



Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 10:35 AM JST

PDB ID : 20ZK / pdb_000020zk
EMDB ID : EMD-67433
Title : Cryo-EM structure of the human neurotensin receptor 1 (hNTSR1)-Gi1 complex in the GTP-bound, AHD-open NC state 3, plunge-frozen 0-5 seconds after GTP addition
Authors : Kobayashi, K.; Matsui, T.E.; Fukuda, M.; Kawakami, K.; Yamashita, K.; Kato, H.E.
Deposited on : 2025-12-03
Resolution : 2.70 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

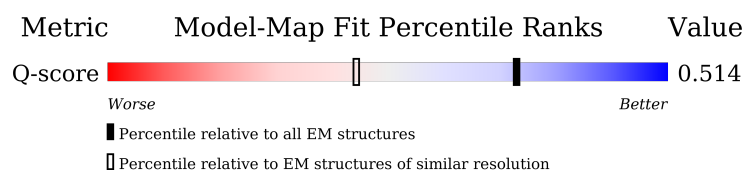
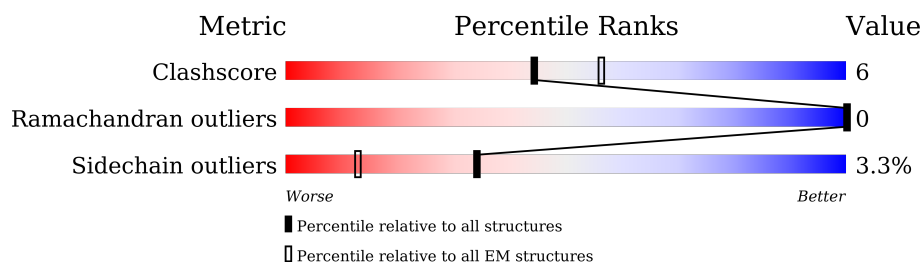
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	354	
2	B	358	
3	C	71	
4	D	259	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	R	436	<div><div></div><div>51%</div><div>17%</div><div>28%</div></div>
6	L	6	<div><div>17%</div><div>33%</div><div>33%</div><div>17%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9076 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	A	218	Total	C	N	O	S	0	0
			1757	1120	293	332	12		

- 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	B	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	HIS	-	expression tag	UNP P62873
B	3	HIS	-	expression tag	UNP P62873
B	4	HIS	-	expression tag	UNP P62873
B	5	HIS	-	expression tag	UNP P62873
B	6	HIS	-	expression tag	UNP P62873
B	7	HIS	-	expression tag	UNP P62873
B	8	LEU	-	expression tag	UNP P62873
B	9	GLU	-	expression tag	UNP P62873
B	10	VAL	-	expression tag	UNP P62873
B	11	LEU	-	expression tag	UNP P62873
B	12	PHE	-	expression tag	UNP P62873
B	13	GLN	-	expression tag	UNP P62873
B	14	GLY	-	expression tag	UNP P62873
B	15	PRO	-	expression tag	UNP P62873
B	16	GLY	-	expression tag	UNP P62873
B	17	SER	-	expression tag	UNP P62873
B	18	SER	-	expression tag	UNP P62873
B	19	GLY	-	expression tag	UNP P62873

- 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	C	54	Total	C	N	O	S	0	0
			413	260	71	79	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	231	Total	C	N	O	S	0	0
			1777	1128	294	345	10		

- Molecule 5 is a protein called Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	312	Total	C	N	O	S	0	0
			2476	1627	414	418	17		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP P30989
R	2	GLY	-	expression tag	UNP P30989
R	3	GLN	-	expression tag	UNP P30989
R	4	PRO	-	expression tag	UNP P30989
R	5	GLY	-	expression tag	UNP P30989
R	6	ASN	-	expression tag	UNP P30989
R	7	GLY	-	expression tag	UNP P30989
R	8	SER	-	expression tag	UNP P30989
R	9	ALA	-	expression tag	UNP P30989
R	10	PHE	-	expression tag	UNP P30989
R	11	LEU	-	expression tag	UNP P30989
R	12	LEU	-	expression tag	UNP P30989
R	13	ALA	-	expression tag	UNP P30989
R	14	PRO	-	expression tag	UNP P30989
R	15	ASN	-	expression tag	UNP P30989
R	16	ARG	-	expression tag	UNP P30989
R	17	SER	-	expression tag	UNP P30989
R	18	HIS	-	expression tag	UNP P30989
R	19	ALA	-	expression tag	UNP P30989
R	20	PRO	-	expression tag	UNP P30989
R	21	ASP	-	expression tag	UNP P30989
R	22	HIS	-	expression tag	UNP P30989

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	23	ASP	-	expression tag	UNP P30989
R	24	VAL	-	expression tag	UNP P30989
R	25	GLU	-	expression tag	UNP P30989
R	26	ASN	-	expression tag	UNP P30989
R	27	LEU	-	expression tag	UNP P30989
R	28	TYR	-	expression tag	UNP P30989
R	29	PHE	-	expression tag	UNP P30989
R	30	GLN	-	expression tag	UNP P30989
R	31	GLY	-	expression tag	UNP P30989
R	97	LEU	ALA	engineered mutation	UNP P30989
R	431	LEU	-	expression tag	UNP P30989
R	432	GLU	-	expression tag	UNP P30989
R	433	VAL	-	expression tag	UNP P30989
R	434	LEU	-	expression tag	UNP P30989
R	435	PHE	-	expression tag	UNP P30989
R	436	GLN	-	expression tag	UNP P30989

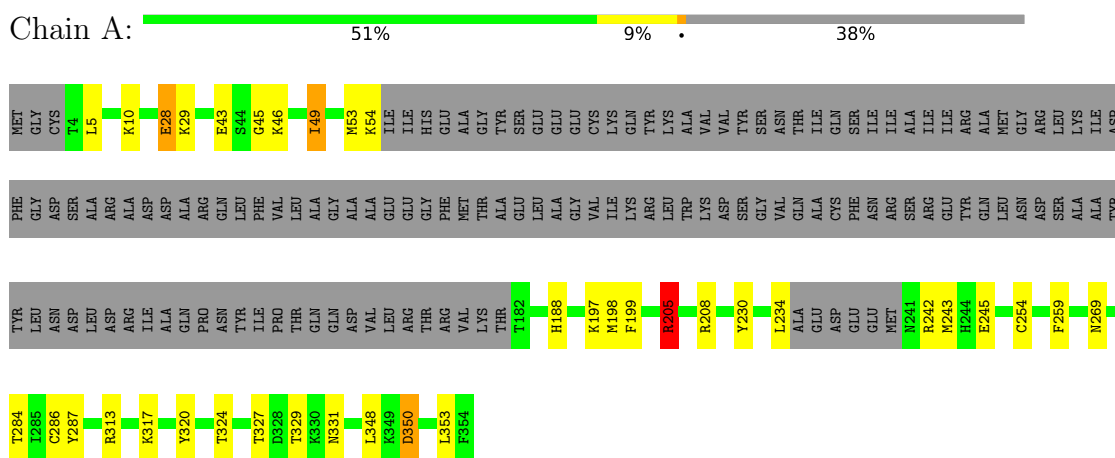
- Molecule 6 is a protein called LYS-LYS-PRO-TYR-ILE-LEU.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	6	Total	C	N	O	0	0
			53	38	8	7		

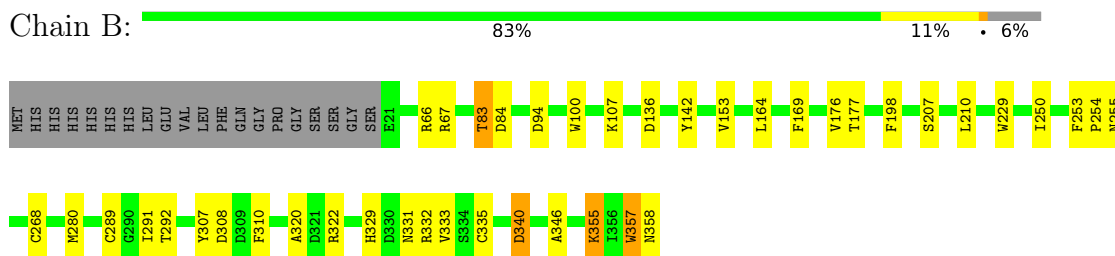
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

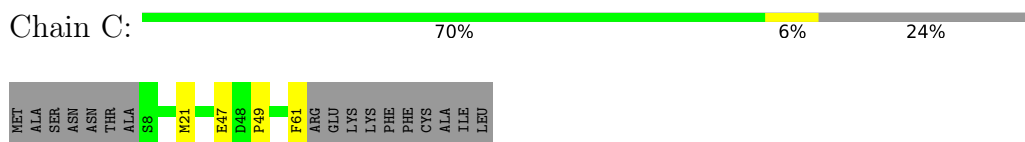
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



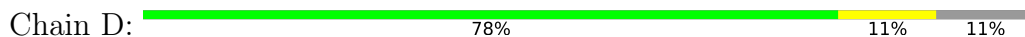
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



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



- Molecule 4: scFv16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288412	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)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.507	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/1786	1.22	8/2395 (0.3%)
2	B	0.86	0/2647	1.15	9/3589 (0.3%)
3	C	0.75	0/419	1.02	1/566 (0.2%)
4	D	0.79	1/1821 (0.1%)	1.04	3/2469 (0.1%)
5	R	0.68	0/2540	1.19	9/3464 (0.3%)
6	L	0.94	0/54	2.31	2/69 (2.9%)
All	All	0.78	1/9267 (0.0%)	1.16	32/12552 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
5	R	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	99	SER	CA-CB	-5.57	1.44	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH2	-17.44	103.50	119.20
6	L	11	TYR	CB-CA-C	-12.26	89.34	109.56
1	A	205	ARG	NE-CZ-NH1	9.68	131.18	121.50
5	R	338	PHE	CB-CA-C	-8.45	96.77	110.79
1	A	208	ARG	N-CA-CB	7.85	122.31	110.22
5	R	191	LEU	N-CA-CB	-7.44	99.12	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	76	LYS	CG-CD-CE	6.94	127.26	111.30
5	R	110	GLN	N-CA-C	-6.67	105.00	113.01
5	R	186	PHE	N-CA-CB	-6.48	100.59	110.12
4	D	76	LYS	CD-CE-NZ	6.33	132.17	111.90
6	L	10	PRO	CA-C-O	-6.29	114.19	121.86
5	R	185	PRO	N-CA-CB	-6.24	96.55	103.23
2	B	357	TRP	CA-C-O	-6.20	113.85	121.78
2	B	83	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	205	ARG	CG-CD-NE	-6.14	98.48	112.00
5	R	110	GLN	N-CA-CB	5.90	120.72	110.39
3	C	21	MET	CB-CG-SD	-5.78	95.36	112.70
1	A	350	ASP	CA-CB-CG	5.75	118.35	112.60
5	R	185	PRO	N-CA-C	5.73	121.67	113.47
5	R	280	ARG	CB-CA-C	-5.71	101.91	110.88
2	B	136	ASP	CA-CB-CG	5.71	118.31	112.60
4	D	114	GLY	CA-C-O	-5.57	118.39	122.23
2	B	94	ASP	CA-CB-CG	5.40	118.00	112.60
2	B	340	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	199	PHE	N-CA-CB	-5.37	102.27	110.65
2	B	346	ALA	CA-C-O	-5.35	114.96	121.28
1	A	28	GLU	CB-CG-CD	5.34	121.67	112.60
5	R	149	GLY	CA-C-O	-5.31	118.33	122.52
2	B	169	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	43	GLU	CB-CA-C	-5.26	104.26	111.73
2	B	329	HIS	CA-CB-CG	5.14	118.94	113.80
2	B	84	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	313	ARG	Sidechain
2	B	322	ARG	Sidechain
2	B	355	LYS	Mainchain
5	R	102	ARG	Sidechain
5	R	306	ARG	Sidechain

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	1757	0	1755	24	0
2	B	2600	0	2505	17	0
3	C	413	0	423	2	0
4	D	1777	0	1712	15	0
5	R	2476	0	2526	58	0
6	L	53	0	63	3	0
All	All	9076	0	8984	115	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 6.

All (115) 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)
2:B:164:LEU:HD11	2:B:177:THR:HB	1.63	0.79
1:A:350:ASP:HB3	5:R:110:GLN:HG2	1.66	0.78
5:R:146:TRP:HE1	5:R:153:CYS:HB2	1.49	0.77
5:R:146:TRP:NE1	5:R:153:CYS:HB2	2.01	0.75
5:R:250:GLN:NE2	5:R:340:TYR:OH	2.21	0.74
1:A:53:MET:HE1	1:A:331:ASN:HB3	1.71	0.72
1:A:188:HIS:CE1	1:A:197:LYS:HE2	2.26	0.70
5:R:108:SER:O	5:R:112:THR:N	2.24	0.70
5:R:377:ASN:HB3	5:R:383:PHE:CE2	2.27	0.69
1:A:259:PHE:O	1:A:317:LYS:NZ	2.26	0.67
4:D:83:MET:HE1	4:D:117:LEU:HD22	1.76	0.66
1:A:188:HIS:HE1	1:A:197:LYS:HE2	1.60	0.66
5:R:168:ALA:HB2	5:R:328:TRP:HZ3	1.60	0.66
1:A:254:CYS:O	1:A:317:LYS:HE3	1.95	0.66
5:R:246:LYS:HG2	5:R:339:CYS:SG	2.36	0.66
5:R:279:VAL:HG13	5:R:307:VAL:HG13	1.77	0.66
2:B:280:MET:SD	2:B:320:ALA:HB2	2.36	0.65
2:B:142:TYR:CE1	2:B:153:VAL:HG22	2.34	0.62
5:R:168:ALA:HB2	5:R:328:TRP:CZ3	2.34	0.62
5:R:108:SER:O	5:R:112:THR:HG23	1.98	0.62
4:D:174:LEU:HD22	4:D:212:PHE:CG	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:378:LEU:HD21	5:R:387:PHE:CD1	2.35	0.60
4:D:32:PHE:CD2	4:D:100:ILE:HB	2.36	0.60
5:R:107:GLN:HB2	5:R:110:GLN:HG3	1.84	0.59
5:R:224:ARG:HB2	5:R:235:VAL:HG21	1.83	0.59
1:A:28:GLU:HG2	5:R:190:THR:HG21	1.83	0.59
2:B:207:SER:OG	2:B:250:ILE:HG22	2.03	0.59
1:A:45:GLY:HA3	1:A:269:ASN:HD22	1.68	0.58
5:R:246:LYS:HA	5:R:339:CYS:SG	2.44	0.57
6:L:11:TYR:O	6:L:12:ILE:C	2.48	0.57
5:R:218:THR:HG22	5:R:240:ILE:CD1	2.34	0.57
5:R:144:HIS:HB2	5:R:145:PRO:HD3	1.86	0.57
4:D:88:SER:O	4:D:91:THR:HG22	2.05	0.56
5:R:377:ASN:HB3	5:R:383:PHE:CD2	2.42	0.55
1:A:350:ASP:CB	5:R:110:GLN:HG2	2.35	0.54
5:R:218:THR:HG21	5:R:248:VAL:HG21	1.90	0.54
5:R:70:THR:HG1	5:R:355:HIS:CE1	2.25	0.54
5:R:174:LEU:HD23	5:R:376:TYR:CE1	2.43	0.53
1:A:234:LEU:HD21	1:A:245:GLU:OE1	2.08	0.52
5:R:218:THR:HG22	5:R:240:ILE:HD13	1.92	0.52
2:B:355:LYS:O	2:B:357:TRP:CD1	2.63	0.52
5:R:373:PRO:O	5:R:377:ASN:HB2	2.10	0.51
4:D:105:SER:O	4:D:191:ARG:NH2	2.37	0.51
5:R:103:LYS:HG2	5:R:386:ILE:HD13	1.95	0.49
2:B:310:PHE:CD1	2:B:331:ASN:C	2.91	0.49
2:B:66:ARG:HE	2:B:358:ASN:HB3	1.78	0.48
5:R:107:GLN:O	5:R:111:SER:HB3	2.13	0.48
5:R:135:GLU:CD	5:R:362:ASN:HD22	2.22	0.47
4:D:12:VAL:HG21	4:D:86:LEU:HD13	1.97	0.47
5:R:134:VAL:HG13	5:R:148:PHE:CE2	2.49	0.47
5:R:144:HIS:HB2	5:R:145:PRO:CD	2.45	0.47
1:A:230:TYR:O	1:A:286:CYS:HB2	2.15	0.46
5:R:152:GLY:O	5:R:153:CYS:C	2.57	0.46
2:B:292:THR:OG1	2:B:333:VAL:O	2.27	0.46
5:R:165:TYR:OH	5:R:252:ASN:HA	2.15	0.46
5:R:282:ALA:HB2	5:R:306:ARG:HE	1.80	0.46
1:A:53:MET:HG3	1:A:198:MET:HE1	1.98	0.46
1:A:230:TYR:HA	1:A:243:MET:CG	2.45	0.46
2:B:100:TRP:CH2	2:B:107:LYS:HE3	2.51	0.46
5:R:154:ARG:NH1	5:R:216:LEU:O	2.40	0.46
5:R:312:HIS:CD2	5:R:315:ARG:HH21	2.34	0.46
6:L:9:LYS:HG3	6:L:10:PRO:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:VAL:HG21	2:B:210:LEU:HD21	1.97	0.45
2:B:268:CYS:SG	2:B:291:ILE:HD13	2.57	0.45
5:R:70:THR:CG2	5:R:359:MET:HE1	2.47	0.45
5:R:96:THR:HG22	5:R:100:LEU:HD12	1.98	0.45
4:D:178:LEU:HD13	4:D:227:TYR:CZ	2.52	0.45
1:A:284:THR:HA	1:A:287:TYR:O	2.16	0.45
2:B:291:ILE:HG12	2:B:307:TYR:CE2	2.52	0.45
5:R:67:ASP:HA	5:R:144:HIS:HE1	1.81	0.44
2:B:198:PHE:HB3	2:B:229:TRP:CE3	2.53	0.44
4:D:83:MET:HB3	4:D:86:LEU:HD21	1.99	0.44
5:R:316:VAL:O	5:R:320:VAL:HG23	2.17	0.44
6:L:11:TYR:C	6:L:13:LEU:N	2.73	0.44
5:R:149:GLY:HA2	5:R:221:GLU:OE1	2.17	0.44
5:R:219:MET:HE1	5:R:238:PRO:HG3	1.98	0.44
5:R:107:GLN:O	5:R:111:SER:N	2.51	0.44
5:R:271:ILE:HG22	5:R:317:LEU:HD11	2.00	0.44
4:D:149:VAL:HG11	4:D:245:LEU:HD11	1.99	0.44
4:D:150:THR:O	4:D:153:GLU:HG2	2.18	0.43
1:A:45:GLY:HA3	1:A:269:ASN:ND2	2.31	0.43
4:D:149:VAL:O	4:D:247:LEU:HA	2.19	0.43
1:A:243:MET:HB2	1:A:286:CYS:SG	2.59	0.43
1:A:320:TYR:CD1	1:A:320:TYR:N	2.86	0.43
4:D:230:MET:SD	4:D:239:PHE:CZ	3.12	0.43
5:R:99:THR:O	5:R:103:LYS:HG3	2.19	0.43
1:A:45:GLY:O	1:A:46:LYS:C	2.62	0.43
1:A:324:THR:HB	1:A:331:ASN:HD21	1.84	0.43
5:R:173:SER:HB2	5:R:200:PHE:HE2	1.83	0.43
5:R:240:ILE:HD12	5:R:244:THR:CG2	2.49	0.42
5:R:66:LEU:HD22	5:R:66:LEU:HA	1.83	0.42
5:R:224:ARG:HB2	5:R:235:VAL:CG2	2.50	0.42
2:B:308:ASP:HA	2:B:332:ARG:HG3	2.00	0.42
1:A:5:LEU:O	1:A:10:LYS:HE3	2.20	0.42
4:D:97:VAL:HG11	4:D:108:PHE:CD2	2.54	0.42
5:R:218:THR:O	5:R:238:PRO:HA	2.20	0.42
5:R:238:PRO:HG2	5:R:338:PHE:HE2	1.85	0.42
5:R:186:PHE:O	5:R:190:THR:OG1	2.37	0.42
5:R:71:ASP:OD1	5:R:71:ASP:N	2.40	0.41
2:B:67:ARG:HH22	3:C:61:PHE:HA	1.85	0.41
1:A:348:LEU:HD22	1:A:353:LEU:HD12	2.01	0.41
2:B:289:CYS:HB2	2:B:308:ASP:HB2	2.03	0.41
5:R:218:THR:HG22	5:R:240:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:89:GLY:HA3	5:R:370:THR:HG22	2.01	0.41
5:R:282:ALA:HB3	5:R:307:VAL:HG22	2.03	0.41
5:R:135:GLU:HA	5:R:139:PHE:CD2	2.56	0.41
2:B:253:PHE:HD2	2:B:255:ASN:OD1	2.03	0.41
4:D:175:TYR:CE2	4:D:190:TYR:HB2	2.56	0.41
1:A:234:LEU:HD23	1:A:242:ARG:HG2	2.02	0.40
4:D:32:PHE:CE2	4:D:100:ILE:HB	2.57	0.40
1:A:49:ILE:HG23	1:A:53:MET:HG2	2.04	0.40
5:R:259:PHE:HB3	5:R:260:PRO:HD3	2.03	0.40
1:A:230:TYR:HA	1:A:243:MET:HG3	2.03	0.40
3:C:47:GLU:O	3:C:49:PRO:HD3	2.21	0.40
5:R:67:ASP:HA	5:R:144:HIS:CE1	2.56	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	212/354 (60%)	208 (98%)	4 (2%)	0	100	100
2	B	336/358 (94%)	326 (97%)	10 (3%)	0	100	100
3	C	52/71 (73%)	52 (100%)	0	0	100	100
4	D	227/259 (88%)	225 (99%)	2 (1%)	0	100	100
5	R	308/436 (71%)	305 (99%)	3 (1%)	0	100	100
6	L	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	1139/1484 (77%)	1119 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/305 (64%)	188 (97%)	6 (3%)	35	65
2	B	281/298 (94%)	277 (99%)	4 (1%)	59	82
3	C	44/58 (76%)	44 (100%)	0	100	100
4	D	196/209 (94%)	196 (100%)	0	100	100
5	R	270/368 (73%)	249 (92%)	21 (8%)	11	29
6	L	6/6 (100%)	4 (67%)	2 (33%)	0	1
All	All	991/1244 (80%)	958 (97%)	33 (3%)	34	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	49	ILE
1	A	54	LYS
1	A	205	ARG
1	A	327	THR
1	A	329	THR
2	B	83	THR
2	B	254	PRO
2	B	335	CYS
2	B	340	ASP
5	R	66	LEU
5	R	68	VAL
5	R	71	ASP
5	R	72	ILE
5	R	102	ARG
5	R	104	LYS
5	R	105	SER
5	R	106	LEU
5	R	107	GLN
5	R	108	SER
5	R	109	LEU
5	R	111	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	142	VAL
5	R	187	LYS
5	R	189	LYS
5	R	190	THR
5	R	235	VAL
5	R	280	ARG
5	R	284	GLU
5	R	285	GLN
5	R	395	CYS
6	L	11	TYR
6	L	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
2	B	34	ASN
2	B	311	ASN
5	R	144	HIS
5	R	222	GLN
5	R	250	GLN
5	R	281	GLN
5	R	285	GLN
5	R	308	GLN
5	R	312	HIS
5	R	332	HIS
5	R	345	GLN
5	R	385	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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.

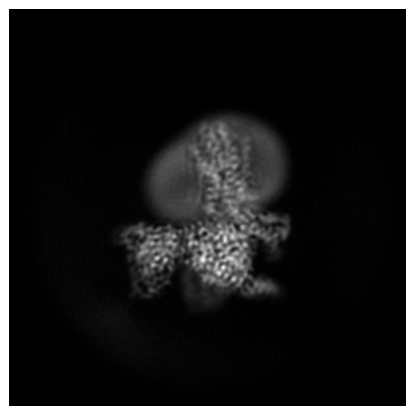
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67433. These allow visual inspection of the internal detail of the map and identification of artifacts.

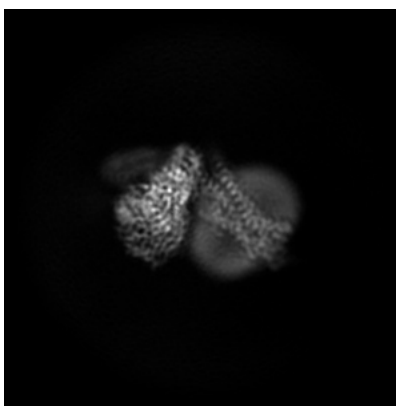
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

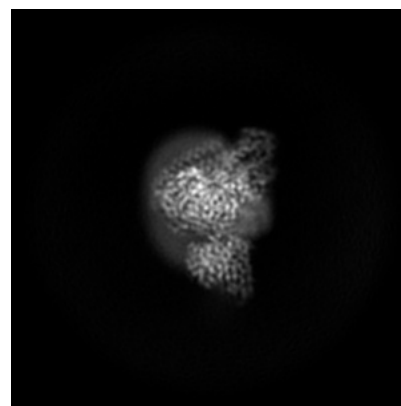
6.1.1 Primary map



X

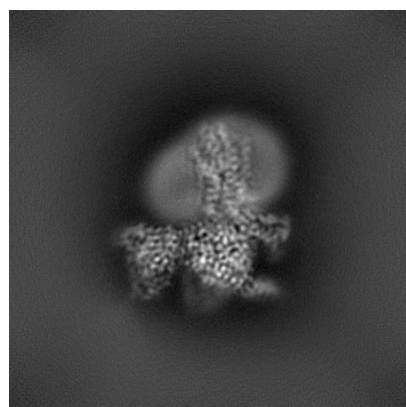


Y

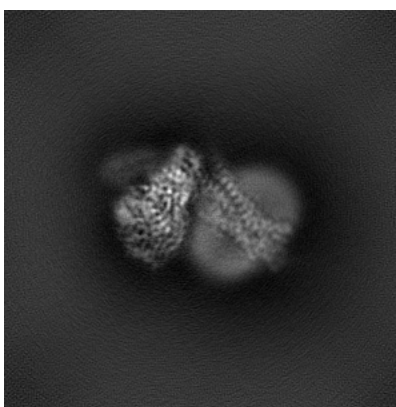


Z

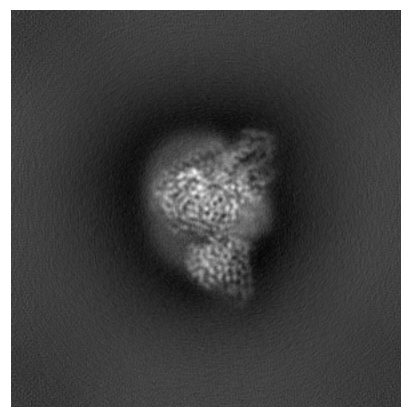
6.1.2 Raw map



X



Y

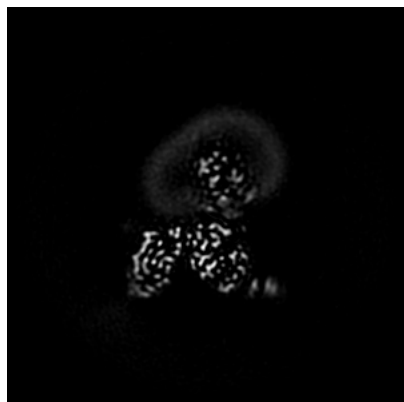


Z

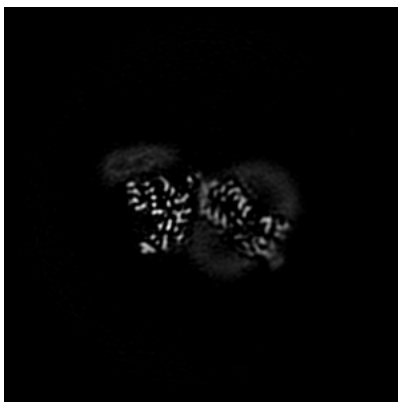
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

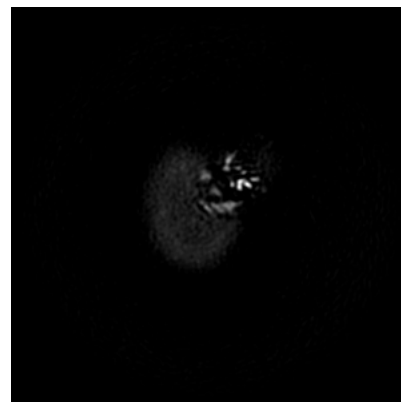
6.2.1 Primary map



X Index: 150

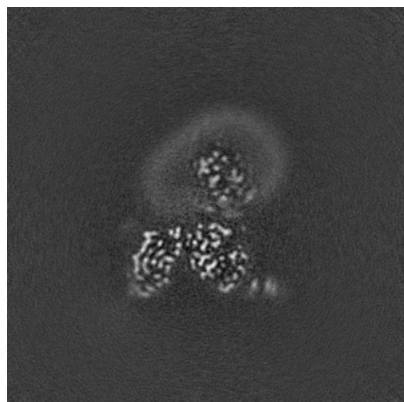


Y Index: 150

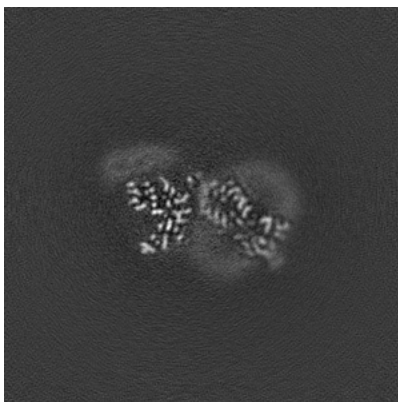


Z Index: 150

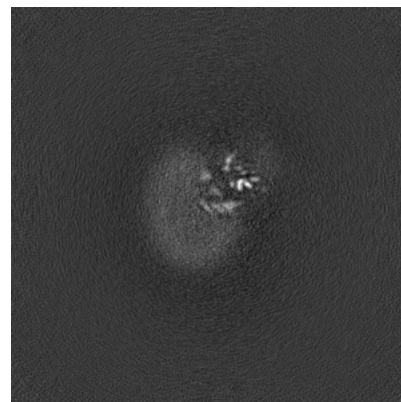
6.2.2 Raw map



X Index: 150



Y Index: 150

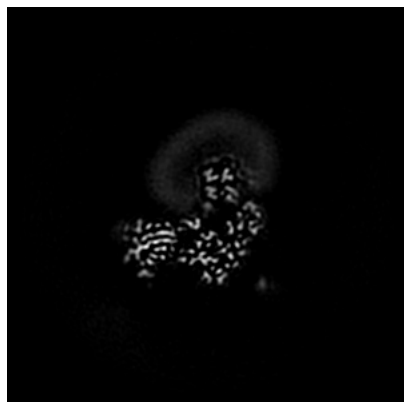


Z Index: 150

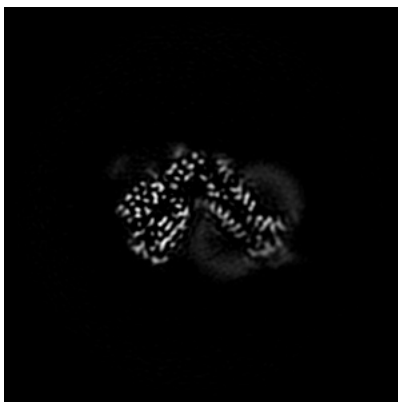
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

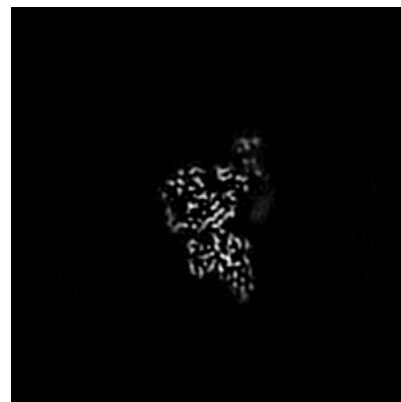
6.3.1 Primary map



X Index: 162

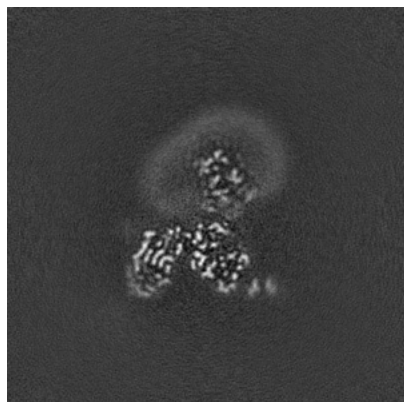


Y Index: 163

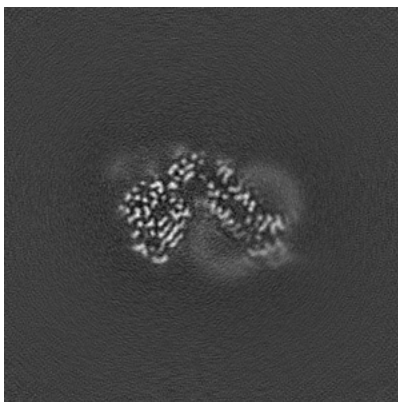


Z Index: 123

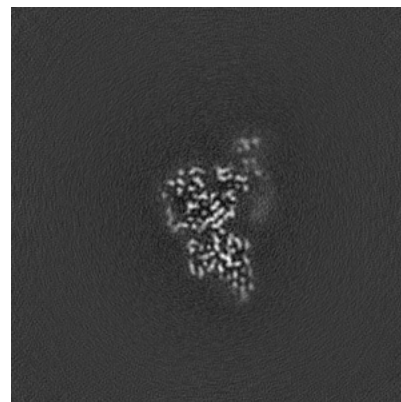
6.3.2 Raw map



X Index: 149



Y Index: 162

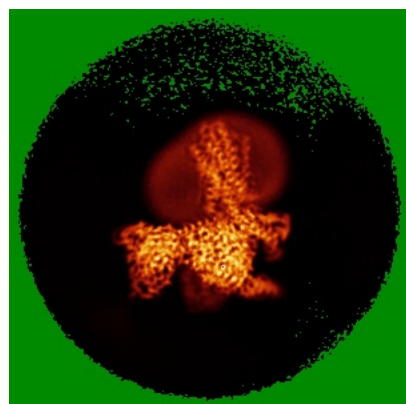


Z Index: 123

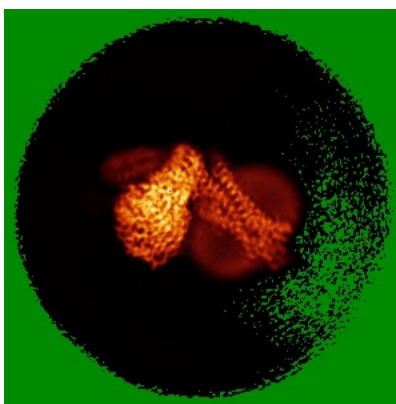
The images above show the largest variance slices of the map in three orthogonal directions.

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

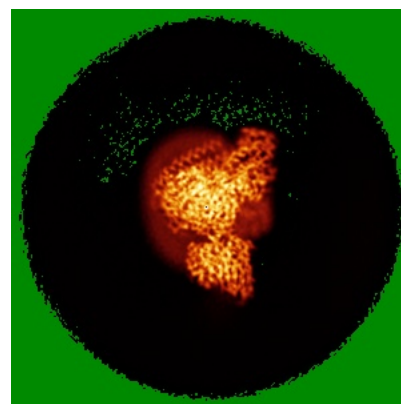
6.4.1 Primary map



X

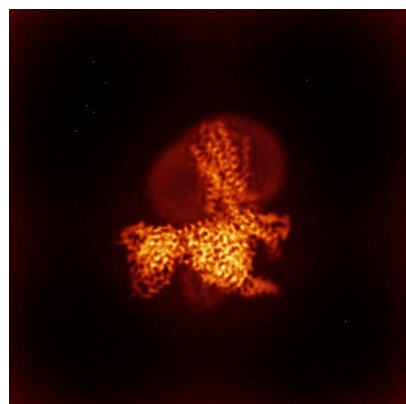


Y

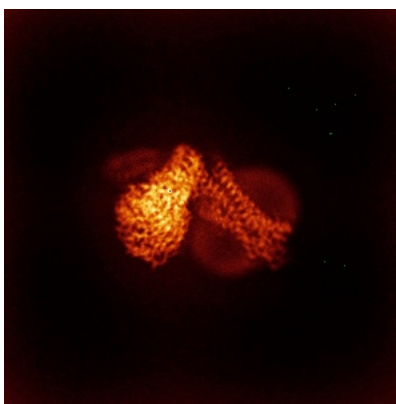


Z

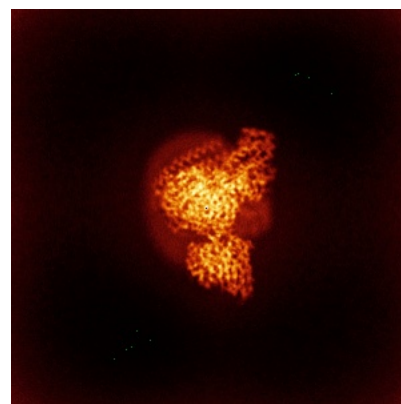
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

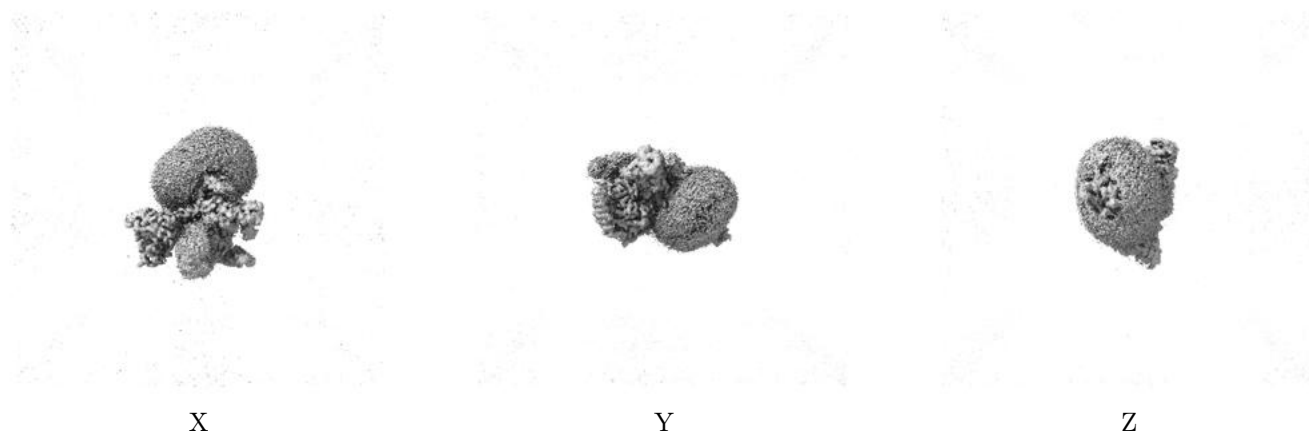
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

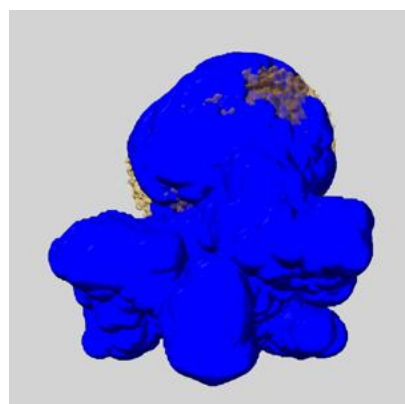
6.6 Mask visualisation [i](#)

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

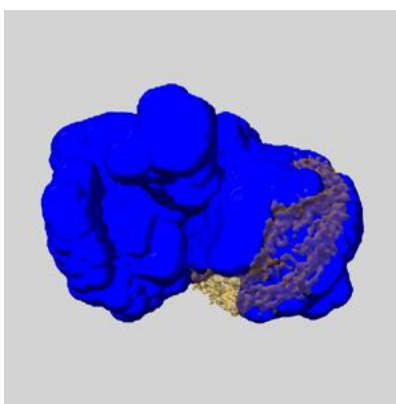
A mask typically either:

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

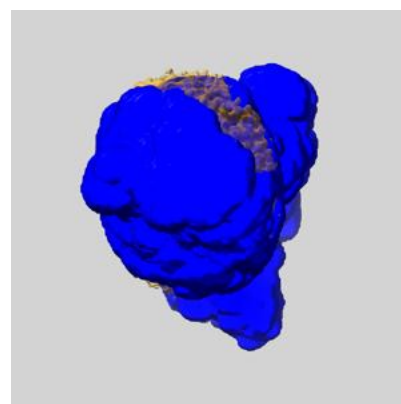
6.6.1 emd_67433_msk_1.map [i](#)



X



Y

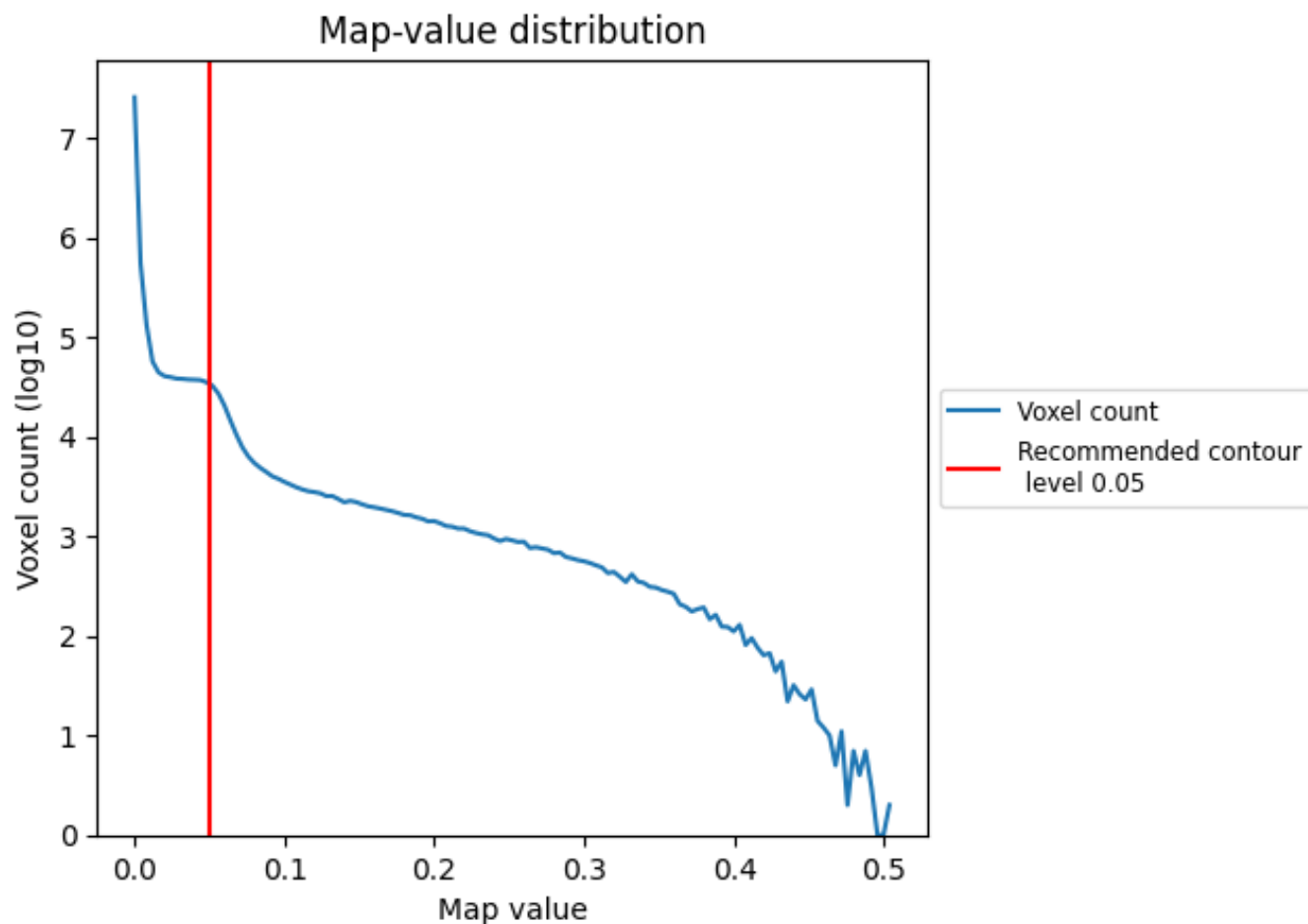


Z

7 Map analysis [i](#)

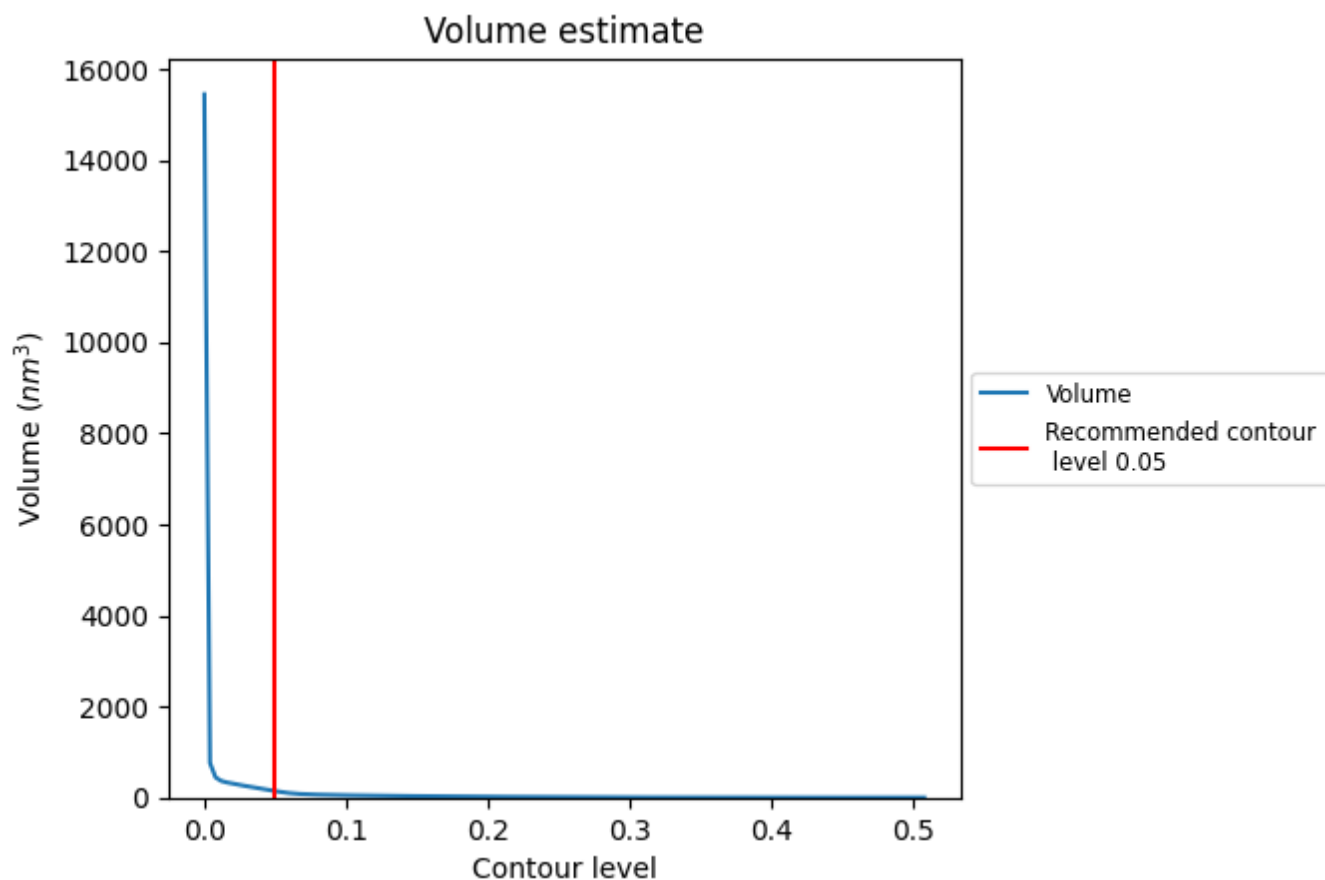
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

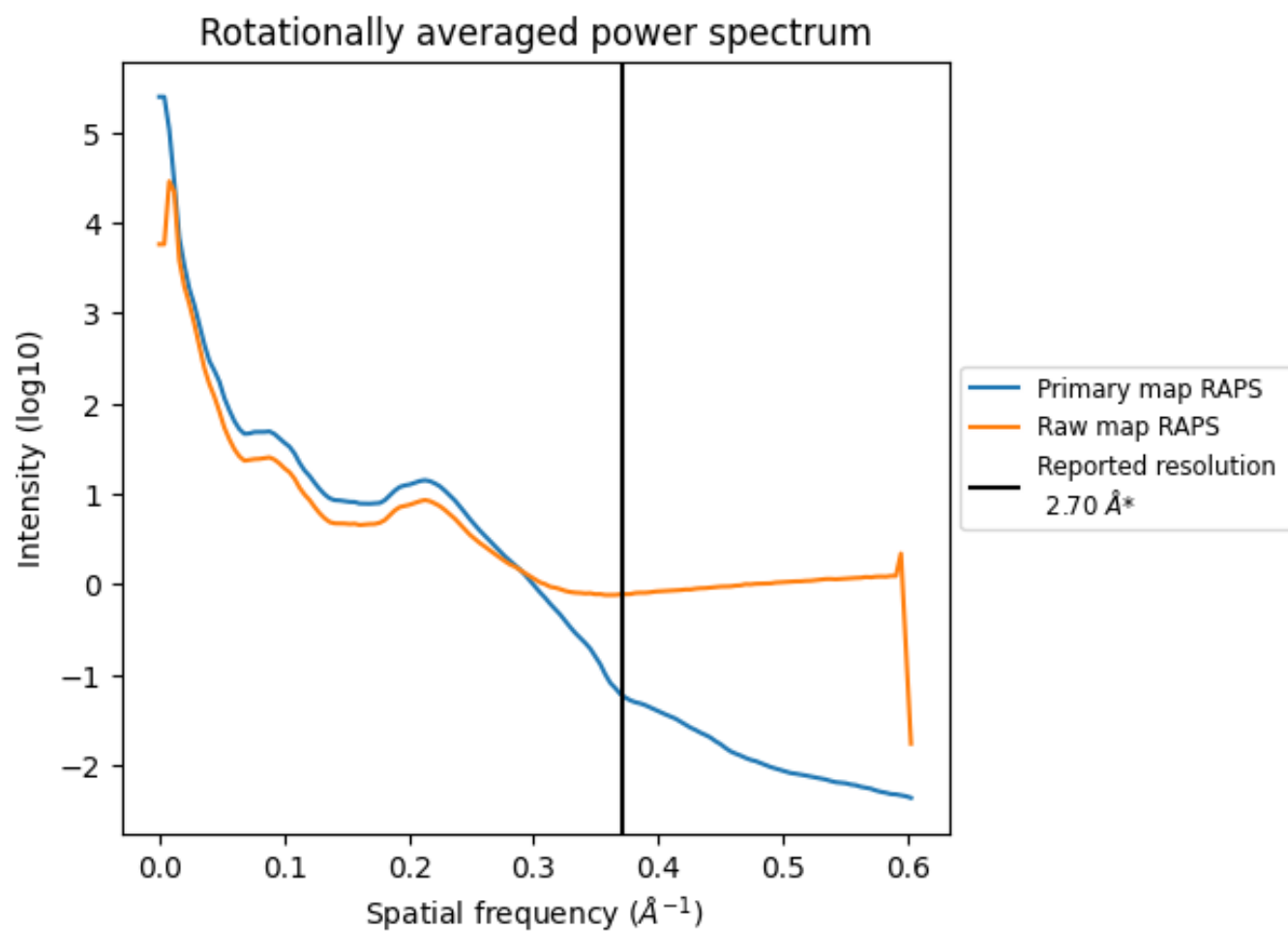
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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 ⓘ

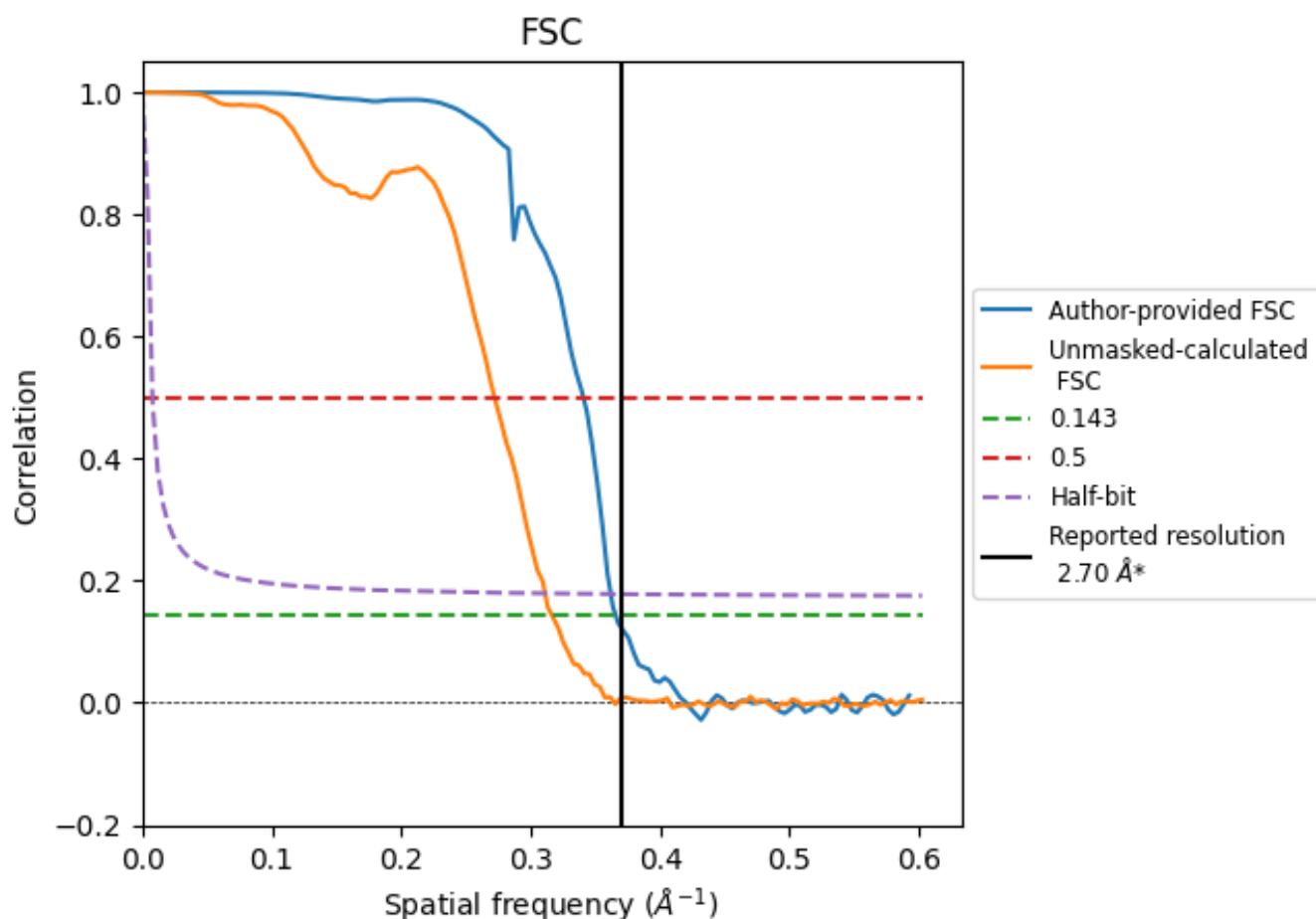


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

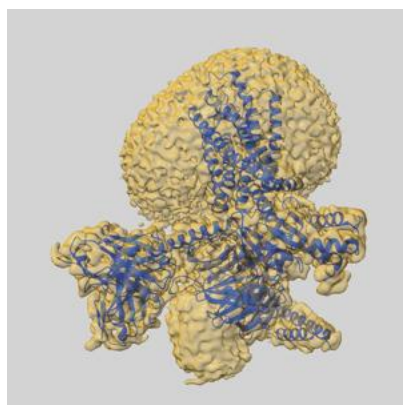
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	2.94	2.76
Unmasked-calculated*	3.16	3.67	3.21

*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 3.16 differs from the reported value 2.7 by more than 10 %

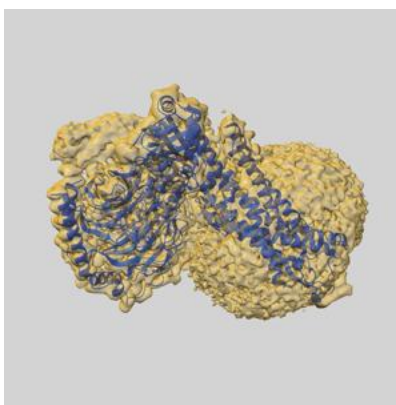
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67433 and PDB model 20ZK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

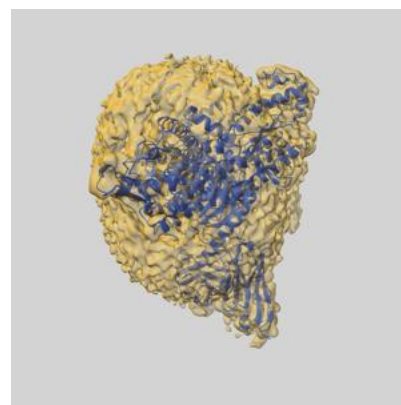
9.1 Map-model overlay [i](#)



X



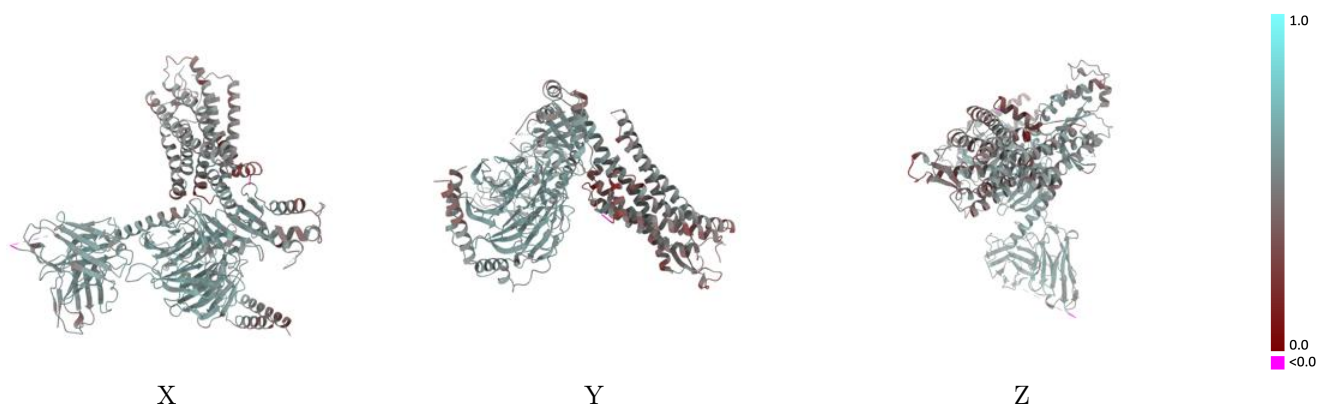
Y



Z

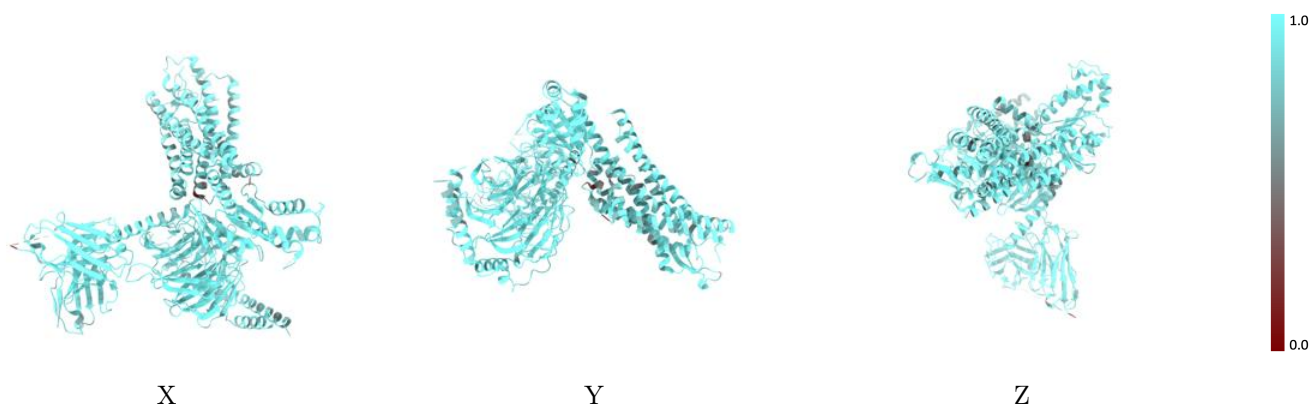
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



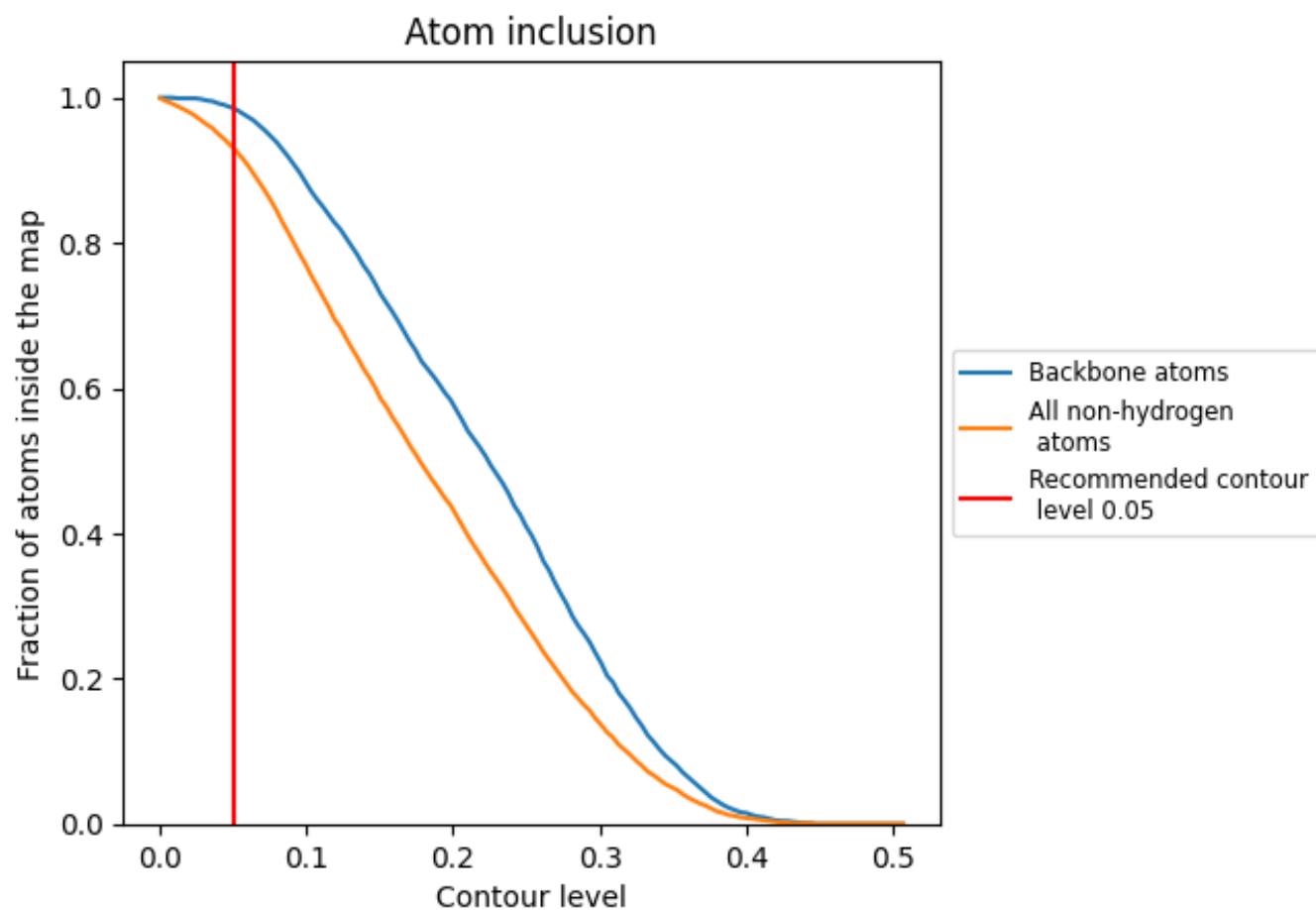
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9300	<div><div></div></div> 0.5140
A	<div><div></div></div> 0.9360	<div><div></div></div> 0.5230
B	<div><div></div></div> 0.9660	<div><div></div></div> 0.5690
C	<div><div></div></div> 0.9090	<div><div></div></div> 0.4970
D	<div><div></div></div> 0.9550	<div><div></div></div> 0.5490
L	<div><div></div></div> 0.9040	<div><div></div></div> 0.4990
R	<div><div></div></div> 0.8740	<div><div></div></div> 0.4290

1.0

0.0

<0.0