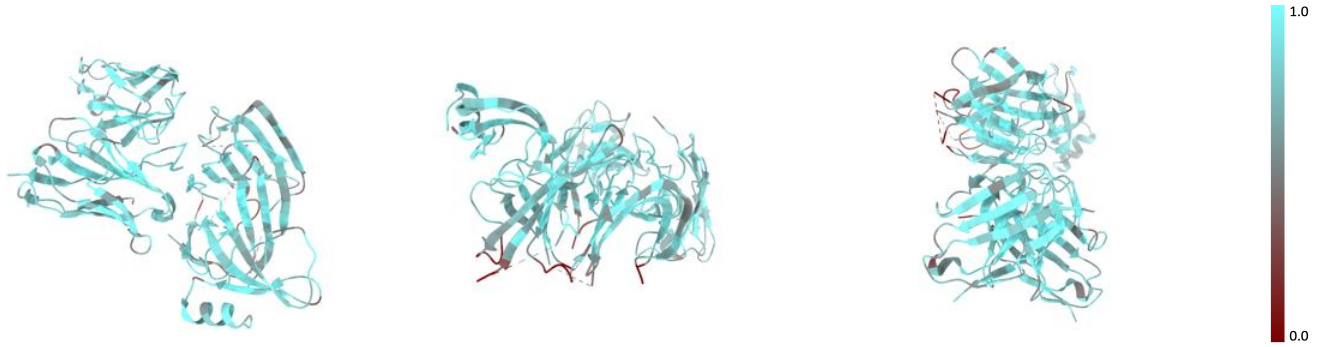
## 9.2 Q-score mapped to coordinate model (i)




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.

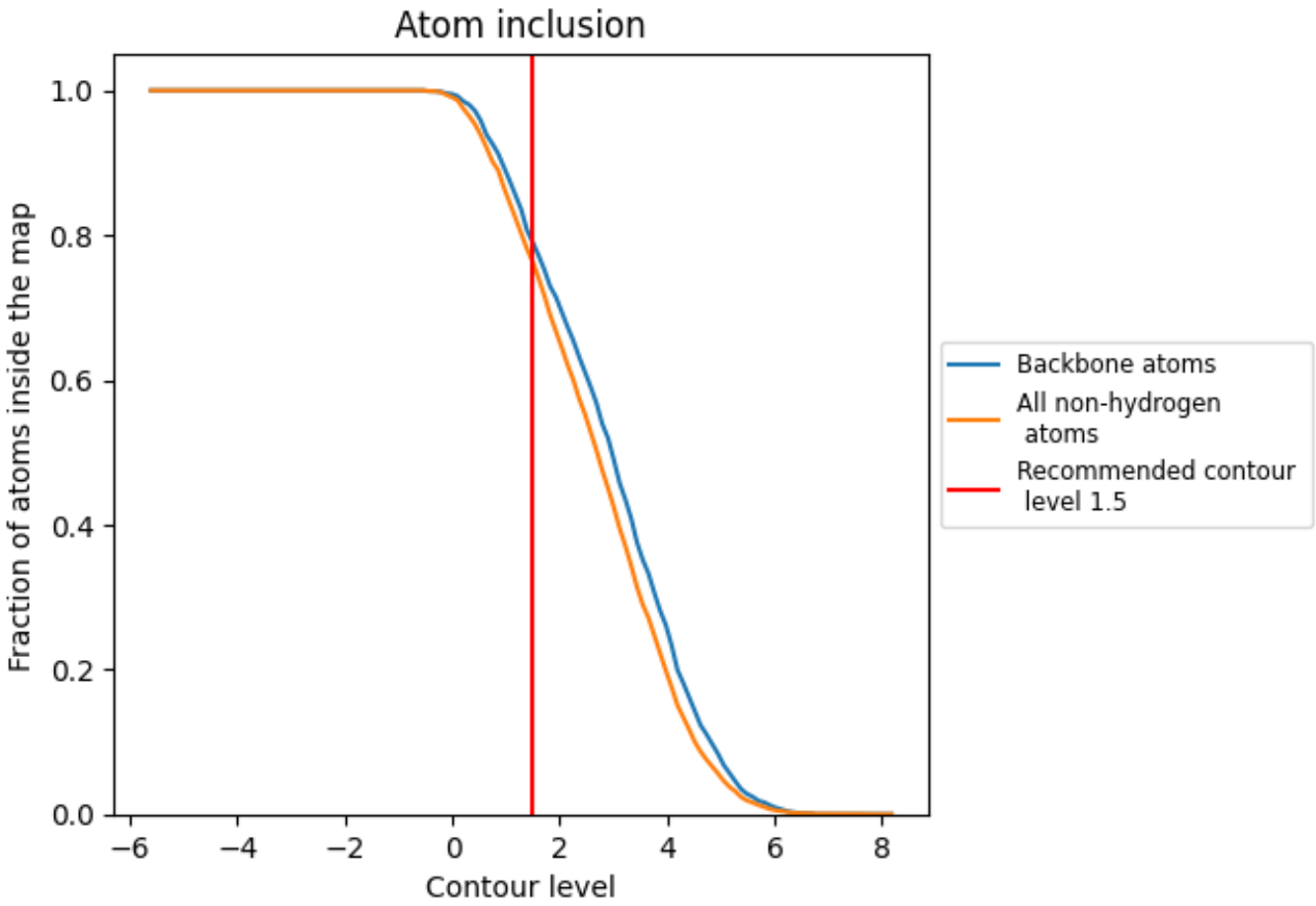
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (1.5).

## 9.4 Atom inclusion (i)




At the recommended contour level, 79% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7627 | 0.5820 |
| A | 0.7279 | 0.5670 |
| H | 0.8000 | 0.6000 |
| L | 0.7975 | 0.5970 |