



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 12:11 PM JST

PDB ID : 9KFI / pdb_00009kfi
EMDB ID : EMD-62297
Title : Cryo-EM structure of the human relaxin family peptide receptor 3 in complex with relaxin-3 and G protein
Authors : Chen, Y.; Zhou, Q.T.; Yan, S.Y.; Yan, J.H.; Yang, D.H.; Chen, J.; Wang, M.W.
Deposited on : 2024-11-06
Resolution : 2.91 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

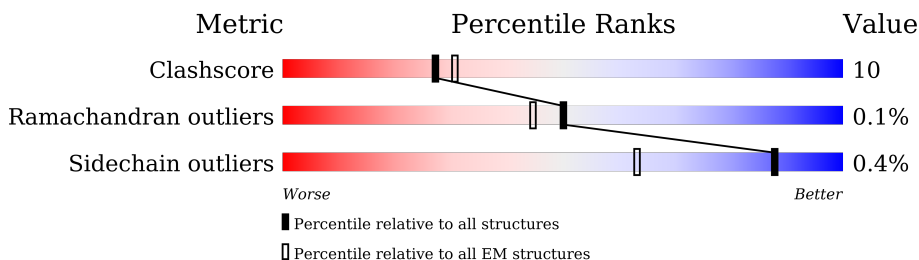
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 $\leq 5\%$. 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 | C | 773 | 5% 24% 16% 60% |
| 2 | G | 55 | 87% 13% |
| 3 | I | 355 | 50% 11% 38% |
| 4 | S | 248 | 77% 15% 7% |
| 5 | T | 338 | 83% 17% |
| 6 | B | 22 | 23% 64% 36% |
| 7 | A | 24 | 83% 92% 8% |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9293 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 Soluble cytochrome b562,Relaxin-3 receptor 1,LgBiT.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | C | 307 | Total | C | N | O | S | 0 | 0 |
| | | | 2435 | 1611 | 410 | 394 | 20 | | |

There are 29 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| C | -130 | MET | - | initiating methionine | UNP P0ABE7 |
| C | -129 | LYS | - | expression tag | UNP P0ABE7 |
| C | -128 | THR | - | expression tag | UNP P0ABE7 |
| C | -127 | ILE | - | expression tag | UNP P0ABE7 |
| C | -126 | ILE | - | expression tag | UNP P0ABE7 |
| C | -125 | ALA | - | expression tag | UNP P0ABE7 |
| C | -124 | LEU | - | expression tag | UNP P0ABE7 |
| C | -123 | SER | - | expression tag | UNP P0ABE7 |
| C | -122 | TYR | - | expression tag | UNP P0ABE7 |
| C | -121 | ILE | - | expression tag | UNP P0ABE7 |
| C | -120 | PHE | - | expression tag | UNP P0ABE7 |
| C | -119 | CYS | - | expression tag | UNP P0ABE7 |
| C | -118 | LEU | - | expression tag | UNP P0ABE7 |
| C | -117 | VAL | - | expression tag | UNP P0ABE7 |
| C | -116 | PHE | - | expression tag | UNP P0ABE7 |
| C | -115 | ALA | - | expression tag | UNP P0ABE7 |
| C | -114 | HIS | - | expression tag | UNP P0ABE7 |
| C | -113 | HIS | - | expression tag | UNP P0ABE7 |
| C | -112 | HIS | - | expression tag | UNP P0ABE7 |
| C | -111 | HIS | - | expression tag | UNP P0ABE7 |
| C | -110 | HIS | - | expression tag | UNP P0ABE7 |
| C | -109 | HIS | - | expression tag | UNP P0ABE7 |
| C | -108 | HIS | - | expression tag | UNP P0ABE7 |
| C | -107 | HIS | - | expression tag | UNP P0ABE7 |
| C | -106 | HIS | - | expression tag | UNP P0ABE7 |
| C | -105 | HIS | - | expression tag | UNP P0ABE7 |
| C | -98 | TRP | MET | engineered mutation | UNP P0ABE7 |
| C | -3 | ILE | HIS | engineered mutation | UNP P0ABE7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| C | 1 | LEU | ARG | engineered mutation | UNP P0ABE7 |

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2 | G | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 424 | 266 | 75 | 80 | 3 | | |

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | I | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1757 | 1120 | 290 | 335 | 12 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| I | 47 | ASN | SER | engineered mutation | UNP P04899 |
| I | 204 | ALA | GLY | engineered mutation | UNP P04899 |
| I | 246 | ALA | GLU | engineered mutation | UNP P04899 |
| I | 327 | SER | ALA | engineered mutation | UNP P04899 |

- Molecule 4 is a protein called scFv16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | S | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1771 | 1125 | 293 | 343 | 10 | | |

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | T | 338 | Total | C | N | O | S | 0 | 0 |
| | | | 2601 | 1604 | 467 | 509 | 21 | | |

- Molecule 6 is a protein called Relaxin-3 B chain.


| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6 | B | 22 | Total | C | N | O | S | 0 | 0 |
| | | | 174 | 110 | 35 | 27 | 2 | | |

- Molecule 7 is a protein called Relaxin-3 A chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 7 | A | 24 | Total | C | N | O | S | 0 | 0 |
| | | | 131 | 76 | 24 | 27 | 4 | | |

GLU
ARG
LEU
ILE
THR
PRO
ASP
GLY
SER
MET
LEU
PHE
ARG
VAL
THR
ILE
ASN
SER

- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:  87% 13%

S8
A23
A34
A35
D36
L50
S57
E58
N59
P60
F61
R62

- Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-2

Chain I:  50% 11% 38%


MET
GLY
CYS
THR
V5
S6
G27
E28
K29
R32
G40
ALA
GLY
GLU
S44
K54
ILE
ILE
HIS
GLU
GLY
ASP
TYR
SER
GLU
GLU
SER
GLY
VAL
ARG
GLN
TYR
ARG
ALA
VAL
TRP
ALA
ASP
TYR
HIS
SER
ASN
THR
ILE
GLN
SER
PHE
ILE
MET
ALA
VAL
LYS
ALA
MET
GLY
ASN
LEU
ILE
ASP

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

TYR
TYR
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GLU
ARG
ILE
ALA
GLN
SER
ASP
TYR
ILE
PRO
THR
GLN
GLN
ASP
VAL
VAL
LEU
ARG
THR
ARG
VAL
LYS
THR
THR
G184
I185
V186
K193
D201
F224
L228
V234
E237
D238
N242
R243
M244
M248
D252
C255
N256
L267
K272

D273
E276
I279
F288
Y291
N295
E299
Q305
S306
K307
F308
E309
D310
L311
K318
H323
F324
F325
C326
D329
F335
F336
V336
F337
D342
K346
C352
F355


- Molecule 4: scFv16

Chain S:  77% 15% 7%

MET
V2
E6
V12
L20
F27
A28
F29
M34
H35
W36
Q39
A40
K43
V48
I51
S52
T57
I58
V64
R67
I70
L79
M83
L86
R87
S88
E89
D90
Y95
T115
S120
ALA
GLY
GLY
GLY
SER
GLY
GLY

GLY
SER
GLY
GLY
GLY
SER
ALA
D137
I157
H167
T172
R180
L188
V199
R202
F212
E220
E222
T243
K244
L245
E246
L247

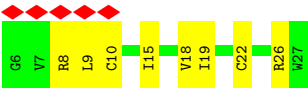
- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain T:  83% 17%

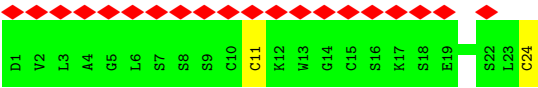
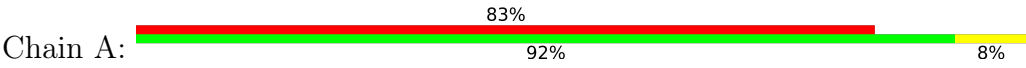
E3
Q6
Q9
I18
R22
C25
A26
D27
L30
T34
D38
I43
Q44
M45
L51
L55
M61
V71
Q75
L79
I93
W99
V100
V112
D118
N119
Y124
T128
N132
V135
G144
L152
D153
Q156

S161
G162
D163
L192
T196
F199
C204
D228
T243
C250
R251
R256
Q259
E260
L261
M262
T263
H266
I269
L270
C271
T274
L286
Y289
D290
V296
L300
V315
S316
C317
M325
A326
V327
L336
W339
R340

- Molecule 6: Relaxin-3 B chain



● Molecule 7: Relaxin-3 A chain



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 364523 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 80 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 2200 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 2.708 | Depositor |
| Minimum map value | -0.002 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.019 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (\AA) | 274.176, 274.176, 274.176 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.071, 1.071, 1.071 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | C | 0.26 | 0/2496 | 0.48 | 0/3389 |
| 2 | G | 0.16 | 0/430 | 0.28 | 0/580 |
| 3 | I | 0.23 | 0/1787 | 0.39 | 0/2397 |
| 4 | S | 0.22 | 0/1815 | 0.40 | 0/2461 |
| 5 | T | 0.27 | 0/2648 | 0.41 | 0/3589 |
| 6 | B | 0.19 | 0/177 | 0.44 | 0/234 |
| 7 | A | 0.17 | 0/130 | 0.52 | 0/175 |
| All | All | 0.24 | 0/9483 | 0.42 | 0/12825 |

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 | C | 2435 | 0 | 2538 | 91 | 0 |
| 2 | G | 424 | 0 | 436 | 6 | 0 |
| 3 | I | 1757 | 0 | 1737 | 27 | 0 |
| 4 | S | 1771 | 0 | 1709 | 22 | 0 |
| 5 | T | 2601 | 0 | 2505 | 39 | 0 |
| 6 | B | 174 | 0 | 173 | 8 | 0 |
| 7 | A | 131 | 0 | 87 | 4 | 0 |
| All | All | 9293 | 0 | 9185 | 177 | 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 10.

The worst 5 of 177 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:I:255:CYS:O | 3:I:318:LYS:NZ | 2.20 | 0.74 |
| 3:I:272:LYS:HD3 | 3:I:324:PHE:HB3 | 1.69 | 0.73 |
| 5:T:161:SER:OG | 5:T:163:ASP:OD1 | 2.07 | 0.73 |
| 1:C:297:ARG:O | 1:C:320:ARG:NH2 | 2.22 | 0.72 |
| 5:T:25:CYS:SG | 5:T:259:GLN:NE2 | 2.65 | 0.70 |

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 | C | 301/773 (39%) | 271 (90%) | 29 (10%) | 1 (0%) | 37 | 65 |
| 2 | G | 53/55 (96%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 3 | I | 213/355 (60%) | 198 (93%) | 15 (7%) | 0 | 100 | 100 |
| 4 | S | 226/248 (91%) | 216 (96%) | 10 (4%) | 0 | 100 | 100 |
| 5 | T | 336/338 (99%) | 322 (96%) | 14 (4%) | 0 | 100 | 100 |
| 6 | B | 20/22 (91%) | 19 (95%) | 1 (5%) | 0 | 100 | 100 |
| 7 | A | 22/24 (92%) | 21 (96%) | 1 (4%) | 0 | 100 | 100 |
| All | All | 1171/1815 (64%) | 1100 (94%) | 70 (6%) | 1 (0%) | 50 | 76 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 145 | ASP |

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 | C | 266/636 (42%) | 264 (99%) | 2 (1%) | 79 | 92 |
| 2 | G | 45/45 (100%) | 45 (100%) | 0 | 100 | 100 |
| 3 | I | 193/309 (62%) | 193 (100%) | 0 | 100 | 100 |
| 4 | S | 195/199 (98%) | 195 (100%) | 0 | 100 | 100 |
| 5 | T | 281/281 (100%) | 279 (99%) | 2 (1%) | 81 | 93 |
| 6 | B | 17/17 (100%) | 17 (100%) | 0 | 100 | 100 |
| 7 | A | 8/21 (38%) | 8 (100%) | 0 | 100 | 100 |
| All | All | 1005/1508 (67%) | 1001 (100%) | 4 (0%) | 88 | 96 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 160 | MET |
| 1 | C | 406 | ARG |
| 5 | T | 243 | THR |
| 5 | T | 250 | CYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | S | 3 | GLN |
| 4 | S | 142 | GLN |
| 5 | T | 340 | ASN |
| 5 | T | 6 | GLN |
| 2 | G | 18 | GLN |

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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.

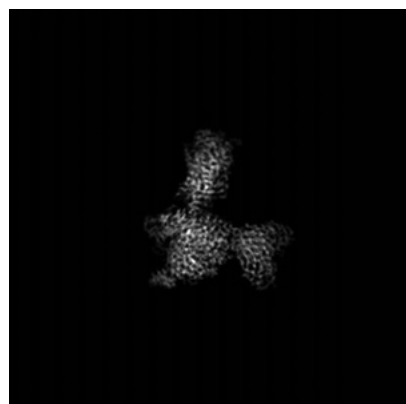
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62297. These allow visual inspection of the internal detail of the map and identification of artifacts.

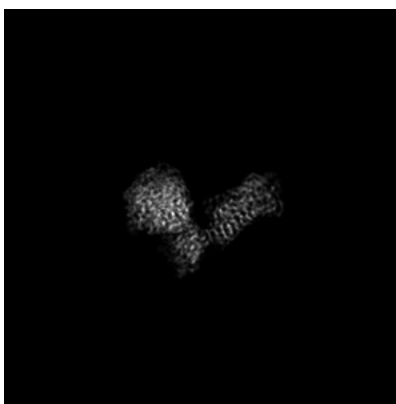
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

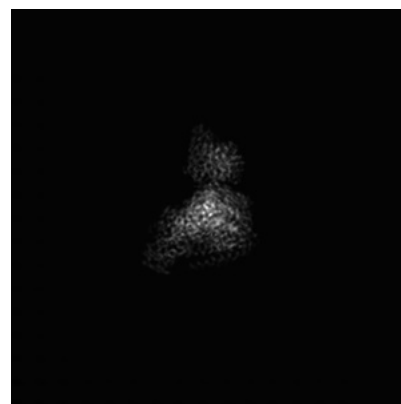
6.1.1 Primary map



X

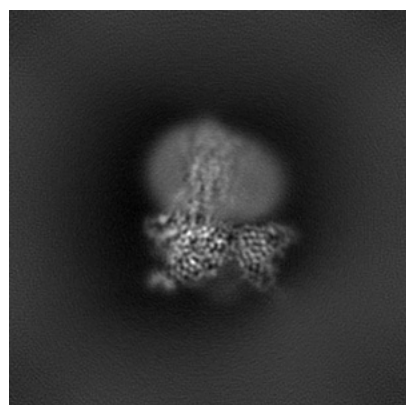


Y

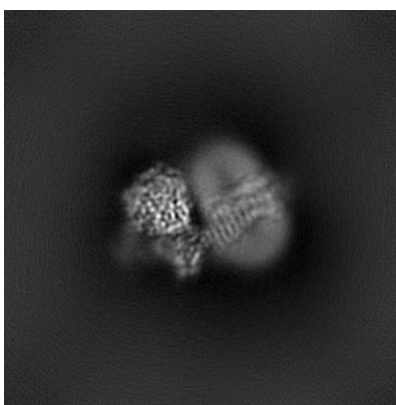


Z

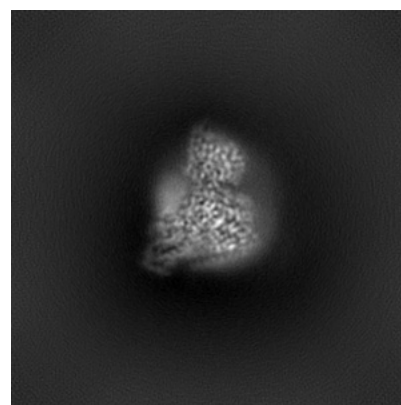
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

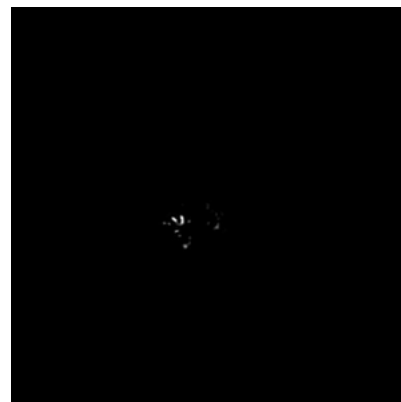
6.2.1 Primary map



X Index: 128

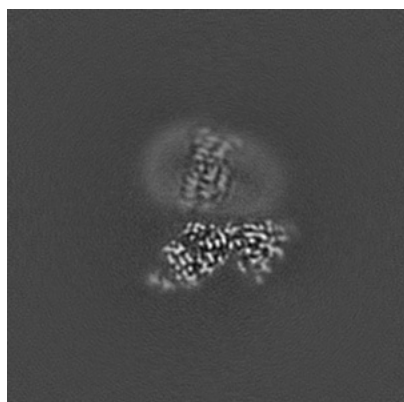


Y Index: 128

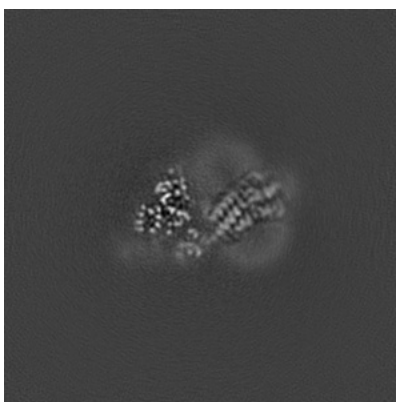


Z Index: 128

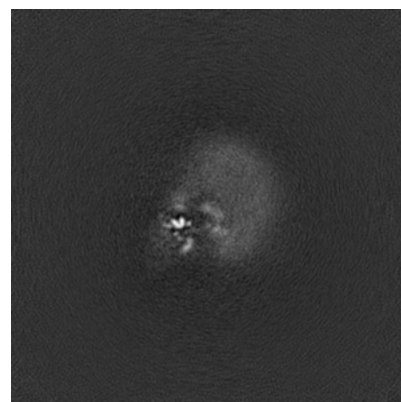
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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: 128

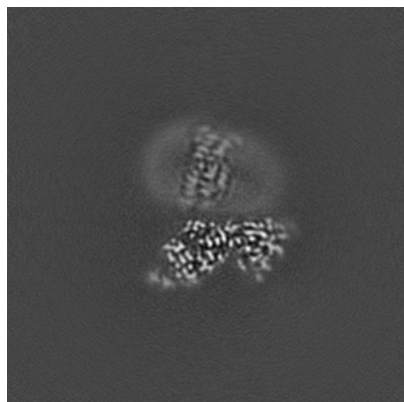


Y Index: 126

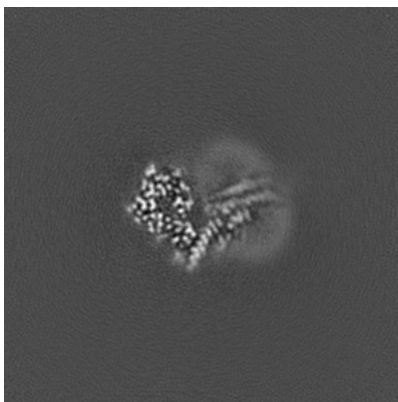


Z Index: 107

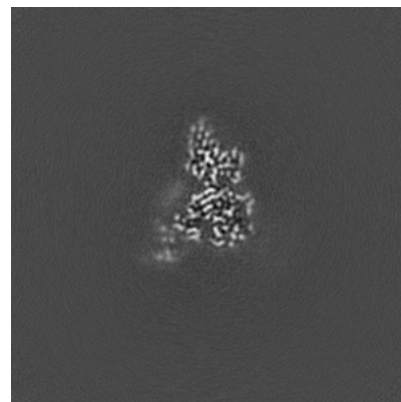
6.3.2 Raw map



X Index: 128



Y Index: 117

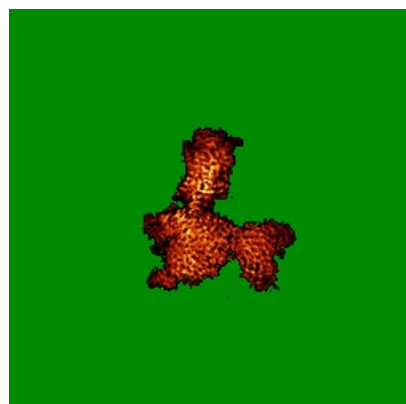


Z Index: 107

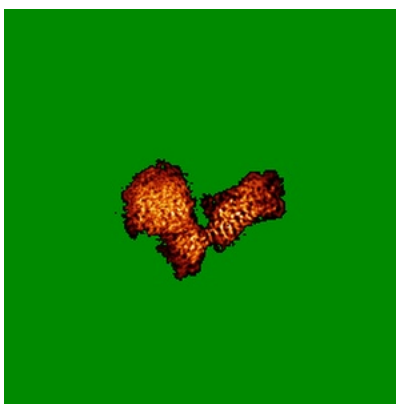
The images above show the largest variance slices of the map in three orthogonal directions.

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

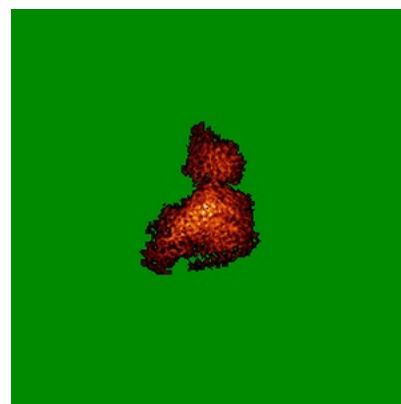
6.4.1 Primary map



X

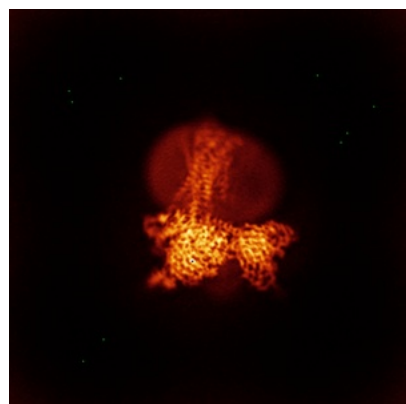


Y

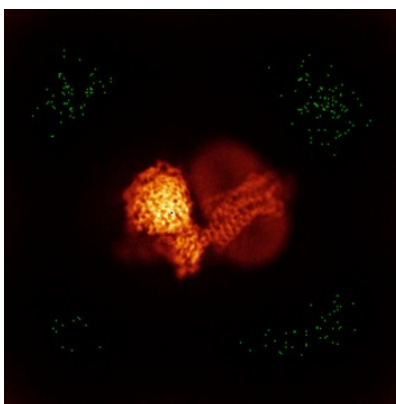


Z

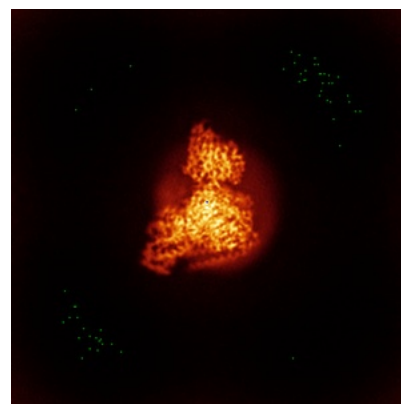
6.4.2 Raw map



X



Y

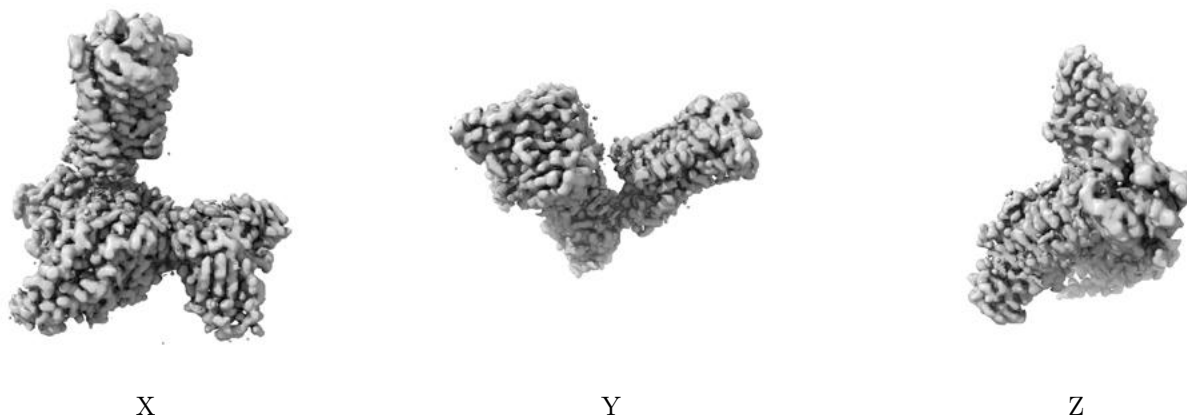


Z

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.

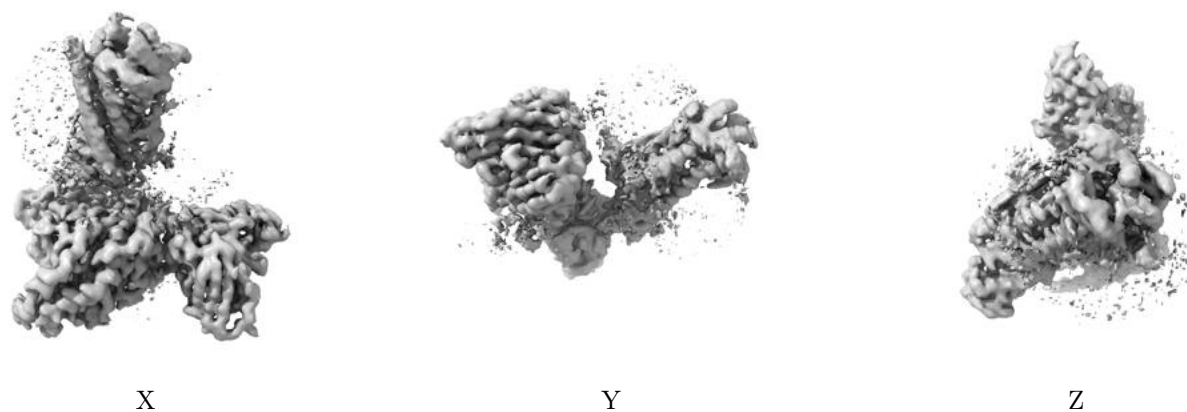
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

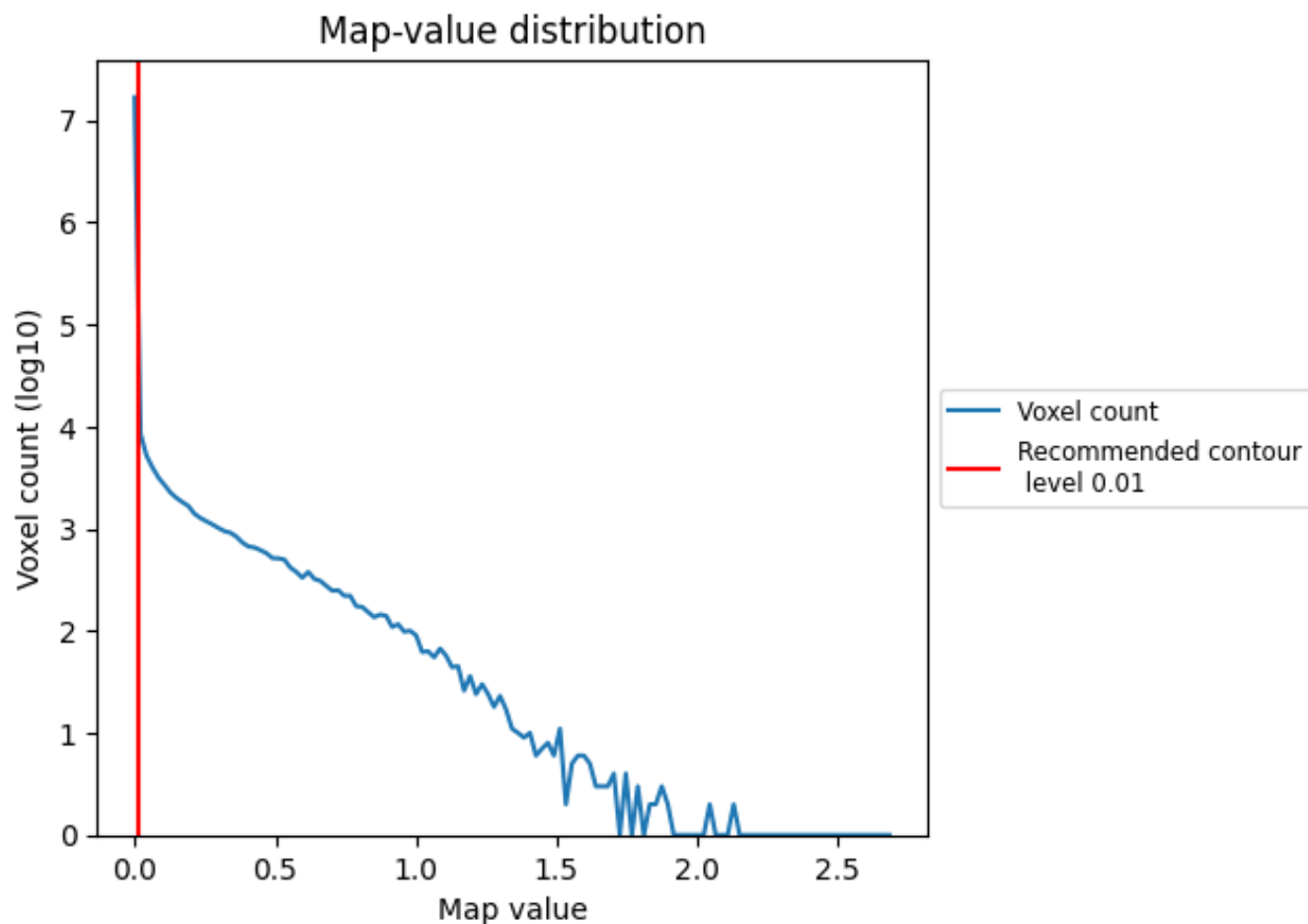
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

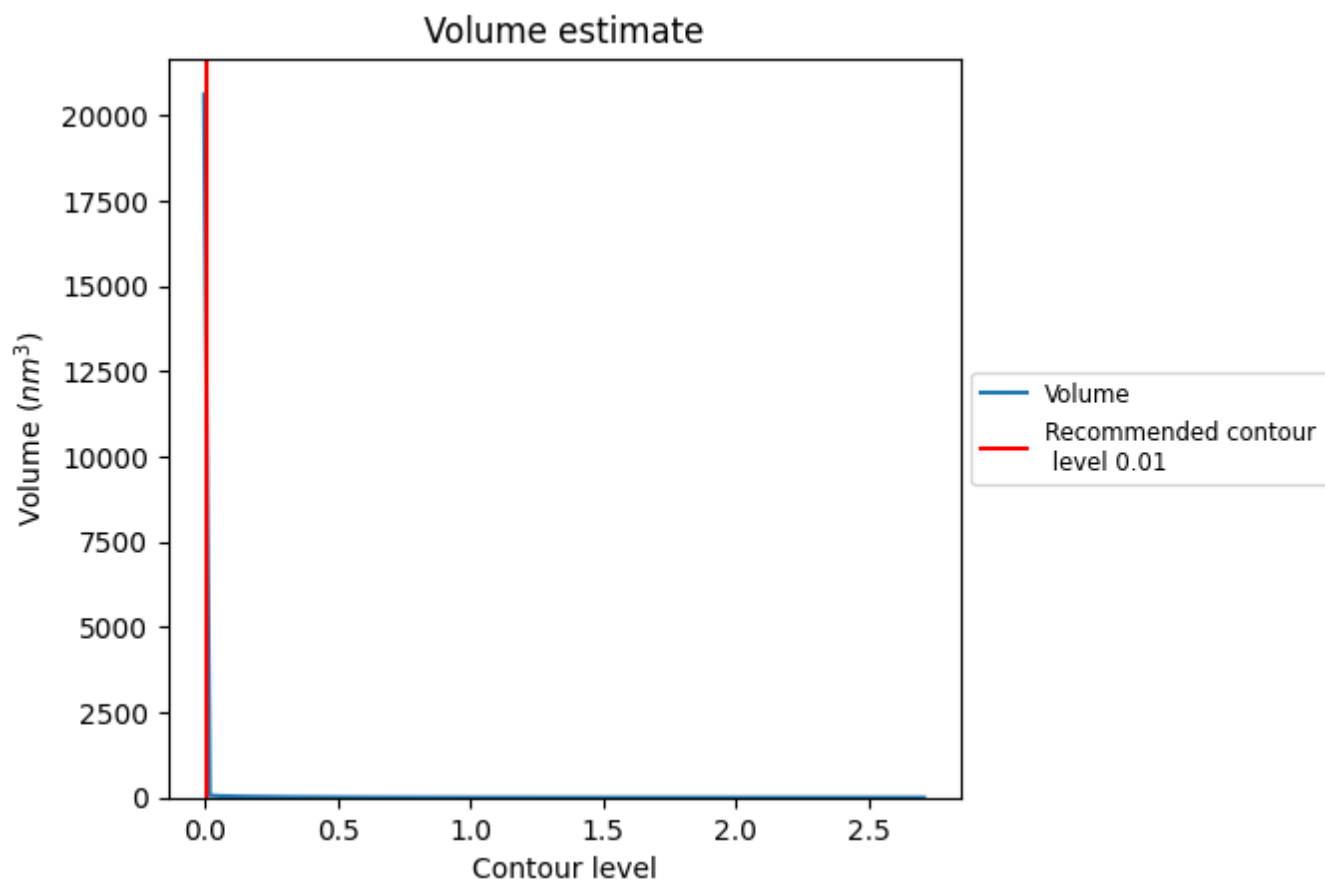
This section contains the results of statistical analysis of the map.

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.

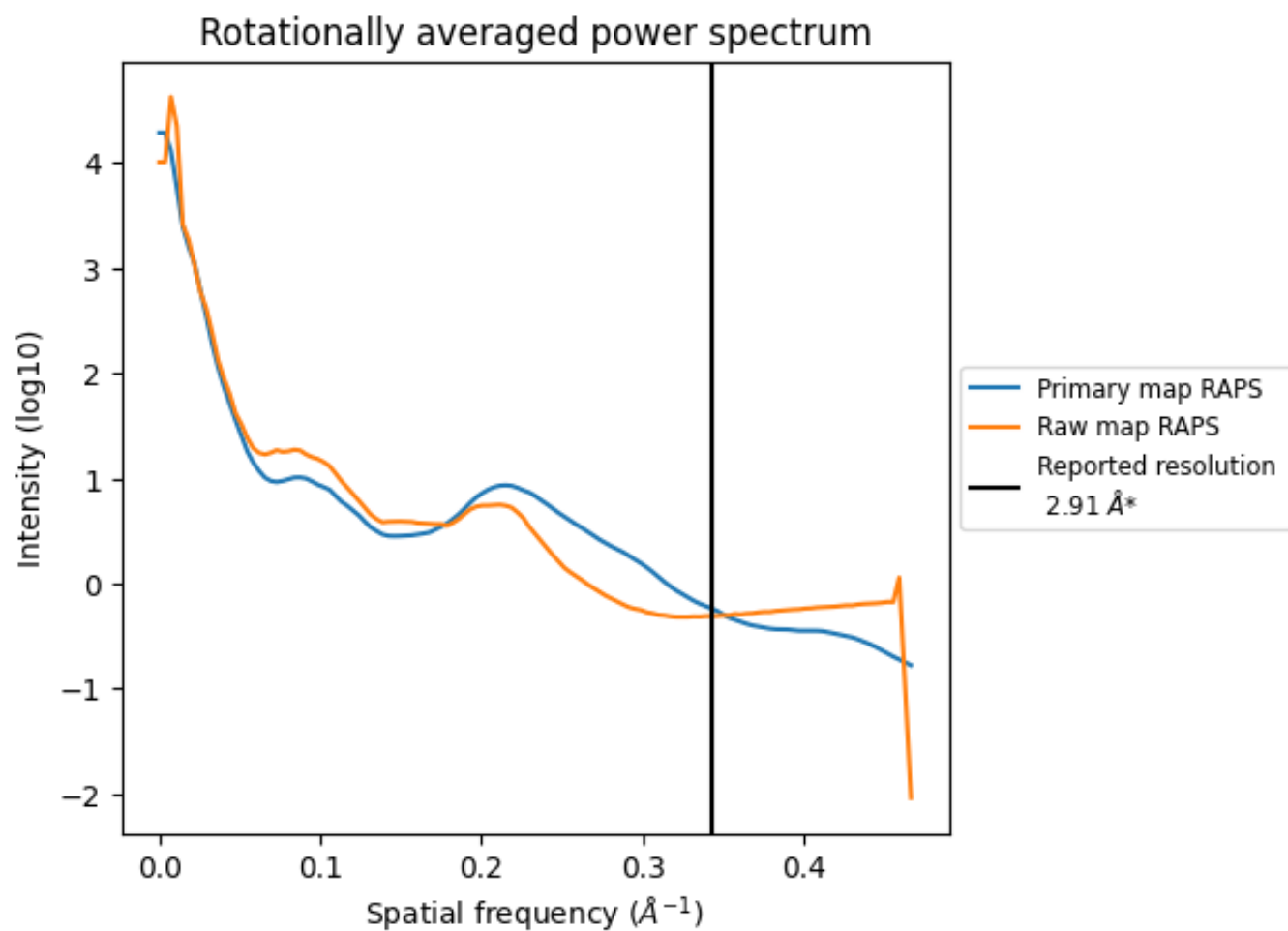
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9180 nm³; this corresponds to an approximate mass of 8293 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 ⓘ

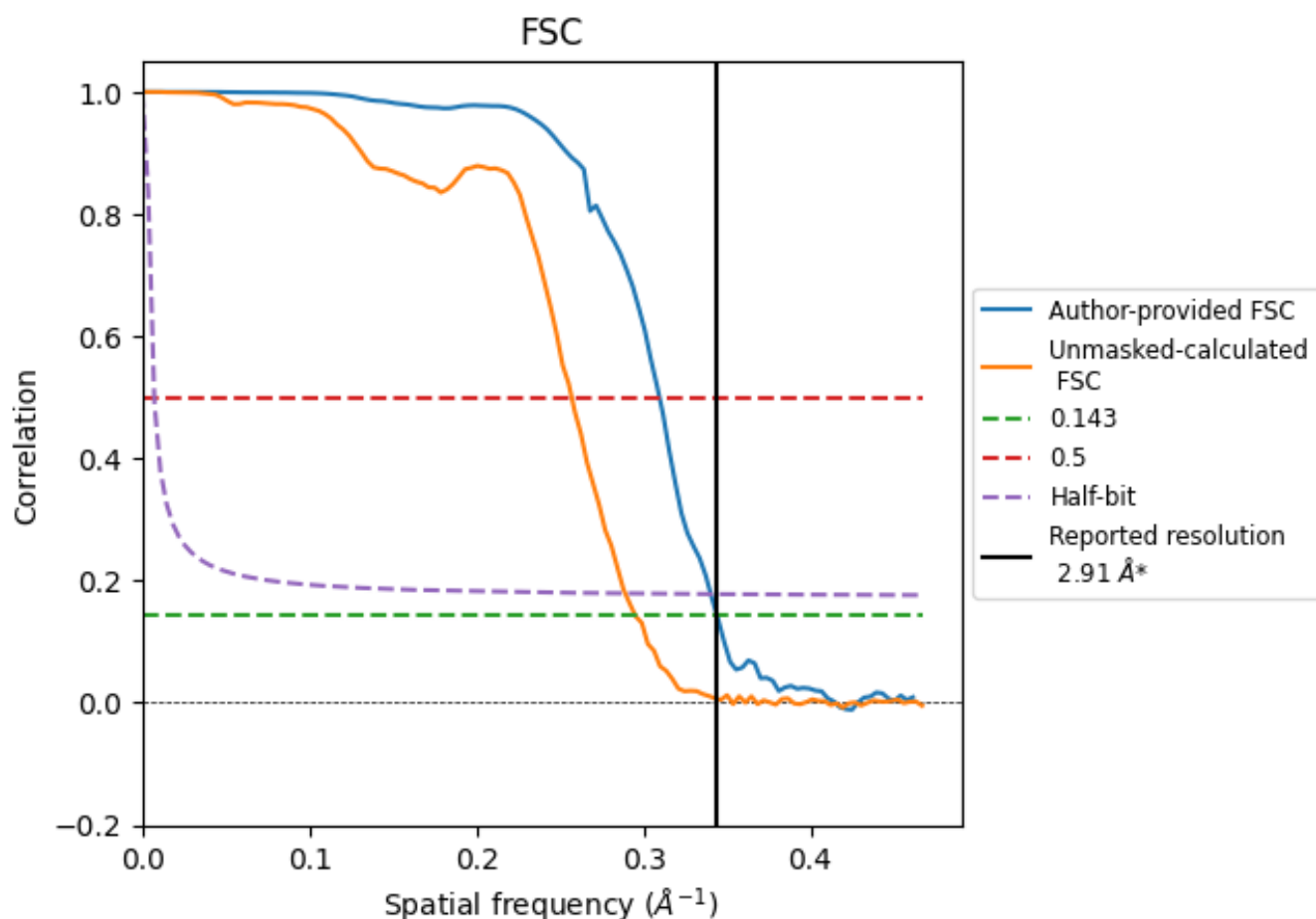


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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 0.344 \AA^{-1}

8.2 Resolution estimates

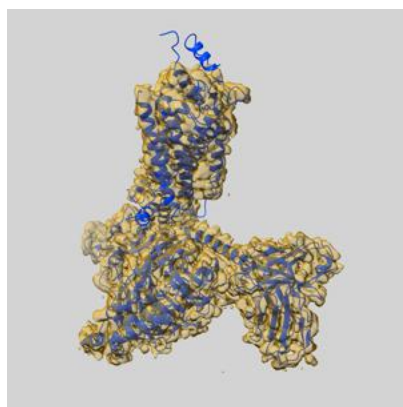
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.91 | - | - |
| Author-provided FSC curve | 2.91 | 3.23 | 2.94 |
| Unmasked-calculated* | 3.39 | 3.89 | 3.46 |

*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 3.39 differs from the reported value 2.91 by more than 10 %

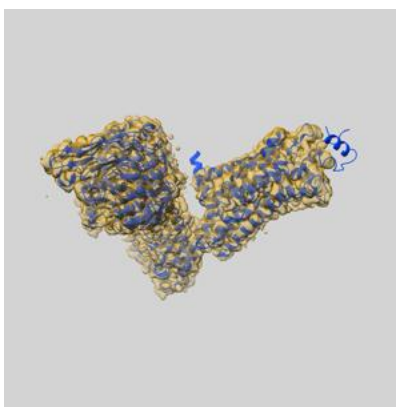
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62297 and PDB model 9KFI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

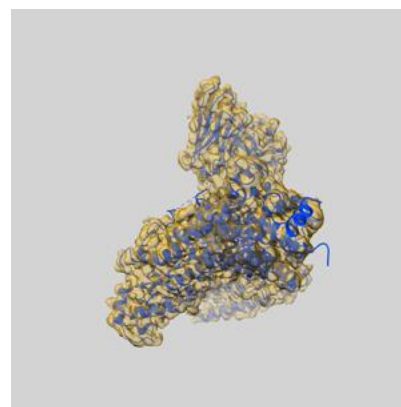
9.1 Map-model overlay [i](#)



X



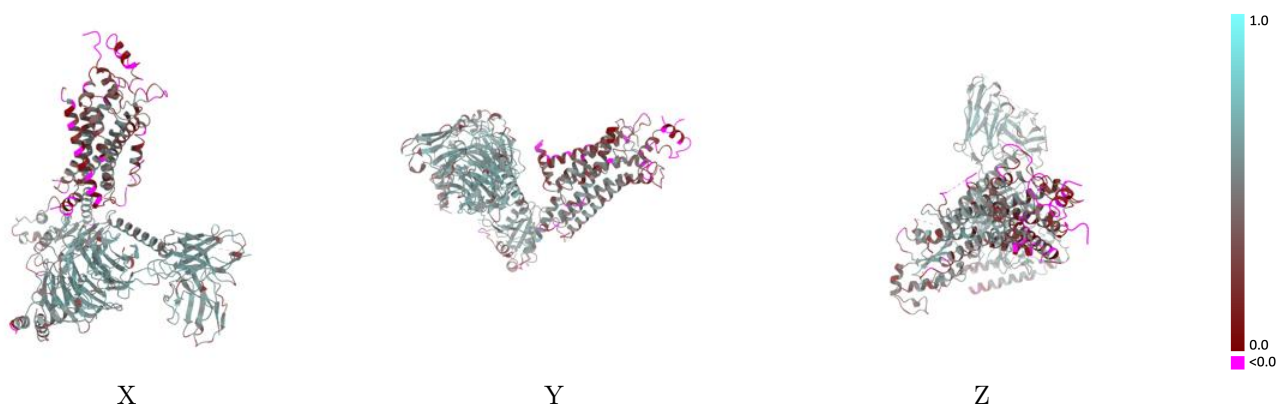
Y



Z

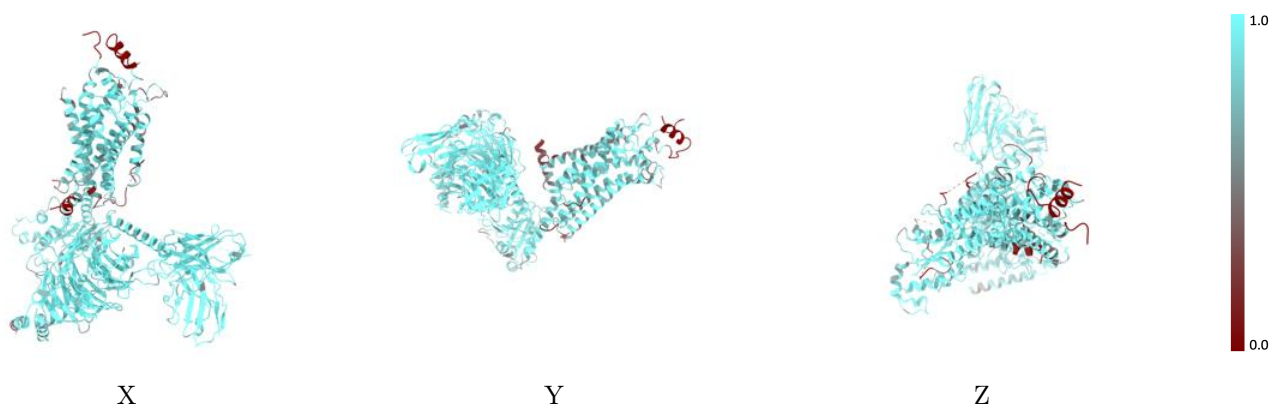
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



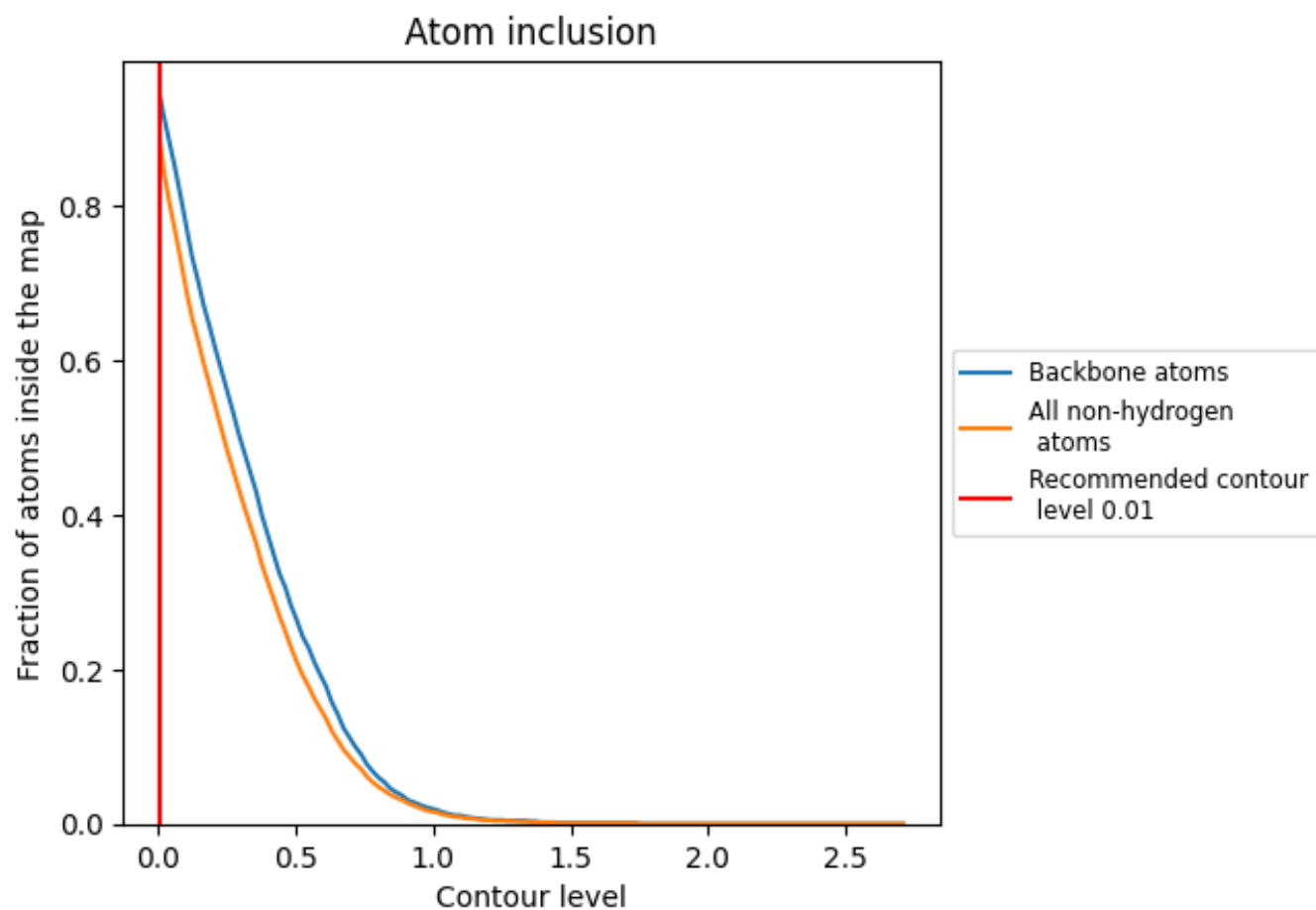
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|---------------------|
| All | <div></div> 0.8790 | <div></div> 0.4540 |
| A | <div></div> 0.1910 | <div></div> -0.0120 |
| B | <div></div> 0.7150 | <div></div> 0.2610 |
| C | <div></div> 0.7810 | <div></div> 0.3000 |
| G | <div></div> 0.8660 | <div></div> 0.4460 |
| I | <div></div> 0.9030 | <div></div> 0.4720 |
| S | <div></div> 0.9450 | <div></div> 0.5370 |
| T | <div></div> 0.9550 | <div></div> 0.5660 |

1.0

0.0

<0.0