



Full wwPDB EM Validation Report ⓘ

Apr 8, 2026 – 07:43 PM UTC

PDB ID : 2IAG / pdb_00002Iag
EMDB ID : EMD-67446
Title : LY334370-bound serotonin 1F (5-HT1F) receptor-miniGoA protein complex
Authors : Cao, C.; Ji, Z.; Wang, Y.
Deposited on : 2025-12-04
Resolution : 3.13 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:

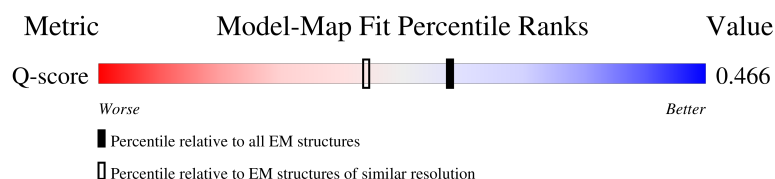
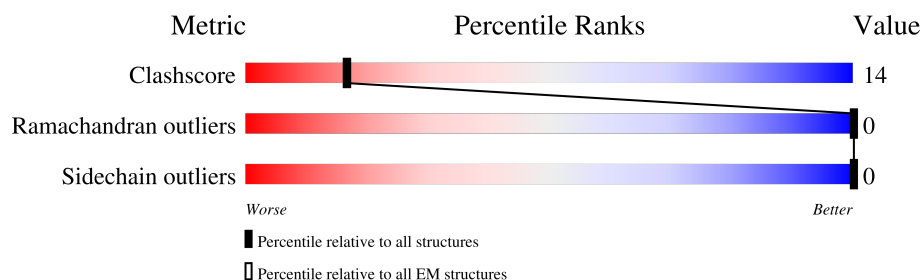
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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	B	358	
2	C	228	
3	G	71	
4	R	366	

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Mol	Chain	Length	Quality of chain
5	S	267	<div><div></div><div>15%</div><div>58%</div><div>28%</div><div>13%</div></div>

ENTRY-COMPOSITION INFOmissingINFO

PHE	MET
CYS	ALA
ALA	SER
ILE	ASN
LEU	ASV
	THR
	A7
	S8
	I9
	A10
	Q11
	A12
	R13
	K14
	L15
	V16
	E17
	Q18
	L19
	K20
	N21
	E22
	A23
	N24
	D25
	D26
	R27
	I28
	K29
	V30
	S31
	K32
	A33
	A34
	A35
	D36
	L37
	M38
	A39
	Y40
	C41
	E42
	K46
	E47
	D48
	P49
	L50
	L51
	T52
	S57
	E58
	F61
	R62
	E63
	K64
	K65
	R66

Y337	LYS	T186	P78	MET
L338	ILE	F187	I81	ASP
N339	SER	Y191	Y82	PHE
I342	THR	I192	Y83	LEU
N343	VAL	P193	I84	ASN
P344	ARG	I197	Y85	SER
L345	SER	Y201	R86	ASP
L346	LEU	K209	W89	GLN
Y347	ARG	H213	Q93	ASN
T348	SER	LYS	Y94	LEU
I349	GLU	ARG	Y95	THR
F350	PHE	GLN	C96	SER
N351	LYS	ALA	D97	GLU
E352	HIS	ALA	I98	LEU
L355	GLU	ARG	R121	ASN
K356	LYS	SER	I125	ARG
K359	TRP	ARG	A128	MET
K360	ARG	ILE	R133	PRO
L361	ARG	LYS	I134	SER
VAL	SER	GLU	R135	K23
ARG	G285	VAL	P137	T24
CYS	T286	ASN	K138	L25
ARG	R287	GLY	I146	V26
CYS	E288	GLN	S155	S27
CYS	R289	VAL	P157	L28
	K290	LEU	P158	T29
	L297	LEU	L159	L30
	T298	GLU	I162	S31
	L299	SER	H163	G32
	C305	GLY	Q164	L33
	F310	LYS	P166	K34
	E313	THR	T166	L35
L314	VAL	SER	S167	N36
V315	V316	TYR	R169	T39
N317	N318	VAL	D170	I40
C319	C320	LEU	E171	M41
K321	K322	LYS	H176	S42
K323	K324	SER	D177	L43
E326	E327	ASP	H178	I44
E328	E329	PRO	I179	V44
N328	S329	THR	V180	V45
S329	N330	ASP	S181	I48
N330	F331	PHE	T182	R52
F331	W334	ASP	I183	H55
			Y184	H56
				P57
				Y60
				C63
				D69
				M77

ALA	V137	Q82	ASP
ALA	T138	M93	V2
LEU			
LEU			
GLU	E141	T84	G8
VAL	S142	S85	G9
LEU		L86	G10
		R87	L11
PHE	I145	S88	V12
GLN	S146		Q13
GLY	C147		P14
PRO			G15
HIS	S150	T91	G16
HIS		A92	S17
HIS	L153	M93	R18
HIS	L154	Y94	C22
HIS	H155	Y95	S23
HIS	S156	C96	A24
HIS		V97	F27
HIS		R98	F32
		S99	G33
		I100	M34
		Y101	H35
		Y102	W36
		G104	V37
		S105	A40
		F108	P41
			E42
			K43
			G44
			L45
			SER
			GLY
			GLY
			GLY
			SER
			GLY
			GLY
			SER
			GLY
			GLY
			S124
			D125
			M128
			A131
			T132
			S133
			S134
			V135
			ALA

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.670	Depositor
Minimum map value	-0.485	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	288.63998, 288.63998, 288.63998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.81999993, 0.81999993, 0.81999993	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1E2G

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	B	0.24	0/2647	0.34	0/3589
2	C	0.15	0/1693	0.24	0/2279
3	G	0.12	0/474	0.25	0/637
4	R	0.20	0/2181	0.33	0/2972
5	S	0.24	0/1817	0.39	0/2464
All	All	0.21	0/8812	0.33	0/11941

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	B	2600	0	2505	95	0
2	C	1664	0	1648	42	0
3	G	467	0	482	20	0
4	R	2130	0	2202	52	0
5	S	1773	0	1710	61	0
6	R	26	0	0	1	0
All	All	8660	0	8547	241	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 14.

All (241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:HG21	1:B:316:SER:HA	1.52	0.90
1:B:286:LEU:HD22	1:B:327:VAL:HG11	1.54	0.88
1:B:51:LEU:HD11	1:B:338:ILE:HD11	1.66	0.76
1:B:274:THR:CG2	1:B:316:SER:HA	2.15	0.76
1:B:160:SER:HB3	1:B:190:LEU:HD23	1.71	0.72
4:R:33:LEU:HD22	4:R:334:TRP:HZ3	1.56	0.69
1:B:161:SER:OG	1:B:163:ASP:OD1	2.12	0.68
1:B:290:ASP:HA	1:B:314:ARG:HG3	1.76	0.67
5:S:175:LEU:HD21	5:S:178:TYR:HB3	1.76	0.67
2:C:205:GLN:HG2	2:C:212:TRP:HZ2	1.60	0.66
1:B:120:ILE:HD12	1:B:140:ALA:HB2	1.77	0.65
2:C:348:LEU:HG	4:R:125:ILE:HD12	1.79	0.65
5:S:166:LEU:HB2	5:S:176:LEU:HD11	1.77	0.65
1:B:61:MET:HE2	1:B:70:LEU:HD12	1.79	0.65
1:B:71:VAL:HG12	1:B:81:ILE:HG12	1.78	0.65
4:R:158:PRO:HA	4:R:176:HIS:CE1	2.31	0.65
4:R:187:PHE:HA	4:R:191:TYR:HB2	1.79	0.65
1:B:283:ARG:HD3	3:G:41:CYS:SG	2.37	0.64
4:R:186:THR:HG23	4:R:310:PHE:HD1	1.63	0.63
2:C:49:ILE:HB	2:C:331:ASN:HD21	1.64	0.62
5:S:37:VAL:HG11	5:S:45:LEU:HD23	1.81	0.62
5:S:91:THR:HG22	5:S:119:VAL:H	1.62	0.62
5:S:40:ALA:HB3	5:S:43:LYS:HB2	1.82	0.62
1:B:95:LEU:HD13	1:B:100:VAL:HG11	1.82	0.61
1:B:283:ARG:HB2	3:G:41:CYS:SG	2.40	0.61
1:B:20:ASP:HA	1:B:23:LYS:HD3	1.81	0.61
2:C:194:ASN:HB3	4:R:133:ARG:HH11	1.64	0.61
1:B:30:LEU:HD22	1:B:262:MET:SD	2.42	0.60
5:S:180:MET:HE3	5:S:200:PHE:CD2	2.37	0.59
4:R:57:PRO:HG2	4:R:135:ARG:HG3	1.83	0.59
1:B:90:VAL:HG13	5:S:102:TYR:HB2	1.85	0.59
2:C:36:LEU:HD13	2:C:223:ILE:HD11	1.85	0.58
4:R:31:SER:HA	4:R:81:ILE:HD13	1.86	0.58
5:S:162:LEU:HD13	5:S:200:PHE:CE1	2.38	0.57
2:C:185:ILE:HD11	2:C:212:TRP:HZ3	1.69	0.57
1:B:126:LEU:HA	1:B:133:VAL:HG22	1.86	0.57
1:B:160:SER:HB2	1:B:187:VAL:CG1	2.35	0.57
5:S:97:VAL:HG11	5:S:108:PHE:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:77:MET:HE2	4:R:337:TYR:HB3	1.88	0.56
4:R:78:PRO:HA	4:R:81:ILE:HD12	1.86	0.56
1:B:248:ALA:H	1:B:272:GLY:HA2	1.70	0.56
5:S:47:TRP:CD1	5:S:225:LEU:HD12	2.40	0.56
5:S:215:TYR:HD1	5:S:215:TYR:H	1.52	0.56
1:B:271:CYS:HB2	1:B:290:ASP:HB2	1.87	0.56
5:S:100:ILE:HG23	5:S:105:SER:HB2	1.87	0.56
5:S:58:ILE:HD13	5:S:70:ILE:HG23	1.87	0.56
1:B:210:LEU:HD13	1:B:255:LEU:HD22	1.88	0.55
4:R:121:ARG:O	4:R:125:ILE:HG12	2.06	0.55
1:B:79:LEU:HB3	1:B:93:ILE:HB	1.88	0.55
1:B:318:LEU:HG	1:B:329:THR:HG22	1.89	0.55
5:S:165:PHE:HE2	5:S:218:MET:HB3	1.72	0.54
1:B:18:ILE:HG22	1:B:22:ARG:HE	1.71	0.54
5:S:51:ILE:HD11	5:S:55:SER:HA	1.89	0.54
2:C:38:LEU:HD23	2:C:223:ILE:HB	1.89	0.54
1:B:99:TRP:HB3	1:B:117:LEU:HD12	1.89	0.54
5:S:83:MET:HB3	5:S:86:LEU:HD21	1.90	0.54
1:B:149:CYS:HB2	1:B:157:ILE:HD11	1.88	0.54
1:B:158:VAL:HG11	1:B:192:LEU:HD21	1.90	0.54
1:B:4:LEU:HD13	3:G:9:ILE:HG22	1.90	0.53
5:S:32:PHE:CE1	5:S:100:ILE:HB	2.44	0.53
1:B:26:ALA:HB2	1:B:259:GLN:HE21	1.74	0.52
1:B:5:ASP:HA	1:B:8:ARG:HE	1.74	0.52
4:R:48:ILE:HD13	4:R:63:CYS:HB2	1.92	0.52
5:S:128:MET:HE1	5:S:153:LEU:HD11	1.92	0.52
4:R:155:SER:C	4:R:158:PRO:HD2	2.35	0.52
1:B:276:VAL:HG13	1:B:285:LEU:HD11	1.91	0.52
4:R:352:GLU:HA	4:R:355:LYS:HD2	1.92	0.52
5:S:32:PHE:CD1	5:S:100:ILE:HB	2.45	0.52
1:B:183:HIS:CE1	1:B:209:LYS:HG3	2.45	0.51
4:R:82:VAL:HA	4:R:85:VAL:HG22	1.92	0.51
1:B:337:LYS:HB2	1:B:339:TRP:NE1	2.25	0.51
4:R:346:ILE:HG13	4:R:347:TYR:CD1	2.46	0.51
4:R:83:TYR:HD2	4:R:89:TRP:HE3	1.58	0.51
4:R:305:CYS:HB3	4:R:339:ASN:HB2	1.91	0.51
1:B:152:LEU:HD23	1:B:192:LEU:HD13	1.93	0.51
2:C:312:ASN:HD21	2:C:317:LYS:HD2	1.76	0.51
3:G:23:ALA:HA	3:G:27:ARG:HH22	1.75	0.51
1:B:121:CYS:HB2	1:B:146:LEU:HD22	1.93	0.50
1:B:160:SER:HB2	1:B:187:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:194:ASN:HB3	4:R:133:ARG:NH1	2.26	0.50
1:B:180:PHE:HB3	1:B:211:TRP:CE3	2.47	0.50
5:S:53:SER:HA	5:S:72:ARG:NH1	2.27	0.50
1:B:101:MET:HE3	2:C:215:CYS:SG	2.51	0.50
5:S:180:MET:HE3	5:S:200:PHE:HD2	1.76	0.49
4:R:179:ILE:HG23	4:R:318:VAL:HG23	1.93	0.49
1:B:163:ASP:O	1:B:165:THR:HG23	2.12	0.49
4:R:313:GLU:O	4:R:317:ASN:HB2	2.12	0.49
1:B:28:ALA:O	3:G:30:VAL:HG11	2.13	0.49
1:B:168:LEU:HD11	1:B:213:VAL:HG13	1.95	0.49
4:R:42:SER:HA	4:R:45:ILE:HD12	1.95	0.48
2:C:339:VAL:HA	2:C:342:ILE:HD12	1.96	0.48
2:C:212:TRP:HE3	2:C:216:PHE:HE2	1.61	0.48
5:S:93:MET:HE2	5:S:116:THR:HB	1.94	0.48
1:B:280:LYS:HB2	1:B:324:GLY:HA3	1.95	0.48
4:R:315:VAL:O	4:R:320:ASP:HB2	2.14	0.48
2:C:312:ASN:ND2	2:C:319:ILE:HD11	2.29	0.48
1:B:120:ILE:HD11	1:B:138:GLU:HB3	1.96	0.47
2:C:340:THR:O	2:C:344:ILE:HG13	2.14	0.47
5:S:22:CYS:SG	5:S:79:LEU:HB3	2.55	0.47
1:B:237:ASN:ND2	1:B:239:ASN:HB2	2.29	0.47
2:C:280:LYS:H	2:C:280:LYS:HG2	1.46	0.47
2:C:351:CYS:O	2:C:353:LEU:HD12	2.15	0.47
1:B:59:TYR:CE2	1:B:75:GLN:HG3	2.49	0.47
1:B:123:ILE:HG23	1:B:151:PHE:HZ	1.79	0.47
4:R:314:LEU:O	4:R:318:VAL:HG12	2.14	0.47
5:S:159:ASN:HB2	5:S:161:TYR:CZ	2.50	0.47
1:B:39:PRO:HB3	1:B:301:LYS:HE3	1.95	0.47
5:S:79:LEU:HD23	5:S:96:CYS:SG	2.55	0.47
1:B:130:GLU:HA	5:S:27:PHE:HB3	1.97	0.47
1:B:69:LEU:HD21	5:S:103:TYR:HD2	1.80	0.47
2:C:44:SER:HB2	2:C:227:ASP:HB2	1.96	0.47
2:C:244:MET:HB3	2:C:287:CYS:SG	2.55	0.47
4:R:197:ILE:O	4:R:201:TYR:HB2	2.15	0.46
5:S:34:MET:HB3	5:S:79:LEU:HD22	1.97	0.46
5:S:147:CYS:O	5:S:200:PHE:HB2	2.15	0.46
5:S:45:LEU:HD13	5:S:216:TYR:CE1	2.51	0.46
5:S:69:THR:HG22	5:S:82:GLN:HB2	1.97	0.46
1:B:162:GLY:HA2	1:B:186:ASP:OD1	2.15	0.46
1:B:232:ILE:HG13	1:B:243:THR:HG22	1.96	0.46
1:B:225:HIS:HD2	1:B:229:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:64:VAL:HG12	5:S:67:ARG:HH21	1.80	0.46
1:B:68:ARG:HD3	5:S:103:TYR:CZ	2.52	0.45
1:B:49:ARG:NH2	3:G:61:PHE:HA	2.31	0.45
1:B:281:SER:HB3	3:G:48:ASP:HB2	1.98	0.45
2:C:305:GLN:HG3	2:C:321:CYS:SG	2.57	0.45
1:B:89:LYS:H	2:C:16:SER:HB2	1.82	0.45
1:B:129:ARG:HD2	1:B:129:ARG:HA	1.78	0.45
2:C:205:GLN:CG	2:C:212:TRP:HZ2	2.27	0.45
5:S:93:MET:HG2	5:S:116:THR:HA	1.99	0.45
2:C:270:ASN:HA	2:C:324:THR:HB	1.97	0.45
2:C:318:GLU:HB3	2:C:320:TYR:CZ	2.51	0.45
5:S:13:GLN:HE22	5:S:16:GLY:HA3	1.82	0.45
1:B:75:GLN:O	1:B:98:SER:HB3	2.16	0.45
2:C:322:HIS:CD2	2:C:334:VAL:HG21	2.51	0.45
1:B:60:ALA:HA	1:B:317:CYS:HB3	1.98	0.45
1:B:283:ARG:HG2	3:G:51:LEU:HD11	1.99	0.45
5:S:145:ILE:O	5:S:201:THR:HA	2.17	0.45
2:C:231:TYR:HE2	2:C:284:LEU:HA	1.82	0.45
2:C:255:CYS:SG	2:C:312:ASN:HA	2.56	0.45
2:C:230:ASP:HB3	2:C:243:ARG:HB3	1.99	0.45
4:R:158:PRO:HA	4:R:176:HIS:HE1	1.77	0.45
4:R:318:VAL:HG13	4:R:319:CYS:H	1.81	0.45
4:R:321:LYS:HA	4:R:321:LYS:HD3	1.78	0.45
1:B:70:LEU:CD2	1:B:82:TRP:HB2	2.47	0.44
1:B:236:PRO:HB2	3:G:40:TYR:CE1	2.52	0.44
2:C:38:LEU:HD21	2:C:199:LEU:HD23	1.99	0.44
1:B:273:ILE:HG21	1:B:276:VAL:HG23	1.99	0.44
4:R:297:LEU:HD13	4:R:350:PHE:HZ	1.82	0.44
1:B:29:THR:HG22	1:B:31:SER:H	1.82	0.44
1:B:55:LEU:HG	2:C:27:GLY:HA3	2.00	0.44
5:S:155:HIS:HD2	5:S:221:LEU:HD22	1.81	0.44
5:S:167:GLN:HB2	5:S:173:PRO:HG3	1.98	0.44
2:C:228:LEU:HA	2:C:244:MET:HE1	1.98	0.44
4:R:52:ARG:HA	4:R:55:HIS:ND1	2.32	0.44
4:R:60:TYR:HE2	4:R:137:PRO:HB3	1.81	0.44
1:B:107:PRO:HD3	1:B:151:PHE:HB3	1.99	0.44
4:R:176:HIS:HB2	6:R:401:A1E2G:C20	2.48	0.44
5:S:162:LEU:HD13	5:S:200:PHE:CD1	2.53	0.44
4:R:85:VAL:HG23	4:R:86:ARG:HG2	1.99	0.44
5:S:50:TYR:HD2	5:S:59:TYR:HD1	1.64	0.44
1:B:326:ALA:HB2	3:G:61:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:183:ILE:HD12	4:R:183:ILE:HA	1.84	0.44
4:R:318:VAL:HG13	4:R:319:CYS:N	2.33	0.44
4:R:349:ILE:HD13	4:R:349:ILE:HA	1.92	0.44
5:S:166:LEU:HD22	5:S:168:ARG:HG3	1.99	0.44
5:S:95:TYR:HD2	5:S:114:GLY:HA3	1.82	0.43
1:B:164:THR:HG22	1:B:185:GLY:O	2.18	0.43
1:B:284:LEU:HD13	3:G:51:LEU:CD2	2.48	0.43
4:R:338:LEU:HD23	4:R:338:LEU:HA	1.87	0.43
5:S:83:MET:HE2	5:S:83:MET:HB2	1.82	0.43
1:B:164:THR:HG22	1:B:185:GLY:C	2.43	0.43
5:S:35:HIS:HB2	5:S:97:VAL:HB	2.00	0.43
1:B:338:ILE:HG21	3:G:61:PHE:CE1	2.53	0.43
4:R:178:HIS:O	4:R:182:THR:HG22	2.19	0.43
5:S:34:MET:HB2	5:S:51:ILE:HG23	2.01	0.43
2:C:184:GLY:HA2	2:C:205:GLN:HE22	1.84	0.43
5:S:53:SER:HA	5:S:72:ARG:HH12	1.83	0.43
1:B:277:SER:HB2	1:B:318:LEU:HD22	2.01	0.43
4:R:157:PRO:HG2	4:R:184:TYR:CE1	2.53	0.43
5:S:51:ILE:HG12	5:S:72:ARG:HB3	2.01	0.43
5:S:166:LEU:HG	5:S:215:TYR:CE1	2.53	0.43
1:B:51:LEU:HD12	1:B:336:LEU:HB2	2.01	0.43
2:C:343:ILE:HG22	4:R:128:ALA:HB1	2.01	0.43
4:R:159:LEU:HA	4:R:159:LEU:HD12	1.76	0.43
5:S:36:TRP:HD1	5:S:70:ILE:HD12	1.84	0.43
3:G:14:LYS:HA	3:G:14:LYS:HD3	1.75	0.42
4:R:209:LYS:HA	4:R:209:LYS:HD2	1.85	0.42
1:B:4:LEU:HD13	3:G:9:ILE:HA	2.01	0.42
1:B:328:ALA:HB2	1:B:338:ILE:HD13	2.00	0.42
2:C:205:GLN:HG2	2:C:212:TRP:CZ2	2.48	0.42
2:C:267:LEU:HD23	2:C:321:CYS:HB2	2.01	0.42
4:R:342:ILE:HG22	4:R:346:ILE:HG23	2.00	0.42
5:S:8:GLY:HA3	5:S:18:ARG:HH22	1.83	0.42
5:S:72:ARG:HE	5:S:72:ARG:HB2	1.59	0.42
1:B:331:SER:HB3	1:B:333:ASP:OD1	2.19	0.42
2:C:193:LYS:HB3	2:C:193:LYS:HE2	1.82	0.42
5:S:138:THR:O	5:S:141:GLU:HG2	2.19	0.42
1:B:18:ILE:HG12	3:G:23:ALA:HB2	2.01	0.42
3:G:47:GLU:O	3:G:49:PRO:HD3	2.20	0.42
4:R:299:LEU:HD23	4:R:299:LEU:HA	1.81	0.42
1:B:70:LEU:HD23	1:B:82:TRP:HB2	2.01	0.42
1:B:102:THR:OG1	1:B:148:CYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LEU:HD13	3:G:51:LEU:HD23	2.01	0.42
2:C:209:ARG:HA	2:C:212:TRP:HD1	1.85	0.42
1:B:198:LEU:HD12	1:B:198:LEU:HA	1.91	0.42
4:R:342:ILE:N	4:R:342:ILE:HD13	2.35	0.42
1:B:180:PHE:CE1	1:B:216:GLY:HA2	2.55	0.41
1:B:197:ARG:HE	1:B:214:ARG:NE	2.17	0.41
2:C:312:ASN:ND2	2:C:317:LYS:HD2	2.35	0.41
4:R:183:ILE:HD13	4:R:314:LEU:HD11	2.01	0.41
2:C:195:LEU:HD23	2:C:195:LEU:HA	1.93	0.41
5:S:24:ALA:HB1	5:S:27:PHE:CE1	2.54	0.41
1:B:237:ASN:HD21	1:B:239:ASN:HB2	1.84	0.41
1:B:278:PHE:CE1	1:B:285:LEU:HB2	2.55	0.41
5:S:68:PHE:CZ	5:S:83:MET:HG2	2.56	0.41
5:S:94:TYR:O	5:S:114:GLY:HA2	2.20	0.41
1:B:56:ALA:HB1	1:B:75:GLN:HB2	2.03	0.41
2:C:48:THR:HA	2:C:51:LYS:HG2	2.02	0.41
2:C:322:HIS:HB2	2:C:334:VAL:HG11	2.02	0.41
1:B:11:ALA:HB2	3:G:16:VAL:HG22	2.02	0.41
1:B:252:LEU:HD21	3:G:37:LEU:HD21	2.01	0.41
1:B:68:ARG:HE	1:B:85:TYR:HB2	1.86	0.41
4:R:52:ARG:HA	4:R:55:HIS:HD1	1.86	0.41
4:R:347:TYR:O	4:R:348:THR:HG22	2.21	0.41
2:C:353:LEU:HD12	2:C:353:LEU:H	1.85	0.41
1:B:43:ILE:HD12	1:B:43:ILE:HA	1.81	0.41
1:B:104:ALA:HB2	1:B:149:CYS:O	2.21	0.41
4:R:192:ILE:HB	4:R:193:PRO:HD3	2.02	0.41
5:S:8:GLY:HA3	5:S:18:ARG:NH2	2.36	0.41
5:S:117:LEU:HD12	5:S:117:LEU:HA	1.76	0.41
5:S:154:LEU:HD23	5:S:155:HIS:O	2.21	0.41
1:B:57:LYS:HB3	1:B:332:TRP:CD1	2.56	0.41
4:R:89:TRP:CD1	4:R:96:CYS:HB2	2.56	0.41
5:S:55:SER:OG	5:S:72:ARG:HG2	2.21	0.41
1:B:37:ILE:HD11	3:G:42:GLU:OE2	2.21	0.40
1:B:59:TYR:OH	2:C:215:CYS:HA	2.21	0.40
1:B:158:VAL:CG1	1:B:192:LEU:HD21	2.51	0.40
4:R:41:ASN:OD1	4:R:344:PRO:HG2	2.22	0.40
5:S:2:VAL:HG13	5:S:27:PHE:CD2	2.56	0.40
4:R:146:ILE:HD13	4:R:146:ILE:HA	1.87	0.40
5:S:99:SER:CB	5:S:108:PHE:H	2.34	0.40

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 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	B	336/358 (94%)	319 (95%)	17 (5%)	0	100	100
2	C	206/228 (90%)	198 (96%)	8 (4%)	0	100	100
3	G	58/71 (82%)	54 (93%)	4 (7%)	0	100	100
4	R	264/366 (72%)	252 (96%)	12 (4%)	0	100	100
5	S	227/267 (85%)	210 (92%)	17 (8%)	0	100	100
All	All	1091/1290 (85%)	1033 (95%)	58 (5%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	B	281/298 (94%)	281 (100%)	0	100	100
2	C	184/196 (94%)	184 (100%)	0	100	100
3	G	49/58 (84%)	49 (100%)	0	100	100
4	R	234/332 (70%)	234 (100%)	0	100	100
5	S	195/216 (90%)	195 (100%)	0	100	100
All	All	943/1100 (86%)	943 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	HIS
1	B	259	GLN
1	B	293	ASN
2	C	257	ASN
2	C	331	ASN
3	G	11	GLN
4	R	56	HIS
4	R	59	ASN
5	S	13	GLN
5	S	167	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

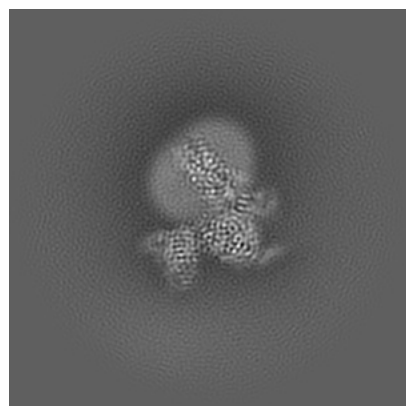
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67446. These allow visual inspection of the internal detail of the map and identification of artifacts.

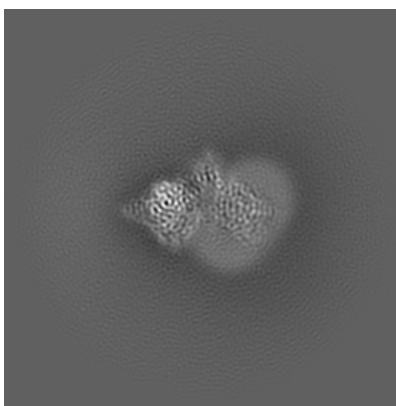
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

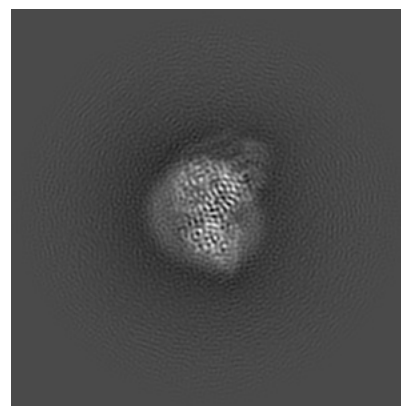
5.1.1 Primary map



X

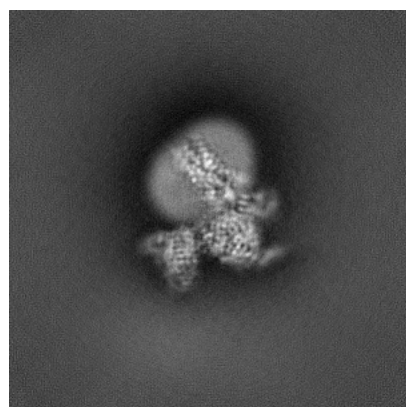


Y

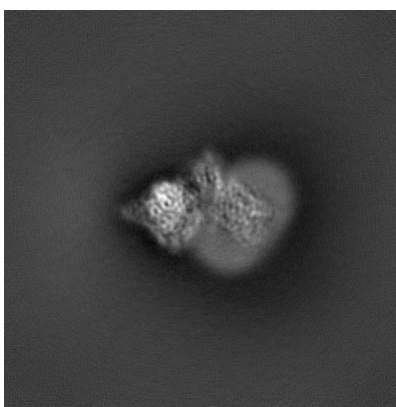


Z

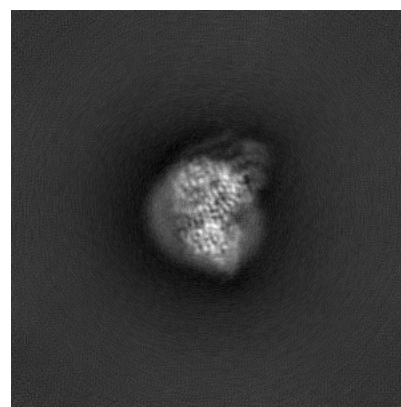
5.1.2 Raw map



X



Y

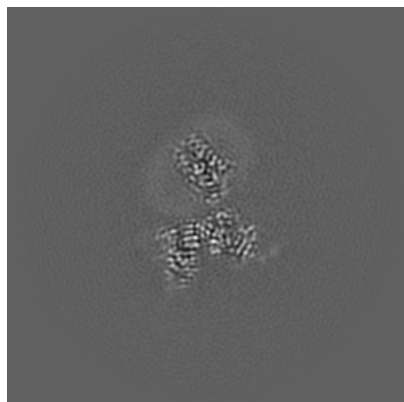


Z

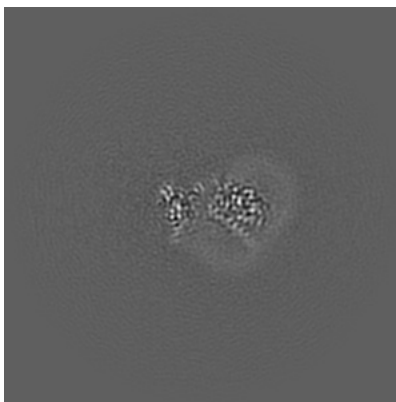
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

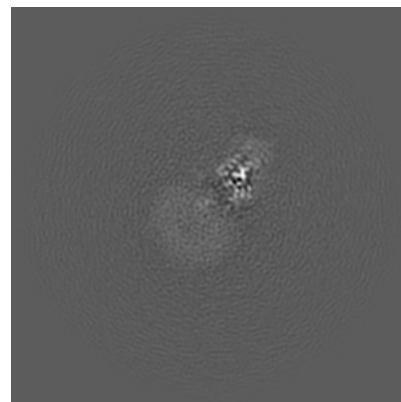
5.2.1 Primary map



X Index: 176

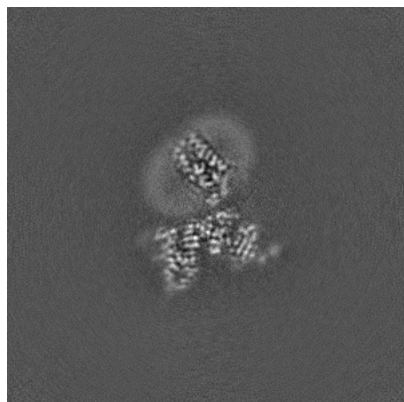


Y Index: 176

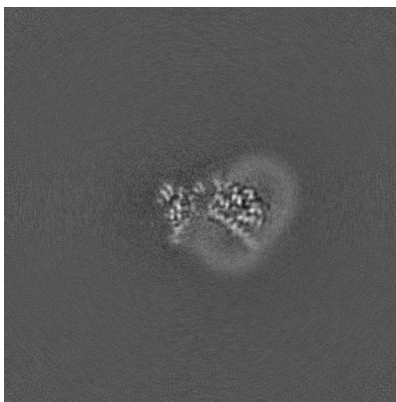


Z Index: 176

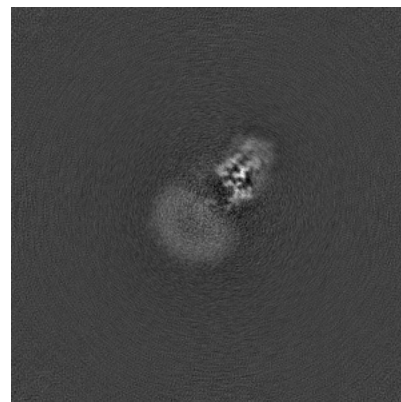
5.2.2 Raw map



X Index: 176



Y Index: 176

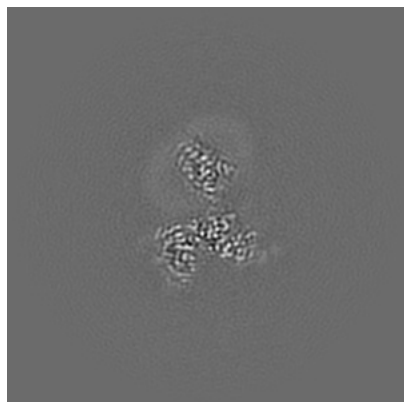


Z Index: 176

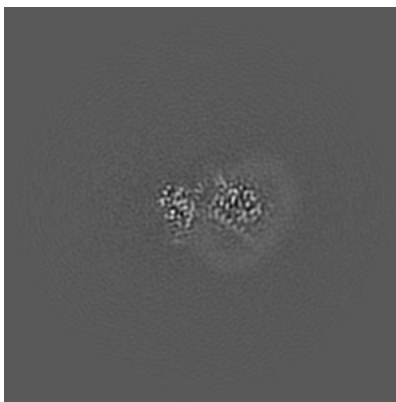
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

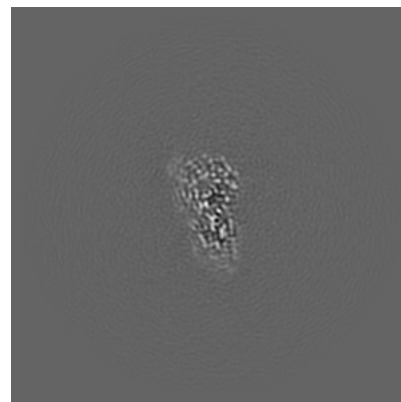
5.3.1 Primary map



X Index: 179

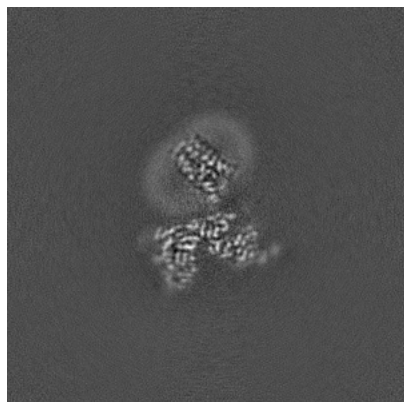


Y Index: 178

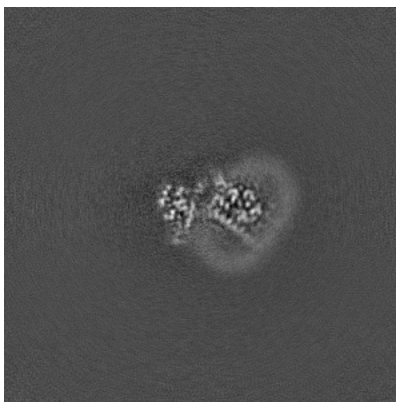


Z Index: 148

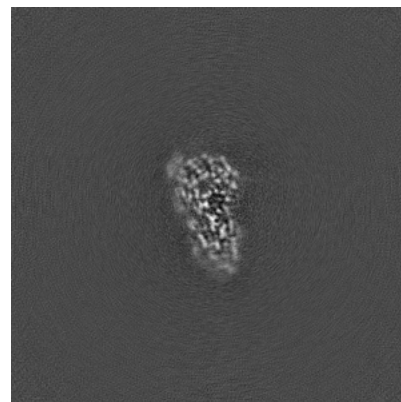
5.3.2 Raw map



X Index: 178



Y Index: 178

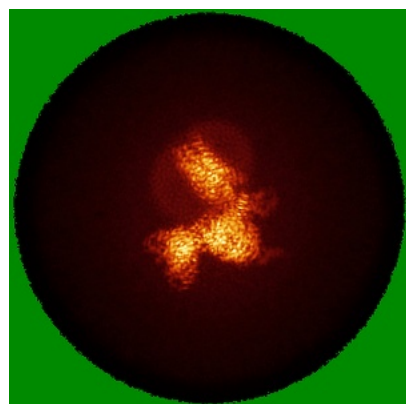


Z Index: 148

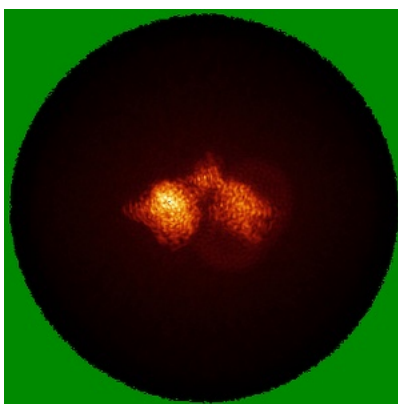
The images above show the largest variance slices of the map in three orthogonal directions.

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

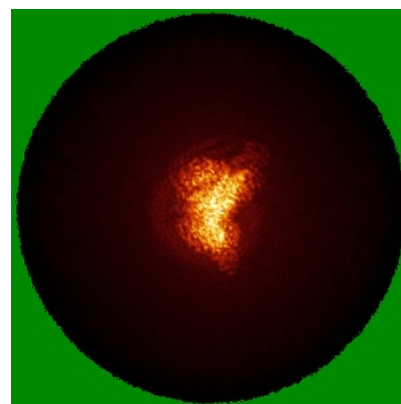
5.4.1 Primary map



X

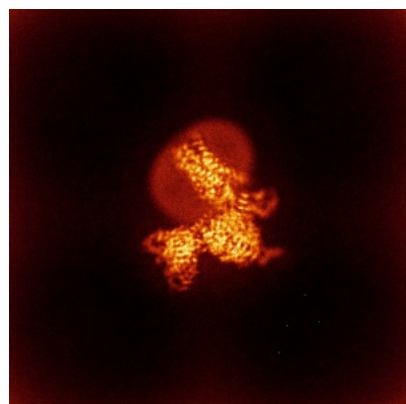


Y

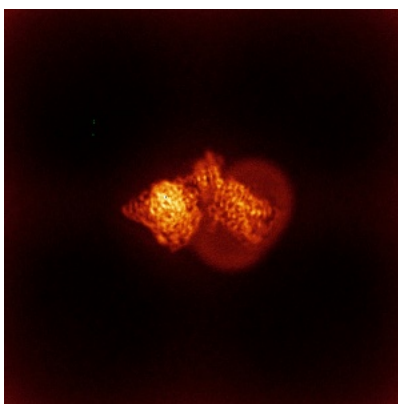


Z

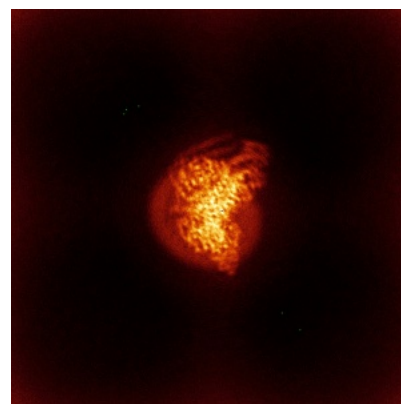
5.4.2 Raw map



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.

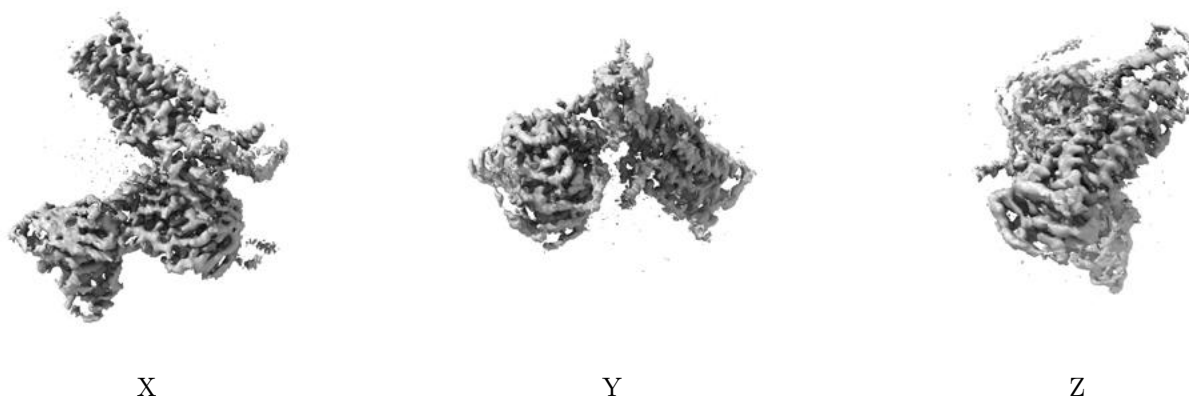
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

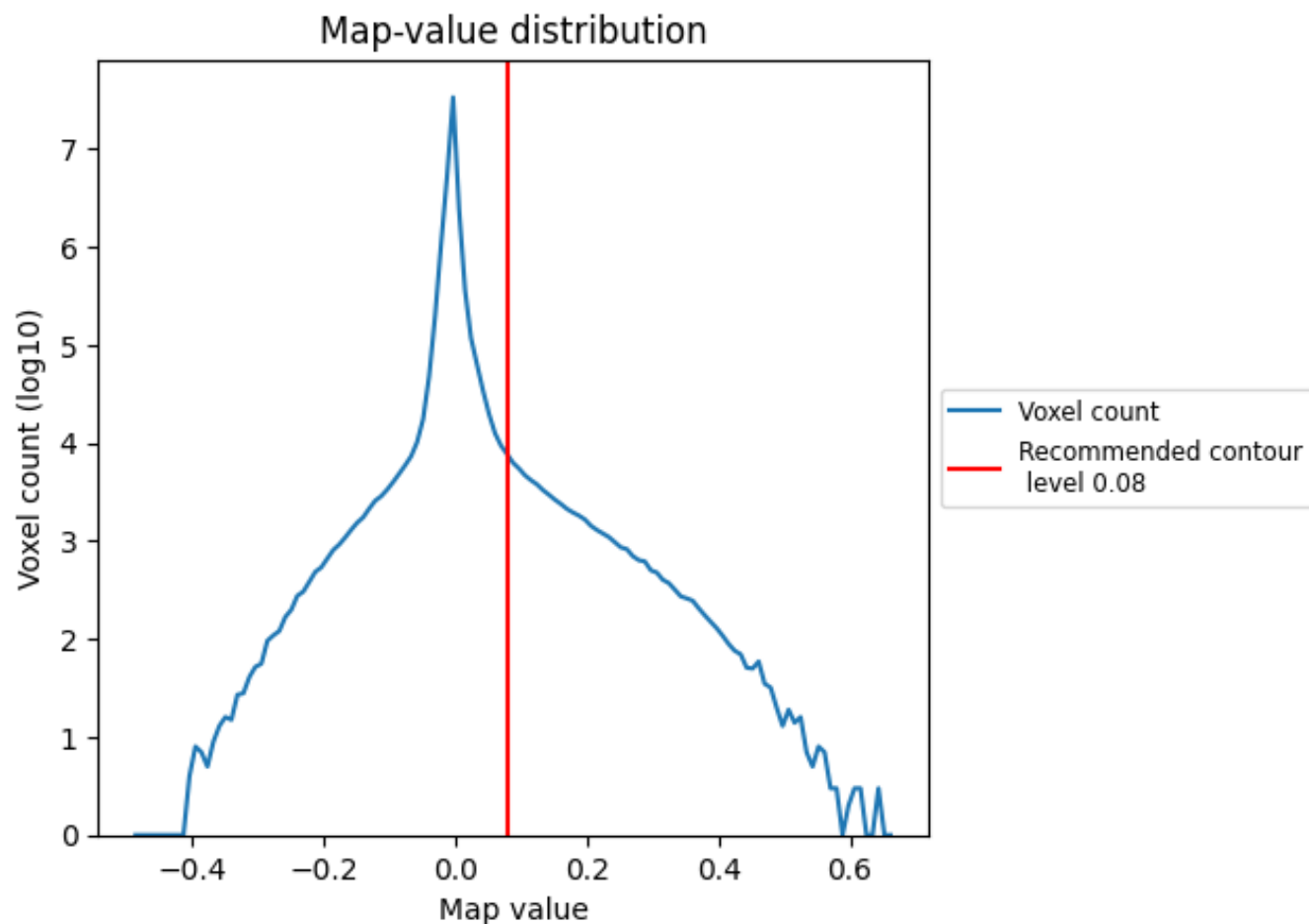
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

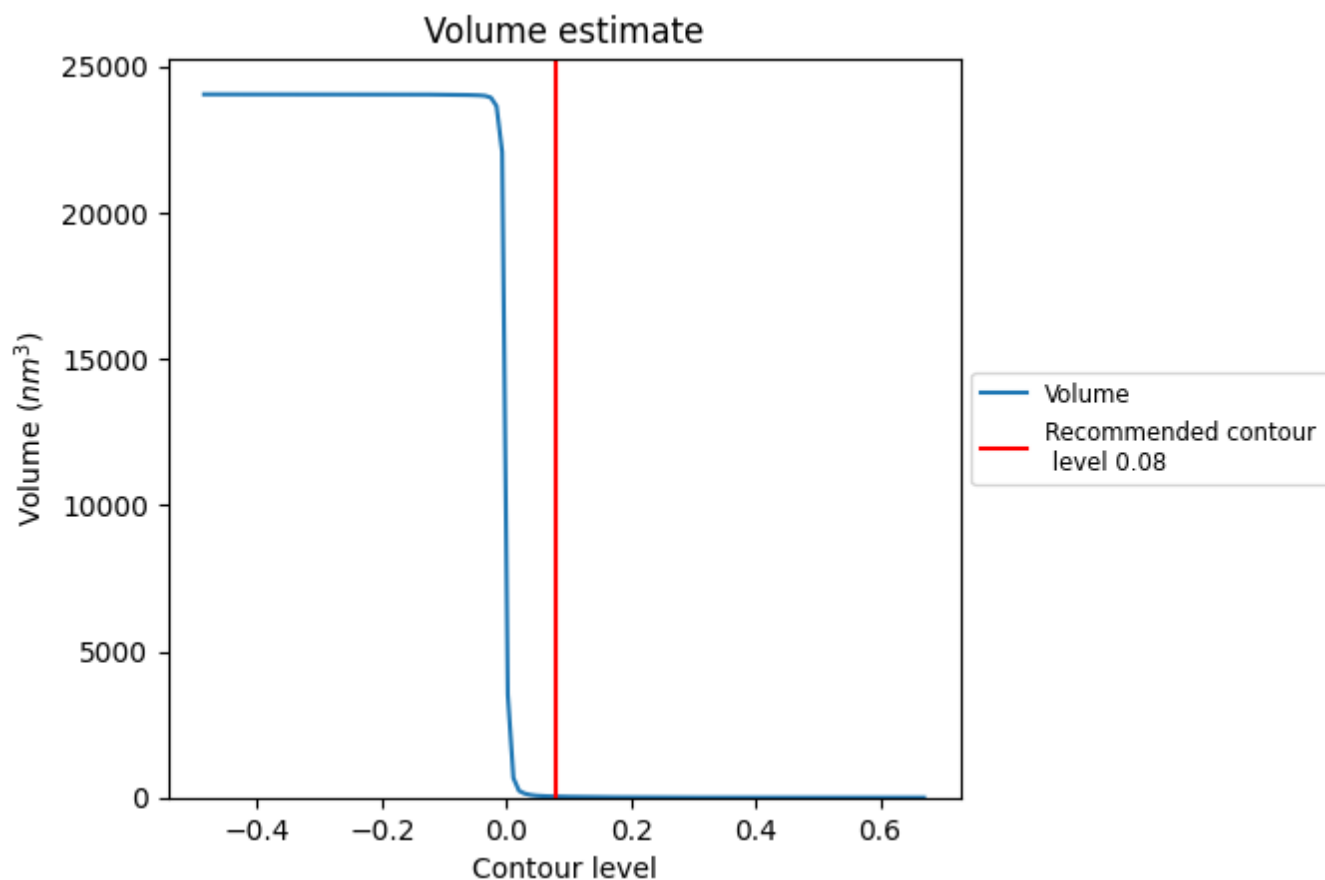
This section contains the results of statistical analysis of the map.

6.1 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.

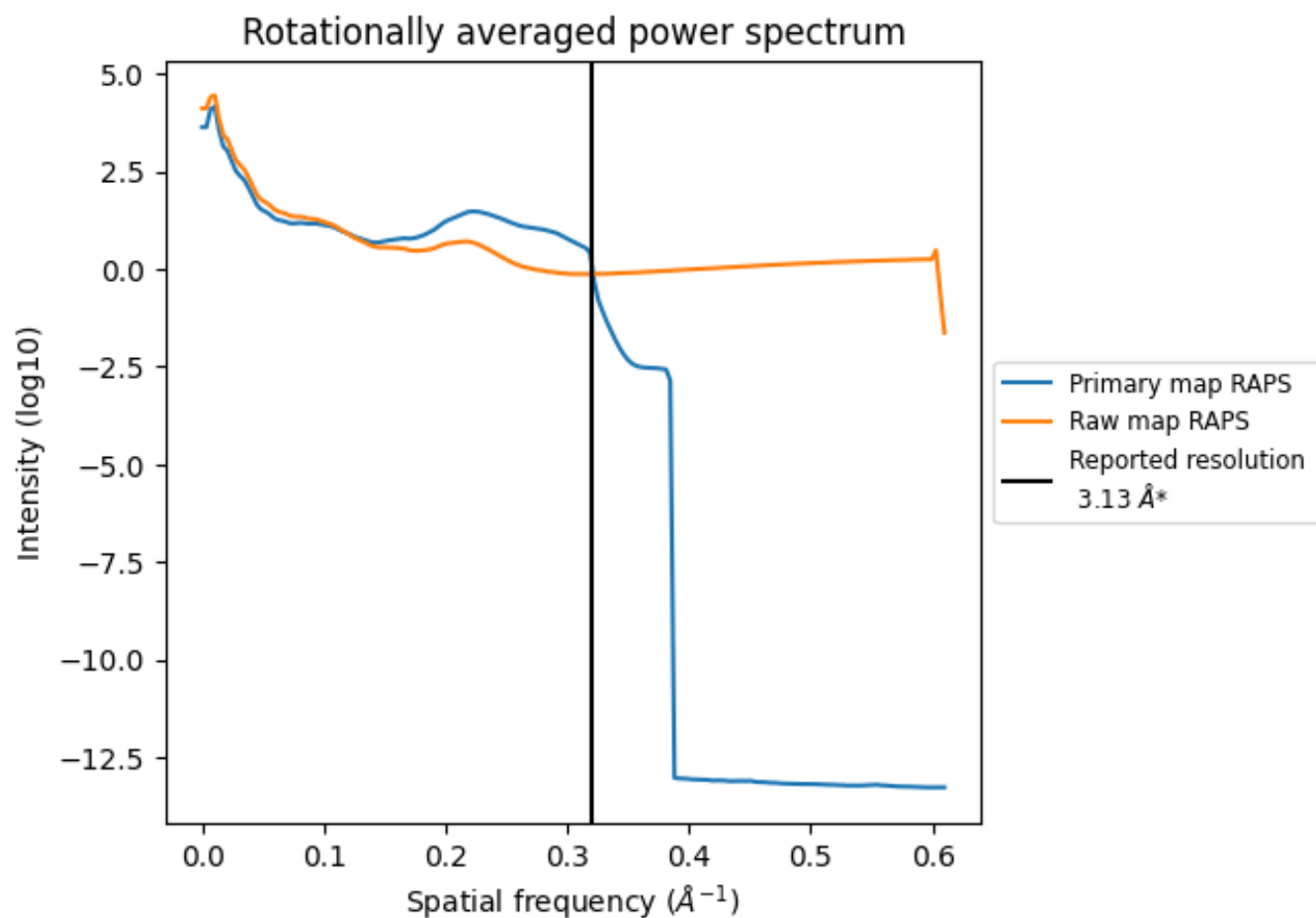
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm³; this corresponds to an approximate mass of 32 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.

6.3 Rotationally averaged power spectrum ⓘ

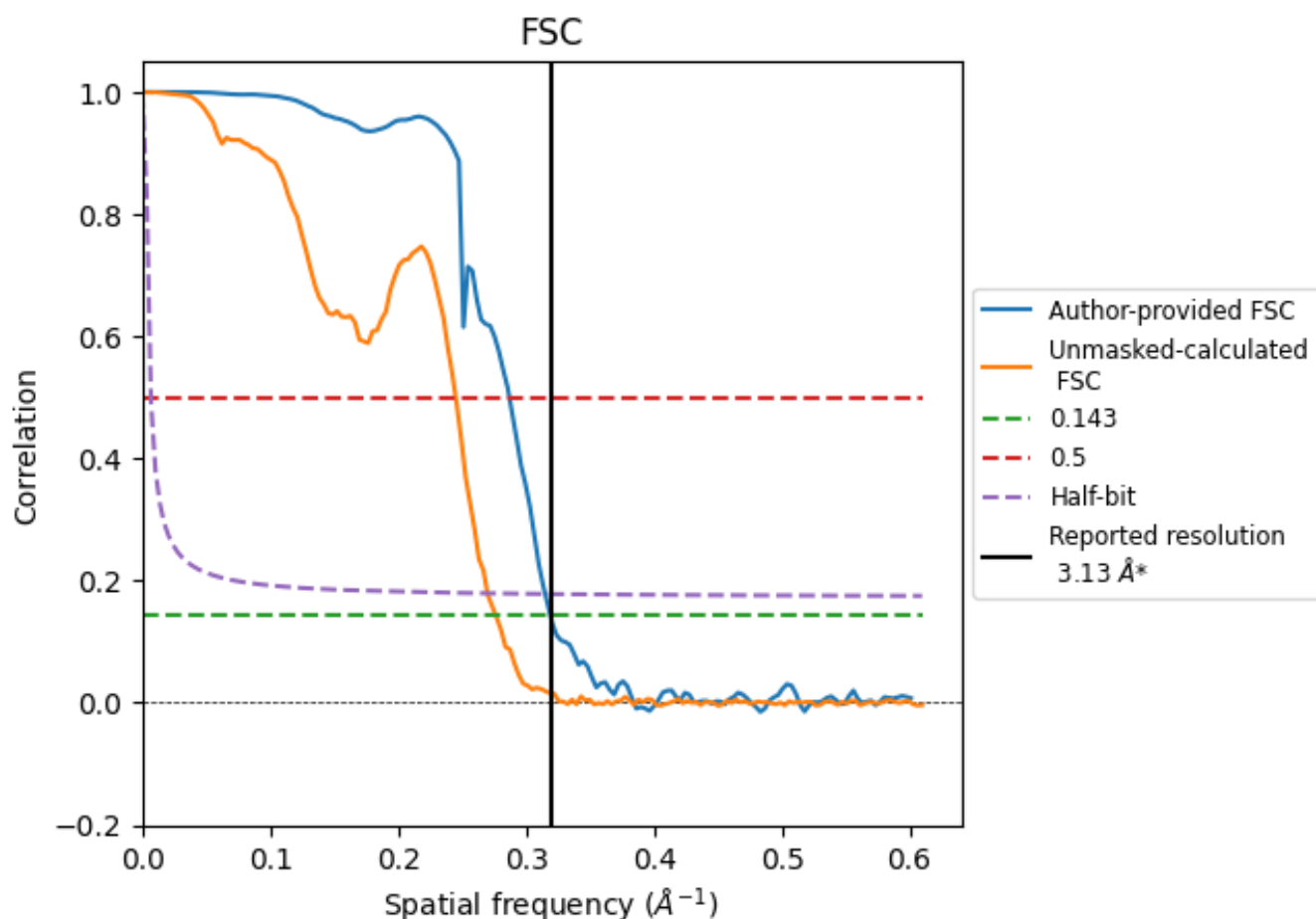


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 \AA^{-1}

7.2 Resolution estimates [i](#)

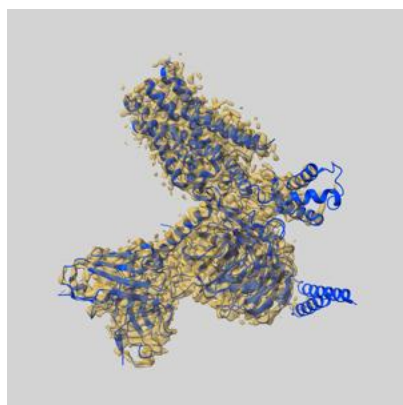
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.48	3.17
Unmasked-calculated*	3.62	4.08	3.70

*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 3.62 differs from the reported value 3.13 by more than 10 %

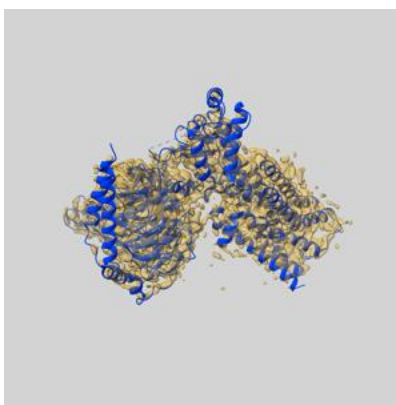
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67446 and PDB model 21AG. Per-residue inclusion information can be found in [section 2](#) on [page 4](#).

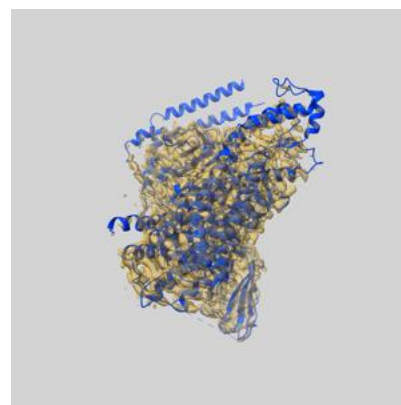
8.1 Map-model overlay [i](#)



X



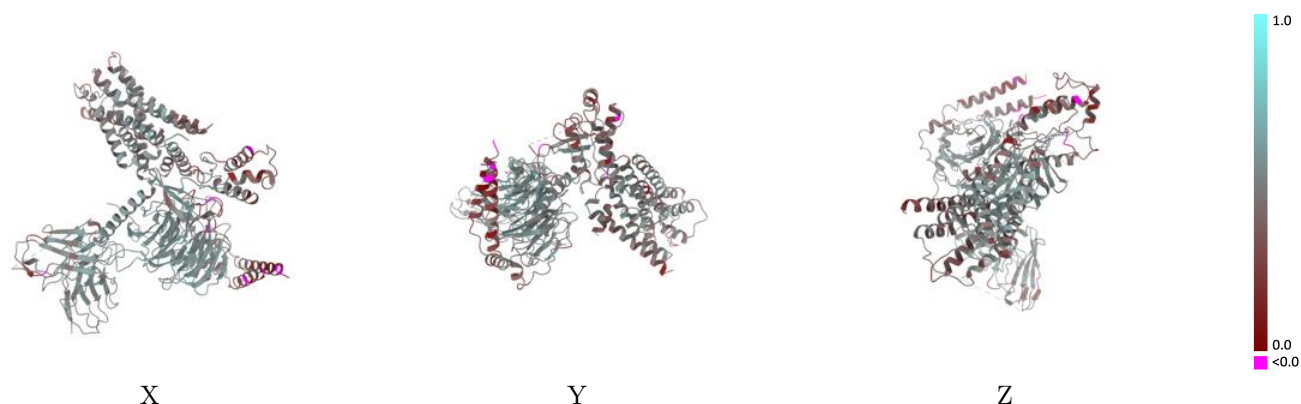
Y



Z

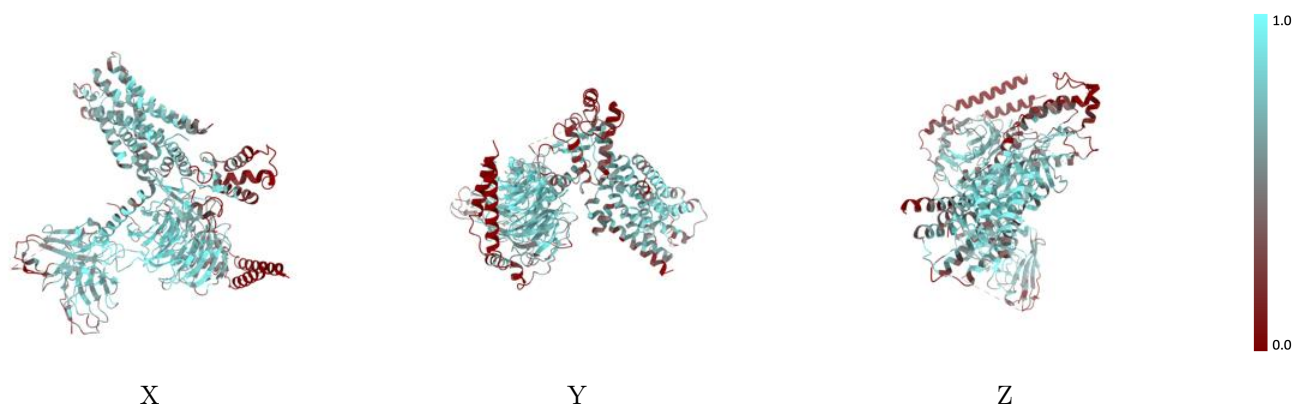
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



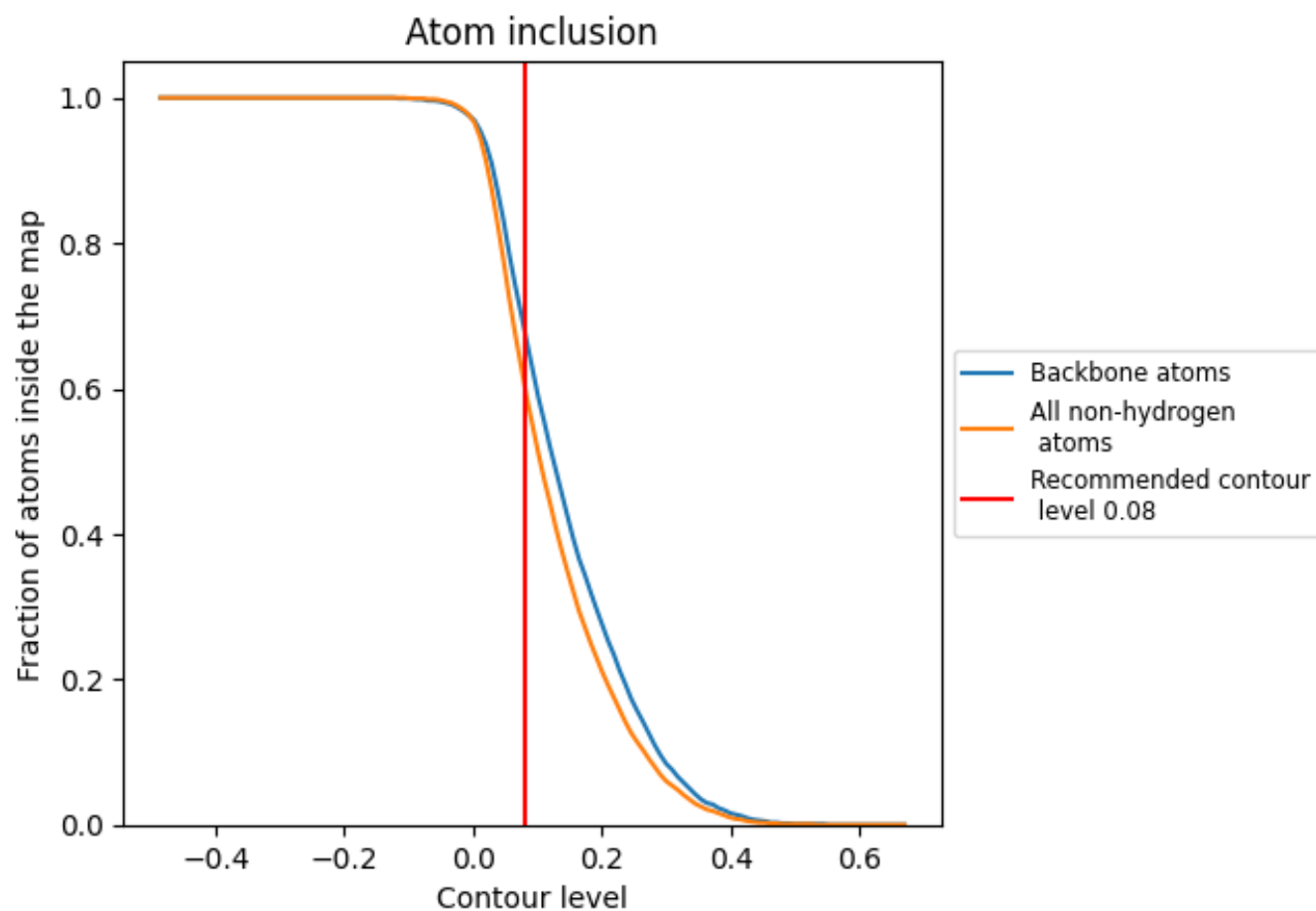
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.08).

8.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6050	<div></div> 0.4660
B	<div></div> 0.6800	<div></div> 0.5040
C	<div></div> 0.4690	<div></div> 0.4290
G	<div></div> 0.3000	<div></div> 0.3780
R	<div></div> 0.6370	<div></div> 0.4490
S	<div></div> 0.6640	<div></div> 0.4900

