



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:45 PM UTC

PDB ID : 8ZBE / pdb_00008zbe
EMDB ID : EMD-39901
Title : cryo-EM structure of the octreotide-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 : 2024-04-26
Resolution : 3.24 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:

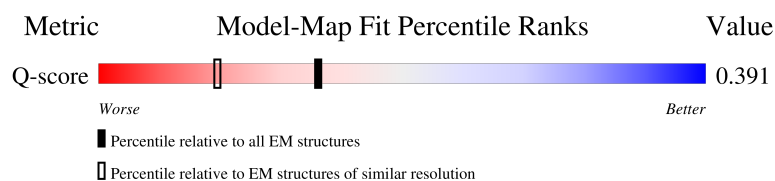
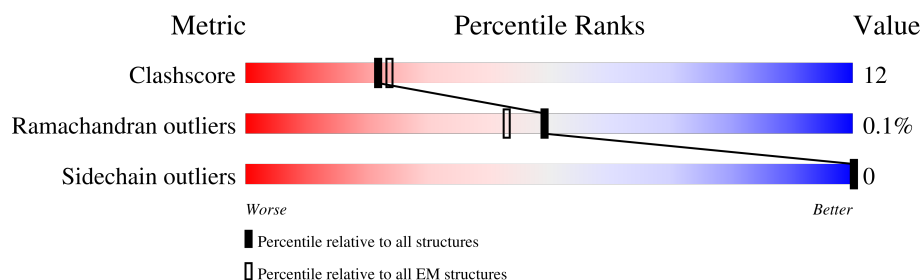
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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

The reported resolution of this entry is 3.24 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	14594 (2.74 - 3.74)

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	A	570	
2	B	354	
3	D	71	
4	E	304	

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Mol	Chain	Length	Quality of chain
5	P	8	25% 25% 25% 25%
6	C	377	10% 64% 27% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7489 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 Beta-2 adrenergic receptor,Somatostatin receptor type 5,lgbt (fusion protein).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	263	1648	1045	293	304	6	0	0

There are 24 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	213	Total	C	N	O	S	0	0
			1414	890	246	272	6		

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 3 is a protein called Guanine nucleotide-binding protein subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	58	Total	C	N	O	S	0	0
			329	203	60	66			

- Molecule 4 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	233	Total	C	N	O	S	0	0
			1602	1009	271	313	9		

- Molecule 5 is a protein called octreotide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	6	Total	C	N	O	S	0	0
			53	36	8	7	2		

- Molecule 6 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	341	Total	C	N	O	S	0	0
			2443	1509	447	475	12		

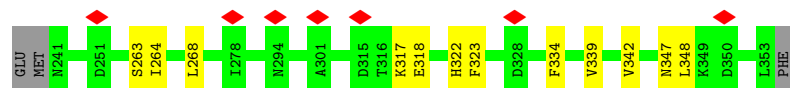
There are 38 discrepancies between the modelled and reference sequences:

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

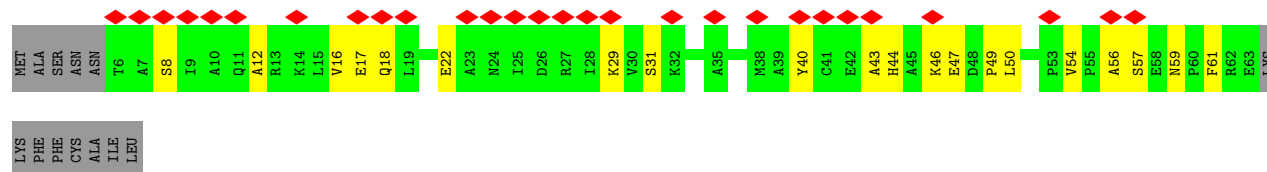
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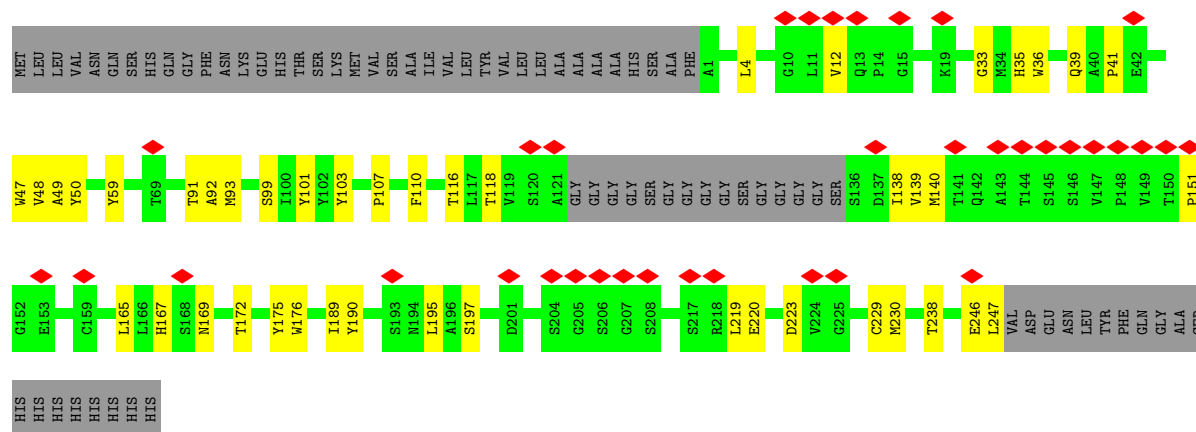
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P54311
C	-4	HIS	-	expression tag	UNP P54311
C	-3	GLY	-	expression tag	UNP P54311
C	-2	SER	-	expression tag	UNP P54311
C	-1	LEU	-	expression tag	UNP P54311
C	0	LEU	-	expression tag	UNP P54311
C	1	GLN	-	expression tag	UNP P54311
C	341	GLY	-	expression tag	UNP P54311
C	342	SER	-	expression tag	UNP P54311
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



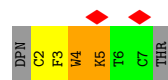
Chain D:



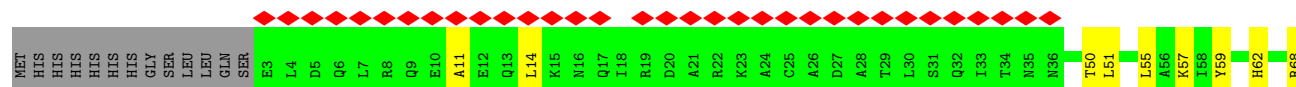
Chain E:

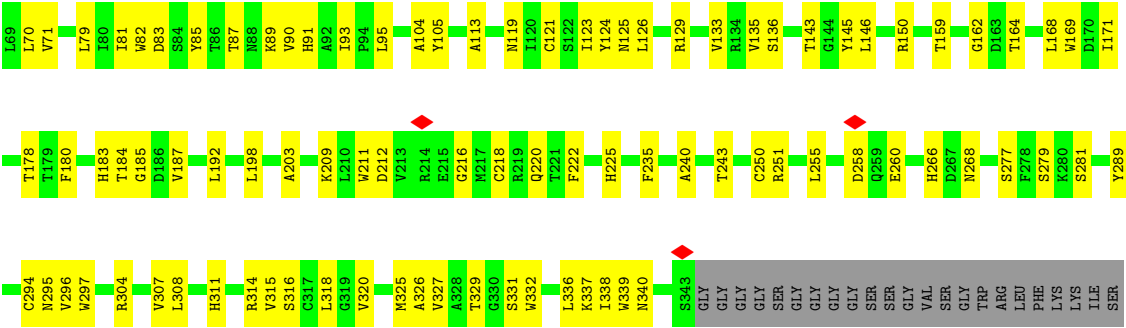


Chain P:



Chain C: 10% 64% 27% 10%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452725	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	4.183	Depositor
Minimum map value	-2.452	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.345	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/1676	0.57	3/2322 (0.1%)
2	B	0.21	0/1433	0.41	0/1960
3	D	0.66	0/334	1.23	2/467 (0.4%)
4	E	0.19	0/1640	0.47	0/2242
5	P	0.51	0/38	1.33	1/47 (2.1%)
6	C	0.22	0/2488	0.46	0/3393
All	All	0.27	0/7609	0.54	6/10431 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	HIS	N-CA-C	6.58	121.99	108.71
3	D	46	LYS	N-CA-C	-6.33	104.43	111.71
1	A	270	VAL	N-CA-C	-6.09	104.91	110.82
5	P	5	LYS	N-CA-CB	5.87	120.47	110.50
3	D	50	LEU	N-CA-C	-5.25	105.73	111.82
1	A	143	HIS	CB-CA-C	-5.24	102.50	111.15

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	A	1648	0	1347	27	0
2	B	1414	0	1155	23	0
3	D	329	0	225	13	0
4	E	1602	0	1367	30	0
5	P	53	0	46	5	0
6	C	2443	0	2191	80	0
All	All	7489	0	6331	160	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 12.

All (160) 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)
6:C:150:ARG:HB2	6:C:192:LEU:HD13	1.68	0.76
6:C:164:THR:HG22	6:C:185:GLY:O	1.87	0.74
6:C:164:THR:HG22	6:C:185:GLY:C	2.13	0.73
6:C:235:PHE:HB2	6:C:240:ALA:HB3	1.75	0.67
1:A:137:ARG:NH1	1:A:221:TYR:OH	2.29	0.66
3:D:56:ALA:HB3	3:D:59:ASN:HA	1.78	0.63
1:A:205:THR:HG21	5:P:4:DTR:HZ3	1.80	0.63
1:A:271:ASN:OD1	5:P:2:CYS:HB3	1.99	0.63
6:C:125:ASN:O	6:C:133:VAL:HG13	1.99	0.63
6:C:311:HIS:NE2	6:C:329:THR:O	2.33	0.61
4:E:93:MET:HA	4:E:116:THR:HA	1.82	0.61
3:D:47:GLU:O	3:D:49:PRO:HD3	2.01	0.61
6:C:222:PHE:HE1	6:C:258:ASP:HA	1.65	0.61
6:C:295:ASN:OD1	6:C:307:VAL:HG23	2.00	0.60
2:B:28:GLU:O	2:B:32:ARG:HG3	2.02	0.60
6:C:121:CYS:HB2	6:C:146:LEU:HD21	1.84	0.59
6:C:187:VAL:HA	6:C:203:ALA:HA	1.85	0.59
1:A:210:PHE:HB2	1:A:261:TRP:HZ3	1.68	0.58
6:C:220:GLN:NE2	6:C:255:LEU:O	2.32	0.58
6:C:126:LEU:HD23	6:C:133:VAL:HG11	1.86	0.57
5:P:4:DTR:CE2	5:P:5:LYS:HE2	2.33	0.57
4:E:167:HIS:HD2	4:E:169:ASN:OD1	1.87	0.57
6:C:326:ALA:HB1	6:C:338:ILE:HG23	1.85	0.57
6:C:183:HIS:CD2	6:C:209:LYS:HD2	2.40	0.57
6:C:146:LEU:HD11	6:C:159:THR:HB	1.86	0.56
6:C:68:ARG:NH2	6:C:83:ASP:OD2	2.38	0.56
2:B:214:CYS:HA	6:C:59:TYR:OH	2.04	0.55
4:E:39:GLN:N	4:E:93:MET:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:HG23	1:A:76:ASN:H	1.72	0.53
6:C:124:TYR:HA	6:C:135:VAL:HA	1.89	0.53
4:E:33:GLY:N	4:E:99:SER:O	2.41	0.53
2:B:339:VAL:HA	2:B:342:VAL:HG12	1.91	0.53
5:P:4:DTR:NE1	5:P:5:LYS:HE2	2.24	0.52
1:A:239:ARG:N	2:B:318:GLU:OE2	2.43	0.52
6:C:337:LYS:HB2	6:C:339:TRP:NE1	2.25	0.52
4:E:138:ILE:HD12	4:E:139:VAL:H	1.75	0.52
6:C:289:TYR:HH	6:C:297:TRP:CD1	2.28	0.52
4:E:246:GLU:O	4:E:247:LEU:C	2.52	0.51
4:E:36:TRP:HB3	4:E:48:VAL:HG22	1.93	0.51
1:A:205:THR:HG21	5:P:4:DTR:CZ3	2.41	0.51
6:C:79:LEU:HB2	6:C:95:LEU:HD21	1.92	0.51
4:E:33:GLY:O	4:E:99:SER:N	2.43	0.50
4:E:47:TRP:HE1	4:E:49:ALA:C	2.20	0.50
2:B:19:ILE:HD12	6:C:89:LYS:O	2.11	0.50
6:C:79:LEU:HD23	6:C:93:ILE:HD13	1.94	0.50
3:D:40:TYR:HA	3:D:43:ALA:HB3	1.94	0.50
6:C:159:THR:OG1	6:C:169:TRP:NE1	2.45	0.50
6:C:87:THR:HG22	6:C:87:THR:O	2.12	0.50
6:C:164:THR:HG21	6:C:184:THR:O	2.12	0.50
3:D:54:VAL:HG22	3:D:56:ALA:H	1.77	0.49
4:E:197:SER:OG	6:C:129:ARG:NH2	2.45	0.49
6:C:51:LEU:N	6:C:336:LEU:O	2.44	0.49
6:C:68:ARG:HG2	6:C:85:TYR:CZ	2.47	0.49
1:A:271:ASN:C	1:A:271:ASN:HD22	2.21	0.49
6:C:180:PHE:CE2	6:C:216:GLY:HA2	2.49	0.48
2:B:34:VAL:HG22	2:B:196:PHE:HA	1.96	0.48
6:C:251:ARG:HB3	6:C:260:GLU:HG3	1.94	0.47
6:C:279:SER:HA	6:C:320:VAL:HG11	1.95	0.47
1:A:202:ILE:HD11	1:A:272:LEU:HD22	1.96	0.47
4:E:4:LEU:HD12	4:E:110:PHE:HD2	1.79	0.47
1:A:93:LEU:HA	1:A:294:TYR:HE2	1.78	0.47
6:C:168:LEU:HD23	6:C:180:PHE:CE1	2.50	0.47
3:D:18:GLN:O	3:D:22:GLU:CB	2.63	0.47
4:E:35:HIS:NE2	4:E:101:TYR:OH	2.42	0.47
6:C:71:VAL:HB	6:C:81:ILE:HD13	1.97	0.47
2:B:27:GLY:HA3	6:C:55:LEU:HD22	1.97	0.47
4:E:165:LEU:HB3	4:E:172:THR:HB	1.97	0.47
6:C:314:ARG:O	6:C:331:SER:HB3	2.15	0.47
3:D:56:ALA:HB3	3:D:59:ASN:CA	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:243:THR:O	6:C:250:CYS:HA	2.15	0.47
6:C:289:TYR:OH	6:C:297:TRP:NE1	2.48	0.47
3:D:61:PHE:HE2	6:C:325:MET:CB	2.28	0.46
1:A:124:PHE:CE1	1:A:205:THR:HG23	2.51	0.46
1:A:258:ALA:O	1:A:262:LEU:HD12	2.15	0.46
6:C:294:CYS:N	6:C:315:VAL:HG21	2.31	0.46
2:B:264:ILE:HG22	2:B:317:LYS:HD3	1.97	0.46
6:C:50:THR:HG23	6:C:337:LYS:HD3	1.97	0.46
6:C:70:LEU:HG	6:C:82:TRP:HB2	1.97	0.46
3:D:61:PHE:HB2	6:C:340:ASN:HD22	1.80	0.46
6:C:62:HIS:ND1	6:C:104:ALA:HA	2.30	0.46
4:E:175:TYR:O	4:E:229:CYS:HA	2.15	0.46
4:E:189:ILE:HG12	4:E:195:LEU:HD12	1.97	0.46
6:C:209:LYS:HB3	6:C:218:CYS:SG	2.55	0.46
6:C:126:LEU:HD23	6:C:133:VAL:CG1	2.46	0.46
2:B:36:LEU:HD11	2:B:339:VAL:HG11	1.98	0.46
6:C:57:LYS:HB3	6:C:332:TRP:HA	1.97	0.46
2:B:208:ARG:O	2:B:212:ILE:HB	2.16	0.46
4:E:91:THR:HG23	4:E:118:THR:HA	1.98	0.45
4:E:151:PRO:HA	4:E:219:LEU:HB2	1.97	0.45
6:C:123:ILE:CD1	6:C:171:ILE:HG12	2.46	0.45
1:A:140:ALA:O	2:B:347:ASN:ND2	2.49	0.45
6:C:289:TYR:HH	6:C:297:TRP:NE1	2.14	0.45
1:A:262:LEU:N	1:A:263:PRO:HD2	2.31	0.45
6:C:198:LEU:HD23	6:C:212:ASP:HA	1.98	0.45
2:B:34:VAL:HG21	2:B:196:PHE:HD1	1.83	0.44
6:C:119:ASN:HA	6:C:146:LEU:HB2	1.99	0.44
6:C:90:VAL:HG12	6:C:91:HIS:CD2	2.53	0.44
1:A:89:TYR:HB2	1:A:122:ASN:CB	2.48	0.44
1:A:190:TRP:O	1:A:193:PRO:HD2	2.18	0.44
6:C:180:PHE:HB3	6:C:211:TRP:CE3	2.51	0.44
6:C:289:TYR:CE1	6:C:295:ASN:HB2	2.53	0.44
2:B:50:VAL:HG11	2:B:200:ASP:OD2	2.18	0.43
6:C:268:ASN:OD1	6:C:268:ASN:N	2.51	0.43
6:C:51:LEU:HB2	6:C:336:LEU:HB2	2.01	0.43
2:B:19:ILE:HG21	6:C:89:LYS:HB3	2.00	0.43
6:C:337:LYS:HB2	6:C:339:TRP:CE2	2.52	0.43
2:B:39:LEU:HG	2:B:40:GLY:N	2.34	0.43
4:E:47:TRP:NE1	4:E:49:ALA:O	2.47	0.43
1:A:98:THR:HA	1:A:101:ALA:HB3	2.00	0.43
2:B:182:THR:OG1	6:C:143:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:220:GLU:N	4:E:220:GLU:OE1	2.52	0.43
6:C:71:VAL:HG12	6:C:105:TYR:HD2	1.83	0.43
6:C:316:SER:H	6:C:331:SER:HA	1.84	0.43
4:E:50:TYR:HD2	4:E:59:TYR:HB2	1.84	0.43
1:A:141:VAL:HG21	2:B:348:LEU:HD23	2.00	0.43
6:C:123:ILE:O	6:C:136:SER:N	2.35	0.43
4:E:41:PRO:HD3	4:E:92:ALA:HA	2.00	0.43
4:E:103:TYR:CZ	6:C:68:ARG:HD3	2.53	0.43
2:B:268:LEU:HG	2:B:323:PHE:HA	2.01	0.42
6:C:164:THR:HG21	6:C:184:THR:C	2.43	0.42
4:E:103:TYR:CE1	6:C:68:ARG:HD3	2.54	0.42
6:C:327:VAL:CG1	6:C:339:TRP:HB2	2.49	0.42
4:E:176:TRP:CZ3	4:E:229:CYS:HB3	2.54	0.42
1:A:264:PHE:CD2	1:A:290:VAL:HG12	2.54	0.42
1:A:303:LEU:HG	1:A:307:LEU:HD12	2.01	0.42
2:B:37:LEU:HD22	2:B:215:PHE:CG	2.54	0.42
4:E:12:VAL:N	4:E:118:THR:O	2.53	0.42
6:C:145:TYR:CD1	6:C:162:GLY:HA3	2.54	0.42
3:D:16:VAL:O	3:D:17:GLU:C	2.61	0.42
4:E:175:TYR:HB2	4:E:230:MET:HB3	2.02	0.42
6:C:289:TYR:CD1	6:C:295:ASN:HB2	2.55	0.42
2:B:27:GLY:HA3	6:C:55:LEU:CD2	2.50	0.42
2:B:263:SER:O	2:B:263:SER:OG	2.32	0.42
3:D:8:SER:O	3:D:12:ALA:N	2.48	0.42
3:D:44:HIS:HB2	6:C:281:SER:HA	2.00	0.42
1:A:210:PHE:CD1	1:A:262:LEU:HD21	2.55	0.41
6:C:113:ALA:HB2	6:C:123:ILE:HG12	2.01	0.41
6:C:251:ARG:HH11	6:C:260:GLU:CD	2.27	0.41
4:E:107:PRO:HD2	4:E:190:TYR:CG	2.55	0.41
6:C:168:LEU:HB2	6:C:178:THR:OG1	2.21	0.41
6:C:11:ALA:HA	6:C:14:LEU:HD12	2.03	0.41
6:C:277:SER:OG	6:C:318:LEU:O	2.30	0.41
1:A:190:TRP:C	1:A:193:PRO:HD2	2.46	0.41
1:A:147:SER:O	1:A:151:ARG:HB2	2.20	0.41
1:A:201:PHE:CD2	1:A:202:ILE:HG23	2.56	0.41
1:A:264:PHE:CD1	1:A:264:PHE:C	2.99	0.41
2:B:322:HIS:HB2	2:B:334:PHE:CE2	2.56	0.41
4:E:220:GLU:H	4:E:223:ASP:HB2	1.85	0.41
6:C:296:VAL:HG23	6:C:308:LEU:HG	2.01	0.41
2:B:38:LEU:HB2	2:B:199:PHE:O	2.21	0.40
3:D:56:ALA:O	3:D:57:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:140:MET:HE1	4:E:238:THR:O	2.21	0.40
4:E:167:HIS:HD2	4:E:169:ASN:CG	2.29	0.40
1:A:73:THR:O	1:A:74:VAL:C	2.63	0.40
3:D:29:LYS:C	3:D:31:SER:N	2.79	0.40
6:C:266:HIS:ND1	6:C:268:ASN:OD1	2.50	0.40
6:C:68:ARG:HG2	6:C:85:TYR:CE1	2.56	0.40
6:C:295:ASN:HB3	6:C:304:ARG:HD3	2.03	0.40
1:A:125:THR:HG21	1:A:164:TRP:CH2	2.57	0.40
6:C:225:HIS:NE2	6:C:243:THR:O	2.45	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	A	257/570 (45%)	240 (93%)	17 (7%)	0	100	100
2	B	207/354 (58%)	194 (94%)	13 (6%)	0	100	100
3	D	56/71 (79%)	51 (91%)	5 (9%)	0	100	100
4	E	229/304 (75%)	219 (96%)	10 (4%)	0	100	100
5	P	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
6	C	339/377 (90%)	316 (93%)	23 (7%)	0	100	100
All	All	1091/1684 (65%)	1021 (94%)	69 (6%)	1 (0%)	49	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	3	PHE

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	A	118/471 (25%)	118 (100%)	0	100	100
2	B	110/306 (36%)	110 (100%)	0	100	100
3	D	15/58 (26%)	15 (100%)	0	100	100
4	E	142/246 (58%)	142 (100%)	0	100	100
5	P	5/6 (83%)	5 (100%)	0	100	100
6	C	229/308 (74%)	229 (100%)	0	100	100
All	All	619/1395 (44%)	619 (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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	310	ASN
2	B	204	GLN
4	E	167	HIS
6	C	176	GLN
6	C	239	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
5	DTR	P	4	5	14,15,16	1.75	2 (14%)	15,20,22	1.75	4 (26%)

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
5	DTR	P	4	5	-	0/5/6/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	4	DTR	CD2-CE2	4.93	1.47	1.41
5	P	4	DTR	CD2-CG	2.54	1.48	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	4	DTR	CZ2-CE2-CD2	-3.76	118.55	122.19
5	P	4	DTR	CE2-NE1-CD1	3.03	111.78	109.08
5	P	4	DTR	CE3-CD2-CE2	2.69	121.63	118.84
5	P	4	DTR	CZ2-CE2-NE1	2.39	134.56	130.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	4	DTR	4	0

5.5 Carbohydrates ⓘ

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.

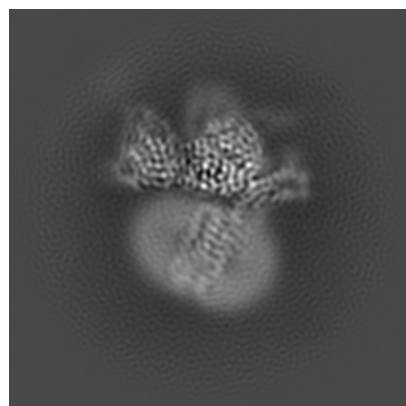
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39901. These allow visual inspection of the internal detail of the map and identification of artifacts.

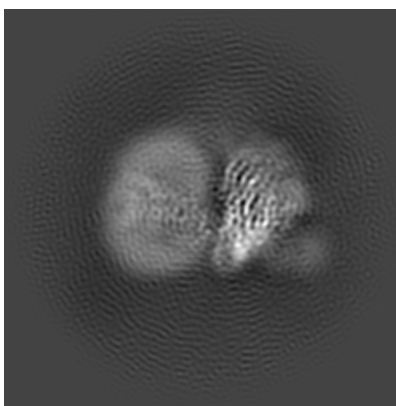
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

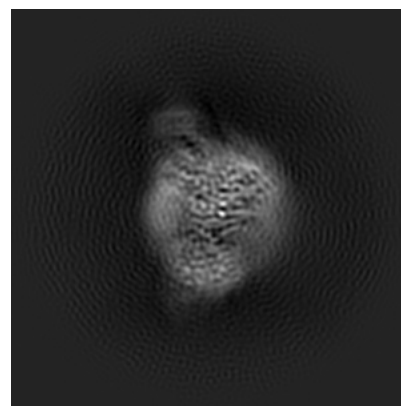
6.1.1 Primary map



X

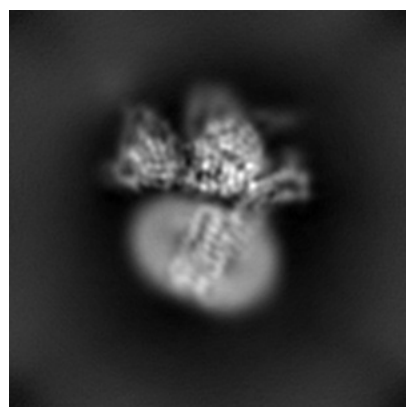


Y

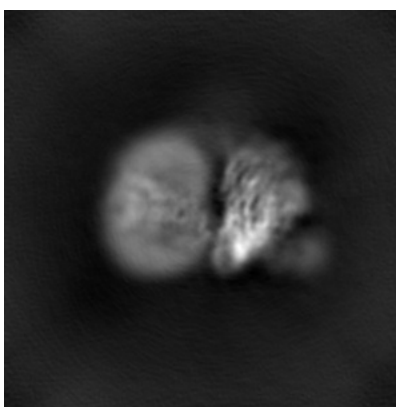


Z

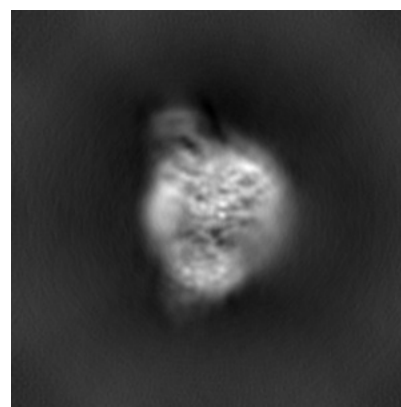
6.1.2 Raw map



X



Y

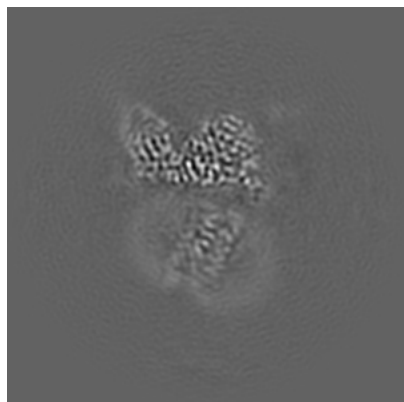


Z

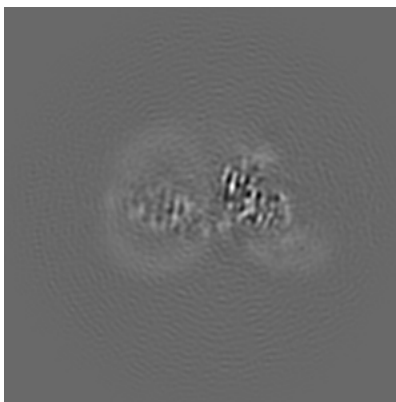
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

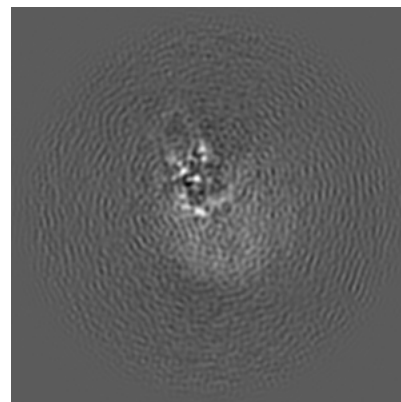
6.2.1 Primary map



X Index: 100

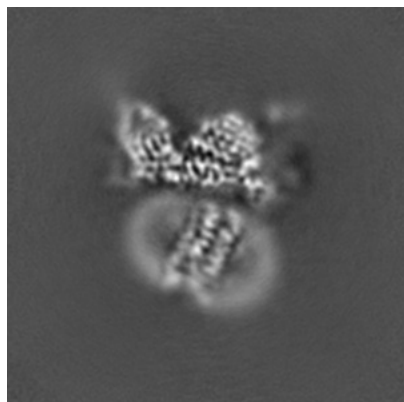


Y Index: 100

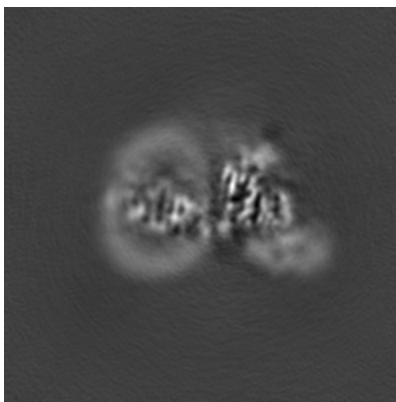


Z Index: 100

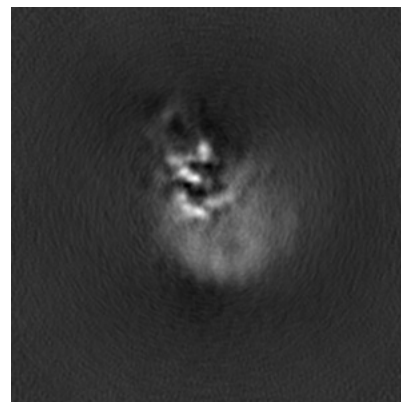
6.2.2 Raw map



X Index: 100



Y Index: 100

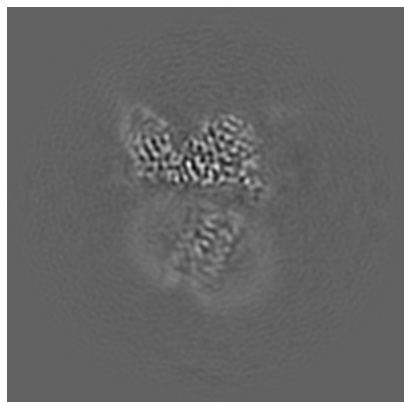


Z Index: 100

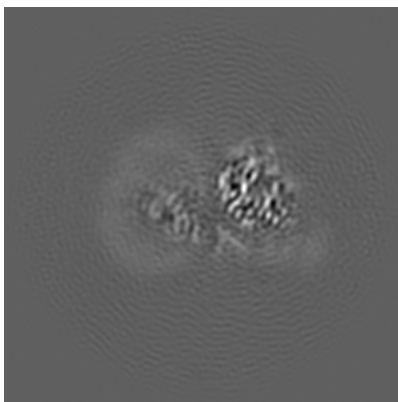
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

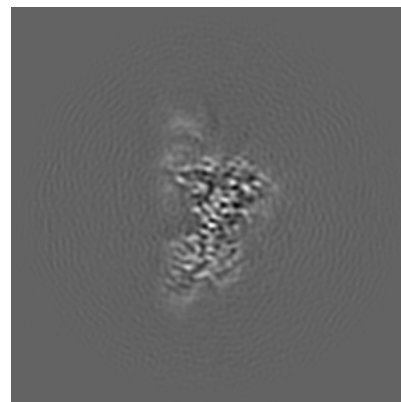
6.3.1 Primary map



X Index: 100

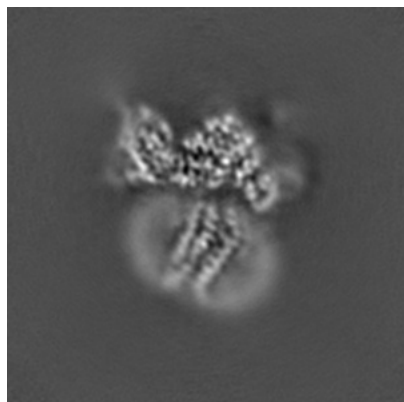


Y Index: 107

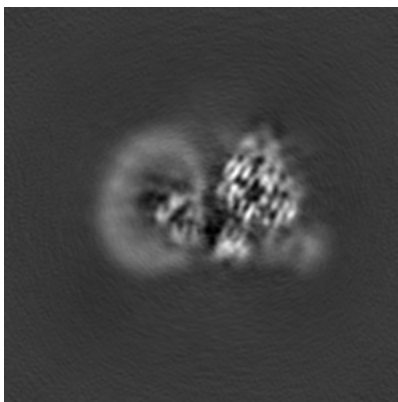


Z Index: 121

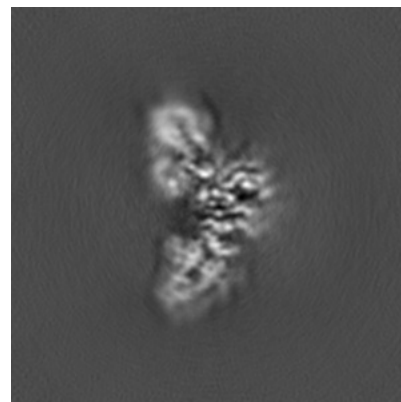
6.3.2 Raw map



X Index: 97



Y Index: 110

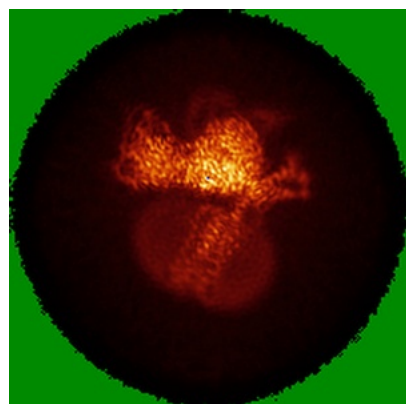


Z Index: 116

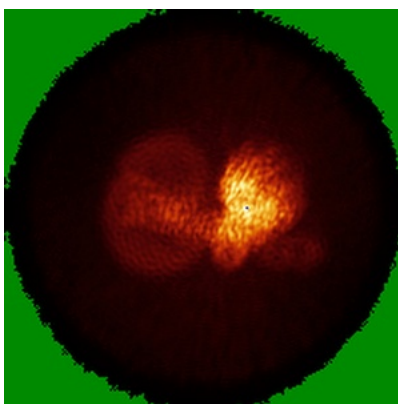
The images above show the largest variance slices of the map in three orthogonal directions.

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

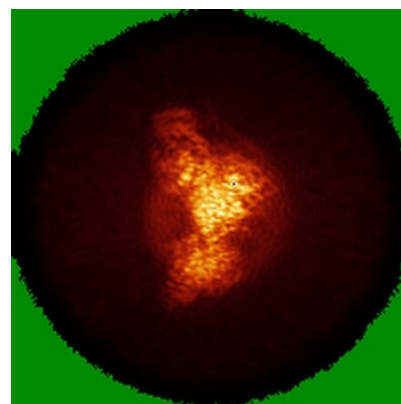
6.4.1 Primary map



X

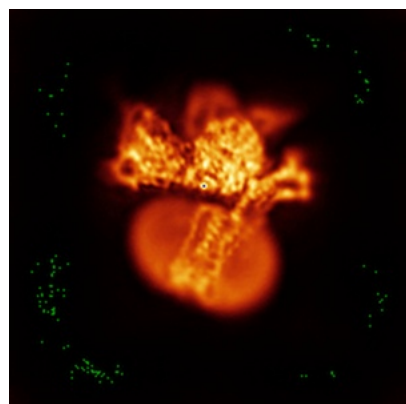


Y

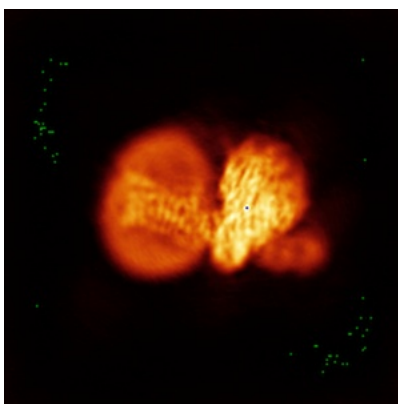


Z

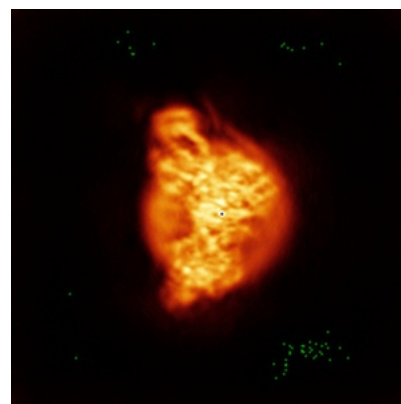
6.4.2 Raw map



X



Y

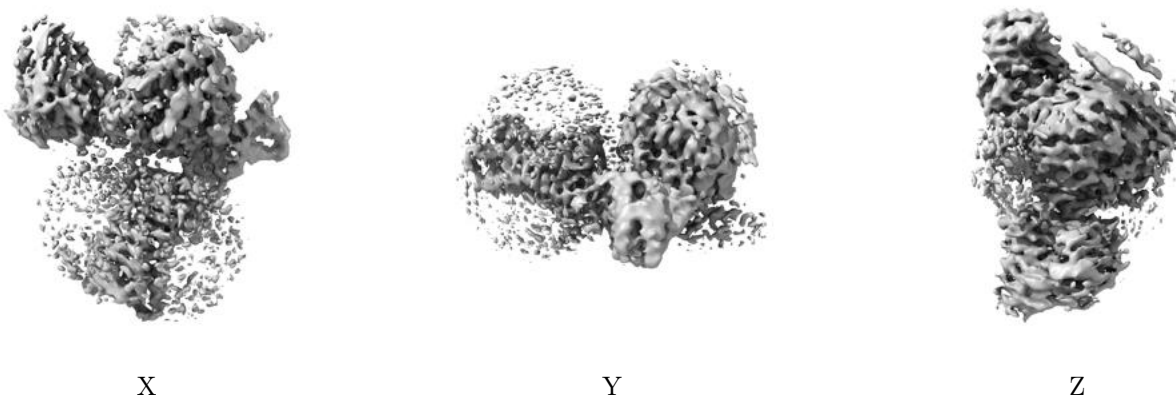


Z

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 0.345. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

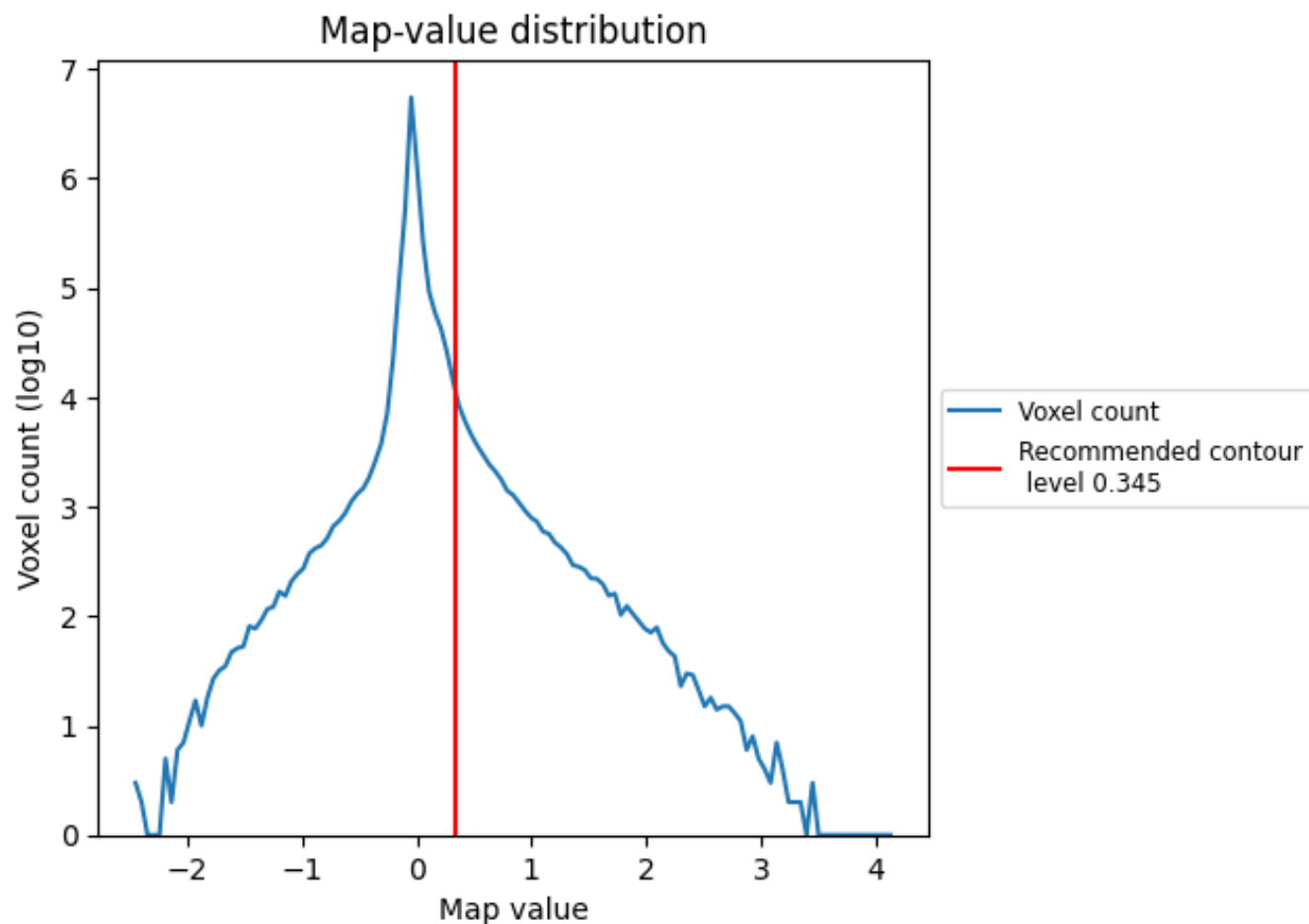
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

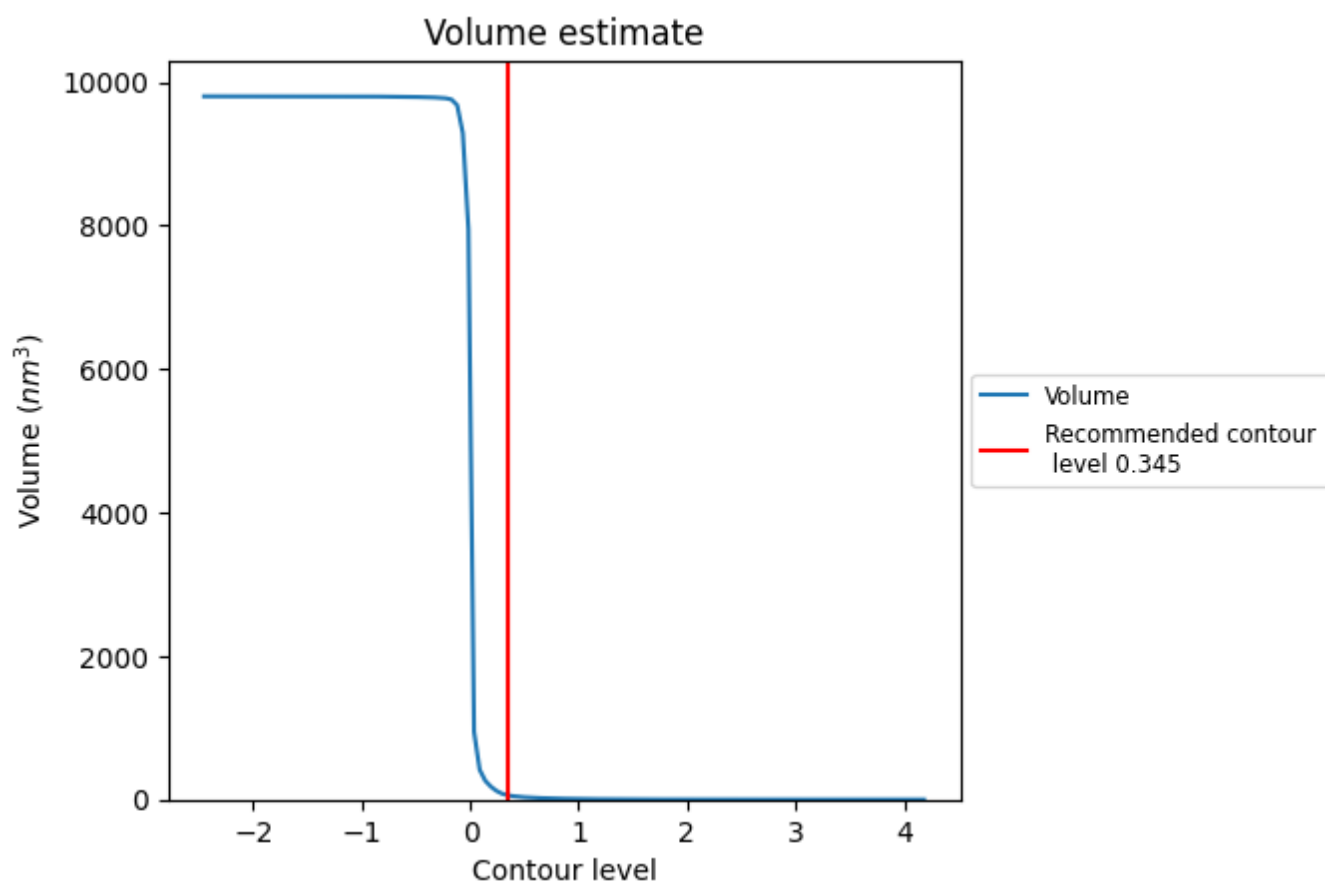
This section contains the results of statistical analysis of the map.

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.

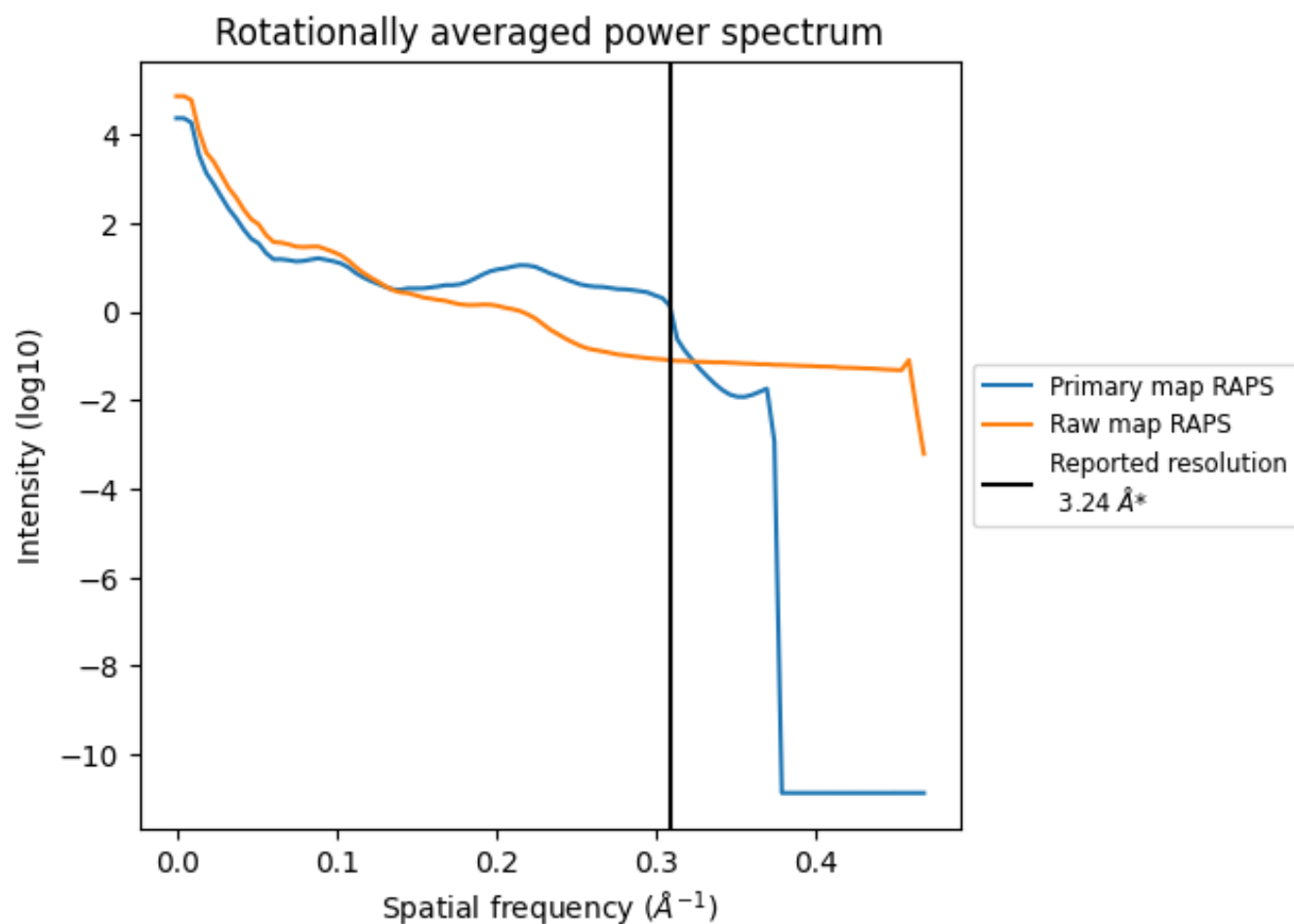
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 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 ⓘ

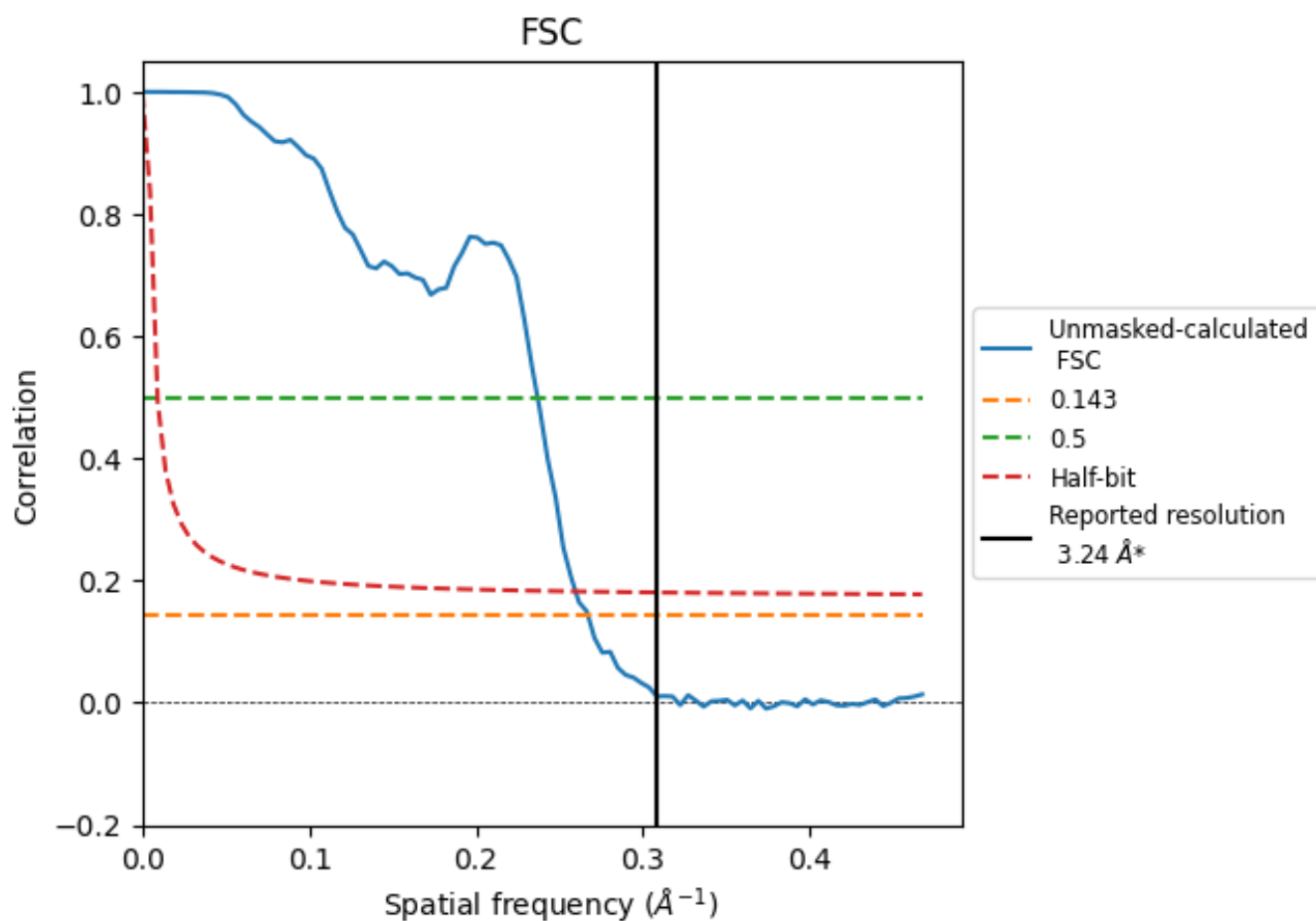


*Reported resolution corresponds to spatial frequency of 0.309 Å⁻¹

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 0.309 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

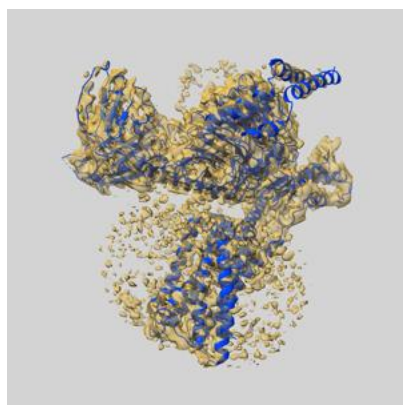
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	4.22	3.85

*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 3.75 differs from the reported value 3.24 by more than 10 %

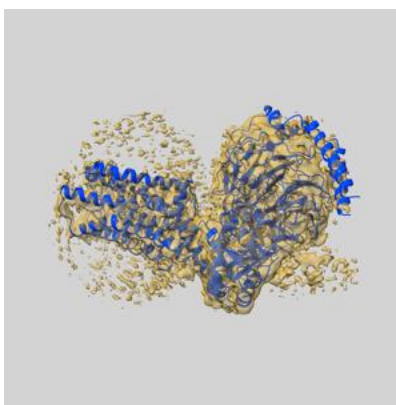
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39901 and PDB model 8ZBE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

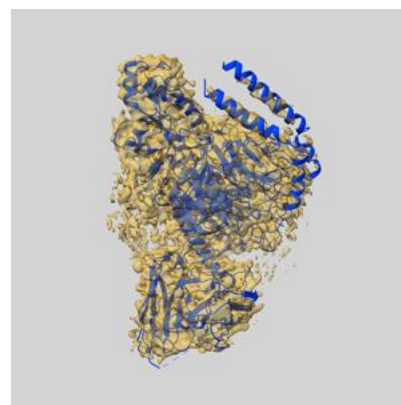
9.1 Map-model overlay [i](#)



X



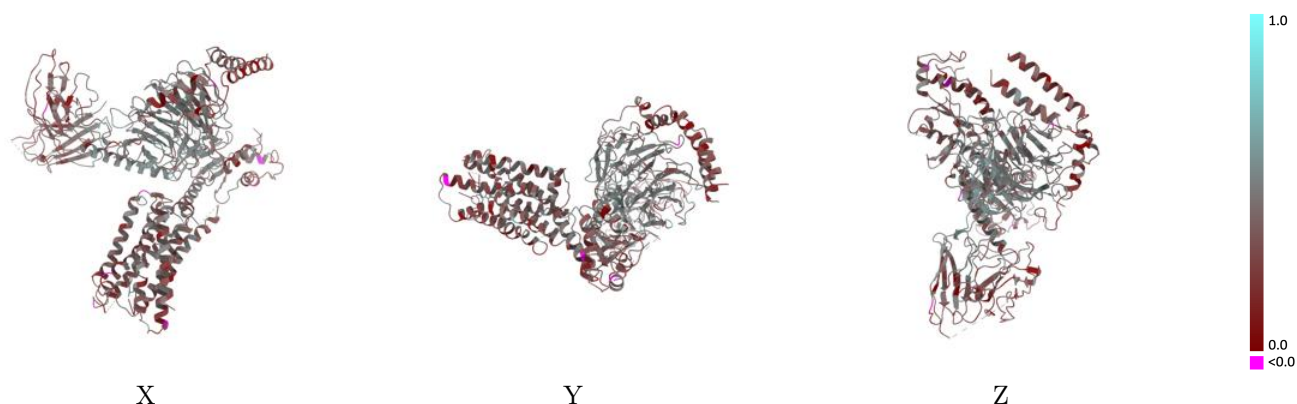
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.345 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](#)

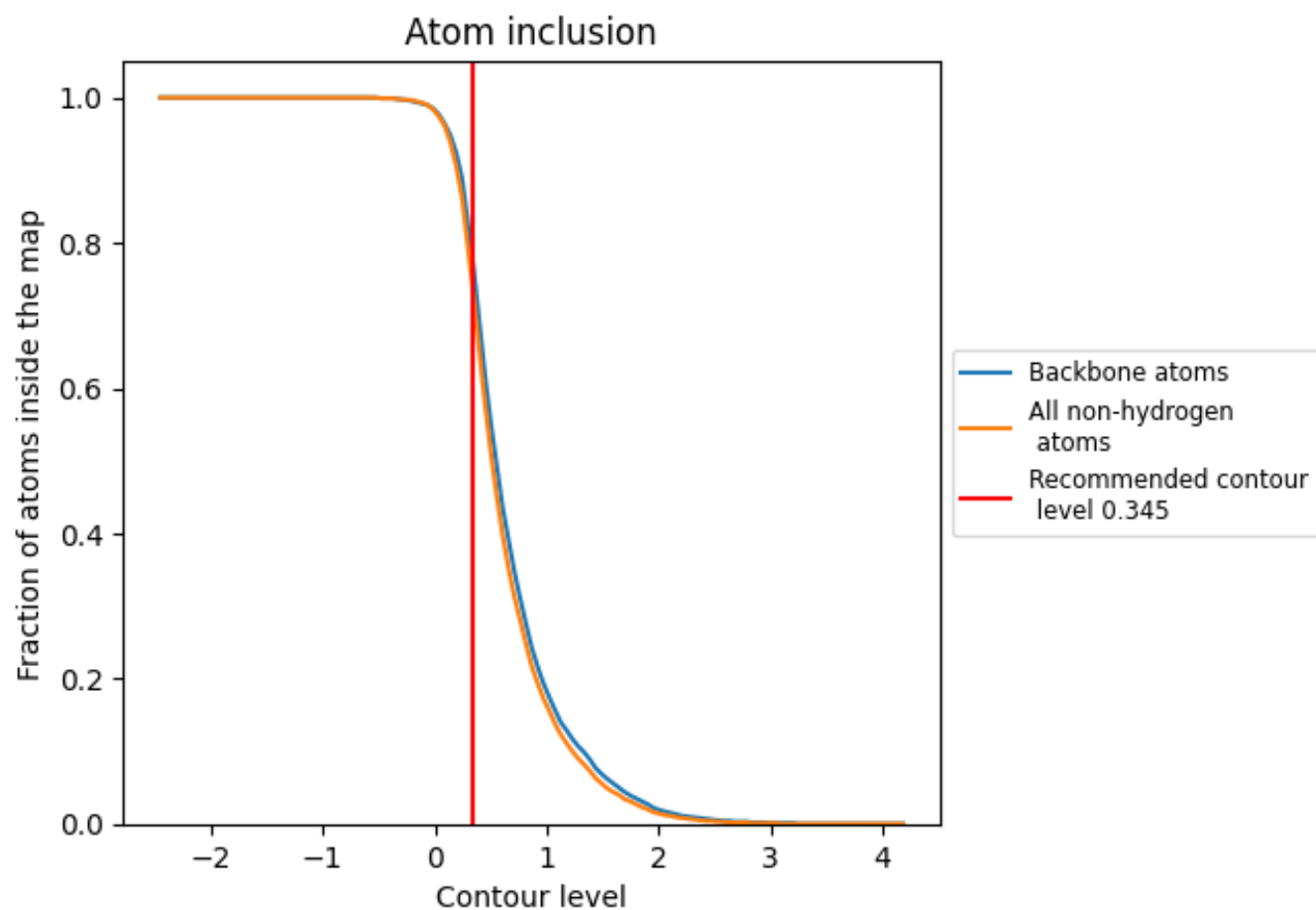


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% 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 (0.345) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.3910
A	0.6320	0.3480
B	0.7950	0.3930
C	0.7910	0.4480
D	0.4980	0.3260
E	0.7160	0.3620
P	0.7120	0.3670

1.0

0.0

<0.0