



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 10:10 PM JST

PDB ID : 25IK / pdb_000025ik
EMDB ID : EMD-80137
Title : Cryo-EM structure of MasR(FL)-Gq
Authors : Suzuki, S.; Nishikawa, K.; Fujiyoshi, Y.
Deposited on : 2026-04-06
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

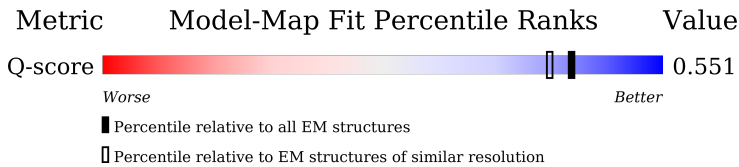
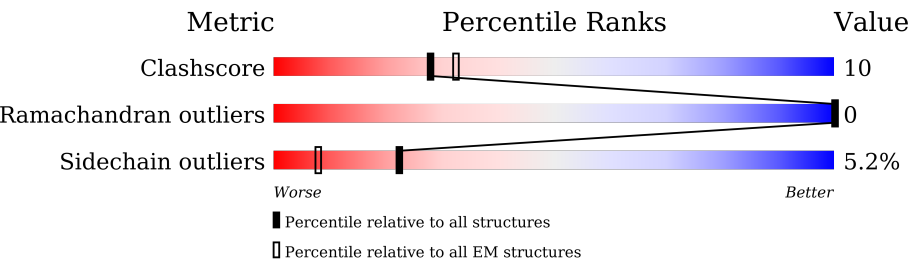
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	R	620	<div><div>9%</div><div>30%10%60%</div></div>
2	A	246	<div><div>8%</div><div>76%14%10%</div></div>
3	B	382	<div><div>27%</div><div>63%24%11%</div></div>
4	C	70	<div><div>73%9%19%</div></div>

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Mol	Chain	Length	Quality of chain
5	S	248	<div><div></div><div>16%</div><div>67%</div><div>26%</div><div>• 6%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8338 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,Proto-oncogene Mas,LgBiT tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	248	Total	C	N	O	S	0	0
			2010	1356	303	335	16		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-124	MET	-	initiating methionine	UNP P0ABE7
R	-123	LYS	-	expression tag	UNP P0ABE7
R	-122	THR	-	expression tag	UNP P0ABE7
R	-121	ILE	-	expression tag	UNP P0ABE7
R	-120	ILE	-	expression tag	UNP P0ABE7
R	-119	ALA	-	expression tag	UNP P0ABE7
R	-118	LEU	-	expression tag	UNP P0ABE7
R	-117	SER	-	expression tag	UNP P0ABE7
R	-116	TYR	-	expression tag	UNP P0ABE7
R	-115	ILE	-	expression tag	UNP P0ABE7
R	-114	PHE	-	expression tag	UNP P0ABE7
R	-113	CYS	-	expression tag	UNP P0ABE7
R	-112	LEU	-	expression tag	UNP P0ABE7
R	-111	VAL	-	expression tag	UNP P0ABE7
R	-110	PHE	-	expression tag	UNP P0ABE7
R	-109	ALA	-	expression tag	UNP P0ABE7
R	-108	ASP	-	expression tag	UNP P0ABE7
R	-107	TYR	-	expression tag	UNP P0ABE7
R	-106	LYS	-	expression tag	UNP P0ABE7
R	-105	ASP	-	expression tag	UNP P0ABE7
R	-104	ASP	-	expression tag	UNP P0ABE7
R	-103	ASP	-	expression tag	UNP P0ABE7
R	-102	ASP	-	expression tag	UNP P0ABE7
R	-101	LYS	-	expression tag	UNP P0ABE7
R	-100	ALA	-	expression tag	UNP P0ABE7
R	-99	ASP	-	expression tag	UNP P0ABE7
R	-94	TRP	MET	engineered mutation	UNP P0ABE7
R	1	ILE	HIS	engineered mutation	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	5	LEU	-	linker	UNP P0ABE7

- Molecule 2 is a protein called Gs-mini-Gq chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	222	Total	C	N	O	S	0	0
			1700	1082	298	313	7		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	339	Total	C	N	O	S	0	0
			2492	1550	440	483	19		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	HIS	-	expression tag	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	GLU	-	expression tag	UNP P62873
B	-5	ASN	-	expression tag	UNP P62873
B	-4	LEU	-	expression tag	UNP P62873
B	-3	TYR	-	expression tag	UNP P62873
B	-2	PHE	-	expression tag	UNP P62873
B	-1	GLN	-	expression tag	UNP P62873
B	0	GLY	-	expression tag	UNP P62873
B	1	SER	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873
B	342	GLY	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873

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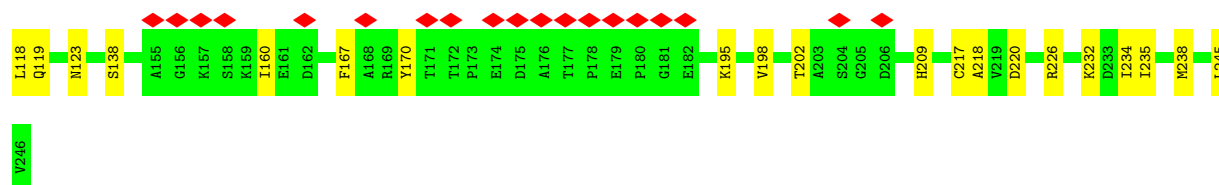
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	SER	-	expression tag	UNP P62873
B	352	SER	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

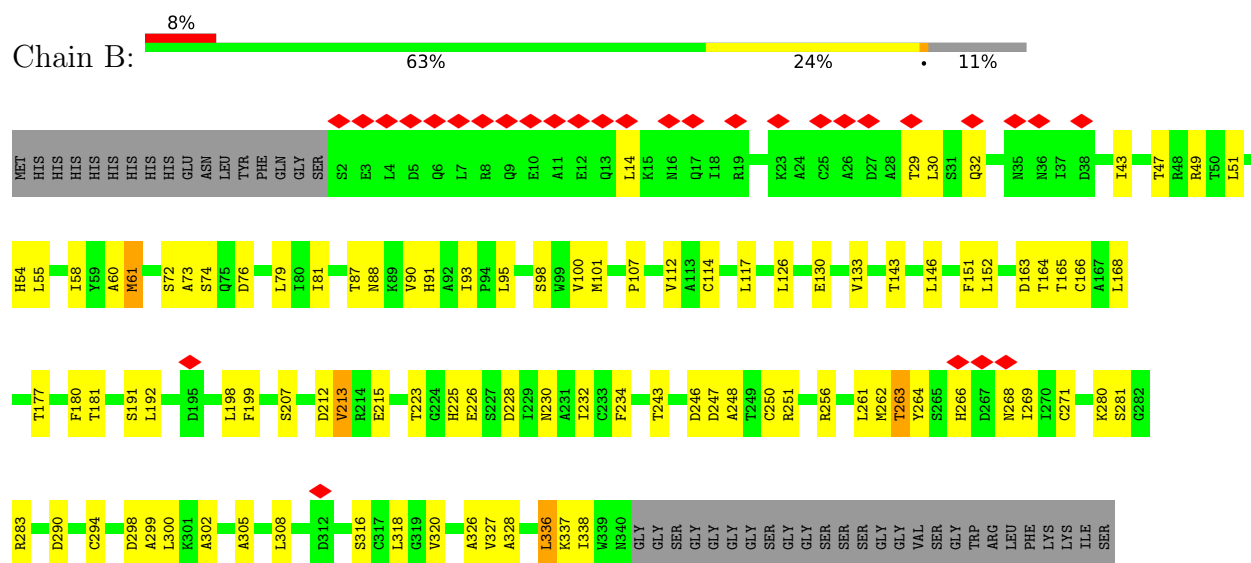
Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	57	Total	C	N	O	S	0	0
			397	249	69	77	2		

- Molecule 5 is a protein called scFv16.

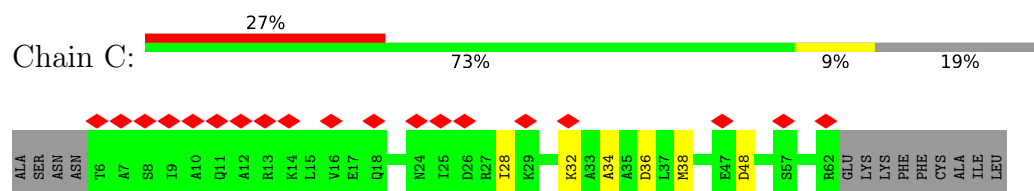
Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	233	Total	C	N	O	S	0	0
			1739	1108	291	331	9		



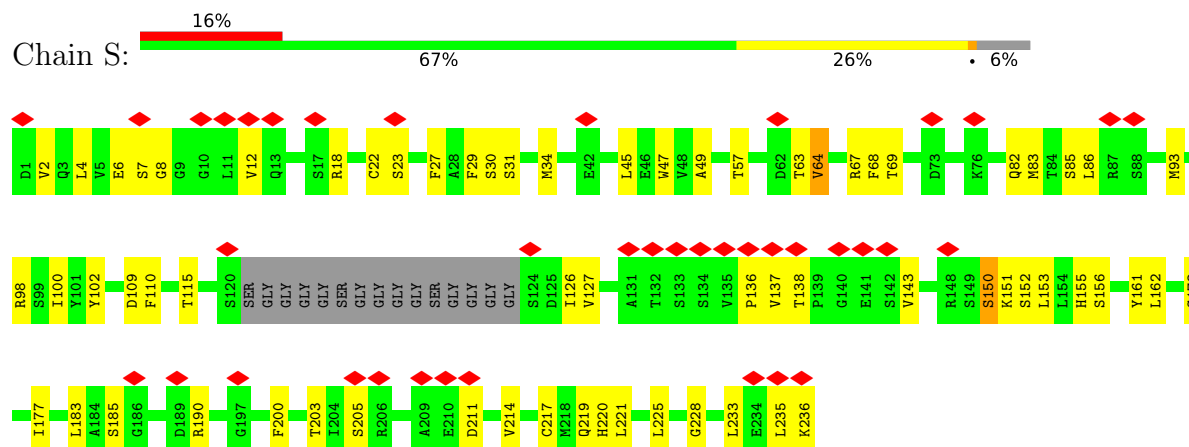
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 5: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.955	Depositor
Minimum map value	-1.832	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.36	Depositor
Map size (\AA)	167.04, 167.04, 167.04	wwPDB
Map dimensions	174, 174, 174	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.96, 0.96, 0.96	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	R	0.11	0/2066	0.29	0/2819
2	A	0.12	0/1731	0.26	0/2346
3	B	0.13	0/2539	0.30	0/3459
4	C	0.08	0/403	0.18	0/552
5	S	0.12	0/1783	0.29	0/2424
All	All	0.12	0/8522	0.28	0/11600

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	R	2010	0	2044	40	0
2	A	1700	0	1614	24	0
3	B	2492	0	2315	62	0
4	C	397	0	370	5	0
5	S	1739	0	1640	42	0
All	All	8338	0	7983	156	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.

All (156) 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:B:271:CYS:HB2	3:B:290:ASP:HB2	1.70	0.71
2:A:119:GLN:O	2:A:123:ASN:ND2	2.25	0.69
3:B:250:CYS:HB3	3:B:264:TYR:HB2	1.74	0.69
2:A:217:CYS:SG	2:A:218:ALA:N	2.65	0.69
1:R:10:VAL:HB	1:R:109:SER:HB2	1.75	0.68
3:B:130:GLU:HG2	5:S:27:PHE:HA	1.76	0.68
5:S:64:VAL:HB	5:S:68:PHE:CD2	2.30	0.67
2:A:160:ILE:HD12	2:A:160:ILE:H	1.58	0.67
2:A:27:GLY:HA3	3:B:55:LEU:HD12	1.75	0.67
2:A:220:ASP:OD2	2:A:226:ARG:NH2	2.28	0.67
3:B:58:ILE:O	3:B:316:SER:OG	2.13	0.64
1:R:188:ILE:HD11	1:R:252:TYR:HB2	1.79	0.64
3:B:266:HIS:ND1	3:B:268:ASN:OD1	2.30	0.64
3:B:192:LEU:HD23	3:B:199:PHE:HB3	1.81	0.63
1:R:138:ILE:HD13	2:A:232:LYS:HG3	1.82	0.62
3:B:256:ARG:NH2	4:C:36:ASP:OD2	2.24	0.62
1:R:204:LEU:HD21	1:R:238:LEU:HD11	1.82	0.62
3:B:49:ARG:HH11	3:B:49:ARG:HG3	1.66	0.61
3:B:300:LEU:HD21	4:C:38:MET:HA	1.81	0.61
1:R:204:LEU:HD11	1:R:238:LEU:HD21	1.83	0.61
5:S:190:ARG:NH1	5:S:211:ASP:OD2	2.34	0.60
2:A:15:ARG:HD3	5:S:102:TYR:HB3	1.84	0.59
5:S:68:PHE:CE1	5:S:83:MET:HG2	2.37	0.59
3:B:93:ILE:HG12	3:B:133:VAL:HG11	1.84	0.59
2:A:115:TYR:HA	2:A:118:LEU:HB2	1.83	0.59
3:B:30:LEU:HD13	4:C:34:ALA:HB1	1.83	0.59
3:B:225:HIS:NE2	3:B:243:THR:OG1	2.36	0.58
5:S:69:THR:HB	5:S:82:GLN:HB3	1.85	0.58
3:B:168:LEU:HD22	3:B:213:VAL:HG12	1.84	0.58
1:R:141:ARG:HG3	2:A:235:ILE:HG23	1.85	0.58
3:B:266:HIS:HB3	3:B:269:ILE:HD12	1.85	0.58
5:S:12:VAL:HG12	5:S:18:ARG:HH21	1.69	0.57
5:S:64:VAL:HB	5:S:68:PHE:HD2	1.69	0.57
5:S:12:VAL:HG21	5:S:86:LEU:HD12	1.85	0.57
5:S:18:ARG:O	5:S:83:MET:HB2	2.05	0.57
3:B:281:SER:OG	4:C:48:ASP:OD2	2.19	0.56
3:B:264:TYR:OH	3:B:299:ALA:O	2.22	0.56
1:R:235:ILE:HG23	1:R:239:ILE:HD12	1.87	0.56
5:S:6:GLU:HG2	5:S:115:THR:HG23	1.88	0.55
1:R:169:VAL:O	1:R:174:ARG:NH1	2.40	0.55
1:R:141:ARG:NH1	1:R:141:ARG:HB3	2.22	0.55
1:R:141:ARG:HB3	1:R:141:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:61:MET:HE3	3:B:328:ALA:HB3	1.87	0.54
1:R:240:PHE:HB3	1:R:272:ASN:HB2	1.89	0.54
5:S:68:PHE:CD1	5:S:83:MET:HG2	2.42	0.54
5:S:69:THR:O	5:S:82:GLN:N	2.40	0.54
3:B:266:HIS:HD1	3:B:268:ASN:H	1.55	0.54
5:S:6:GLU:HA	5:S:22:CYS:HA	1.89	0.54
2:A:6:SER:OG	5:S:161:TYR:OH	2.26	0.53
1:R:116:TYR:HE2	1:R:245:ARG:HG2	1.73	0.53
5:S:143:VAL:HG11	5:S:233:LEU:HD21	1.91	0.53
1:R:242:MET:N	1:R:243:PRO:HD2	2.23	0.53
1:R:234:ILE:O	1:R:238:LEU:HD12	2.10	0.52
5:S:7:SER:OG	5:S:8:GLY:N	2.42	0.52
3:B:74:SER:OG	3:B:76:ASP:OD2	2.24	0.52
5:S:2:VAL:HG12	5:S:27:PHE:HB3	1.91	0.52
4:C:28:ILE:HD12	4:C:32:LYS:HB3	1.92	0.51
3:B:54:HIS:NE2	3:B:72:SER:OG	2.38	0.51
3:B:30:LEU:HD22	3:B:261:LEU:HD23	1.93	0.51
1:R:230:ILE:O	1:R:233:THR:OG1	2.25	0.50
3:B:51:LEU:HB2	3:B:336:LEU:HB2	1.93	0.50
5:S:67:ARG:NH1	5:S:85:SER:O	2.45	0.50
2:A:14:GLU:OE2	5:S:57:THR:OG1	2.27	0.50
3:B:79:LEU:HB2	3:B:93:ILE:HB	1.94	0.50
5:S:126:ILE:HG12	5:S:151:LYS:HD3	1.92	0.50
3:B:95:LEU:HD13	3:B:100:VAL:HG11	1.94	0.50
2:A:73:LYS:HE3	2:A:82:HIS:CG	2.47	0.49
2:A:198:VAL:O	2:A:202:THR:OG1	2.23	0.49
3:B:166:CYS:HB2	3:B:180:PHE:HB2	1.95	0.49
3:B:294:CYS:HB2	3:B:308:LEU:HB2	1.95	0.49
1:R:64:ASN:N	1:R:64:ASN:OD1	2.45	0.49
2:A:105:ALA:HB2	2:A:234:ILE:HD13	1.95	0.49
5:S:220:HIS:HA	5:S:225:LEU:HD22	1.93	0.49
1:R:50:ASN:HB3	1:R:78:ILE:HG12	1.95	0.48
5:S:136:PRO:HB2	5:S:236:LYS:HD3	1.95	0.48
1:R:71:THR:HG23	1:R:72:HIS:HD2	1.79	0.48
1:R:236:ILE:HD12	1:R:279:ILE:HD12	1.96	0.48
3:B:126:LEU:HA	3:B:133:VAL:HG22	1.94	0.48
3:B:320:VAL:HG22	3:B:327:VAL:HG22	1.95	0.48
1:R:80:LEU:HD12	1:R:116:TYR:HB2	1.94	0.48
3:B:248:ALA:HB1	3:B:269:ILE:HG22	1.95	0.48
1:R:13:PHE:HE1	1:R:251:TYR:HB2	1.79	0.48
3:B:163:ASP:O	3:B:164:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:230:ASN:ND2	3:B:246:ASP:OD1	2.43	0.47
3:B:191:SER:HB2	3:B:232:ILE:HG23	1.97	0.47
5:S:127:VAL:HG12	5:S:150:SER:HB3	1.95	0.47
1:R:193:ILE:HA	1:R:197:LEU:HD21	1.96	0.47
3:B:326:ALA:HB1	3:B:338:ILE:HG23	1.96	0.47
5:S:126:ILE:HG23	5:S:151:LYS:HG2	1.97	0.47
2:A:234:ILE:O	2:A:238:MET:HG3	2.13	0.47
1:R:205:VAL:O	1:R:209:ILE:HG13	2.14	0.47
3:B:54:HIS:HE2	3:B:72:SER:HG	1.55	0.46
3:B:143:THR:N	3:B:163:ASP:OD2	2.47	0.46
3:B:212:ASP:HB3	3:B:215:GLU:HG2	1.97	0.46
5:S:153:LEU:HB3	5:S:221:LEU:HD13	1.97	0.46
3:B:47:THR:HG23	3:B:337:LYS:HB3	1.96	0.46
3:B:247:ASP:O	3:B:247:ASP:OD1	2.34	0.46
3:B:152:LEU:HD23	3:B:152:LEU:HA	1.82	0.45
1:R:42:ILE:HG22	1:R:270:THR:HG22	1.97	0.45
5:S:100:ILE:HG12	5:S:102:TYR:CE2	2.51	0.45
2:A:99:CYS:SG	3:B:101:MET:HE2	2.56	0.45
5:S:153:LEU:HD23	5:S:221:LEU:HB2	1.99	0.45
3:B:43:ILE:HD12	3:B:305:ALA:HB1	1.98	0.45
1:R:163:VAL:O	1:R:167:GLU:HG2	2.16	0.45
1:R:210:LEU:HD21	2:A:245:LEU:HD21	1.99	0.45
2:A:38:LEU:O	2:A:39:LEU:HD23	2.16	0.45
3:B:262:MET:HG2	3:B:302:ALA:HB2	1.97	0.45
5:S:177:ILE:HG12	5:S:183:LEU:HD23	1.98	0.45
1:R:36:HIS:HB2	1:R:263:HIS:CE1	2.52	0.45
2:A:167:PHE:HA	2:A:170:TYR:HB2	1.98	0.45
5:S:190:ARG:HG3	5:S:205:SER:O	2.17	0.44
3:B:283:ARG:NE	3:B:298:ASP:OD2	2.49	0.44
3:B:107:PRO:HD3	3:B:151:PHE:HB3	2.00	0.44
1:R:72:HIS:ND1	1:R:153:CYS:HB3	2.32	0.43
3:B:250:CYS:O	3:B:264:TYR:N	2.42	0.43
5:S:47:TRP:NE1	5:S:49:ALA:O	2.51	0.43
3:B:60:ALA:HB3	3:B:73:ALA:HB3	1.99	0.43
3:B:226:GLU:OE1	3:B:226:GLU:N	2.52	0.43
5:S:217:CYS:O	5:S:228:GLY:N	2.52	0.43
1:R:245:ARG:HH21	1:R:249:LEU:HG	1.84	0.43
5:S:4:LEU:HD12	5:S:110:PHE:HD2	1.84	0.43
1:R:247:LEU:O	1:R:251:TYR:N	2.50	0.43
3:B:81:ILE:HD12	3:B:91:HIS:HB2	2.01	0.43
3:B:88:ASN:HD22	3:B:88:ASN:HA	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:112:VAL:HG13	3:B:126:LEU:HD11	1.99	0.43
3:B:198:LEU:HD23	3:B:212:ASP:HA	2.01	0.43
1:R:121:TYR:HB3	1:R:156:LEU:HD22	2.00	0.43
3:B:165:THR:HG22	3:B:181:THR:HG22	2.01	0.43
3:B:49:ARG:HD3	3:B:87:THR:OG1	2.19	0.43
3:B:262:MET:HE2	3:B:262:MET:HB2	1.88	0.43
2:A:38:LEU:HB2	2:A:83:MET:HG2	2.01	0.42
1:R:60:ARG:HE	1:R:60:ARG:HB3	1.68	0.42
5:S:235:LEU:H	5:S:235:LEU:HD23	1.83	0.42
2:A:6:SER:HB3	5:S:155:HIS:CE1	2.55	0.42
1:R:275:ALA:O	1:R:279:ILE:HG22	2.20	0.42
2:A:138:SER:HA	2:A:209:HIS:HB2	2.01	0.42
3:B:130:GLU:CG	5:S:27:PHE:HA	2.48	0.42
3:B:168:LEU:O	3:B:177:THR:N	2.53	0.42
2:A:195:LYS:HA	2:A:198:VAL:HG22	2.02	0.41
1:R:230:ILE:HD11	2:A:245:LEU:HD23	2.02	0.41
3:B:207:SER:HB2	3:B:223:THR:HG22	2.01	0.41
1:R:14:VAL:HG22	1:R:263:HIS:CD2	2.56	0.41
5:S:155:HIS:CD2	5:S:156:SER:N	2.88	0.41
1:R:102:TYR:O	1:R:106:VAL:HG23	2.20	0.41
1:R:174:ARG:HA	1:R:174:ARG:HD2	1.81	0.41
1:R:258:PHE:CD1	1:R:258:PHE:N	2.88	0.41
1:R:106:VAL:HG13	1:R:168:TYR:OH	2.20	0.41
5:S:162:LEU:HD22	5:S:200:PHE:CG	2.56	0.41
3:B:90:VAL:HG13	5:S:102:TYR:HB2	2.02	0.41
3:B:251:ARG:HG2	3:B:263:THR:HG23	2.03	0.41
5:S:98:ARG:NE	5:S:109:ASP:OD1	2.32	0.41
5:S:29:PHE:HE1	5:S:34:MET:HE2	1.86	0.41
5:S:219:GLN:HE21	5:S:225:LEU:HA	1.85	0.40
1:R:54:LEU:HD23	1:R:54:LEU:HA	1.95	0.40
3:B:14:LEU:HD12	3:B:14:LEU:HA	1.89	0.40
3:B:101:MET:HE3	3:B:117:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	240/620 (39%)	233 (97%)	7 (3%)	0	100	100
2	A	216/246 (88%)	211 (98%)	5 (2%)	0	100	100
3	B	337/382 (88%)	326 (97%)	11 (3%)	0	100	100
4	C	55/70 (79%)	55 (100%)	0	0	100	100
5	S	229/248 (92%)	221 (96%)	8 (4%)	0	100	100
All	All	1077/1566 (69%)	1046 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	R	227/553 (41%)	213 (94%)	14 (6%)	16	49
2	A	170/213 (80%)	167 (98%)	3 (2%)	51	77
3	B	251/313 (80%)	238 (95%)	13 (5%)	21	55
4	C	36/57 (63%)	36 (100%)	0	100	100
5	S	182/201 (90%)	167 (92%)	15 (8%)	10	37
All	All	866/1337 (65%)	821 (95%)	45 (5%)	22	55

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	10	VAL
1	R	13	PHE
1	R	15	VAL
1	R	57	LEU
1	R	74	SER
1	R	127	SER

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Mol	Chain	Res	Type
1	R	161	CYS
1	R	170	MET
1	R	187	VAL
1	R	230	ILE
1	R	242	MET
1	R	244	MET
1	R	248	TYR
1	R	274	SER
2	A	5	VAL
2	A	22	ASN
2	A	76	VAL
3	B	29	THR
3	B	32	GLN
3	B	61	MET
3	B	98	SER
3	B	114	CYS
3	B	146	LEU
3	B	213	VAL
3	B	228	ASP
3	B	234	PHE
3	B	263	THR
3	B	280	LYS
3	B	318	LEU
3	B	336	LEU
5	S	23	SER
5	S	30	SER
5	S	31	SER
5	S	45	LEU
5	S	63	THR
5	S	64	VAL
5	S	93	MET
5	S	137	VAL
5	S	138	THR
5	S	150	SER
5	S	152	SER
5	S	172	SER
5	S	185	SER
5	S	203	THR
5	S	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	260	ASN
2	A	119	GLN
2	A	123	ASN
3	B	75	GLN
3	B	110	ASN
4	C	18	GLN
5	S	113	GLN
5	S	155	HIS
5	S	171	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

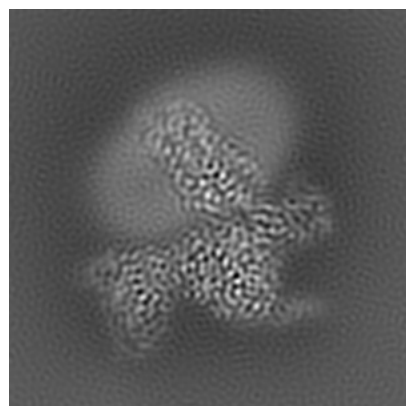
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-80137. These allow visual inspection of the internal detail of the map and identification of artifacts.

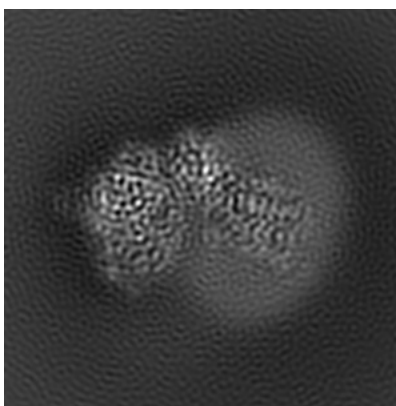
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

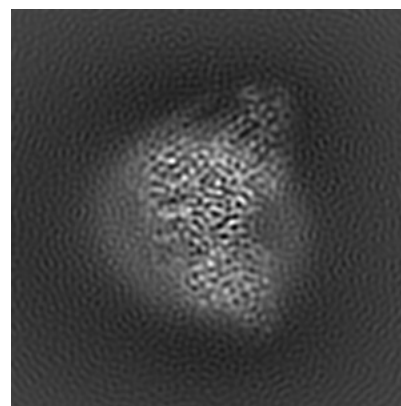
6.1.1 Primary map



X

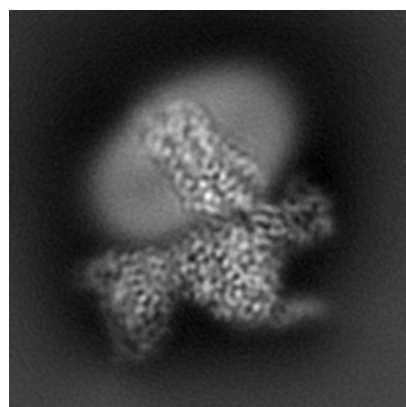


Y

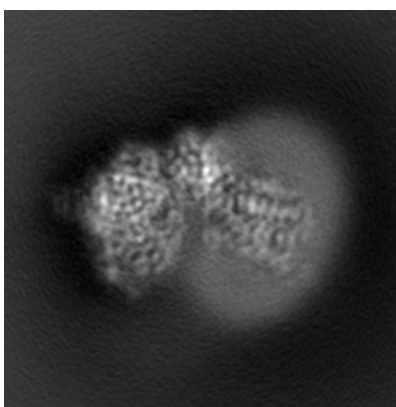


Z

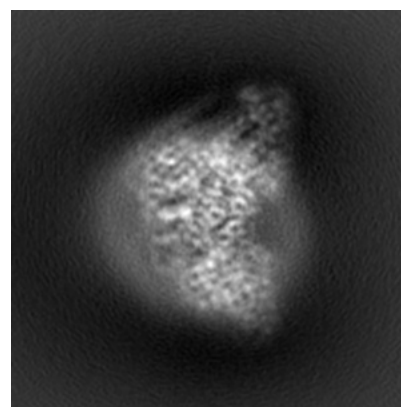
6.1.2 Raw map



X



Y

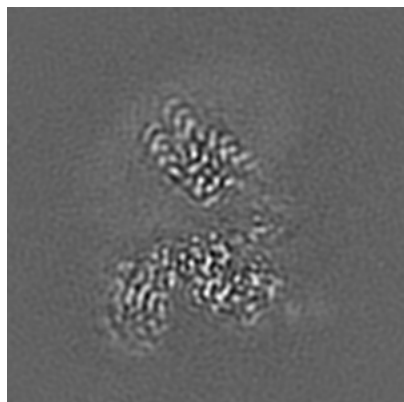


Z

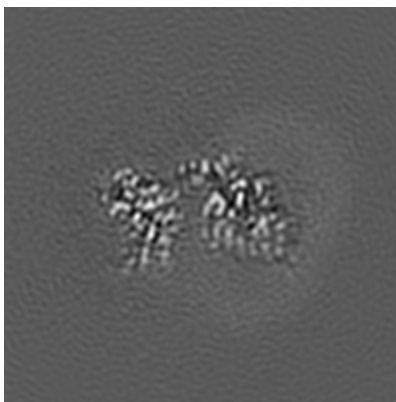
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

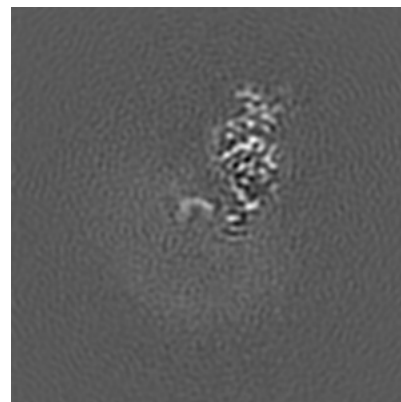
6.2.1 Primary map



X Index: 87

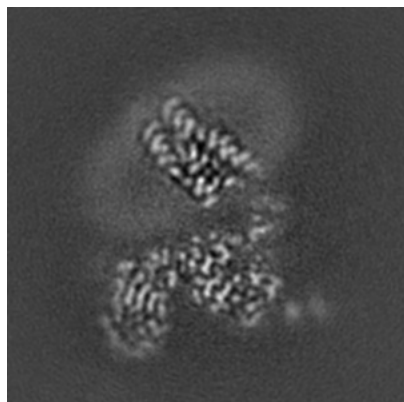


Y Index: 87

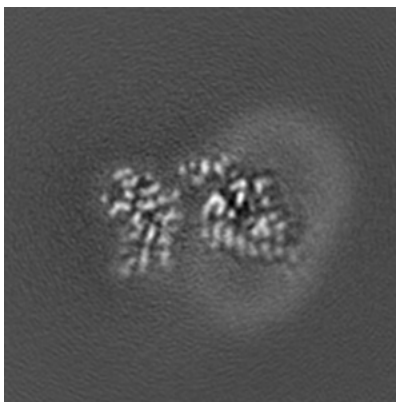


Z Index: 87

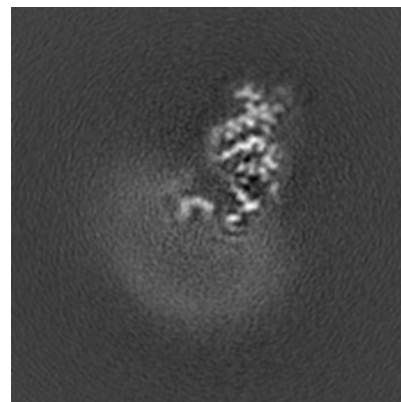
6.2.2 Raw map



X Index: 87



Y Index: 87

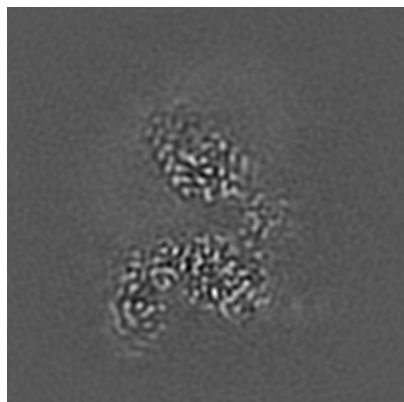


Z Index: 87

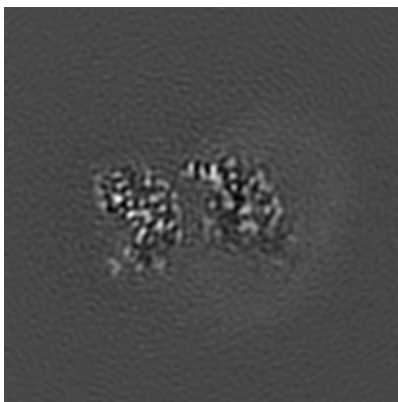
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

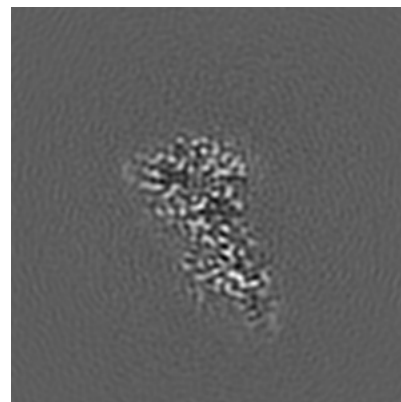
6.3.1 Primary map



X Index: 90

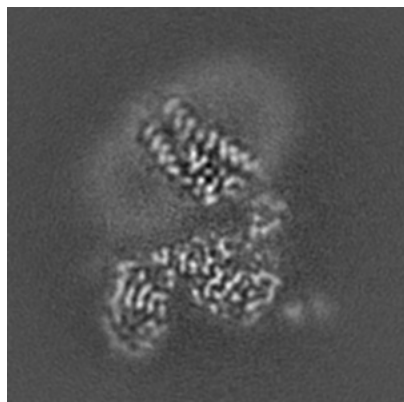


Y Index: 90

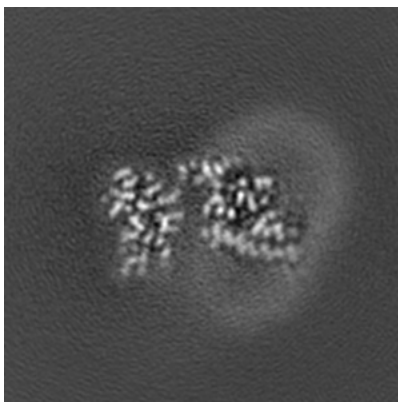


Z Index: 57

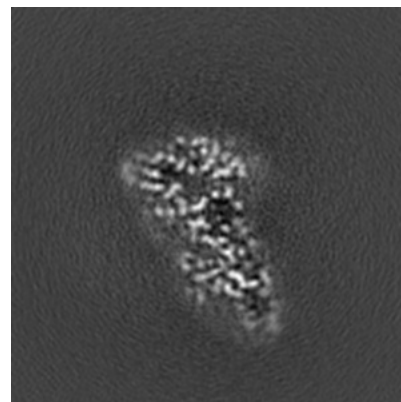
6.3.2 Raw map



X Index: 88



Y Index: 86

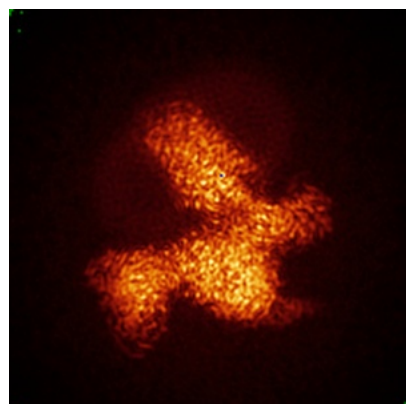


Z Index: 57

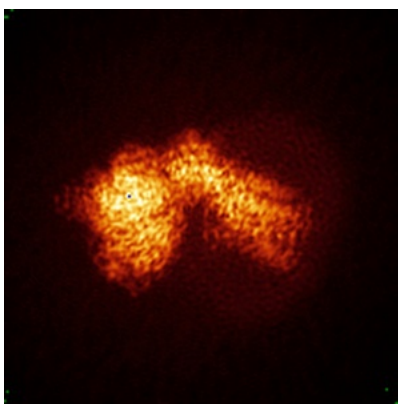
The images above show the largest variance slices of the map in three orthogonal directions.

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

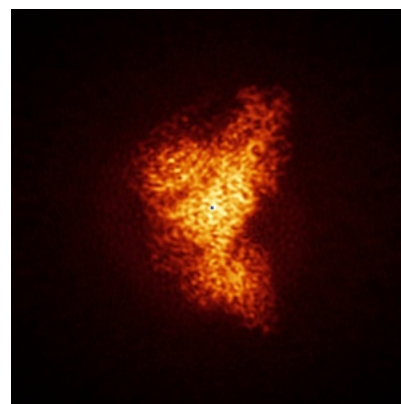
6.4.1 Primary map



X

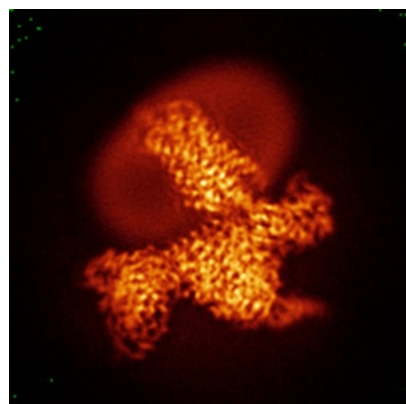


Y

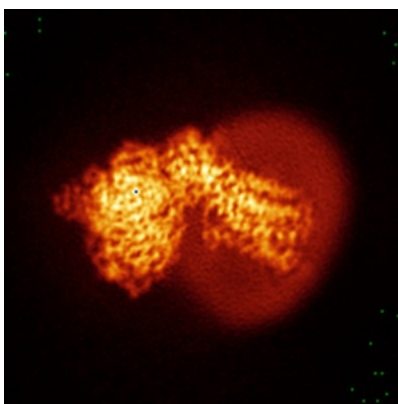


Z

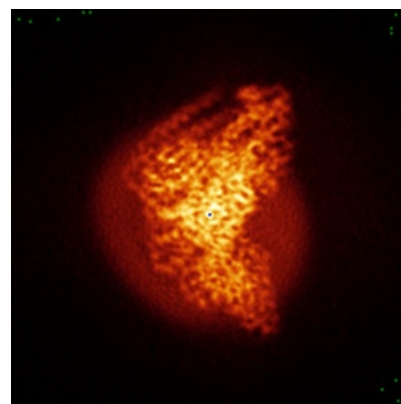
6.4.2 Raw map



X



Y

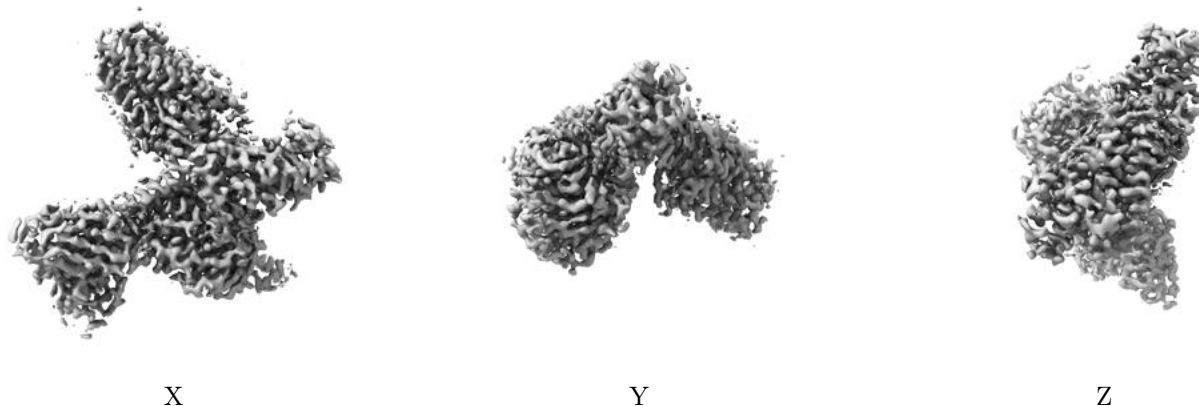


Z

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.

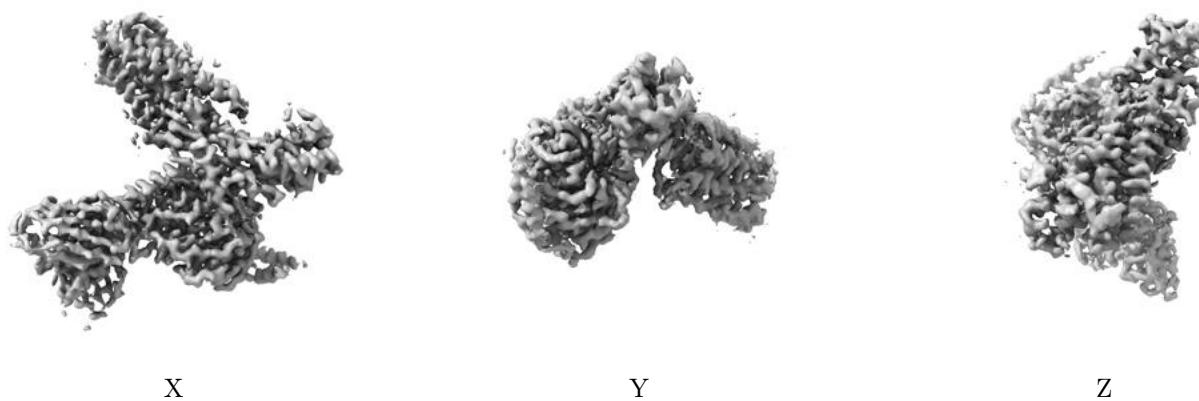
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. 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.

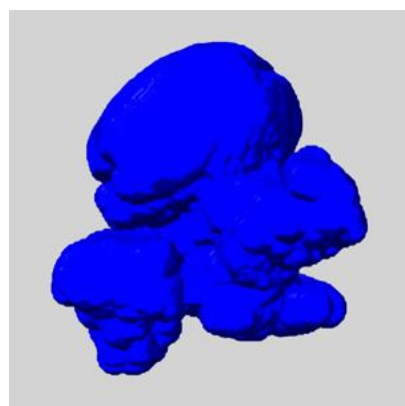
6.6 Mask visualisation [i](#)

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

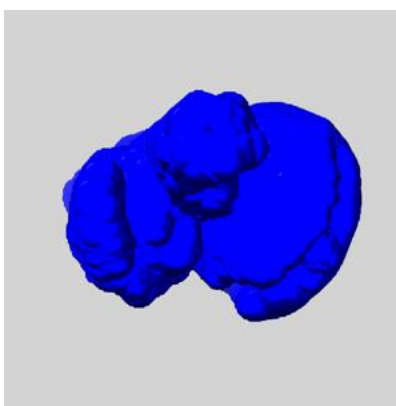
A mask typically either:

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

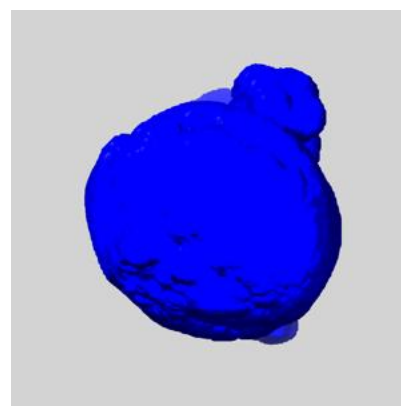
6.6.1 emd_80137_msk_1.map [i](#)



X



Y

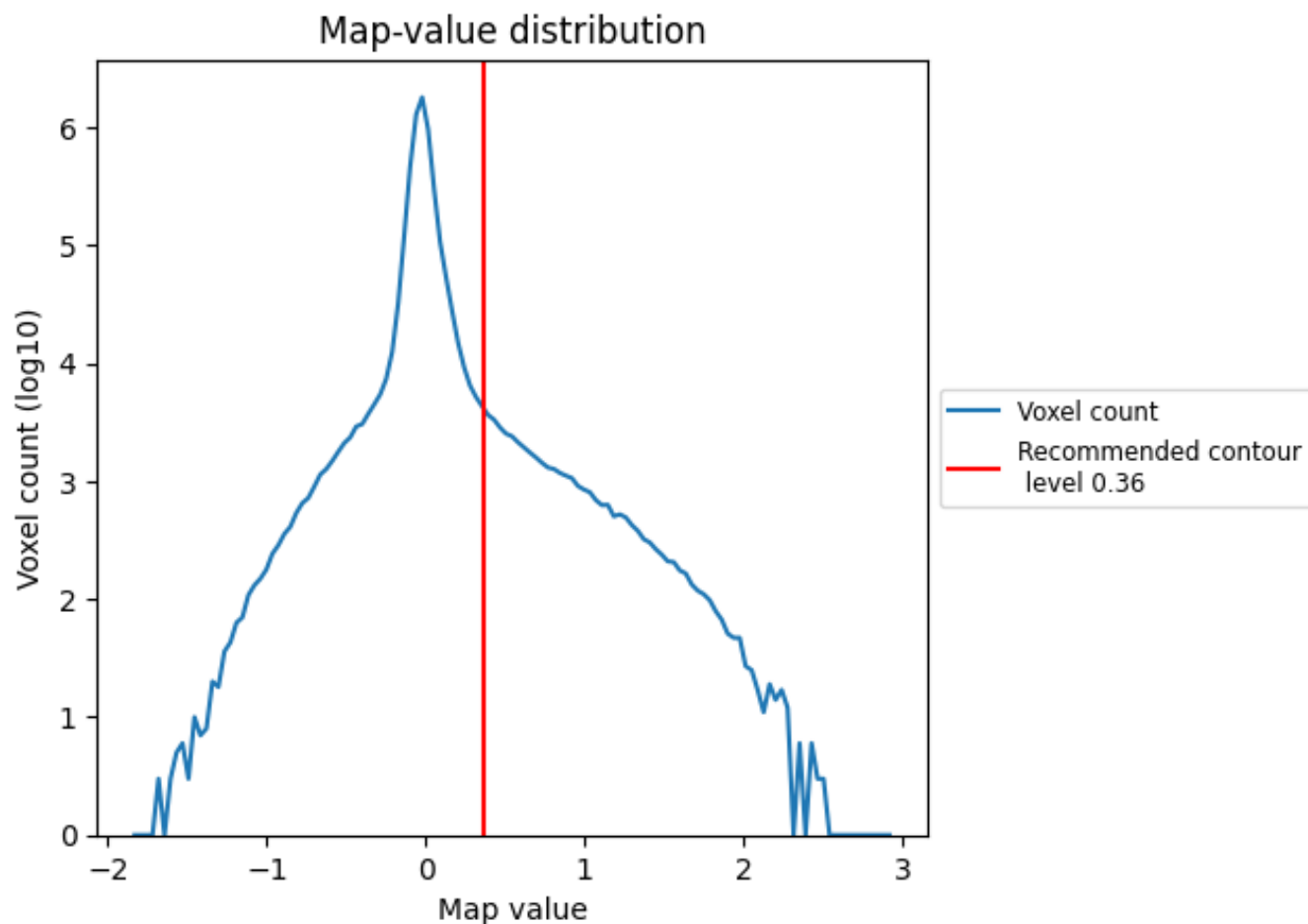


Z

7 Map analysis [i](#)

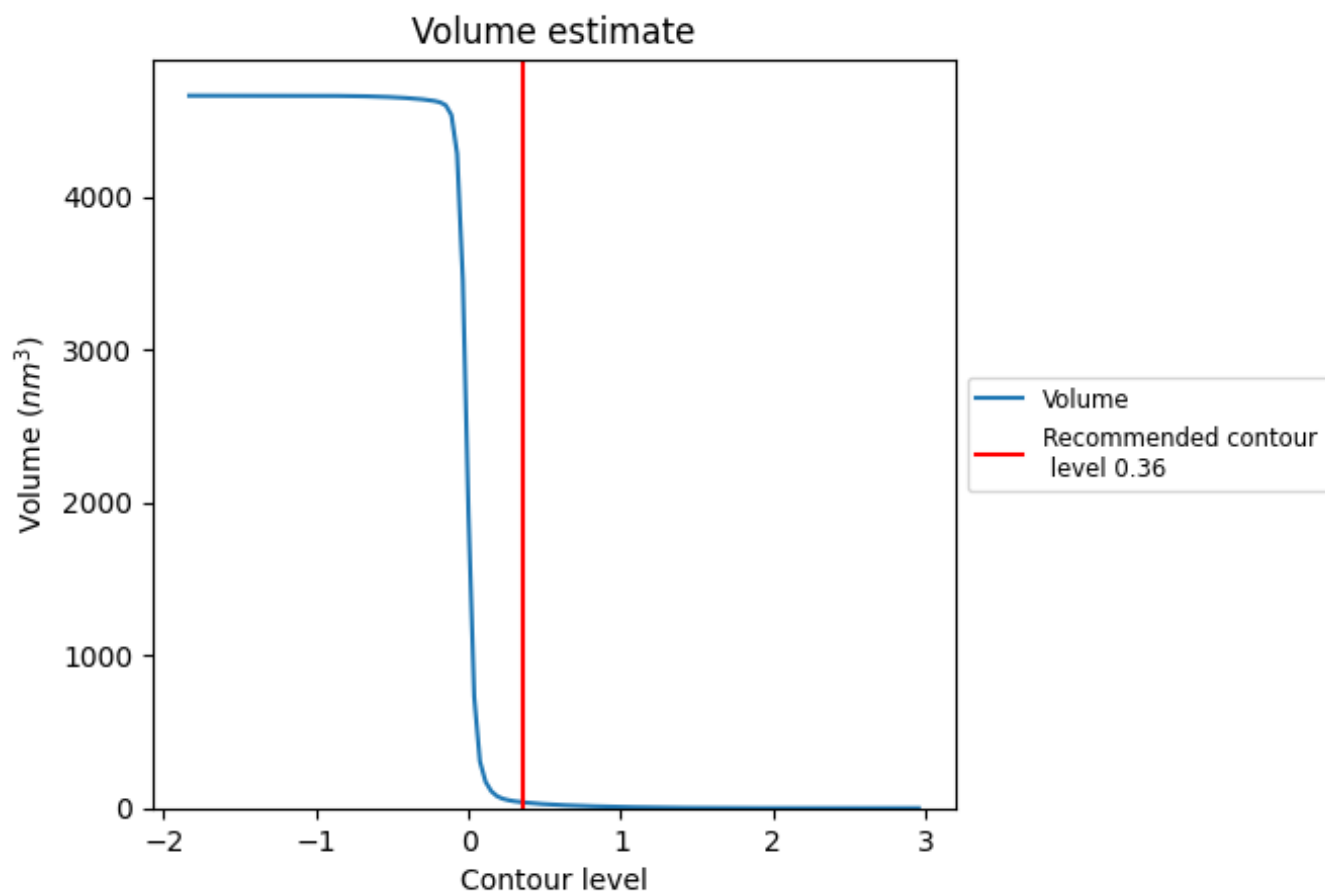
This section contains the results of statistical analysis of the map.

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.

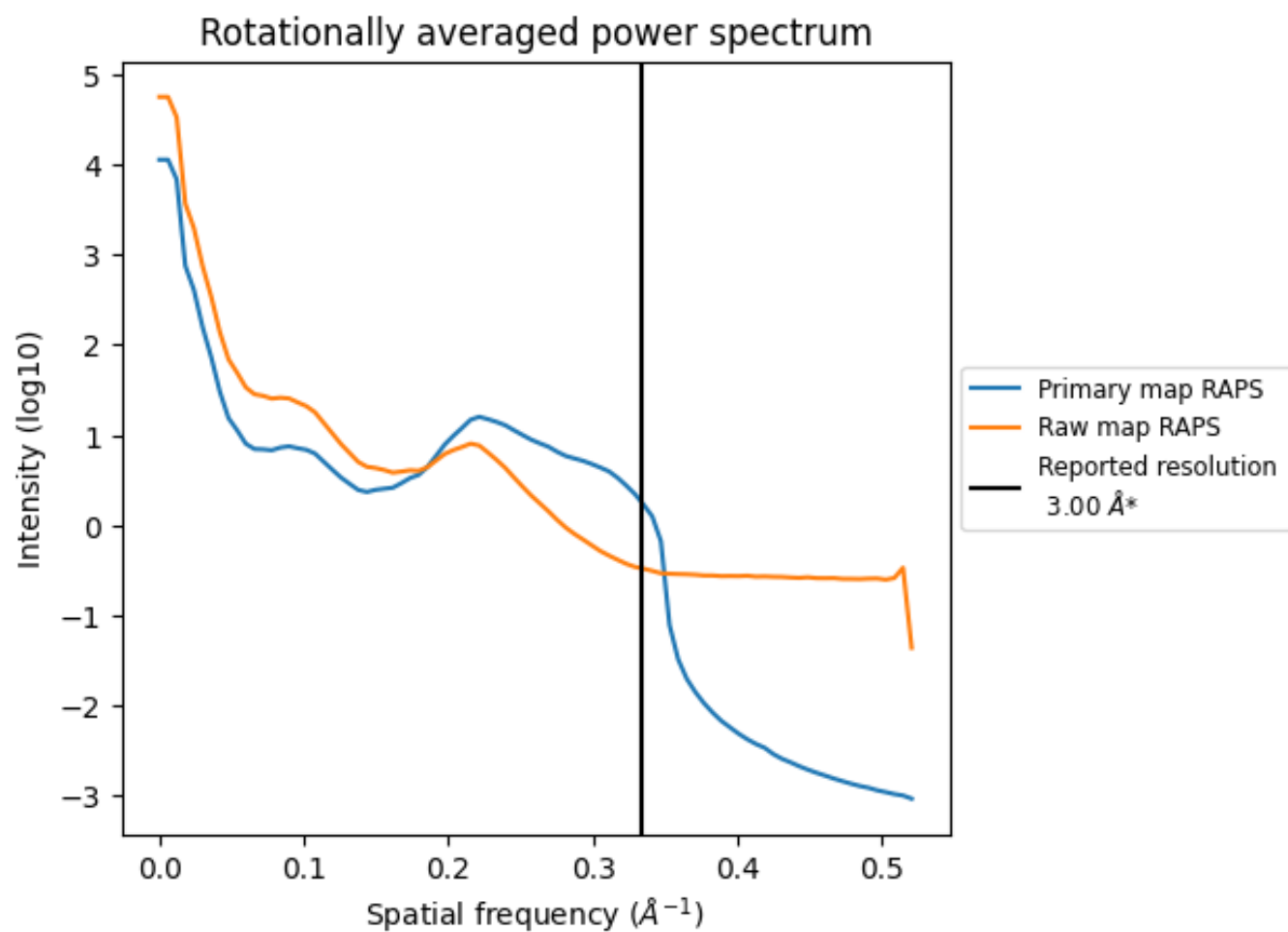
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm^3 ; this corresponds to an approximate mass of 34 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 ⓘ

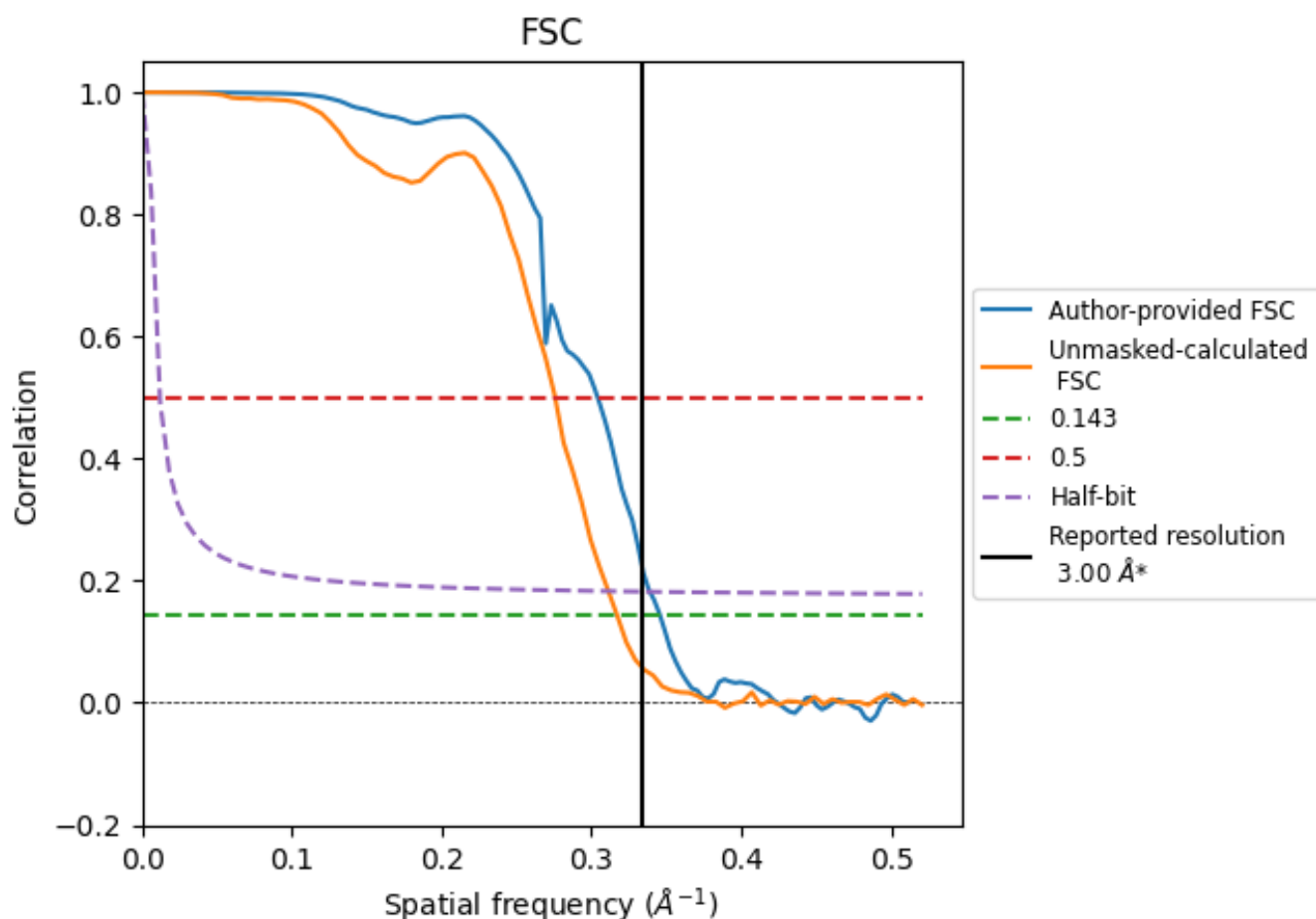


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

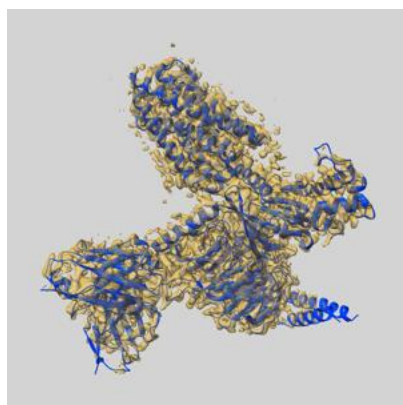
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.89	3.29	2.94
Unmasked-calculated*	3.15	3.63	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

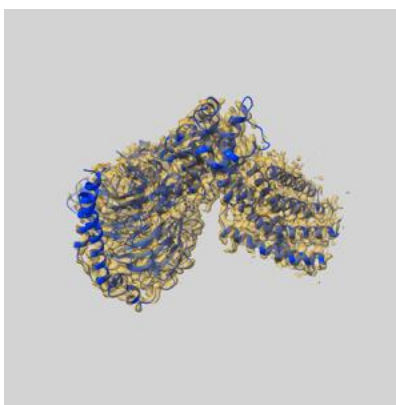
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-80137 and PDB model 25IK. Per-residue inclusion information can be found in section 3 on page 7.

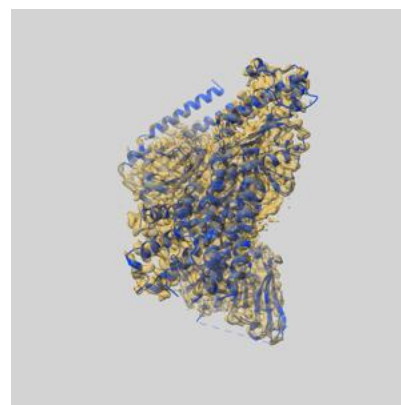
9.1 Map-model overlay [i](#)



X



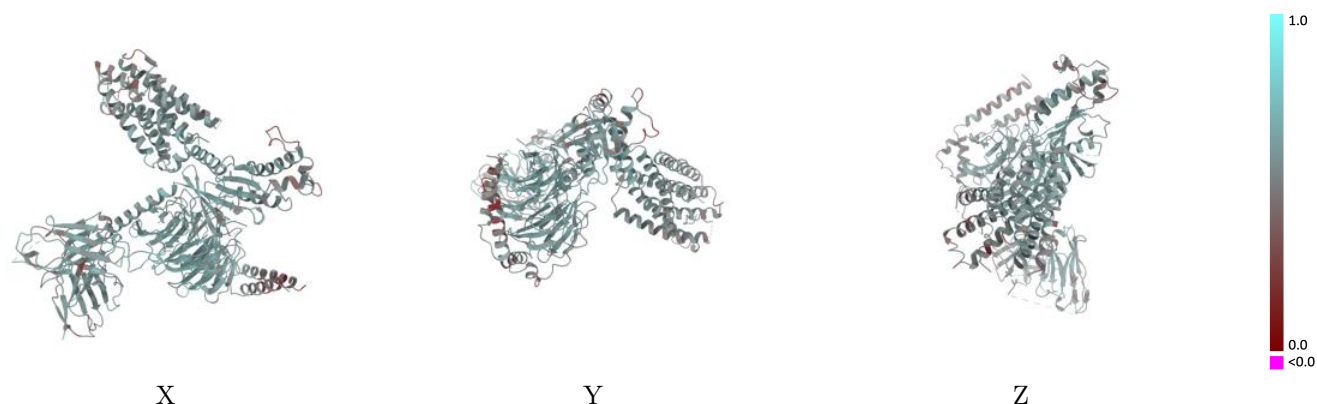
Y



Z

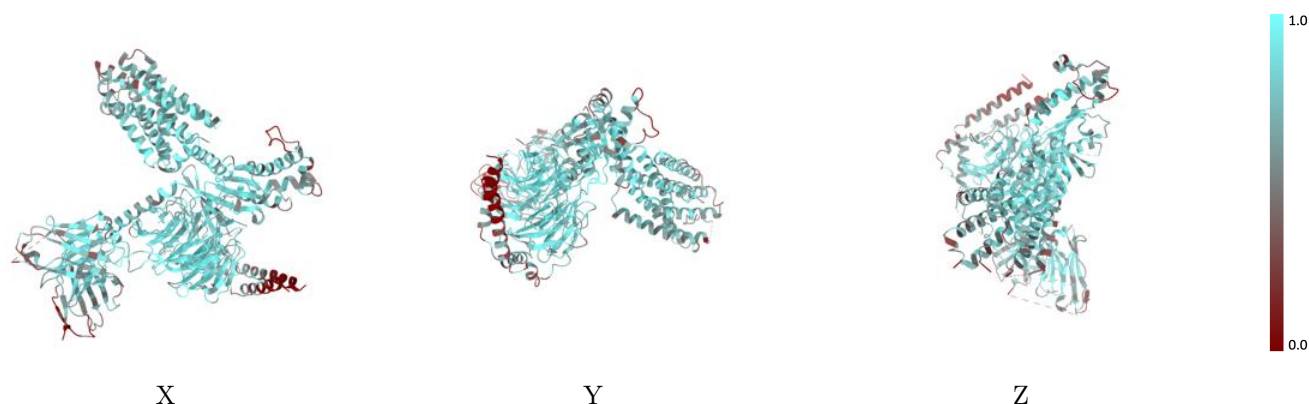
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



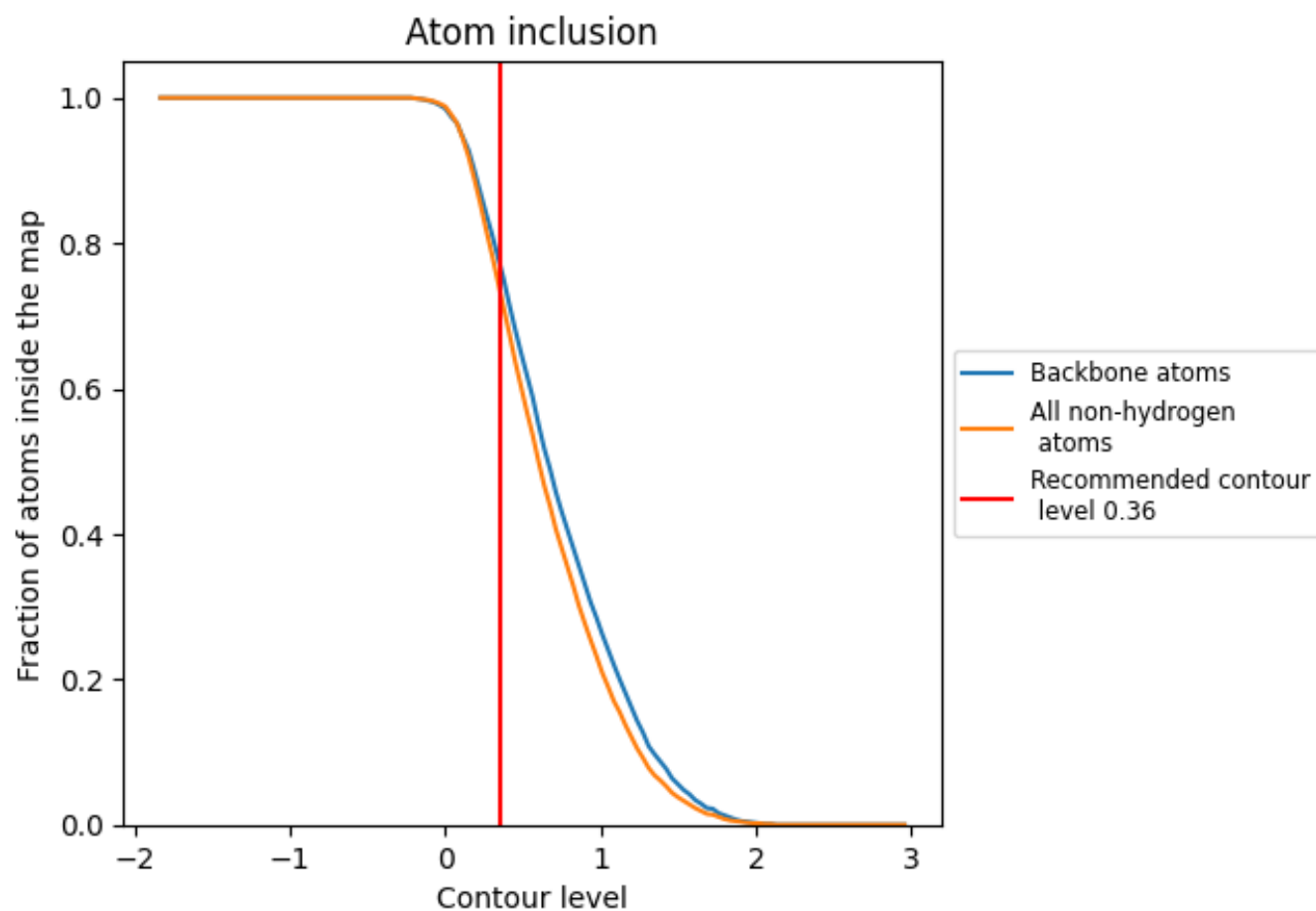
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7270	<div></div> 0.5510
A	<div></div> 0.7410	<div></div> 0.5570
B	<div></div> 0.7990	<div></div> 0.5770
C	<div></div> 0.5030	<div></div> 0.4960
R	<div></div> 0.7060	<div></div> 0.5270
S	<div></div> 0.6840	<div></div> 0.5510

