



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:39 AM UTC

PDB ID : 8ZCJ / pdb_00008zcj
EMDB ID : EMD-39931
Title : Cryo-EM structure of the pasireotide-bound SSTR5-Gi complex
Authors : Li, Y.G.; Meng, X.Y.; Yang, X.R.; Ling, S.L.; Shi, P.; Tian, C.L.; Yang, F.
Deposited on : 2024-04-29
Resolution : 3.09 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:

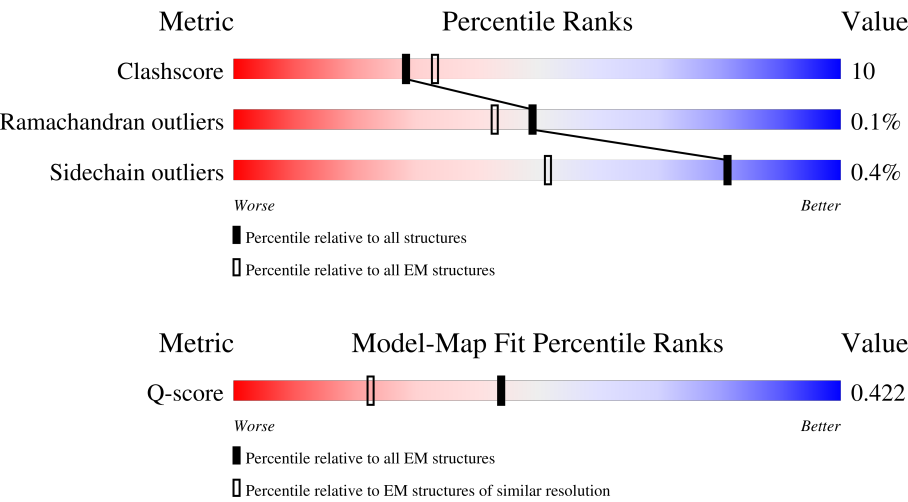
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.09 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.



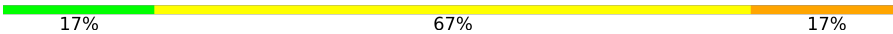
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14003 (2.59 - 3.59)

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	354	
2	C	377	
3	D	71	
4	E	304	

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Mol	Chain	Length	Quality of chain
5	G	570	
6	A	6	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7808 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(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	222	Total	C	N	O	S	0	0
			1556	985	264	297	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	ALA	GLY	conflict	UNP P63096
B	326	SER	ALA	conflict	UNP P63096

- 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
2	C	341	Total	C	N	O	S	0	0
			2369	1471	430	457	11		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP P54311
C	-9	HIS	-	expression tag	UNP P54311
C	-8	HIS	-	expression tag	UNP P54311
C	-7	HIS	-	expression tag	UNP P54311
C	-6	HIS	-	expression tag	UNP P54311
C	-5	HIS	-	expression tag	UNP P54311
C	-4	HIS	-	expression tag	UNP P54311
C	-3	GLY	-	expression tag	UNP P54311
C	-2	SER	-	expression tag	UNP P54311
C	-1	LEU	-	expression tag	UNP P54311
C	0	LEU	-	expression tag	UNP P54311
C	1	GLN	-	expression tag	UNP P54311
C	341	GLY	-	expression tag	UNP P54311
C	342	SER	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
C	343	SER	-	expression tag	UNP P54311
C	344	GLY	-	expression tag	UNP P54311
C	345	GLY	-	expression tag	UNP P54311
C	346	GLY	-	expression tag	UNP P54311
C	347	GLY	-	expression tag	UNP P54311
C	348	SER	-	expression tag	UNP P54311
C	349	GLY	-	expression tag	UNP P54311
C	350	GLY	-	expression tag	UNP P54311
C	351	GLY	-	expression tag	UNP P54311
C	352	GLY	-	expression tag	UNP P54311
C	353	SER	-	expression tag	UNP P54311
C	354	SER	-	expression tag	UNP P54311
C	355	GLY	-	expression tag	UNP P54311
C	356	VAL	-	expression tag	UNP P54311
C	357	SER	-	expression tag	UNP P54311
C	358	GLY	-	expression tag	UNP P54311
C	359	TRP	-	expression tag	UNP P54311
C	360	ARG	-	expression tag	UNP P54311
C	361	LEU	-	expression tag	UNP P54311
C	362	PHE	-	expression tag	UNP P54311
C	363	LYS	-	expression tag	UNP P54311
C	364	LYS	-	expression tag	UNP P54311
C	365	ILE	-	expression tag	UNP P54311
C	366	SER	-	expression tag	UNP P54311

- 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
3	D	50	Total	C	N	O	0	0
			296	187	53	56		

- Molecule 4 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	233	Total	C	N	O	S	0	0
			1705	1080	281	336	8		

- Molecule 5 is a protein called Beta-2 adrenergic receptor,Somatostatin receptor type 5,lgbit (fusion protein).

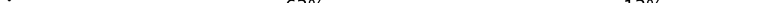
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	275	Total	C	N	O	S	0	0
			1818	1174	308	324	12		

There are 24 discrepancies between the modelled and reference sequences:

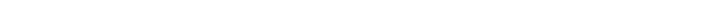
Chain	Residue	Modelled	Actual	Comment	Reference
G	-47	MET	-	initiating methionine	UNP P07550
G	-46	LYS	-	expression tag	UNP P07550
G	-45	THR	-	expression tag	UNP P07550
G	-44	ILE	-	expression tag	UNP P07550
G	-43	ILE	-	expression tag	UNP P07550
G	-42	ALA	-	expression tag	UNP P07550
G	-41	LEU	-	expression tag	UNP P07550
G	-40	SER	-	expression tag	UNP P07550
G	-39	TYR	-	expression tag	UNP P07550
G	-38	ILE	-	expression tag	UNP P07550
G	-37	PHE	-	expression tag	UNP P07550
G	-36	CYS	-	expression tag	UNP P07550
G	-35	LEU	-	expression tag	UNP P07550
G	-34	VAL	-	expression tag	UNP P07550
G	-33	PHE	-	expression tag	UNP P07550
G	-32	ALA	-	expression tag	UNP P07550
G	-31	ASP	-	expression tag	UNP P07550
G	-30	TYR	-	expression tag	UNP P07550
G	-29	LYS	-	expression tag	UNP P07550
G	-28	ASP	-	expression tag	UNP P07550
G	-27	ASP	-	expression tag	UNP P07550
G	-26	ASP	-	expression tag	UNP P07550
G	-25	ASP	-	expression tag	UNP P07550
G	-24	LYS	-	expression tag	UNP P07550

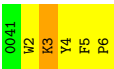
- Molecule 6 is a protein called 004-DTR-LYS-TYR-PHA-HYP.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	6	Total	C	N	O	0	0
			64	48	8	8		

Chain E:  8% 63% 13% 23%

Chain G: 

Chain A:  17% 67% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1227503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.227	Depositor
Minimum map value	-2.610	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.41	Depositor
Map size ($\text{\AA}$)	214.00002, 214.00002, 214.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTR, 004, HYP, PHA

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	0.31	0/1579	0.61	3/2148 (0.1%)
2	C	0.25	0/2416	0.55	3/3306 (0.1%)
3	D	0.15	0/302	0.52	0/422
4	E	0.19	0/1747	0.46	0/2381
5	G	0.25	0/1856	0.56	3/2562 (0.1%)
6	A	3.02	1/21 (4.8%)	1.73	1/26 (3.8%)
All	All	0.29	1/7921 (0.0%)	0.55	10/10845 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3	LYS	C-N	12.68	1.51	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	LYS	N-CA-C	-8.59	101.84	111.71
5	G	143	HIS	CA-C-N	-6.71	113.00	120.45
5	G	143	HIS	C-N-CA	-6.71	113.00	120.45
2	C	186	ASP	N-CA-C	6.10	118.39	108.63
2	C	118	ASP	N-CA-C	-5.96	105.99	113.20
1	B	39	LEU	N-CA-CB	-5.92	102.67	111.43
5	G	190	TRP	N-CA-C	-5.36	100.83	109.40
1	B	43	GLU	N-CA-C	-5.27	105.50	112.24
6	A	4	TYR	CA-CB-CG	-5.21	104.52	113.90
2	C	104	ALA	N-CA-C	5.04	115.19	108.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1556	0	1365	30	0
2	C	2369	0	2017	47	0
3	D	296	0	204	3	0
4	E	1705	0	1562	24	0
5	G	1818	0	1619	39	0
6	A	64	0	54	2	0
All	All	7808	0	6821	139	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 (139) 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:G:147:SER:O	5:G:151:ARG:N	2.26	0.68
5:G:89:TYR:HB2	5:G:122:ASN:HB3	1.78	0.65
5:G:74:VAL:HG21	5:G:151:ARG:HD3	1.83	0.61
5:G:81:ASN:ND2	5:G:160:SER:OG	2.34	0.61
5:G:127:VAL:HG12	5:G:213:PRO:HB2	1.83	0.60
5:G:123:GLN:HE22	5:G:265:PHE:HZ	1.51	0.58
5:G:218:CYS:SG	5:G:254:VAL:HG22	2.44	0.57
1:B:339:VAL:O	1:B:343:ILE:HG13	2.05	0.57
2:C:103:CYS:SG	2:C:104:ALA:N	2.79	0.56
4:E:140:MET:HG3	4:E:240:GLY:HA3	1.86	0.56
4:E:175:TYR:HB2	4:E:230:MET:HB3	1.88	0.56
4:E:37:VAL:HG11	4:E:45:LEU:HD23	1.86	0.56
4:E:6:GLU:N	4:E:6:GLU:OE1	2.39	0.55
2:C:321:THR:OG1	2:C:325:MET:N	2.40	0.55
2:C:102:THR:HG21	2:C:148:CYS:HA	1.88	0.55
5:G:210:PHE:HE1	5:G:261:TRP:CD1	2.25	0.55
1:B:263:SER:OG	1:B:342:VAL:HG21	2.07	0.55
1:B:339:VAL:HG12	1:B:343:ILE:CD1	2.37	0.54
2:C:180:PHE:HB3	2:C:211:TRP:NE1	2.22	0.54
2:C:180:PHE:HB3	2:C:211:TRP:CD1	2.43	0.54
2:C:50:THR:HG22	2:C:52:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:TYR:O	2:C:162:GLY:N	2.42	0.53
4:E:230:MET:HE3	4:E:237:LEU:HB3	1.89	0.53
5:G:142:VAL:HG22	5:G:227:LYS:HE2	1.91	0.53
4:E:88:SER:HA	4:E:119:VAL:HG21	1.90	0.53
1:B:311:ASN:HD22	1:B:319:ILE:HG12	1.74	0.53
1:B:194:LEU:HD22	1:B:196:PHE:CE2	2.43	0.53
4:E:12:VAL:HG21	4:E:18:ARG:HD3	1.90	0.53
5:G:125:THR:HA	5:G:128:PHE:HB2	1.91	0.52
1:B:266:LEU:HB3	1:B:321:THR:HG22	1.91	0.52
2:C:86:THR:OG1	2:C:88:ASN:OD1	2.28	0.52
2:C:113:ALA:H	2:C:151:PHE:HE2	1.57	0.52
5:G:116:MET:HG3	5:G:186:CYS:HB3	1.91	0.51
2:C:80:ILE:HG21	2:C:89:LYS:HD3	1.93	0.51
2:C:81:ILE:HD12	2:C:91:HIS:HB2	1.93	0.51
5:G:140:ALA:HB2	5:G:151:ARG:HH22	1.75	0.51
5:G:267:VAL:HG21	5:G:286:TYR:HE1	1.74	0.50
2:C:144:GLY:HA3	2:C:163:ASP:H	1.76	0.50
2:C:126:LEU:HA	2:C:133:VAL:HG22	1.93	0.50
1:B:34:VAL:CG2	1:B:194:LEU:HD21	2.41	0.50
1:B:40:GLY:HA3	1:B:224:CYS:HB2	1.94	0.49
2:C:105:TYR:HE1	2:C:126:LEU:HD11	1.76	0.49
4:E:100:ILE:O	4:E:105:SER:OG	2.28	0.49
1:B:264:ILE:HB	1:B:319:ILE:HD12	1.94	0.49
1:B:45:GLY:O	1:B:49:ILE:HG12	2.13	0.49
4:E:173:TYR:HD2	4:E:233:LEU:HD22	1.77	0.49
2:C:107:PRO:HD3	2:C:151:PHE:HB3	1.93	0.49
1:B:27:GLY:HA3	2:C:55:LEU:HD22	1.95	0.49
5:G:257:PHE:O	5:G:261:TRP:HB2	2.13	0.49
4:E:231:GLN:NE2	4:E:233:LEU:HB2	2.28	0.48
4:E:138:ILE:HD11	4:E:163:LYS:HE2	1.94	0.48
2:C:286:LEU:HD22	2:C:327:VAL:HG21	1.94	0.48
4:E:39:GLN:HB3	4:E:93:MET:HB3	1.96	0.47
1:B:47:SER:HA	1:B:50:VAL:HG22	1.95	0.47
4:E:180:ARG:HB2	4:E:183:GLN:HB2	1.95	0.47
2:C:294:CYS:HA	2:C:315:VAL:HG11	1.95	0.47
1:B:196:PHE:HE1	1:B:339:VAL:HG21	1.79	0.47
1:B:320:TYR:HB3	1:B:334:PHE:CZ	2.49	0.47
2:C:102:THR:HG21	2:C:148:CYS:CA	2.45	0.47
2:C:307:VAL:O	2:C:308:LEU:HD12	2.14	0.47
5:G:295:ALA:HA	5:G:298:CYS:SG	2.55	0.47
5:G:278:GLN:HA	6:A:5:PHA:HZ	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:232:HIS:HA	4:E:237:LEU:HD22	1.97	0.46
2:C:232:ILE:HD11	2:C:241:PHE:CD2	2.50	0.46
4:E:38:ARG:N	4:E:46:GLU:O	2.36	0.46
5:G:122:ASN:HA	5:G:125:THR:HG22	1.98	0.46
2:C:284:LEU:HD23	2:C:286:LEU:HD11	1.98	0.46
3:D:48:ASP:OD1	3:D:51:LEU:HB2	2.17	0.45
1:B:34:VAL:HB	1:B:194:LEU:HD21	1.97	0.45
2:C:38:ASP:N	2:C:39:PRO:HD3	2.31	0.45
5:G:263:PRO:HA	5:G:266:THR:OG1	2.16	0.45
5:G:135:VAL:O	5:G:139:LEU:HG	2.16	0.45
2:C:187:VAL:HA	2:C:203:ALA:HA	1.99	0.45
1:B:194:LEU:HD22	1:B:196:PHE:CD2	2.51	0.45
5:G:129:CYS:HA	5:G:132:VAL:HG22	1.99	0.45
2:C:60:ALA:HB2	2:C:102:THR:HA	1.98	0.45
1:B:45:GLY:C	1:B:47:SER:N	2.73	0.45
4:E:178:LEU:HB2	4:E:188:LEU:HD11	1.98	0.44
1:B:47:SER:C	1:B:49:ILE:N	2.73	0.44
4:E:35:HIS:HB2	4:E:97:VAL:HG13	1.98	0.44
4:E:171:ASN:HB2	4:E:173:TYR:CZ	2.53	0.44
1:B:8:GLU:OE2	4:E:232:HIS:ND1	2.51	0.44
4:E:226:VAL:HA	4:E:244:LYS:HA	2.00	0.44
4:E:2:VAL:HG12	4:E:27:PHE:HB3	1.99	0.44
2:C:106:ALA:HB2	2:C:111:TYR:HB2	2.00	0.44
5:G:221:TYR:HB3	5:G:250:VAL:HG13	2.00	0.44
5:G:262:LEU:N	5:G:263:PRO:HD2	2.33	0.44
2:C:189:SER:CB	2:C:232:ILE:HG22	2.48	0.44
1:B:254:CYS:O	1:B:317:LYS:NZ	2.50	0.44
1:B:339:VAL:HG12	1:B:343:ILE:HD11	1.99	0.44
2:C:76:ASP:OD1	2:C:76:ASP:N	2.50	0.43
5:G:58:ASN:HB3	5:G:87:VAL:HB	1.98	0.43
5:G:268:ASN:HA	5:G:271:ASN:ND2	2.33	0.43
1:B:339:VAL:HG12	1:B:343:ILE:HD12	2.00	0.43
1:B:339:VAL:CG1	1:B:343:ILE:HD11	2.48	0.43
5:G:282:SER:HB3	6:A:5:PHA:HE1	2.00	0.43
5:G:107:PHE:C	5:G:109:PRO:HD2	2.42	0.43
2:C:189:SER:HB2	2:C:232:ILE:HG22	2.00	0.43
5:G:144:PRO:HA	5:G:147:SER:OG	2.19	0.43
2:C:136:SER:OG	2:C:137:ARG:N	2.52	0.43
1:B:337:ASP:O	1:B:340:THR:HG22	2.18	0.43
2:C:106:ALA:HB2	2:C:111:TYR:O	2.20	0.42
2:C:209:LYS:HB2	2:C:211:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:199:PHE:HA	2:C:234:PHE:HE2	1.84	0.42
5:G:55:LEU:HA	5:G:87:VAL:HG23	2.01	0.42
2:C:54:HIS:ND1	2:C:58:ILE:HD11	2.34	0.42
4:E:187:LEU:HD21	4:E:190:TYR:HB3	2.02	0.42
2:C:137:ARG:NH2	2:C:173:THR:O	2.52	0.42
2:C:241:PHE:CZ	2:C:253:PHE:HB2	2.54	0.42
1:B:34:VAL:HG21	1:B:194:LEU:HD21	2.02	0.42
2:C:108:SER:O	2:C:109:GLY:C	2.62	0.42
2:C:144:GLY:HA3	2:C:163:ASP:N	2.35	0.42
1:B:196:PHE:CE1	1:B:339:VAL:HG21	2.55	0.42
5:G:221:TYR:CD1	5:G:250:VAL:HG22	2.54	0.42
2:C:101:MET:SD	2:C:117:LEU:HD11	2.59	0.41
5:G:90:MET:HA	5:G:294:TYR:HE1	1.85	0.41
5:G:203:ILE:HD12	5:G:203:ILE:HA	1.86	0.41
1:B:265:ILE:HG23	1:B:334:PHE:HE2	1.85	0.41
2:C:292:PHE:HA	2:C:314:ARG:HA	2.01	0.41
2:C:295:ASN:OD1	2:C:304:ARG:HD2	2.21	0.41
2:C:110:ASN:HA	2:C:126:LEU:HB2	2.02	0.41
4:E:165:LEU:HB3	4:E:172:THR:HB	2.02	0.41
5:G:139:LEU:HB2	5:G:151:ARG:HH21	1.85	0.41
5:G:60:LEU:O	5:G:64:VAL:HG23	2.21	0.41
1:B:221:ILE:HD11	1:B:259:PHE:CD1	2.56	0.41
2:C:155:ASN:OD1	2:C:172:GLU:N	2.52	0.41
2:C:85:TYR:CE2	3:D:60:PRO:HB3	2.55	0.41
5:G:202:ILE:HD13	5:G:202:ILE:HA	1.90	0.41
1:B:38:LEU:HD21	1:B:46:LYS:HB3	2.03	0.40
5:G:51:CYS:HA	5:G:294:TYR:CZ	2.56	0.40
5:G:82:LEU:HD21	5:G:300:ASN:ND2	2.36	0.40
5:G:217:ILE:O	5:G:220:CYS:HB3	2.20	0.40
2:C:83:ASP:O	2:C:87:THR:N	2.55	0.40
2:C:324:GLY:O	3:D:49:PRO:HD2	2.20	0.40
1:B:35:LYS:HB3	1:B:199:PHE:CE2	2.56	0.40
4:E:36:TRP:HD1	4:E:70:ILE:HD12	1.86	0.40
5:G:142:VAL:HG12	5:G:143:HIS:ND1	2.37	0.40
2:C:277:SER:HB3	2:C:318:LEU:HD12	2.04	0.40
5:G:185:THR:OG1	5:G:186:CYS:N	2.55	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	B	218/354 (62%)	210 (96%)	8 (4%)	0	100	100
2	C	339/377 (90%)	318 (94%)	21 (6%)	0	100	100
3	D	48/71 (68%)	45 (94%)	3 (6%)	0	100	100
4	E	229/304 (75%)	221 (96%)	8 (4%)	0	100	100
5	G	273/570 (48%)	253 (93%)	19 (7%)	1 (0%)	30	61
6	A	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1109/1682 (66%)	1049 (95%)	59 (5%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	193	PRO

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	B	139/306 (45%)	139 (100%)	0	100	100
2	C	202/308 (66%)	202 (100%)	0	100	100
3	D	14/58 (24%)	14 (100%)	0	100	100
4	E	174/247 (70%)	174 (100%)	0	100	100
5	G	150/471 (32%)	148 (99%)	2 (1%)	61	77
6	A	2/2 (100%)	1 (50%)	1 (50%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	681/1392 (49%)	678 (100%)	3 (0%)	81	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	99	GLN
5	G	261	TRP
6	A	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	169	ASN
4	E	171	ASN
4	E	179	GLN
5	G	99	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	DTR	A	2	6	14,15,16	1.72	3 (21%)	15,20,22	1.21	2 (13%)
6	HYP	A	6	6	7,8,9	4.76	4 (57%)	5,10,12	1.08	0
6	004	A	1	6	9,10,11	0.84	0	9,12,14	1.00	0
6	PHA	A	5	6	10,11,11	0.55	0	8,13,13	1.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DTR	A	2	6	-	2/5/6/8	0/2/2/2
6	HYP	A	6	6	-	0/0/11/13	0/1/1/1
6	004	A	1	6	-	1/4/6/8	0/1/1/1
6	PHA	A	5	6	-	0/5/6/6	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6	HYP	CB-CA	-8.92	1.34	1.54
6	A	6	HYP	CA-N	7.18	1.61	1.48
6	A	6	HYP	CD-N	-4.41	1.32	1.47
6	A	2	DTR	CD2-CE2	-4.13	1.36	1.41
6	A	2	DTR	CD1-NE1	-2.70	1.32	1.37
6	A	2	DTR	CB-CG	2.56	1.55	1.50
6	A	6	HYP	OD1-CG	-2.47	1.36	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2	DTR	CG-CD1-NE1	-2.22	107.87	110.31
6	A	2	DTR	CZ2-CE2-CD2	-2.07	120.18	122.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2	DTR	CA-CB-CG-CD1
6	A	2	DTR	CA-CB-CG-CD2
6	A	1	004	C-CA-CB-CG1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5	PHA	2	0

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.

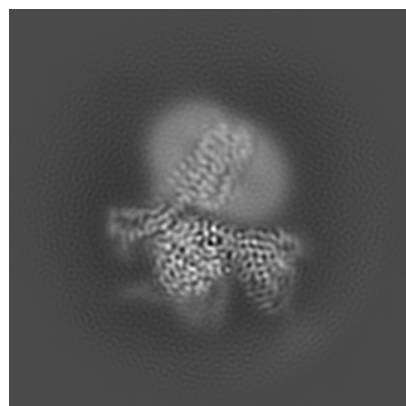
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39931. These allow visual inspection of the internal detail of the map and identification of artifacts.

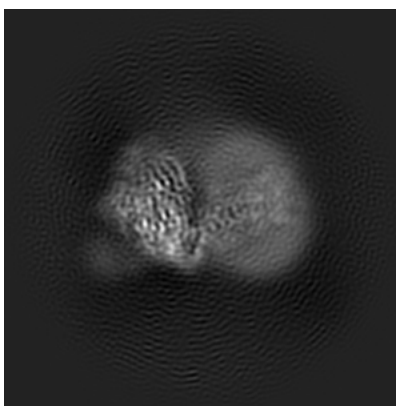
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

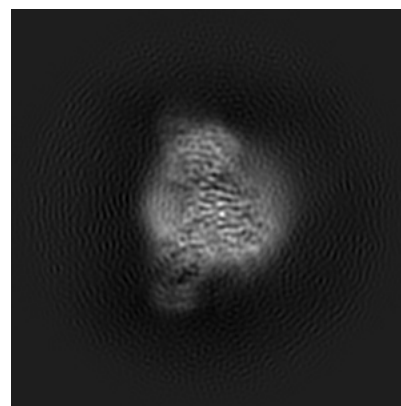
6.1.1 Primary map



X

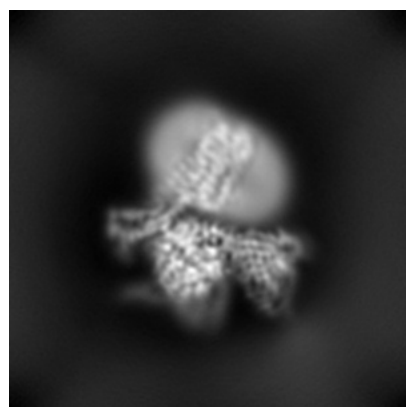


Y

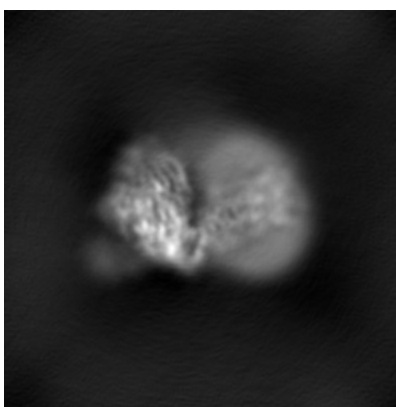


Z

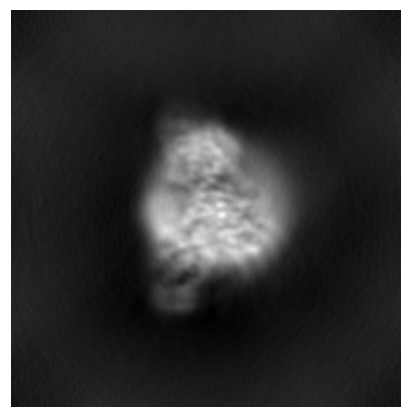
6.1.2 Raw map



X



Y

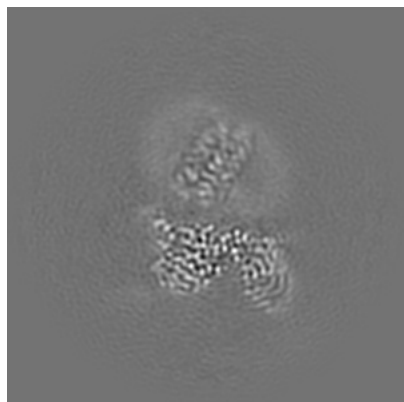


Z

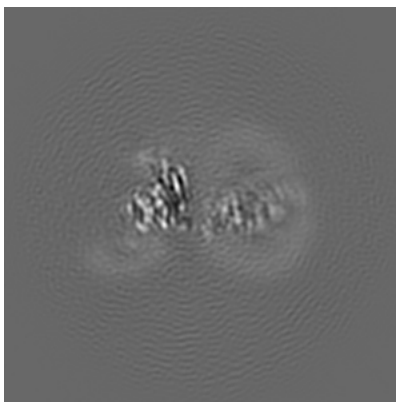
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

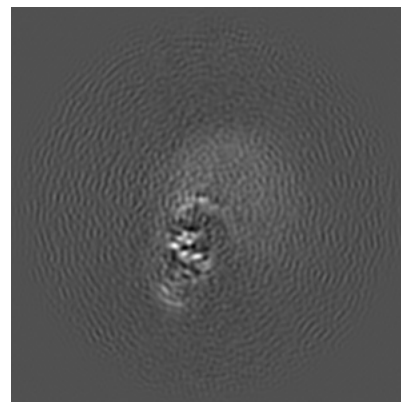
6.2.1 Primary map



X Index: 100

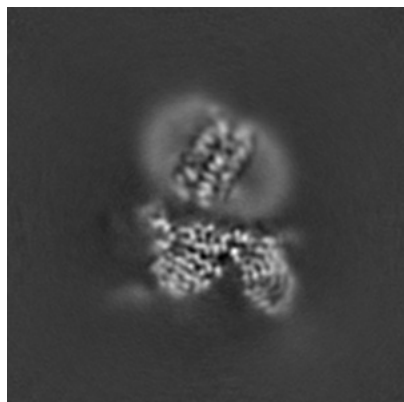


Y Index: 100

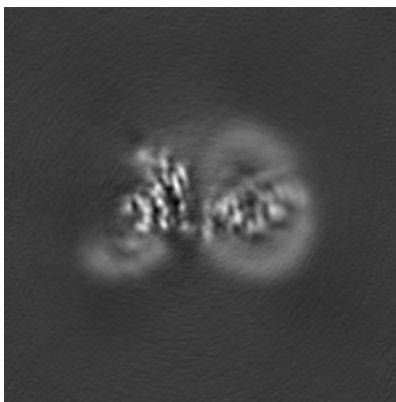


Z Index: 100

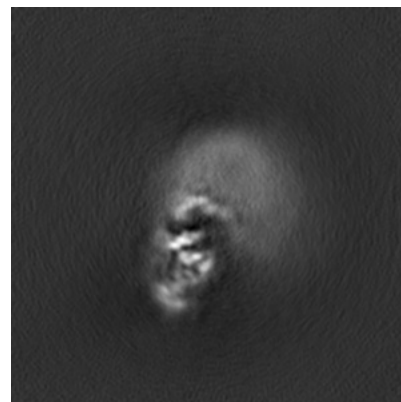
6.2.2 Raw map



X Index: 100



Y Index: 100

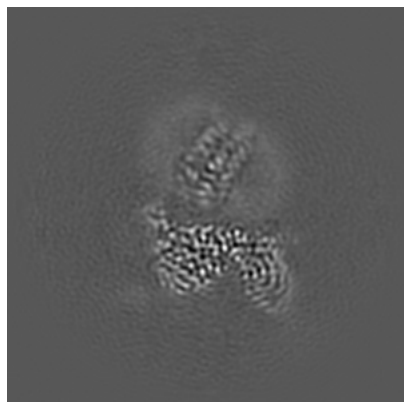


Z Index: 100

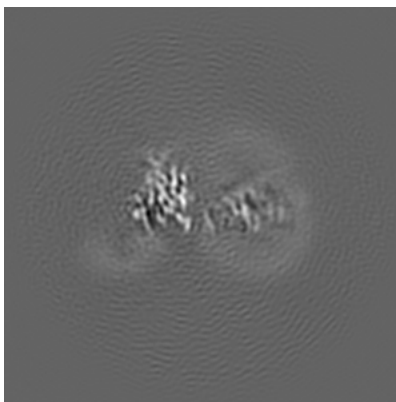
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

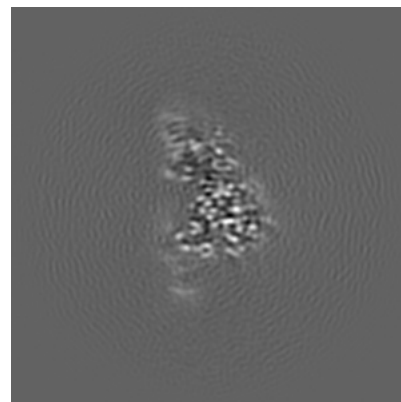
6.3.1 Primary map



X Index: 99

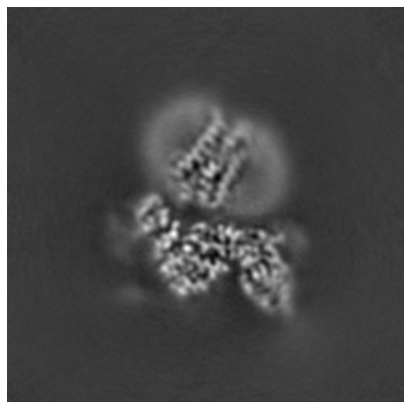


Y Index: 102

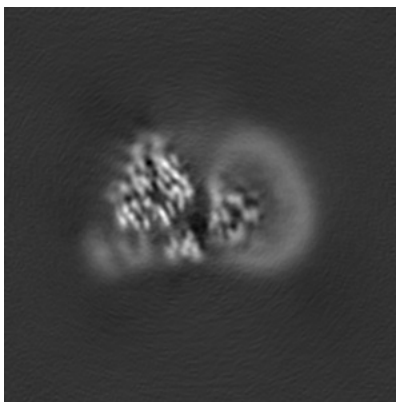


Z Index: 81

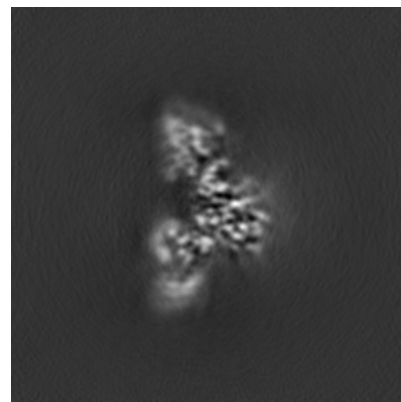
6.3.2 Raw map



X Index: 96



Y Index: 89

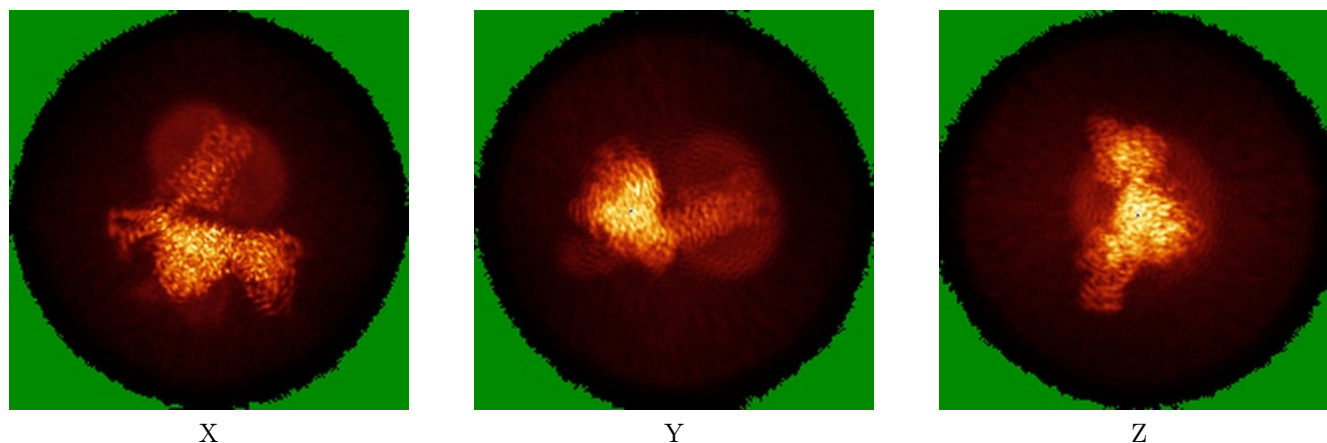


Z Index: 85

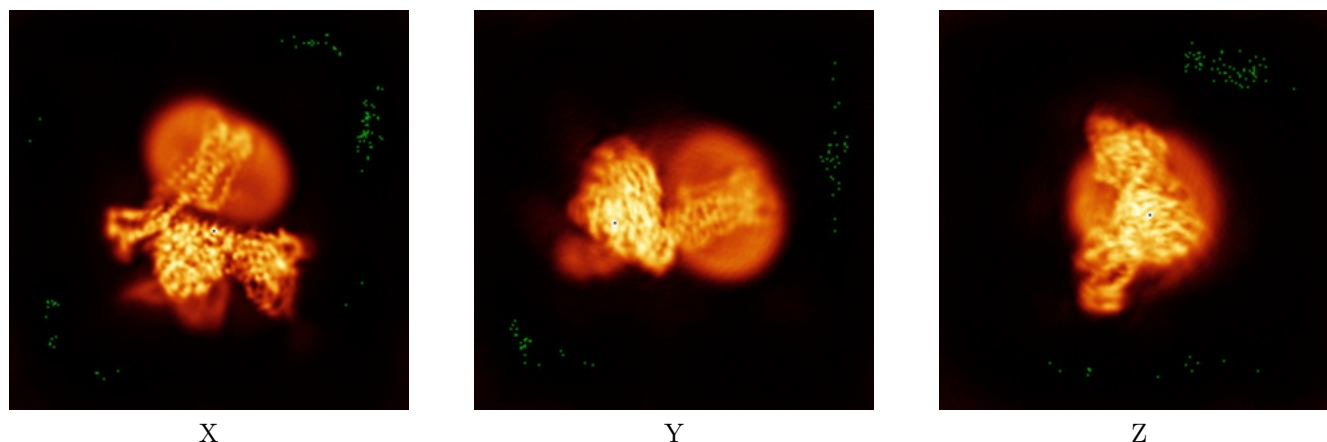
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

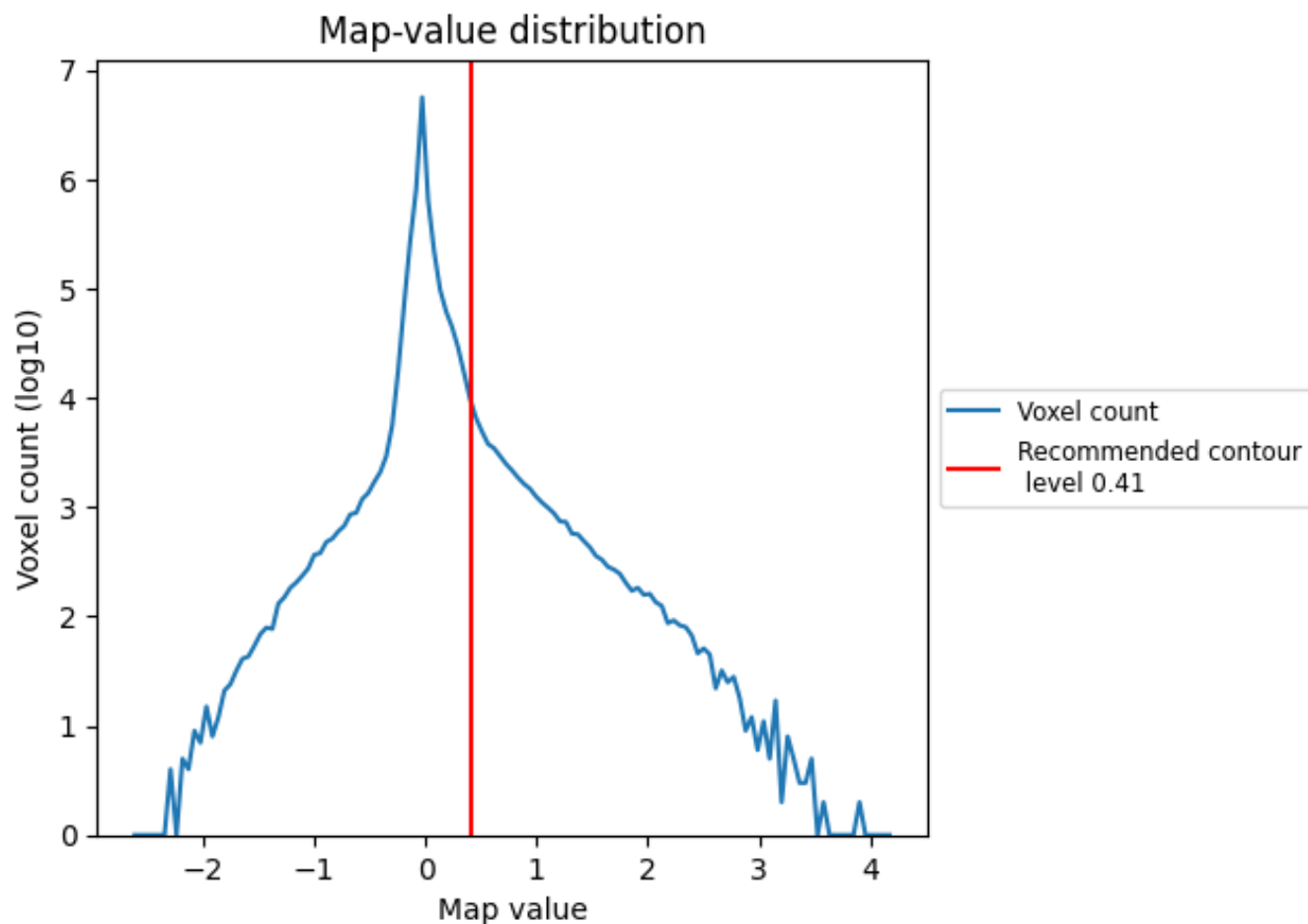
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

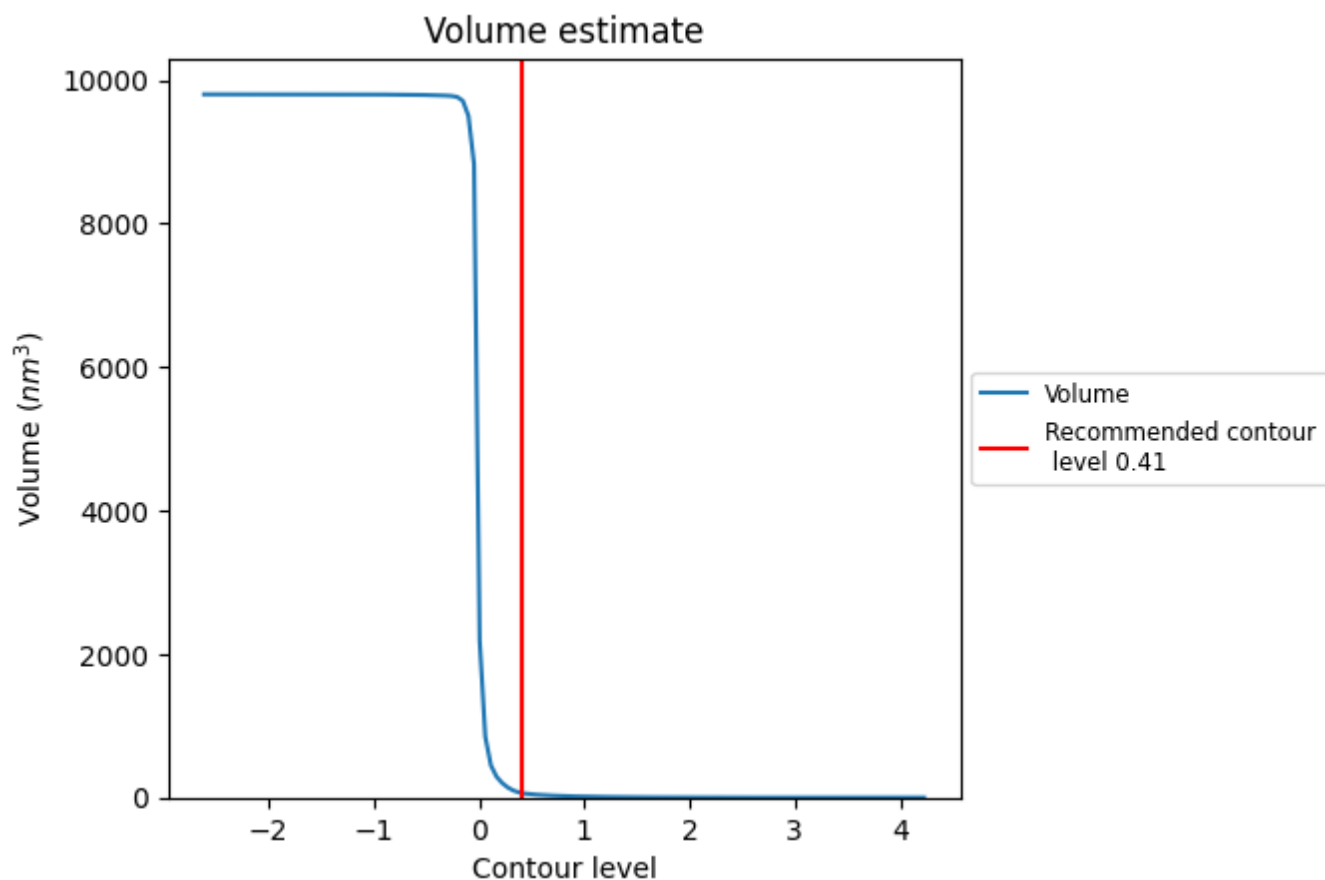
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

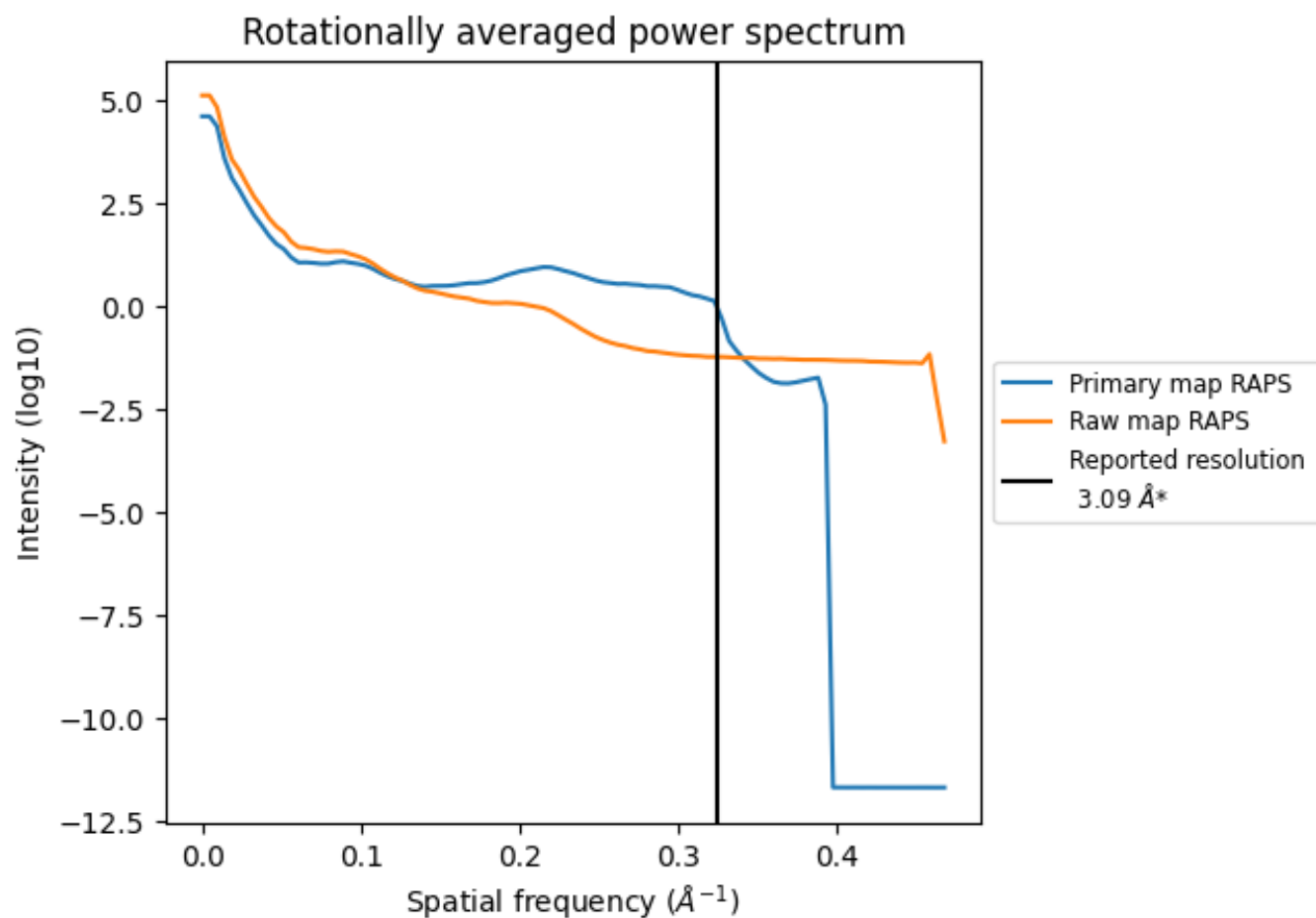
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm^3 ; this corresponds to an approximate mass of 57 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 ⓘ

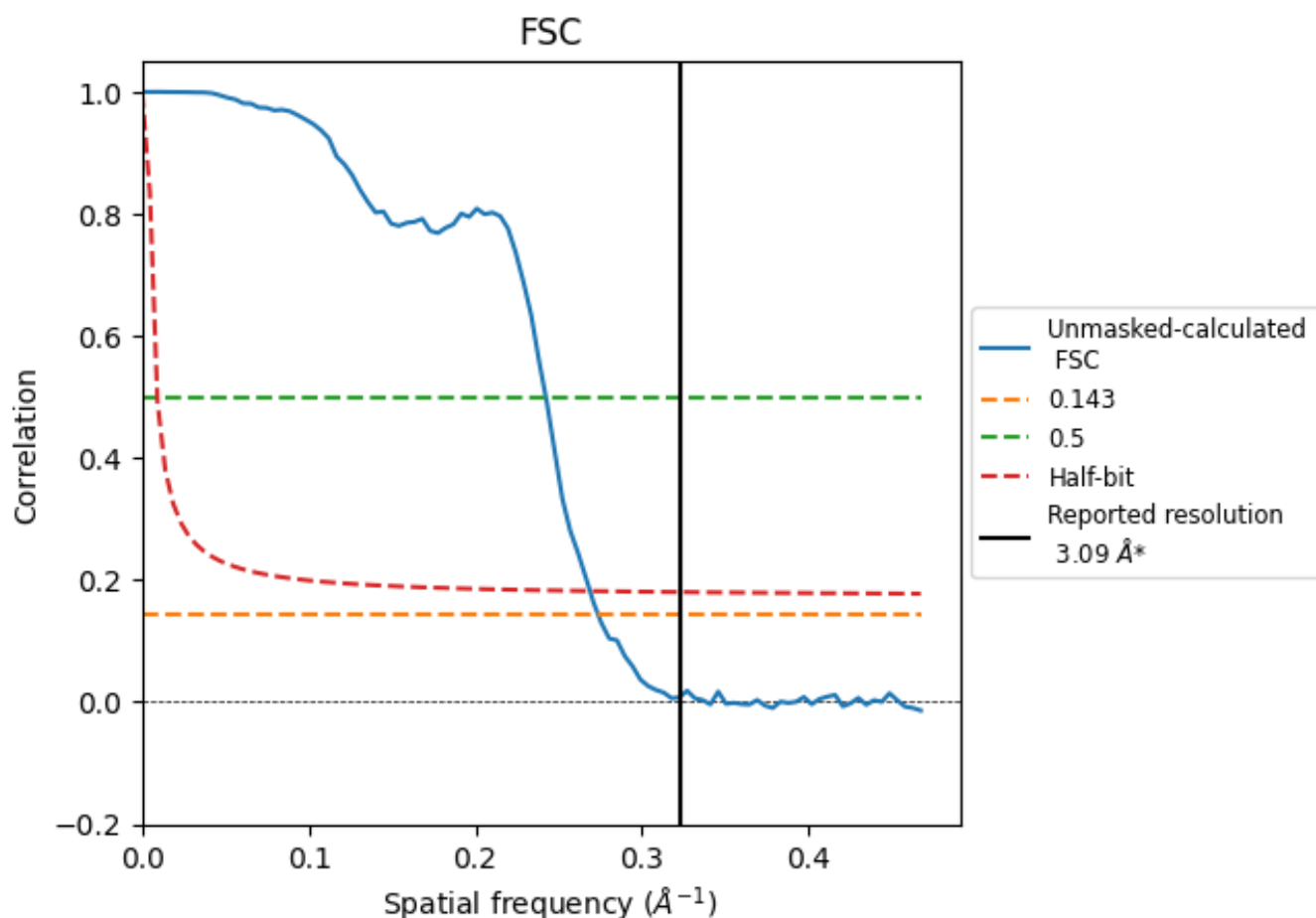


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

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 $0.324 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

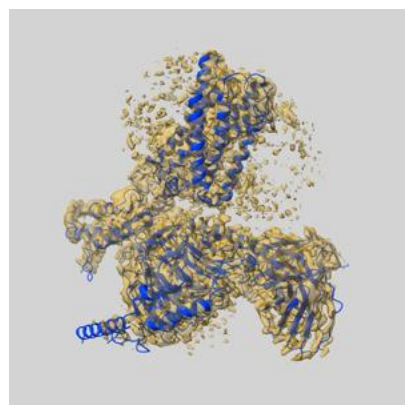
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.13	3.72

*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 3.65 differs from the reported value 3.09 by more than 10 %

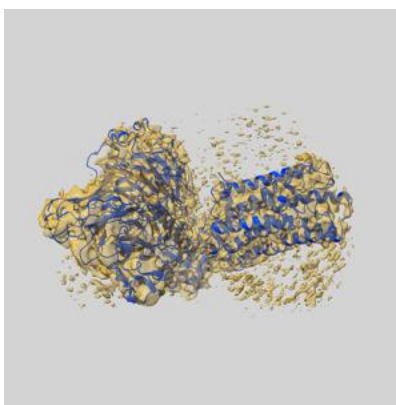
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39931 and PDB model 8ZCJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

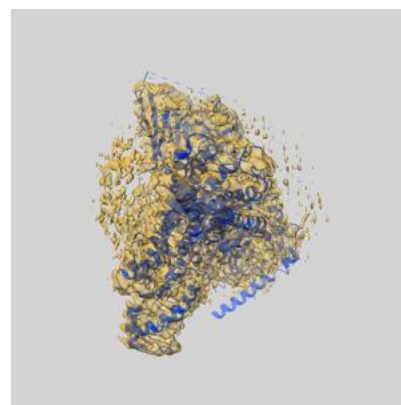
9.1 Map-model overlay [i](#)



X



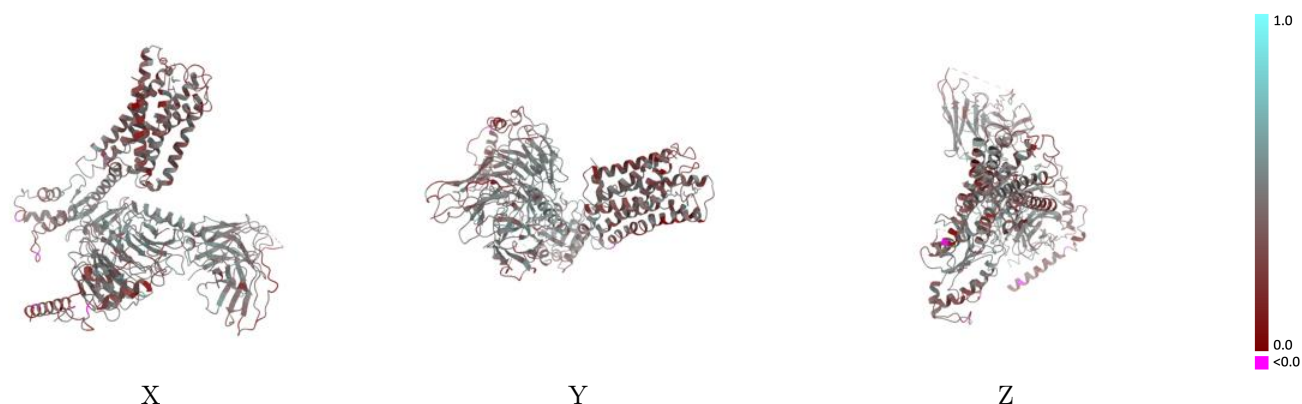
Y



Z

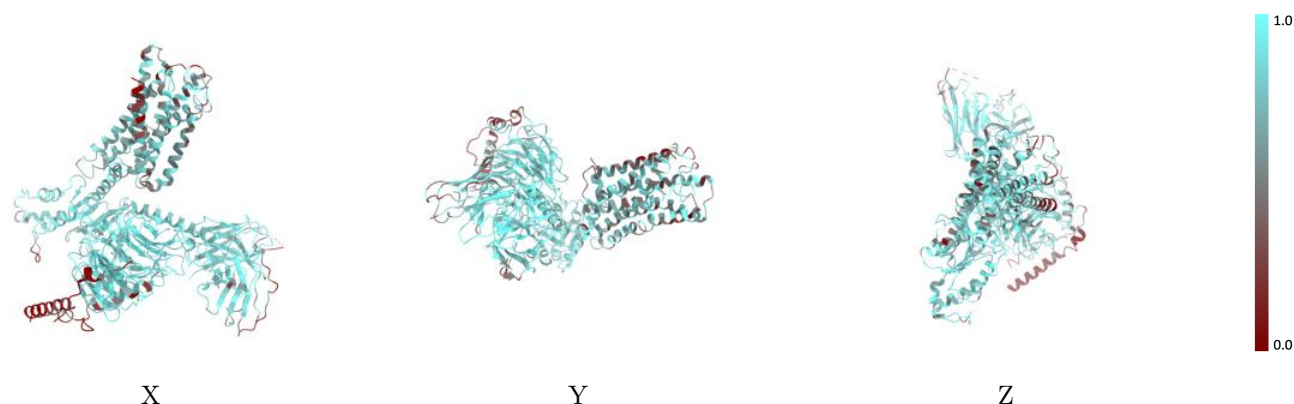
The images above show the 3D surface view of the map at the recommended contour level 0.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



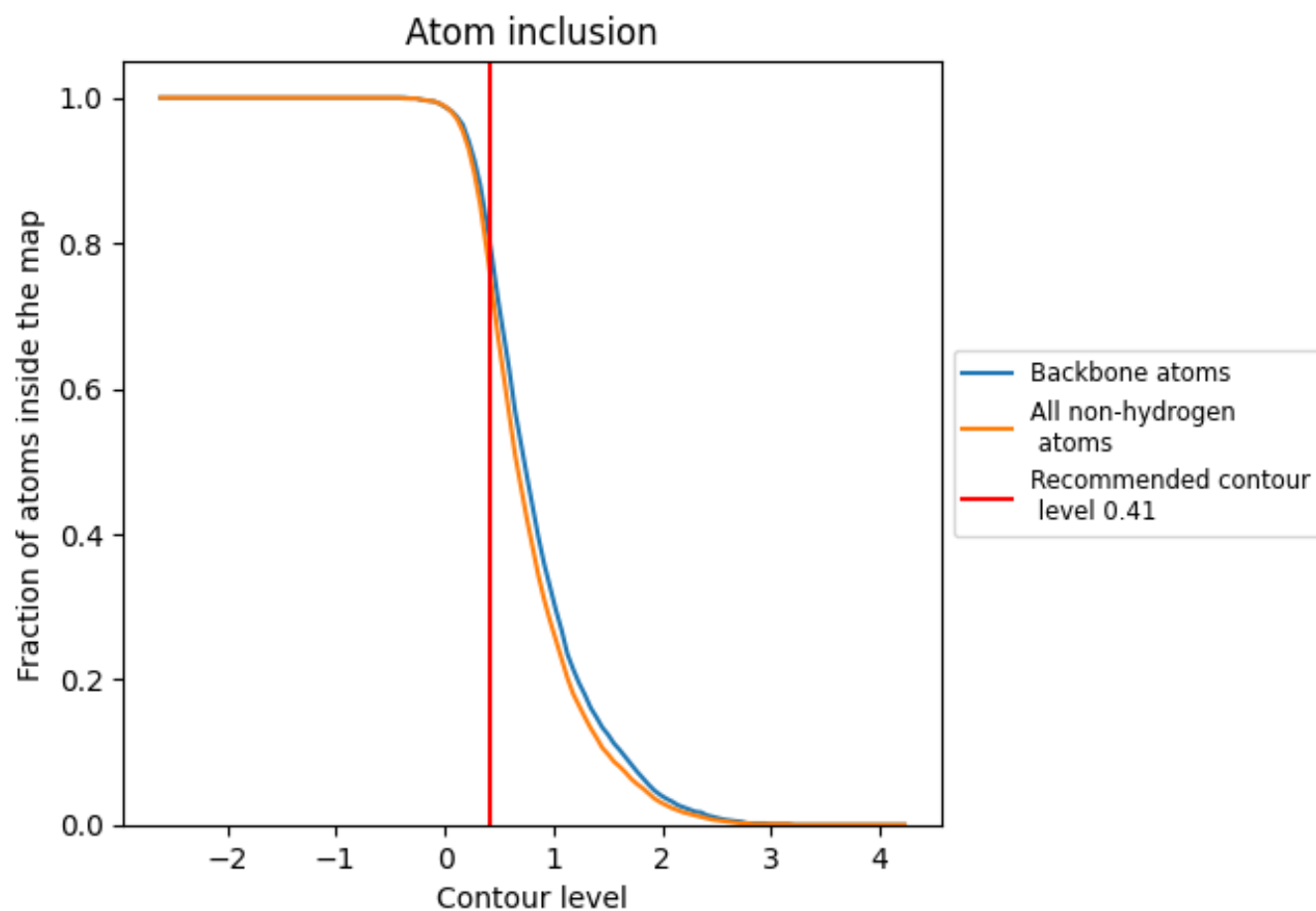
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.41).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.4220
A	0.8710	0.4380
B	0.8080	0.4330
C	0.8250	0.4630
D	0.5390	0.3340
E	0.7950	0.4320
G	0.6650	0.3650

1.0

0.0

<0.0