wwPDB EM Validation Summary Report (i)

Jan 11, 2024 – 04:14 PM JST

PDB ID	:	8JHI
EMDB ID	:	EMD-36266
Title	:	FZD3-Gs complex
Authors	:	Xu, F.; Zhang, Z.
Deposited on	:	2023-05-23
Resolution	:	3.20 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.

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

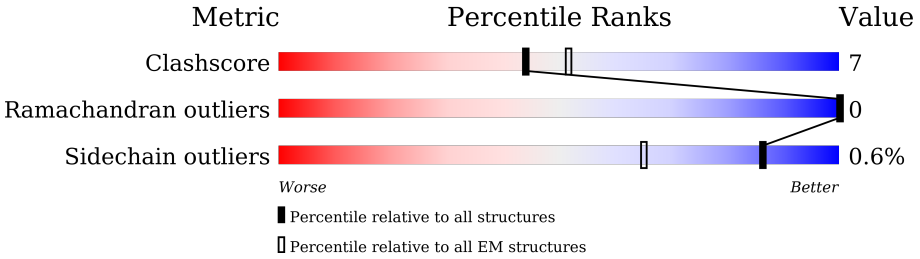
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	248	85% 10% 5%
2	B	337	79% 21%
3	C	57	14% 88% 12%
4	N	126	75% 25%
5	R	520	6% 50% 12% 38%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8562 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	235	1953	1230	355	358	10	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	expression tag	UNP Q5JWF2
A	2	SER	-	expression tag	UNP Q5JWF2
A	3	LYS	-	expression tag	UNP Q5JWF2
A	4	THR	-	expression tag	UNP Q5JWF2
A	5	GLU	-	expression tag	UNP Q5JWF2
A	6	ASP	-	expression tag	UNP Q5JWF2
A	44	ASP	GLY	engineered mutation	UNP Q5JWF2
A	45	ASN	GLU	engineered mutation	UNP Q5JWF2
A	196	GLY	-	linker	UNP Q5JWF2
A	197	GLY	-	linker	UNP Q5JWF2
A	198	SER	-	linker	UNP Q5JWF2
A	199	GLY	-	linker	UNP Q5JWF2
A	200	GLY	-	linker	UNP Q5JWF2
A	201	SER	-	linker	UNP Q5JWF2
A	202	GLY	-	linker	UNP Q5JWF2
A	203	GLY	-	linker	UNP Q5JWF2
A	249	ASP	ALA	engineered mutation	UNP Q5JWF2
A	252	ASP	SER	engineered mutation	UNP Q5JWF2
A	?	-	ASN	deletion	UNP Q5JWF2
A	?	-	MET	deletion	UNP Q5JWF2
A	?	-	VAL	deletion	UNP Q5JWF2
A	?	-	ILE	deletion	UNP Q5JWF2
A	?	-	ARG	deletion	UNP Q5JWF2
A	?	-	GLU	deletion	UNP Q5JWF2
A	?	-	ASP	deletion	UNP Q5JWF2
A	?	-	ASN	deletion	UNP Q5JWF2
A	?	-	GLN	deletion	UNP Q5JWF2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q5JWF2
A	372	ALA	ILE	engineered mutation	UNP Q5JWF2
A	375	ILE	VAL	engineered mutation	UNP Q5JWF2

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	337	2592	1599	466	506	21	0	0

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	57	436	273	77	83	3	0	0

- Molecule 4 is a protein called Nb35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	126	962	599	168	189	6	0	0

- Molecule 5 is a protein called Frizzled-3.

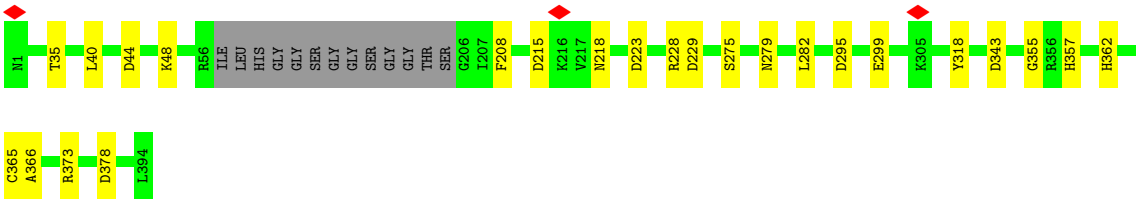
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	322	2619	1753	413	430	23	1	0

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.

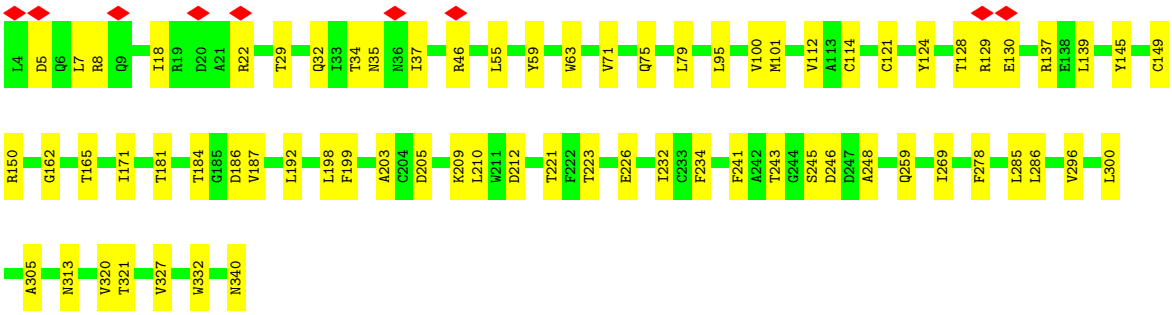
• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas

Chain A:



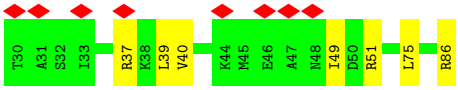
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



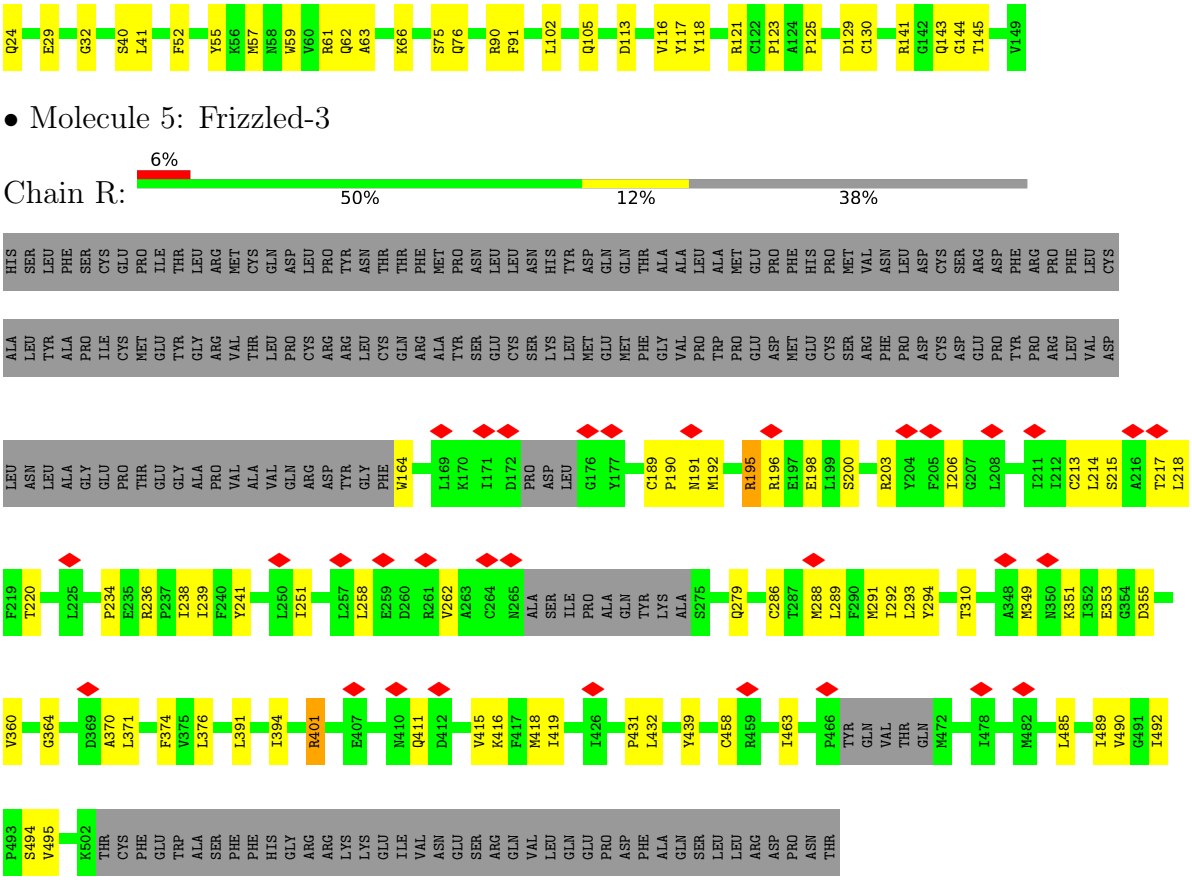
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



• Molecule 4: Nb35

Chain N:


Q24 E29 G32 S40 L41 F52 Y55 K56 M57 N58 W59 V60 R61 Q62 A63 K66 S75 Q76 R90 F91 L102 Q105 D113 V116 Y117 Y118 R121 C122 P123 A124 P125 D129 C130 R141 G142 Q143 G144 T145 V149
• Molecule 5: Frizzled-3
Chain R:
6%
50%
12%
38%
HIS SER LEU PHE SER CYS GLU PRO ILE THR LEU ARG MET CYS GLN ASP LEU PRO TYR ASN THR THR PHE MET PRO ASN LEU LEU ASN HIS TYR ASP GLN GLN THR ALA ALA LEU ALA MET GLU PRO PHE HIS PRO MET VAL ASN LEU ASP CYS SER ARG ASP PHE ARG PRO PHE LEU CYS
ALA LEU TYR ALA PRO ILE CYS MET GLU TYR GLY ARG VAL THR LEU PRO CYS ARG ARG LEU CYS GLN ARG ALA TYR SER GLU CYS SER LYS LEU MET GLU MET PHE GLY VAL PRO TRP PRO GLU ASP MET GLU CYS SER ARG PHE PRO ASP CYS ASP GLU PRO TYR PRO ARG LEU VAL ASP
LEU ASN LEU ALA GLY GLU PRO THR GLU GLY ALA PRO VAL ALA VAL GLN ARG ASP TYR GLY PHE W164 L169 K170 I171 D172 PRO ASP LEU G176 Y177 C189 P190 N191 M192 R195 R196 E197 E198 L199 S200 R203 Y204 F205 I206 G207 L208 I211 I212 C213 L214 S215 A216 T217 L218
F219 T220 L225 P234 E235 R236 P237 I238 I239 F240 Y241 L250 I251 L257 L258 E259 D260 R261 V262 A263 C264 N265 ALA SER ILE PRO ALA GLN TYR LYS ALA S275 Q279 C286 T287 M288 L289 F290 M291 I292 L293 Y294 T310 A348 M349 N350 K351 I352 E353 G354 D355
V360 G364 D369 A370 L371 F374 V375 L376 L391 I394 R401 E407 M410 Q411 D412 V415 K416 F417 M418 I419 T426 P431 L432 Y439 C458 R459 I463 P466 TYR GLN VAL THR GLN M472 I478 M482 L485 I489 V490 G491 I492
P493 S494 V495 K502 THR CYS PHE GLU TRP ALA SER PHE PHE HIS GLY ARG ARG LYS LYS GLU ILE VAL ASN GLU SER ARG GLN VAL LEU GLN GLU PRO ASP PHE ALA GLN SER LEU LEU ARG ASP PRO ASN THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141786	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 ($e^-/Å^2$)	20	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	0.756	Depositor
Minimum map value	-0.466	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.074	Depositor
Map size (Å)	239.616, 239.616, 239.616	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	A	0.26	0/1990	0.53	0/2670
2	B	0.28	0/2639	0.55	0/3577
3	C	0.24	0/442	0.50	0/597
4	N	0.32	0/982	0.56	0/1329
5	R	0.28	0/2680	0.57	1/3635 (0.0%)
All	All	0.28	0/8733	0.55	1/11808 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	286	CYS	CA-CB-SG	5.18	123.33	114.00

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	A	1953	0	1943	15	0
2	B	2592	0	2499	45	0
3	C	436	0	448	5	0
4	N	962	0	925	22	0
5	R	2619	0	2678	38	0
All	All	8562	0	8493	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 118 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)
5:R:292:ILE:C	5:R:293:LEU:CA	2.45	0.85
5:R:215:SER:O	5:R:218:LEU:HB3	1.83	0.79
5:R:251:ILE:HD11	5:R:292:ILE:HG23	1.77	0.66
4:N:32:GLY:HA2	4:N:41:LEU:HD21	1.78	0.65
4:N:55:TYR:HE1	4:N:125:PRO:HA	1.61	0.65

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	231/248 (93%)	221 (96%)	10 (4%)	0	100	100
2	B	335/337 (99%)	319 (95%)	16 (5%)	0	100	100
3	C	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
4	N	124/126 (98%)	118 (95%)	6 (5%)	0	100	100
5	R	313/520 (60%)	289 (92%)	24 (8%)	0	100	100
All	All	1058/1288 (82%)	1001 (95%)	57 (5%)	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	212/219 (97%)	212 (100%)	0	100	100
2	B	280/280 (100%)	277 (99%)	3 (1%)	73	88
3	C	46/46 (100%)	45 (98%)	1 (2%)	52	79
4	N	104/104 (100%)	104 (100%)	0	100	100
5	R	285/464 (61%)	283 (99%)	2 (1%)	84	94
All	All	927/1113 (83%)	921 (99%)	6 (1%)	86	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	86	ARG
5	R	195	ARG
5	R	401	ARG
2	B	129	ARG
2	B	46	ARG

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)

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.

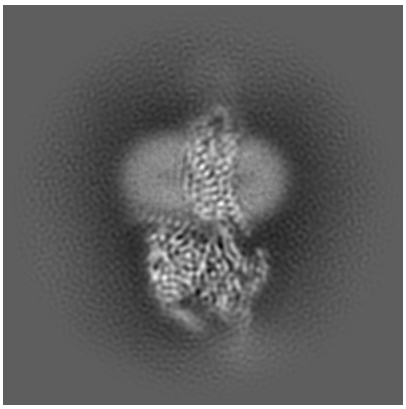
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-36266. These allow visual inspection of the internal detail of the map and identification of artifacts.

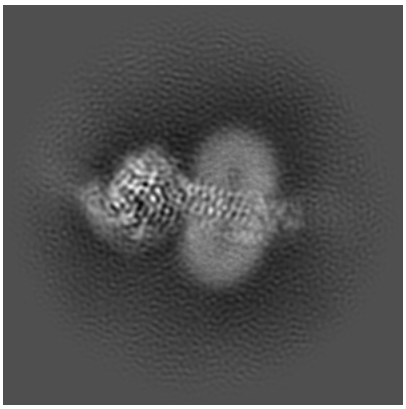
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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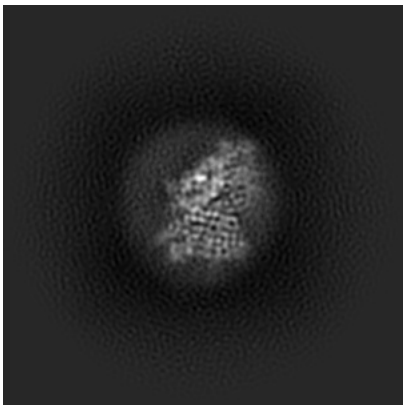
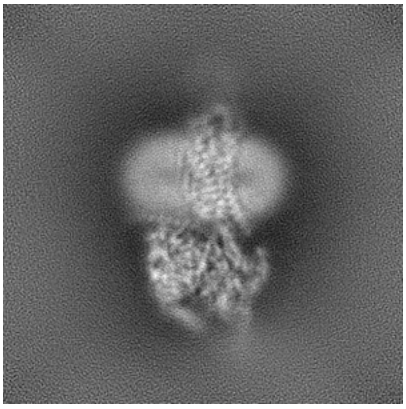


Z

6.1.2 Raw map



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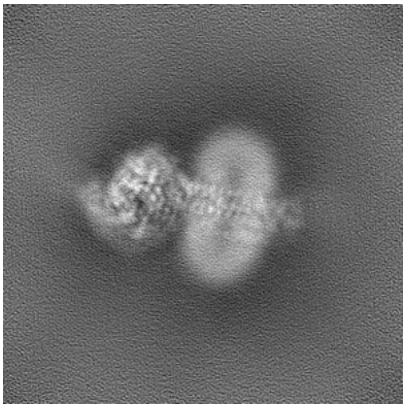
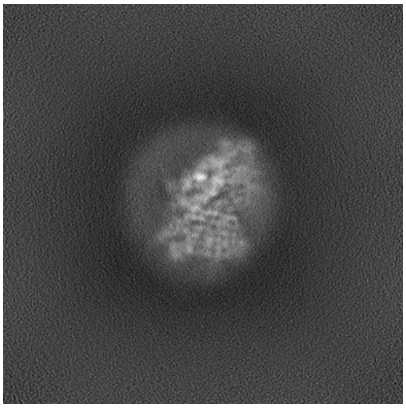


Y

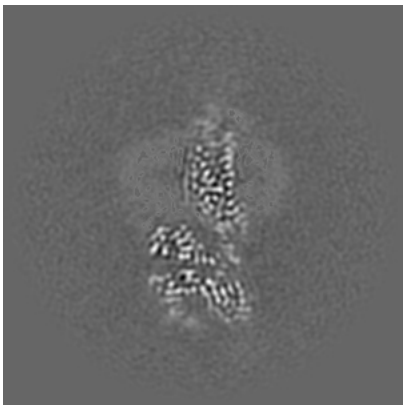


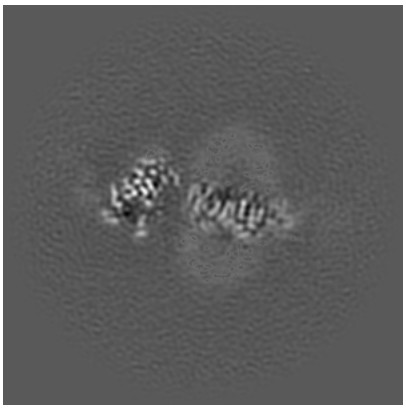
Z

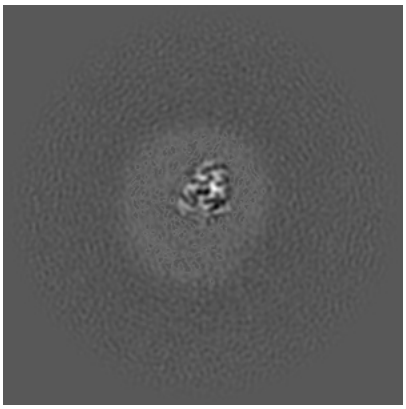
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 144


Y Index: 144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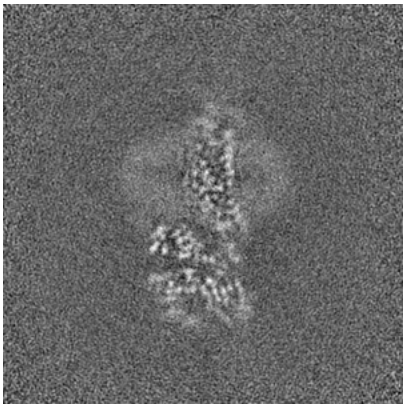
6.2.2 Raw map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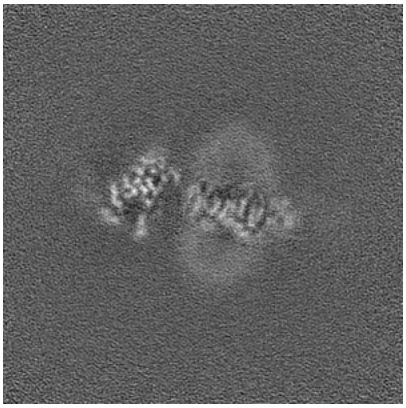
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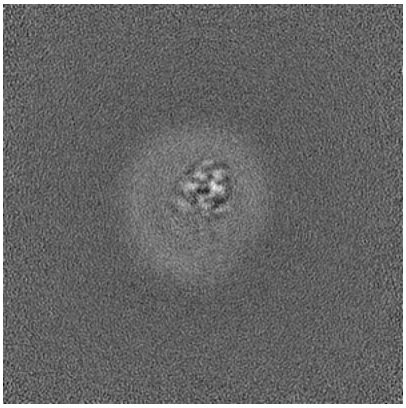
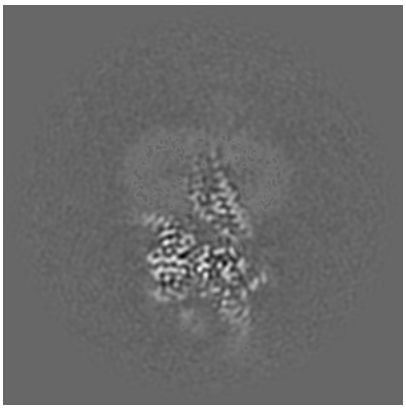

Z Index: 144

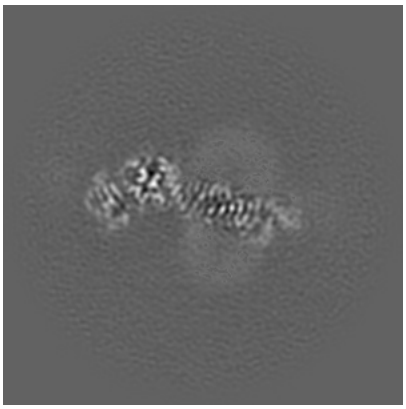
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

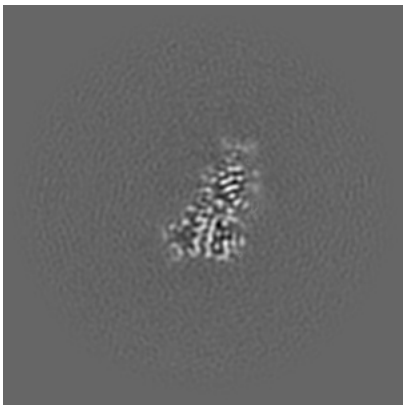
6.3.1 Primary map



X Index: 155

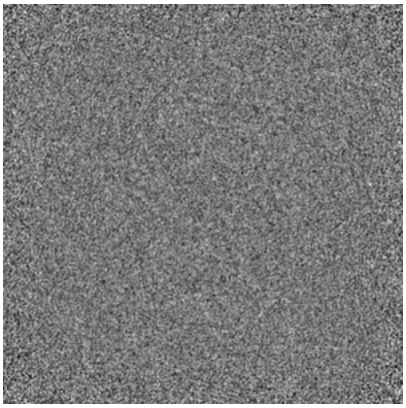


Y Index: 160

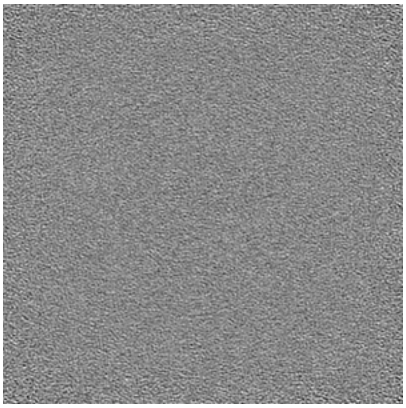


Z Index: 107

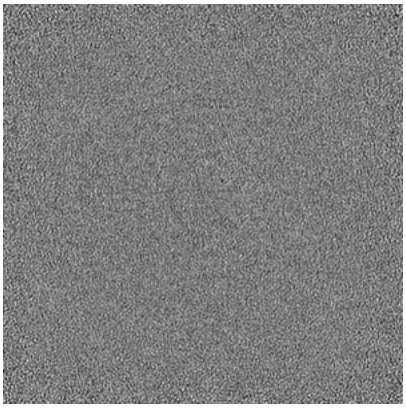
6.3.2 Raw map



X Index: 0



Y Index: 0

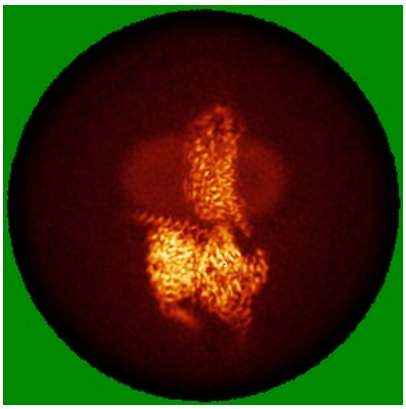


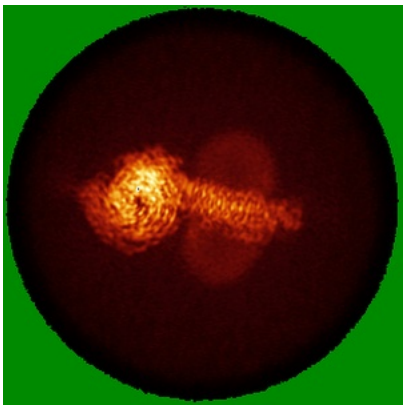
Z Index: 287

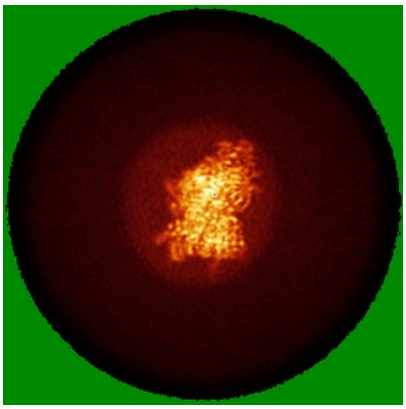
The images above show the largest variance slices of the map in three orthogonal directions.

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

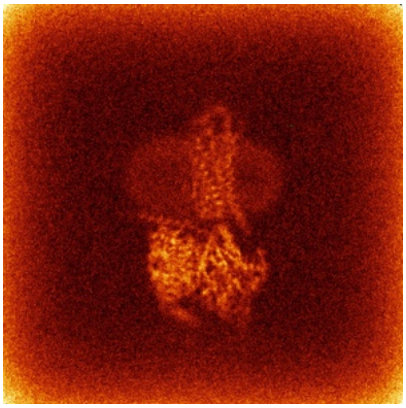
6.4.1 Primary map

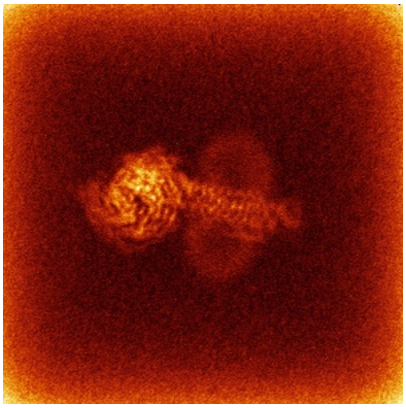

X

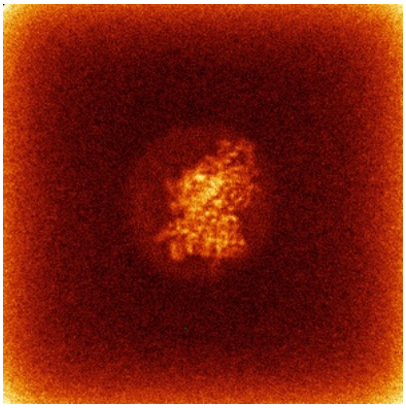

Y


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.

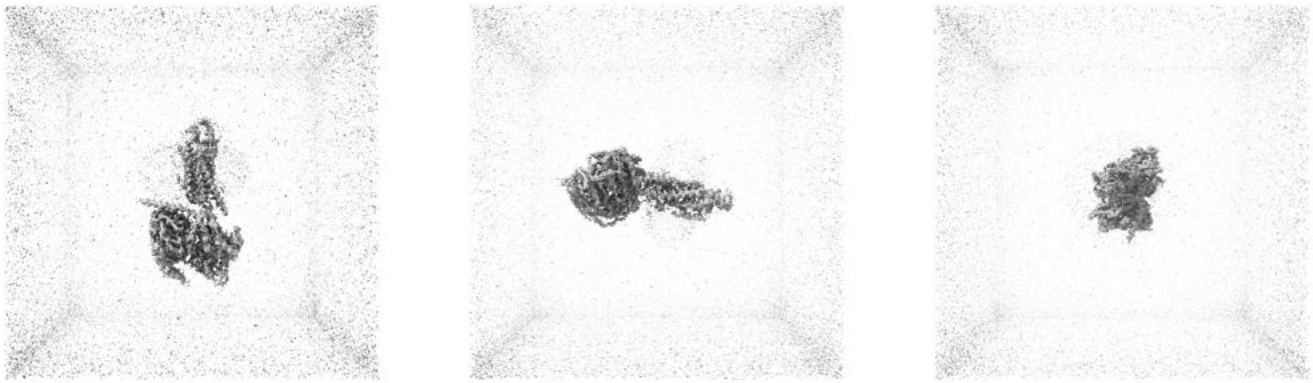
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.074. 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



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.

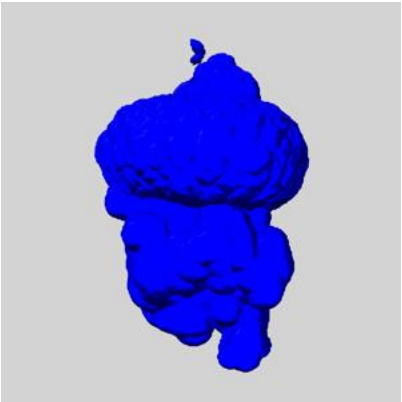
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

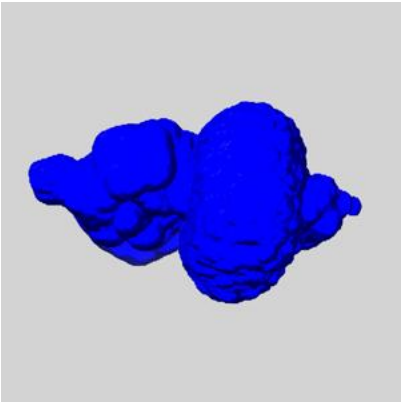
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

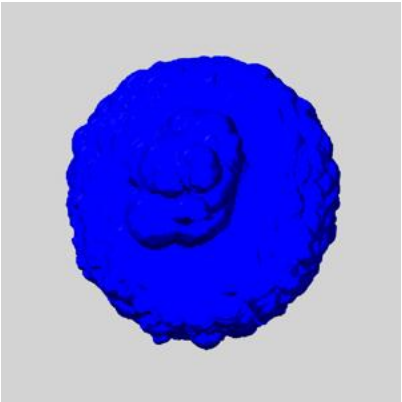
6.6.1 emd_36266_msk_1.map (i)



X



Y

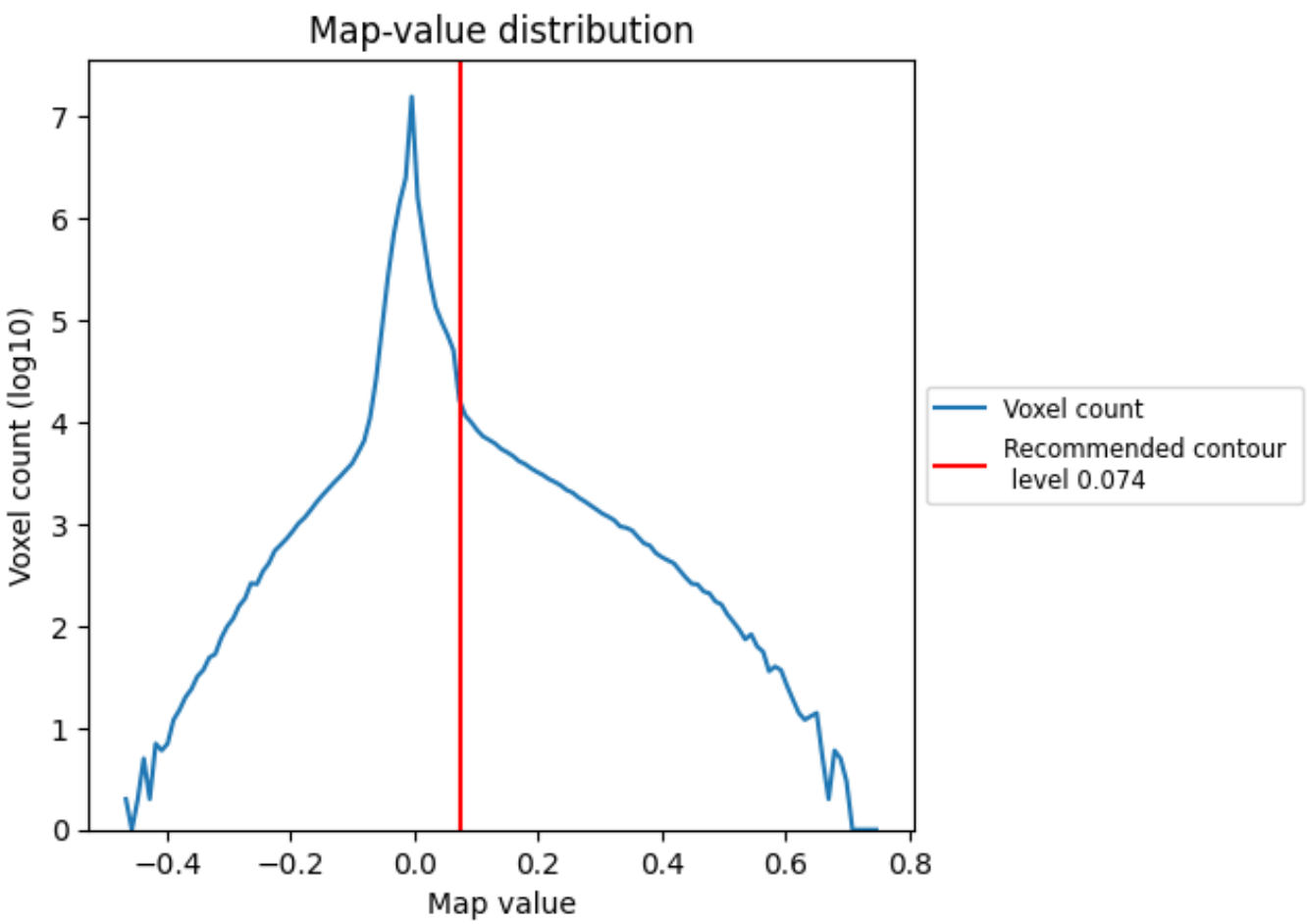


Z

7 Map analysis (i)

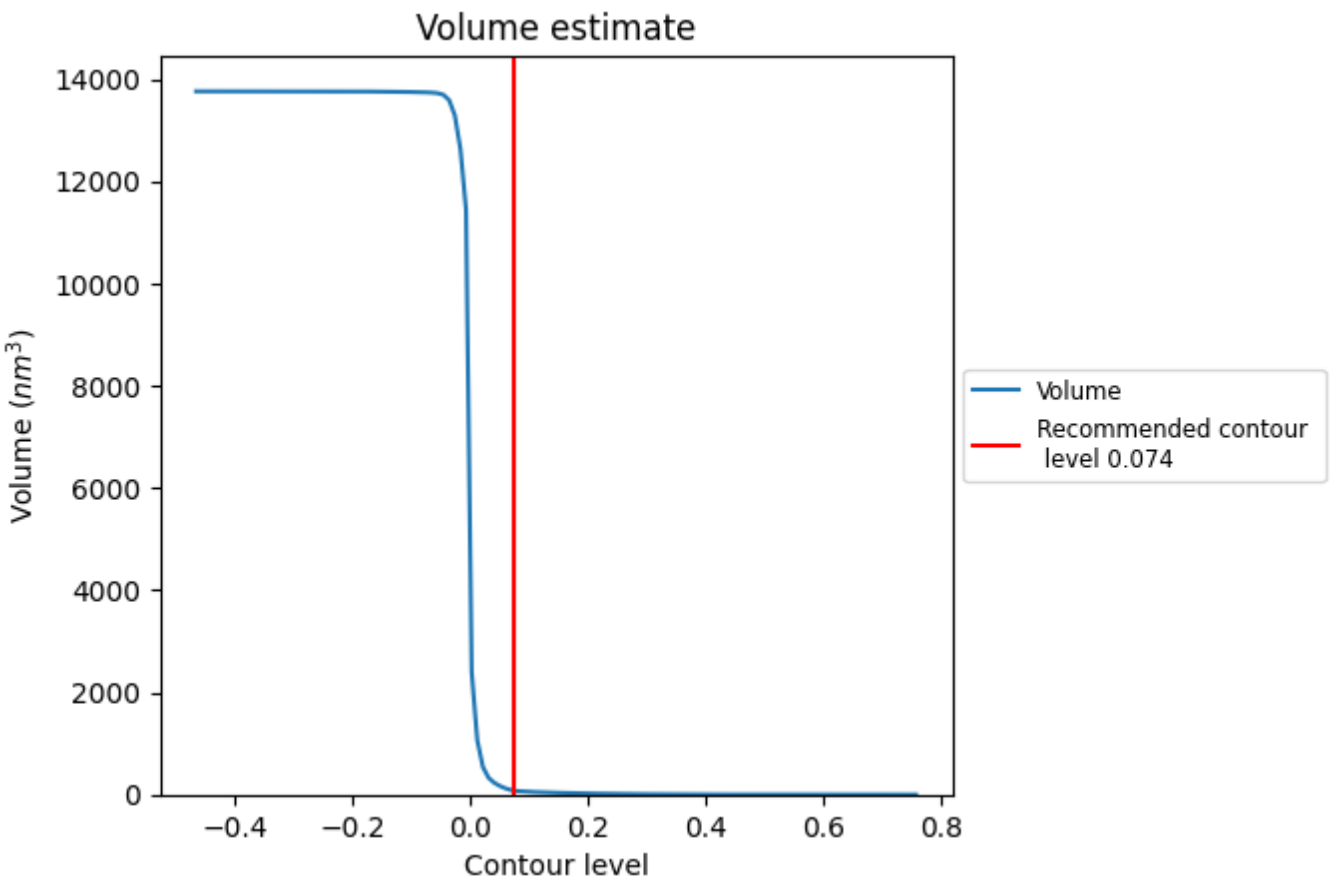
This section contains the results of statistical analysis of the map.

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.

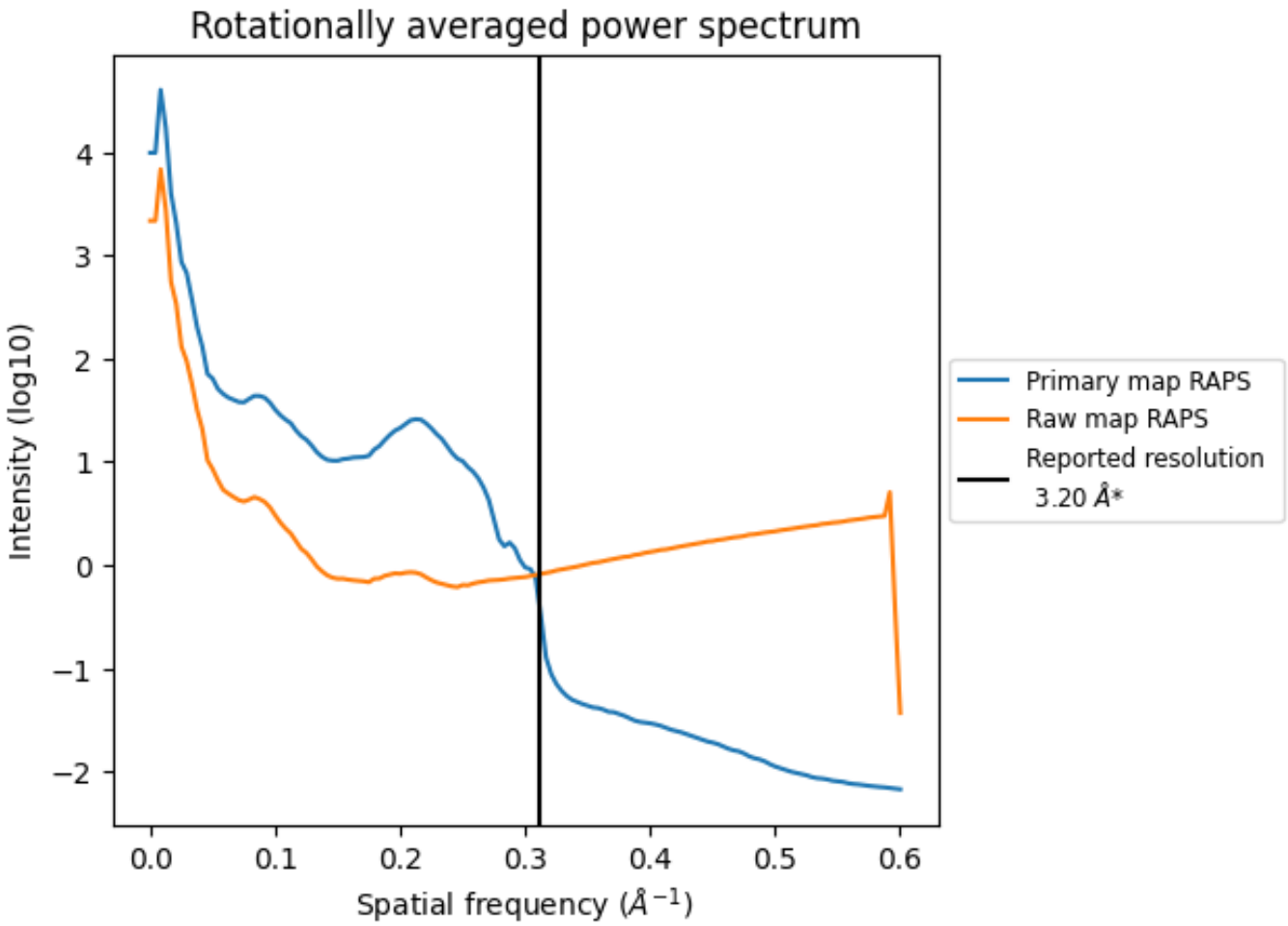
7.2 Volume estimate (i)



The volume at the recommended contour level is 77 nm^3; this corresponds to an approximate mass of 70 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)

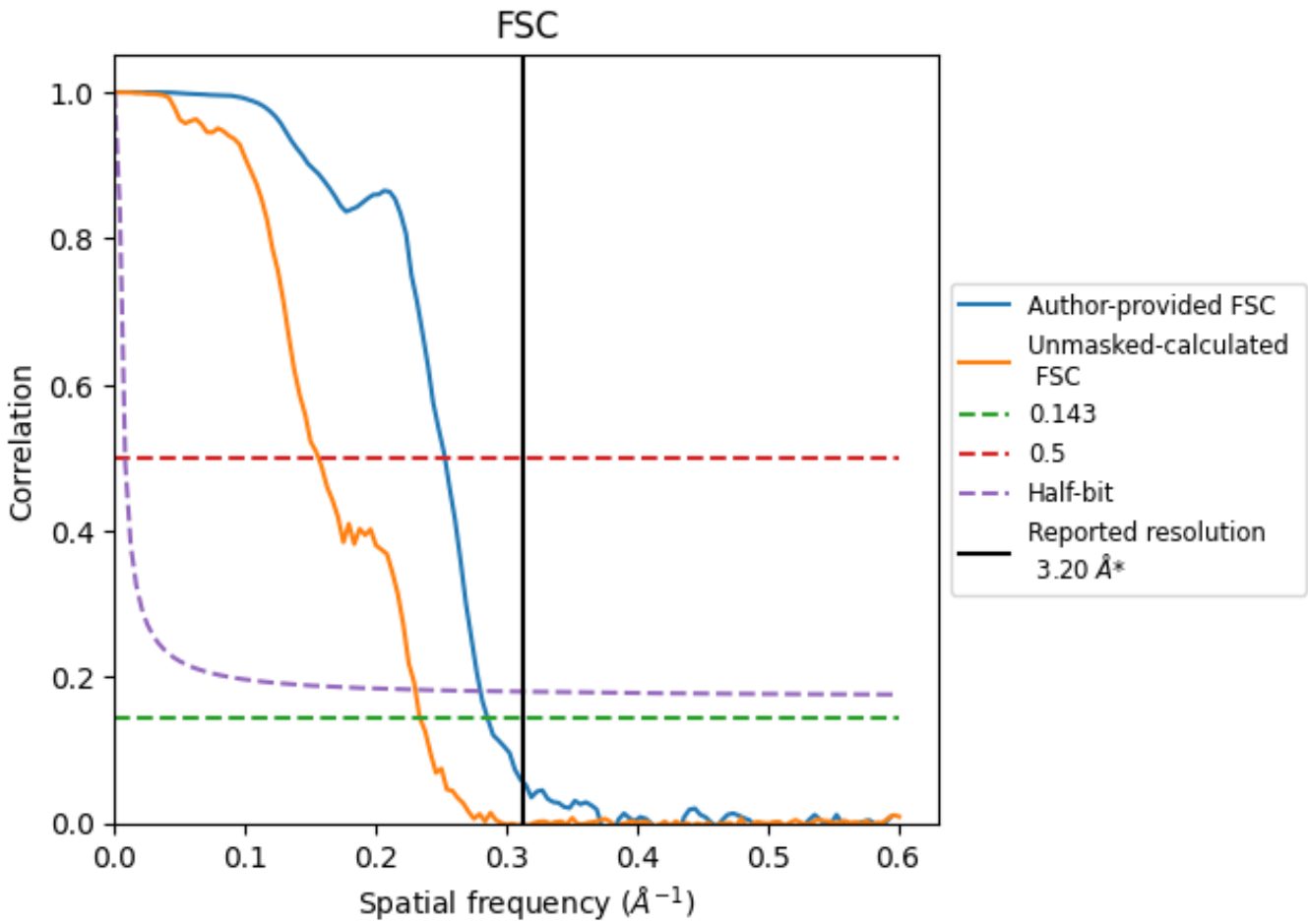


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

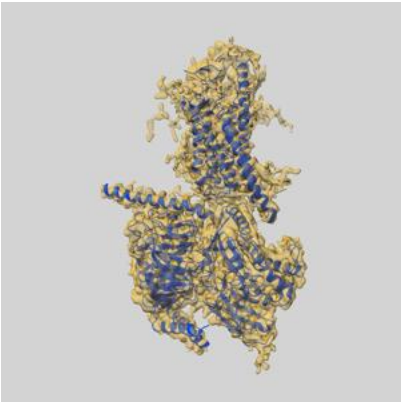
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.50	3.95	3.57
Unmasked-calculated*	4.27	6.41	4.34

*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 4.27 differs from the reported value 3.2 by more than 10 %

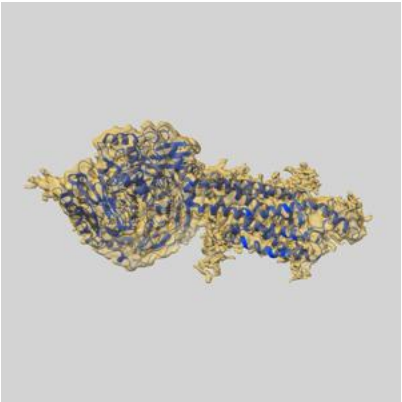
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-36266 and PDB model 8JHI. Per-residue inclusion information can be found in section 3 on page 5.

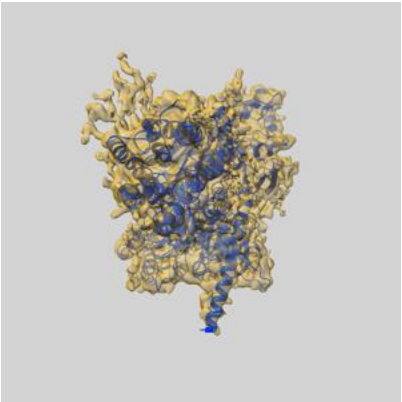
9.1 Map-model overlay (i)



X



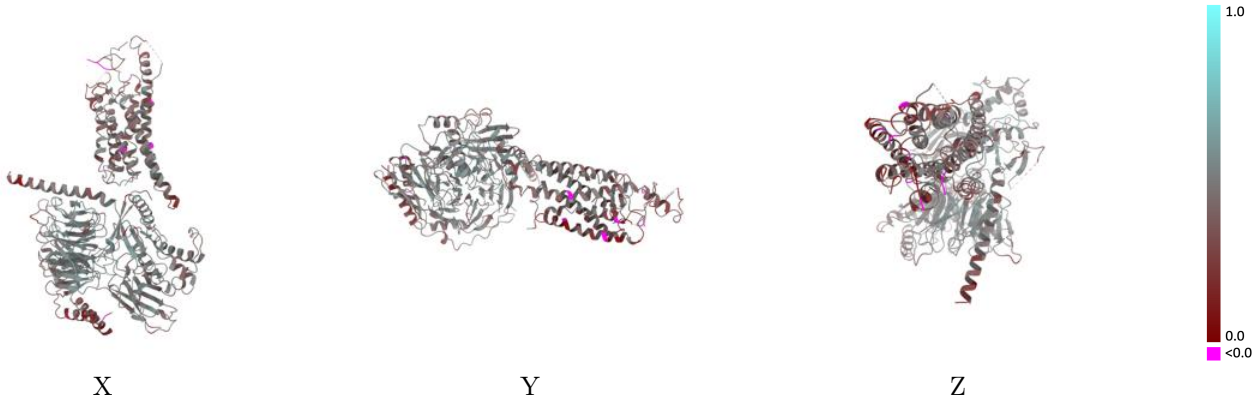
Y



Z

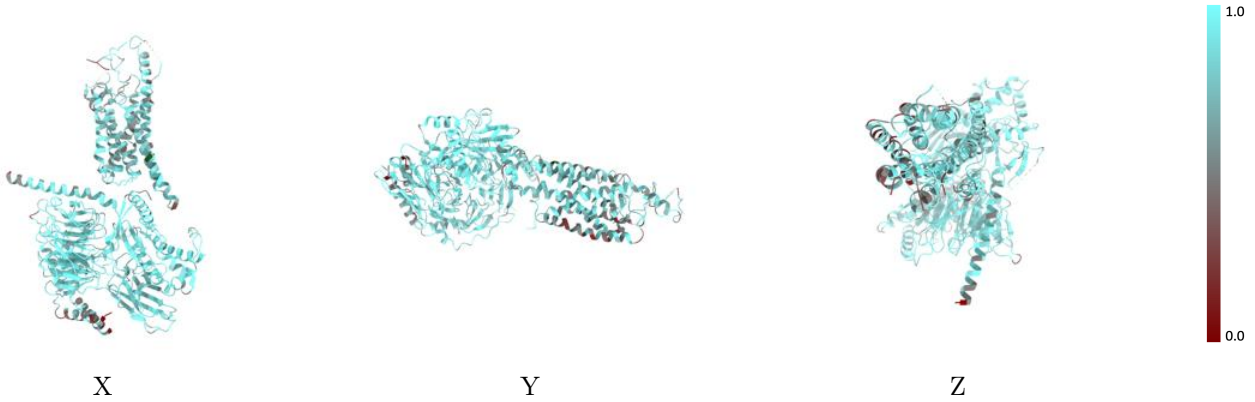
The images above show the 3D surface view of the map at the recommended contour level 0.074 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



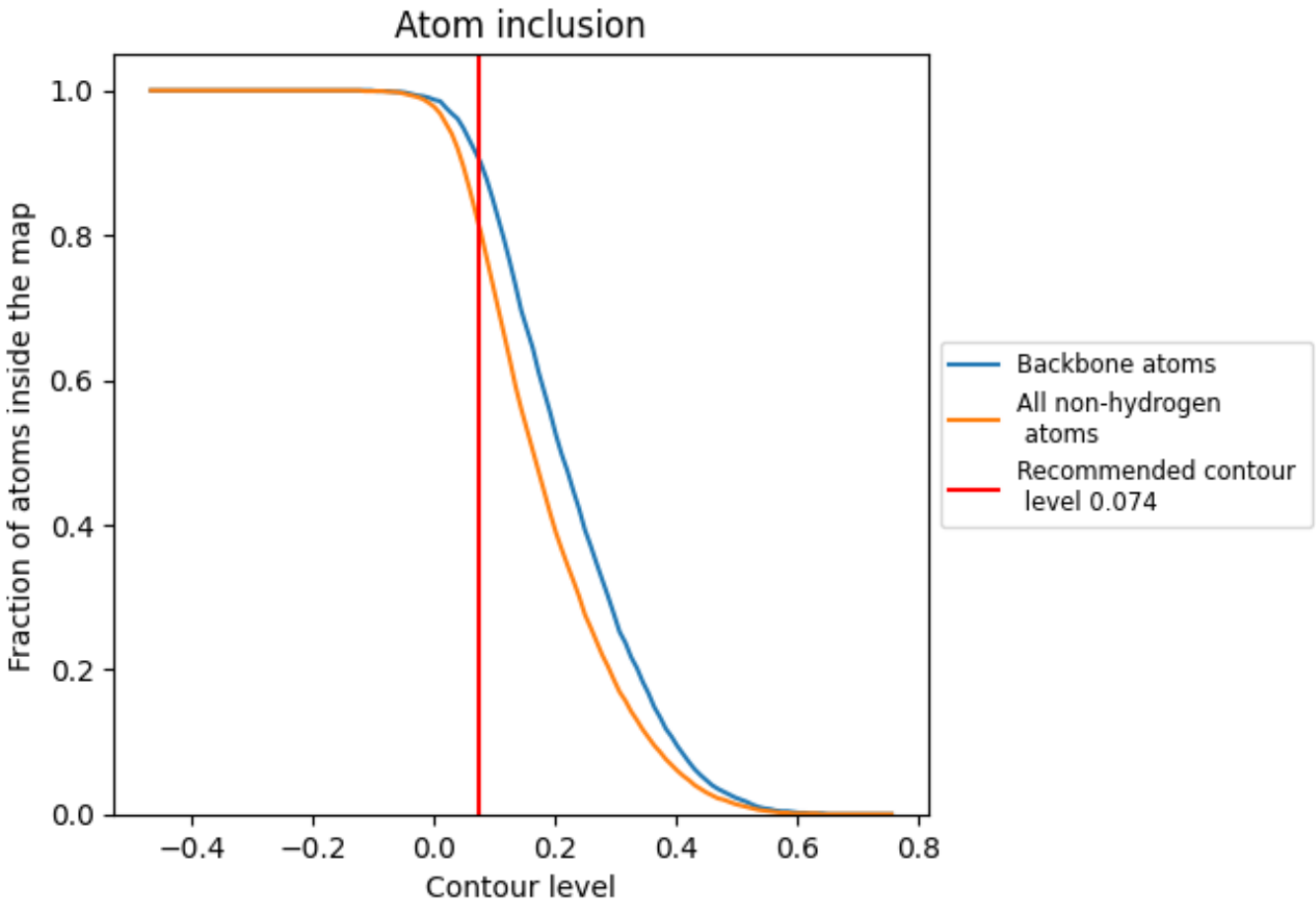
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.074).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.074) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.4230
A	0.8680	0.4610
B	0.8540	0.4590
C	0.7370	0.3460
N	0.8700	0.4560
R	0.7370	0.3590