



Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 10:26 AM JST

PDB ID : 20ZC / pdb_000020zc
EMDB ID : EMD-67426
Title : Cryo-EM structure of human Neurotensin Receptor 1 (hNTSR1)-Gi1 (delipidated) complex in nucleotide-free C state
Authors : Kobayashi, K.; Matsui, T.E.; Fukuda, M.; Kawakami, K.; Yamashita, K.; Kato, H.E.
Deposited on : 2025-12-03
Resolution : 2.60 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

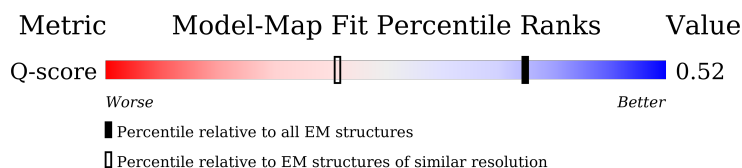
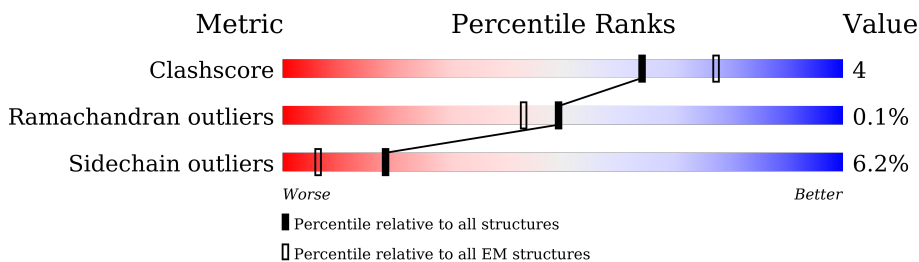
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	

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Mol	Chain	Length	Quality of chain
5	L	6	<div><div></div><div>83%</div><div>17%</div></div>
6	R	436	<div><div></div><div>60%</div><div>9%</div><div>30%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8932 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
			1747	1112	292	331	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	engineered mutation	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	B	338	Total	C	N	O	S	0	0
			2584	1595	462	506	21		

There are 19 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	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	53	Total	C	N	O	S	0	0
			404	256	70	75	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	68	SER	CYS	engineered mutation	UNP P59768

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	231	Total	C	N	O	S	0	0
			1762	1121	294	337	10		

- Molecule 5 is a protein called LYS-LYS-PRO-TYR-ILE-LEU.

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

- Molecule 6 is a protein called Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	306	Total	C	N	O	S	0	0
			2382	1562	395	410	15		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-11	MET	-	initiating methionine	UNP P30989
R	-10	GLY	-	expression tag	UNP P30989
R	-9	GLN	-	expression tag	UNP P30989

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-8	PRO	-	expression tag	UNP P30989
R	-7	GLY	-	expression tag	UNP P30989
R	-6	ASN	-	expression tag	UNP P30989
R	-5	GLY	-	expression tag	UNP P30989
R	-4	SER	-	expression tag	UNP P30989
R	-3	ALA	-	expression tag	UNP P30989
R	-2	PHE	-	expression tag	UNP P30989
R	-1	LEU	-	expression tag	UNP P30989
R	0	LEU	-	expression tag	UNP P30989
R	1	ALA	-	expression tag	UNP P30989
R	2	PRO	-	expression tag	UNP P30989
R	3	ASN	-	expression tag	UNP P30989
R	4	ARG	-	expression tag	UNP P30989
R	5	SER	-	expression tag	UNP P30989
R	6	HIS	-	expression tag	UNP P30989
R	7	ALA	-	expression tag	UNP P30989
R	8	PRO	-	expression tag	UNP P30989
R	9	ASP	-	expression tag	UNP P30989
R	10	HIS	-	expression tag	UNP P30989
R	11	ASP	-	expression tag	UNP P30989
R	12	VAL	-	expression tag	UNP P30989
R	13	GLU	-	expression tag	UNP P30989
R	14	ASN	-	expression tag	UNP P30989
R	15	LEU	-	expression tag	UNP P30989
R	16	TYR	-	expression tag	UNP P30989
R	17	PHE	-	expression tag	UNP P30989
R	18	GLN	-	expression tag	UNP P30989
R	19	GLY	-	expression tag	UNP P30989
R	85	LEU	ALA	engineered mutation	UNP P30989
R	419	LEU	-	expression tag	UNP P30989
R	420	GLU	-	expression tag	UNP P30989
R	421	VAL	-	expression tag	UNP P30989
R	422	LEU	-	expression tag	UNP P30989
R	423	PHE	-	expression tag	UNP P30989
R	424	GLN	-	expression tag	UNP P30989

- Molecule 5: LYS-LYS-PRO-TYR-ILE-LEU

- Molecule 6: Neurotensin receptor type 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	520529	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	0.494	Depositor
Minimum map value	-0.255	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	258.3, 258.3, 258.3	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86099994, 0.86099994, 0.86099994	Depositor

5 Model quality

5.1 Standard geometry

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	0.69	0/1776	1.48	14/2382 (0.6%)
2	B	0.98	2/2631 (0.1%)	1.63	25/3569 (0.7%)
3	C	0.63	0/410	1.32	1/554 (0.2%)
4	D	0.83	0/1806	1.33	10/2450 (0.4%)
5	L	0.67	0/54	1.02	0/69
6	R	0.70	1/2443 (0.0%)	1.40	14/3339 (0.4%)
All	All	0.81	3/9120 (0.0%)	1.47	64/12363 (0.5%)

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
2	B	0	3
6	R	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	174	PHE	CG-CD1	12.44	1.65	1.38
2	B	161	SER	CA-CB	-5.31	1.45	1.53
2	B	106	ALA	CA-CB	-5.03	1.45	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	151	PHE	CA-CB-CG	16.48	130.28	113.80
2	B	106	ALA	O-C-N	-16.46	102.39	121.32
2	B	106	ALA	CA-C-O	-16.12	98.07	120.16
6	R	174	PHE	CB-CG-CD2	11.50	140.24	120.70
2	B	48	ARG	CB-CA-C	11.27	128.52	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	179	ARG	CB-CA-C	9.04	128.42	110.42
2	B	52	ARG	N-CA-C	8.70	123.20	112.59
6	R	174	PHE	CD1-CG-CD2	-8.31	106.14	118.60
2	B	151	PHE	N-CA-CB	8.16	123.38	110.57
6	R	326	PHE	CA-CB-CG	8.09	121.89	113.80
1	A	51	LYS	N-CA-CB	7.96	121.82	110.12
4	D	68	PHE	CA-CB-CG	7.21	121.02	113.80
3	C	49	PRO	N-CA-C	6.67	122.31	113.57
6	R	95	GLN	N-CA-C	-6.53	104.48	113.56
1	A	14	GLU	CB-CG-CD	6.51	123.66	112.60
1	A	354	PHE	CA-CB-CG	-6.47	107.33	113.80
1	A	216	GLU	CB-CA-C	6.42	120.62	109.65
1	A	353	LEU	N-CA-CB	6.42	119.37	110.07
2	B	323	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	210	LYS	N-CA-CB	-6.37	100.02	110.40
2	B	76	ASP	CA-CB-CG	6.22	118.82	112.60
6	R	182	ARG	CA-CB-CG	-6.16	101.78	114.10
6	R	148	ARG	CA-CB-CG	6.15	126.40	114.10
6	R	174	PHE	CB-CG-CD1	-6.14	110.25	120.70
6	R	200	ALA	CA-C-N	6.14	124.11	120.24
6	R	200	ALA	C-N-CA	6.14	124.11	120.24
2	B	305	ALA	N-CA-C	6.02	117.92	111.36
1	A	201	VAL	N-CA-CB	-5.93	103.43	112.15
6	R	100	THR	N-CA-C	-5.92	104.82	111.28
4	D	178	TYR	CA-CB-CG	5.88	124.48	113.90
4	D	179	ARG	CA-C-O	-5.85	112.14	120.51
6	R	133	PRO	N-CA-CB	-5.84	97.12	103.25
4	D	73	ASP	CA-CB-CG	5.83	118.43	112.60
4	D	41	PRO	N-CA-C	5.72	121.49	113.53
1	A	324	THR	CA-CB-OG1	-5.72	101.02	109.60
6	R	205	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	354	PHE	CB-CA-C	5.68	120.90	110.10
1	A	259	PHE	CA-CB-CG	5.64	119.44	113.80
6	R	174	PHE	CG-CD2-CE2	5.63	130.27	120.70
2	B	54	HIS	CA-CB-CG	5.61	119.41	113.80
2	B	340	ASN	CA-CB-CG	5.60	118.20	112.60
2	B	278	PHE	CA-CB-CG	5.58	119.38	113.80
2	B	333	ASP	CA-CB-CG	5.51	118.11	112.60
2	B	225	HIS	CA-CB-CG	5.50	119.30	113.80
2	B	186	ASP	CA-CB-CG	5.49	118.09	112.60
2	B	298	ASP	CA-CB-CG	5.48	118.08	112.60
2	B	66	ASP	CA-CB-CG	5.47	118.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	LEU	N-CA-CB	-5.47	101.31	110.99
4	D	220	HIS	CA-CB-CG	5.46	119.26	113.80
2	B	83	ASP	CA-CB-CG	5.34	117.94	112.60
6	R	354	TYR	CB-CA-C	5.34	120.92	110.67
4	D	107	PRO	N-CA-C	5.33	119.41	111.41
4	D	179	ARG	N-CA-C	-5.27	99.57	110.80
2	B	119	ASN	CA-CB-CG	5.24	117.84	112.60
2	B	236	PRO	N-CA-C	5.23	121.55	113.75
1	A	200	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	223	PHE	CA-CB-CG	5.12	118.92	113.80
4	D	161	TYR	N-CA-CB	-5.10	103.00	110.49
1	A	193	ASP	CA-CB-CG	5.09	117.69	112.60
2	B	46	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	B	154	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	51	LYS	CB-CA-C	-5.01	102.47	110.79
2	B	227	SER	CA-C-N	5.01	127.97	120.90
2	B	227	SER	C-N-CA	5.01	127.97	120.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	ALA	Mainchain
2	B	107	PRO	Peptide
2	B	48	ARG	Peptide
6	R	90	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1747	0	1731	20	0
2	B	2584	0	2475	23	0
3	C	404	0	416	5	0
4	D	1762	0	1696	9	0
5	L	53	0	63	0	0
6	R	2382	0	2382	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8932	0	8763	71	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 4.

All (71) 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:46:ARG:HB2	2:B:48:ARG:HE	1.42	0.83
4:D:147:CYS:HG	4:D:217:CYS:HG	0.85	0.81
1:A:348:LEU:HB2	1:A:354:PHE:HA	1.71	0.72
1:A:348:LEU:HD12	1:A:349:LYS:N	2.05	0.71
2:B:105:TYR:O	2:B:106:ALA:O	2.09	0.71
2:B:110:ASN:HA	2:B:127:LYS:HE3	1.73	0.70
1:A:348:LEU:HB2	1:A:354:PHE:CA	2.22	0.69
1:A:53:MET:HE3	1:A:198:MET:HE1	1.76	0.68
1:A:353:LEU:HD21	6:R:166:ARG:NE	2.09	0.67
1:A:348:LEU:HB2	1:A:354:PHE:C	2.20	0.67
1:A:39:LEU:HD13	1:A:253:ILE:HD13	1.76	0.66
6:R:93:SER:HB3	6:R:99:SER:HB2	1.78	0.65
2:B:142:HIS:CD2	2:B:161:SER:HB2	2.32	0.64
6:R:177:LYS:HD3	6:R:180:MET:SD	2.38	0.63
6:R:176:ALA:O	6:R:180:MET:HG3	1.98	0.63
4:D:162:LEU:O	4:D:179:ARG:O	2.18	0.60
1:A:340:THR:HG23	6:R:174:PHE:CE2	2.38	0.59
2:B:338:ILE:HG22	3:C:61:PHE:CZ	2.39	0.58
4:D:130:GLN:HG3	4:D:230:GLY:H	1.69	0.58
1:A:340:THR:HG23	6:R:174:PHE:HE2	1.70	0.56
1:A:353:LEU:CD2	6:R:166:ARG:NE	2.69	0.56
2:B:331:SER:OG	2:B:332:TRP:N	2.37	0.55
1:A:322:HIS:NE2	1:A:325:CYS:SG	2.80	0.55
6:R:115:THR:HG22	6:R:151:CYS:HB3	1.88	0.55
4:D:91:THR:HG23	4:D:118:THR:HA	1.89	0.54
6:R:98:GLN:HG2	6:R:102:HIS:CE1	2.42	0.53
2:B:79:LEU:HD11	2:B:93:ILE:HD12	1.91	0.53
1:A:345:LYS:O	1:A:348:LEU:HG	2.09	0.52
2:B:290:ASP:HA	2:B:314:ARG:HG3	1.93	0.51
6:R:96:SER:O	6:R:97:LEU:HB3	2.10	0.50
2:B:121:CYS:SG	2:B:149:CYS:SG	3.03	0.50
6:R:70:TYR:HE1	6:R:351:ALA:HA	1.77	0.49
6:R:101:VAL:O	6:R:102:HIS:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD13	1:A:354:PHE:CD2	2.47	0.49
2:B:333:ASP:O	2:B:334:SER:OG	2.27	0.49
6:R:112:ASP:O	6:R:115:THR:OG1	2.26	0.48
1:A:353:LEU:O	1:A:354:PHE:HB2	2.13	0.48
6:R:97:LEU:O	6:R:97:LEU:HG	2.14	0.47
2:B:47:THR:O	2:B:47:THR:OG1	2.30	0.47
2:B:90:VAL:HG23	2:B:91:HIS:CD2	2.50	0.46
2:B:180:PHE:HE1	2:B:216:GLY:HA2	1.80	0.46
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.49	0.46
1:A:343:ILE:HD12	6:R:174:PHE:HE1	1.81	0.46
6:R:74:PHE:HA	6:R:116:LEU:HD21	1.97	0.45
1:A:322:HIS:HE2	1:A:325:CYS:HG	1.57	0.45
4:D:83:MET:HE1	4:D:117:LEU:HD13	1.99	0.44
2:B:58:ILE:HD11	2:B:330:GLY:HA3	1.98	0.44
6:R:71:LEU:HD13	6:R:71:LEU:HA	1.81	0.44
2:B:340:ASN:HB2	3:C:61:PHE:CD2	2.53	0.44
2:B:185:GLY:N	2:B:205:ASP:OD1	2.50	0.44
2:B:250:CYS:HB2	2:B:264:TYR:HB2	2.00	0.44
2:B:284:LEU:HD11	3:C:50:LEU:HD22	1.99	0.43
4:D:40:ALA:HB3	4:D:43:LYS:HB2	1.98	0.43
6:R:120:MET:HE3	6:R:124:LEU:HD11	2.01	0.43
2:B:51:LEU:HB2	2:B:336:LEU:HB2	2.01	0.43
4:D:137:VAL:HG11	4:D:207:LEU:HG	2.01	0.42
6:R:101:VAL:HG13	6:R:165:GLU:OE2	2.20	0.42
6:R:362:ILE:HA	6:R:366:LEU:HB3	2.01	0.42
1:A:18:MET:HG3	1:A:21:ARG:NH2	2.34	0.42
6:R:70:TYR:HB3	6:R:120:MET:HE1	2.02	0.42
1:A:38:LEU:HB3	1:A:46:LYS:HD2	2.02	0.42
4:D:178:TYR:O	4:D:179:ARG:C	2.61	0.42
4:D:180:MET:HB3	4:D:180:MET:HE2	1.73	0.42
2:B:105:TYR:C	2:B:106:ALA:O	2.60	0.41
1:A:353:LEU:CD2	6:R:166:ARG:CZ	2.97	0.41
2:B:45:MET:SD	3:C:50:LEU:HD21	2.61	0.41
2:B:162:GLY:HA2	2:B:186:ASP:HB2	2.03	0.41
6:R:123:GLU:HA	6:R:127:PHE:HD2	1.86	0.41
3:C:60:PRO:HG2	3:C:61:PHE:CE2	2.56	0.40
6:R:116:LEU:O	6:R:120:MET:HB3	2.21	0.40
2:B:45:MET:HE3	2:B:308:LEU:HD11	2.02	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%)	211 (100%)	1 (0%)	0	100	100
2	B	336/358 (94%)	328 (98%)	8 (2%)	0	100	100
3	C	51/71 (72%)	51 (100%)	0	0	100	100
4	D	227/259 (88%)	224 (99%)	3 (1%)	0	100	100
5	L	4/6 (67%)	4 (100%)	0	0	100	100
6	R	302/436 (69%)	295 (98%)	6 (2%)	1 (0%)	36	58
All	All	1132/1484 (76%)	1113 (98%)	18 (2%)	1 (0%)	49	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	133	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	A	191/305 (63%)	168 (88%)	23 (12%)	5	10
2	B	277/298 (93%)	262 (95%)	15 (5%)	20	42
3	C	42/58 (72%)	41 (98%)	1 (2%)	43	70
4	D	191/209 (91%)	183 (96%)	8 (4%)	26	52
5	L	6/6 (100%)	5 (83%)	1 (17%)	2	4
6	R	254/368 (69%)	242 (95%)	12 (5%)	23	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	961/1244 (77%)	901 (94%)	60 (6%)	18	36

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	10	LYS
1	A	18	MET
1	A	23	LEU
1	A	25	GLU
1	A	28	GLU
1	A	29	LYS
1	A	46	LYS
1	A	51	LYS
1	A	54	LYS
1	A	204	GLN
1	A	205	ARG
1	A	216	GLU
1	A	266	LEU
1	A	267	PHE
1	A	279	LYS
1	A	310	LEU
1	A	327	THR
1	A	335	VAL
1	A	341	ASP
1	A	343	ILE
1	A	348	LEU
1	A	353	LEU
2	B	15	LYS
2	B	48	ARG
2	B	58	ILE
2	B	90	VAL
2	B	108	SER
2	B	127	LYS
2	B	142	HIS
2	B	151	PHE
2	B	169	TRP
2	B	195	ASP
2	B	252	LEU
2	B	280	LYS
2	B	286	LEU
2	B	290	ASP

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Mol	Chain	Res	Type
2	B	308	LEU
3	C	50	LEU
4	D	51	ILE
4	D	117	LEU
4	D	160	THR
4	D	177	ILE
4	D	183	LEU
4	D	185	SER
4	D	194	SER
4	D	206	ARG
5	L	13	LEU
6	R	83	VAL
6	R	97	LEU
6	R	99	SER
6	R	130	VAL
6	R	132	HIS
6	R	164	VAL
6	R	165	GLU
6	R	179	LEU
6	R	304	VAL
6	R	325	MET
6	R	326	PHE
6	R	356	SER

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	195	HIS
2	B	17	GLN
2	B	75	GLN
2	B	88	ASN
2	B	91	HIS
2	B	119	ASN
2	B	156	GLN
2	B	220	GLN
2	B	259	GLN
2	B	340	ASN
4	D	39	GLN
4	D	167	GLN
6	R	81	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

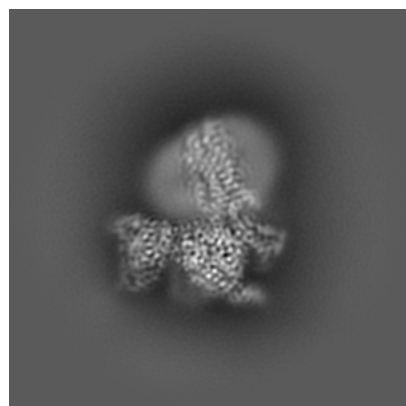
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67426. These allow visual inspection of the internal detail of the map and identification of artifacts.

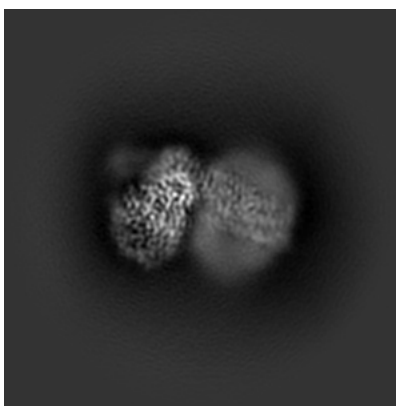
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

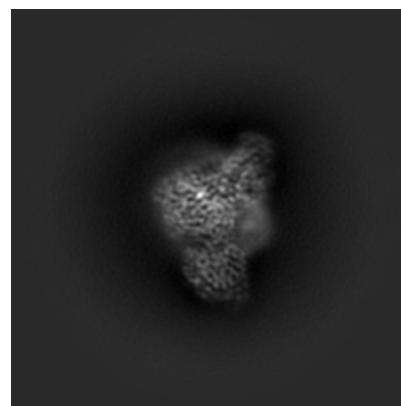
6.1.1 Primary map



X

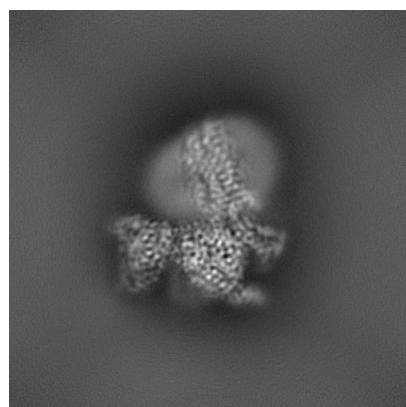


Y

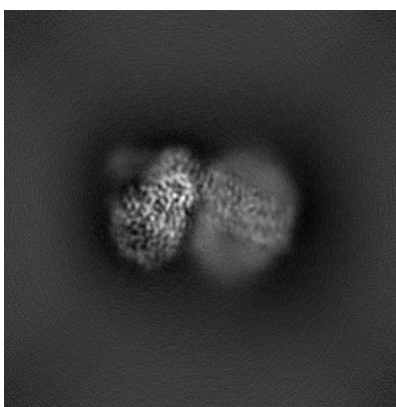


Z

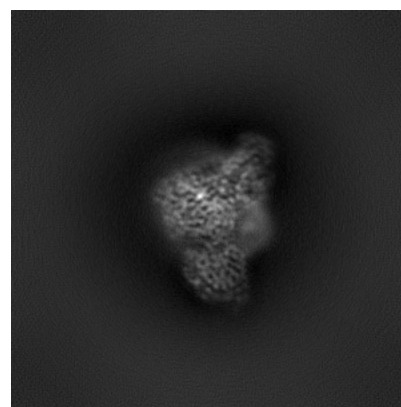
6.1.2 Raw map



X



Y

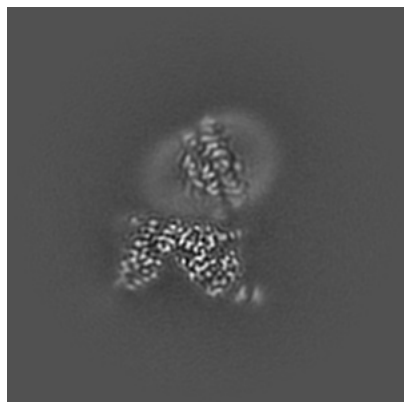


Z

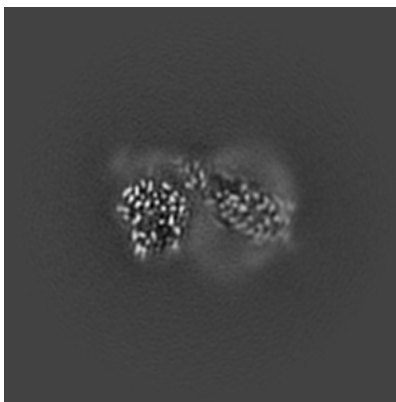
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

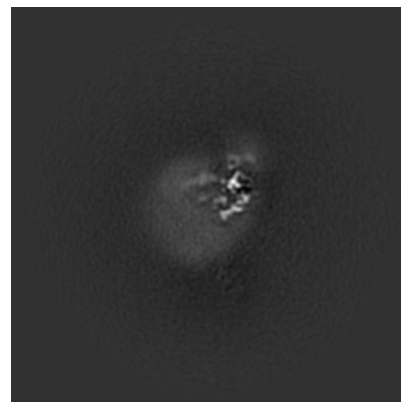
6.2.1 Primary map



X Index: 150

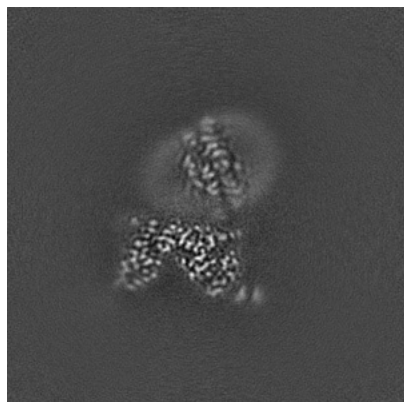


Y Index: 150

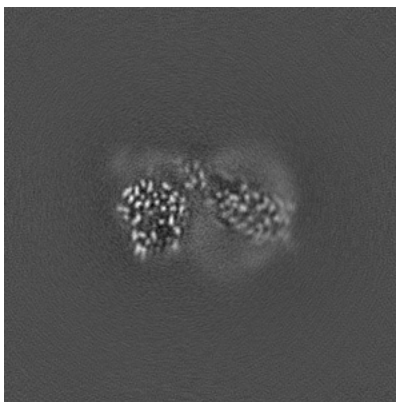


Z Index: 150

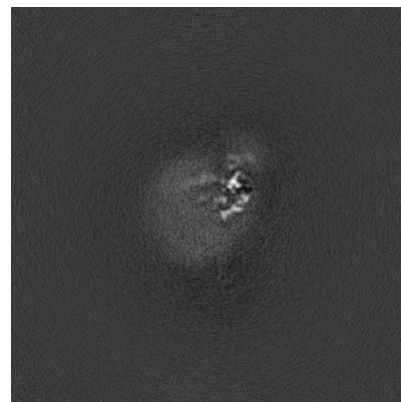
6.2.2 Raw map



X Index: 150



Y Index: 150

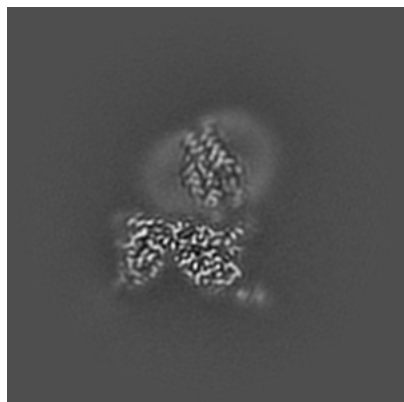


Z Index: 150

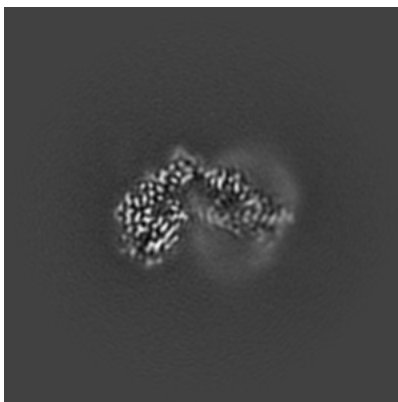
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

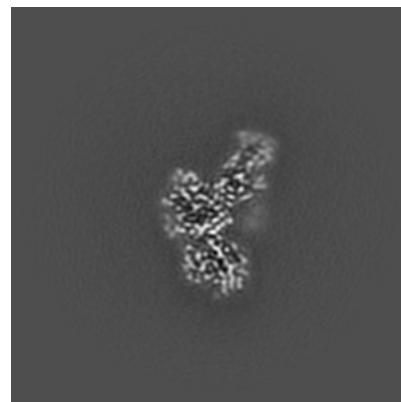
6.3.1 Primary map



X Index: 153

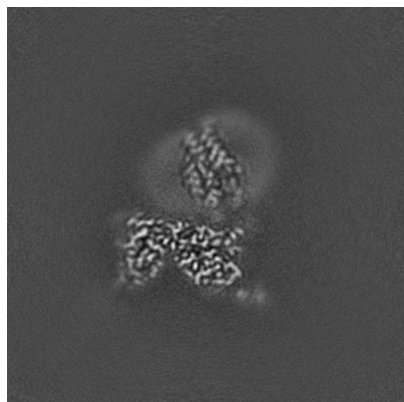


Y Index: 159

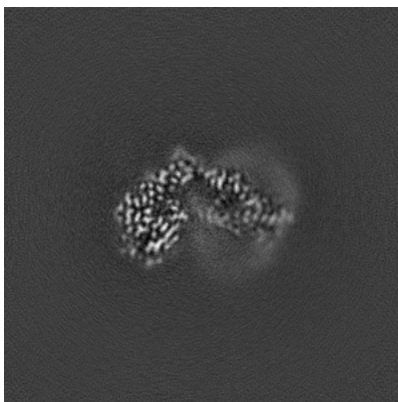


Z Index: 124

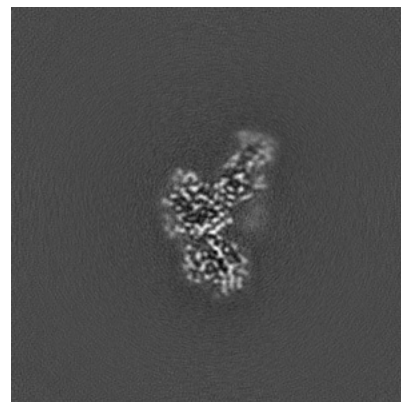
6.3.2 Raw map



X Index: 153



Y Index: 159

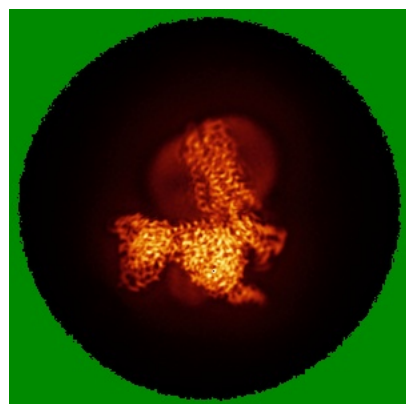


Z Index: 124

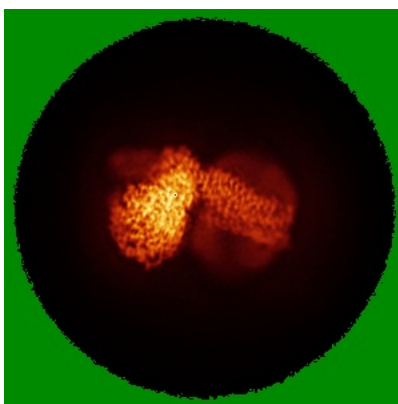
The images above show the largest variance slices of the map in three orthogonal directions.

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

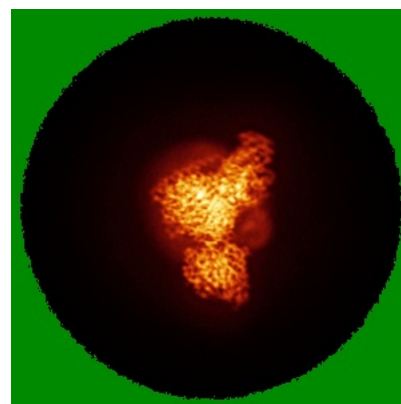
6.4.1 Primary map



X

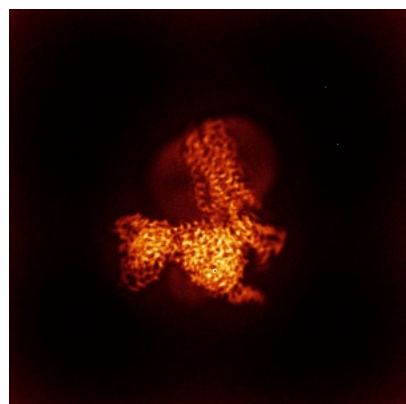


Y

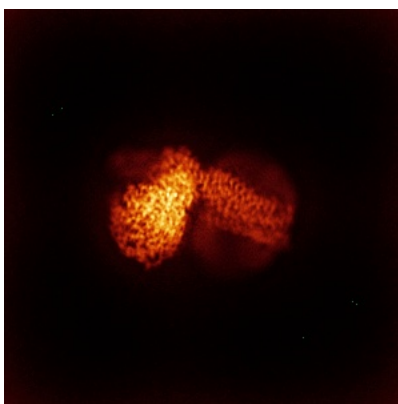


Z

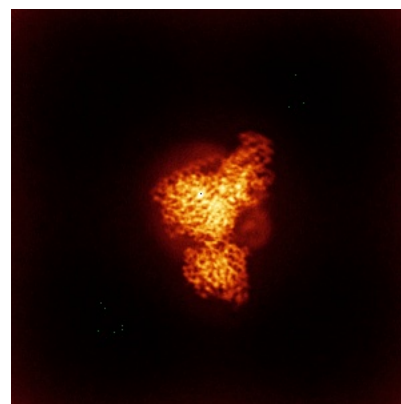
6.4.2 Raw map



X



Y

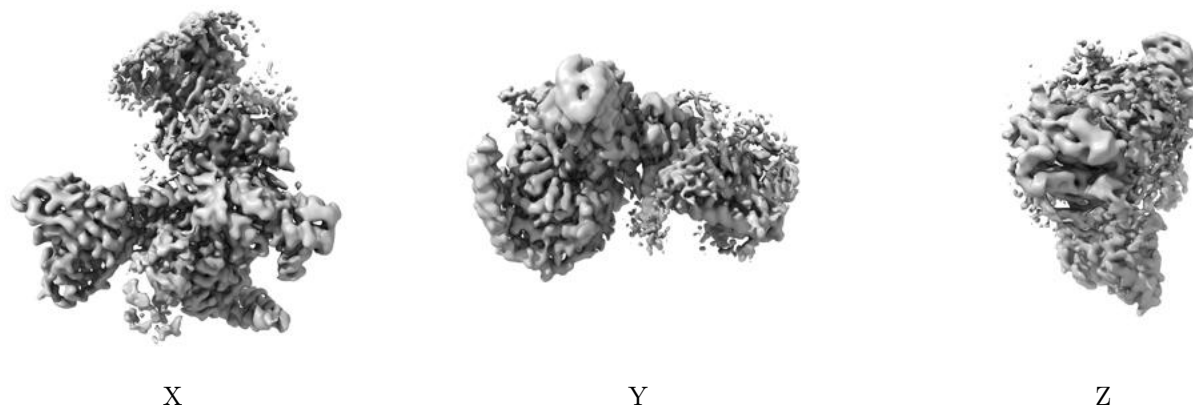


Z

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.

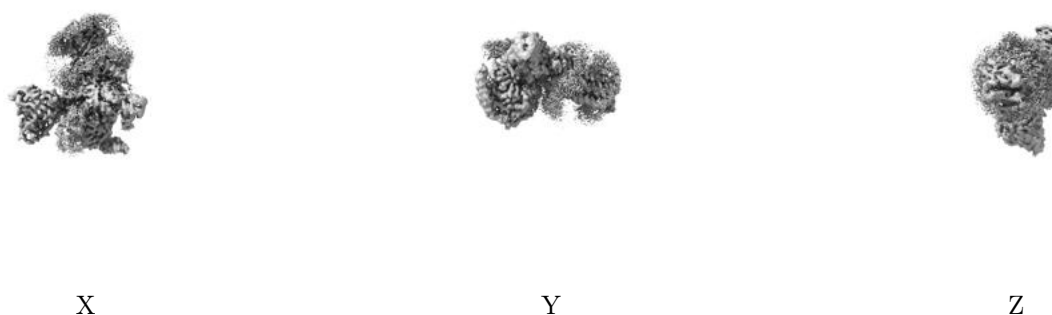
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

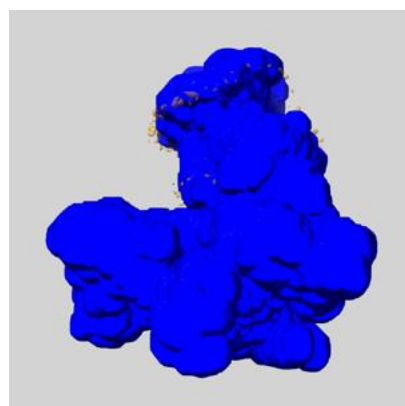
6.6 Mask visualisation [i](#)

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

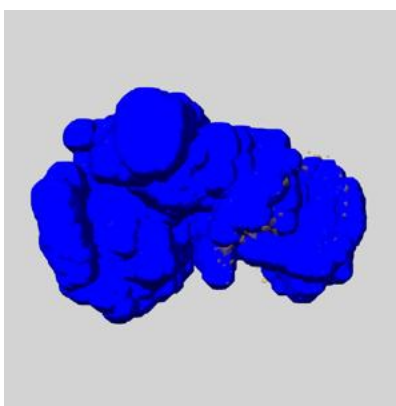
A mask typically either:

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

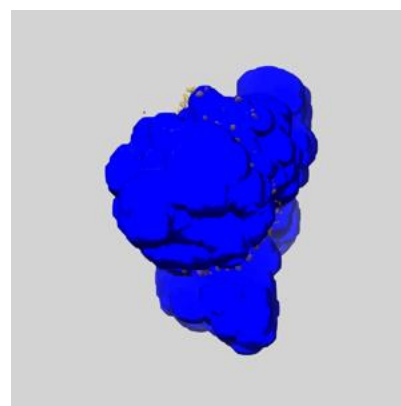
6.6.1 emd_67426_msk_1.map [i](#)



X



Y

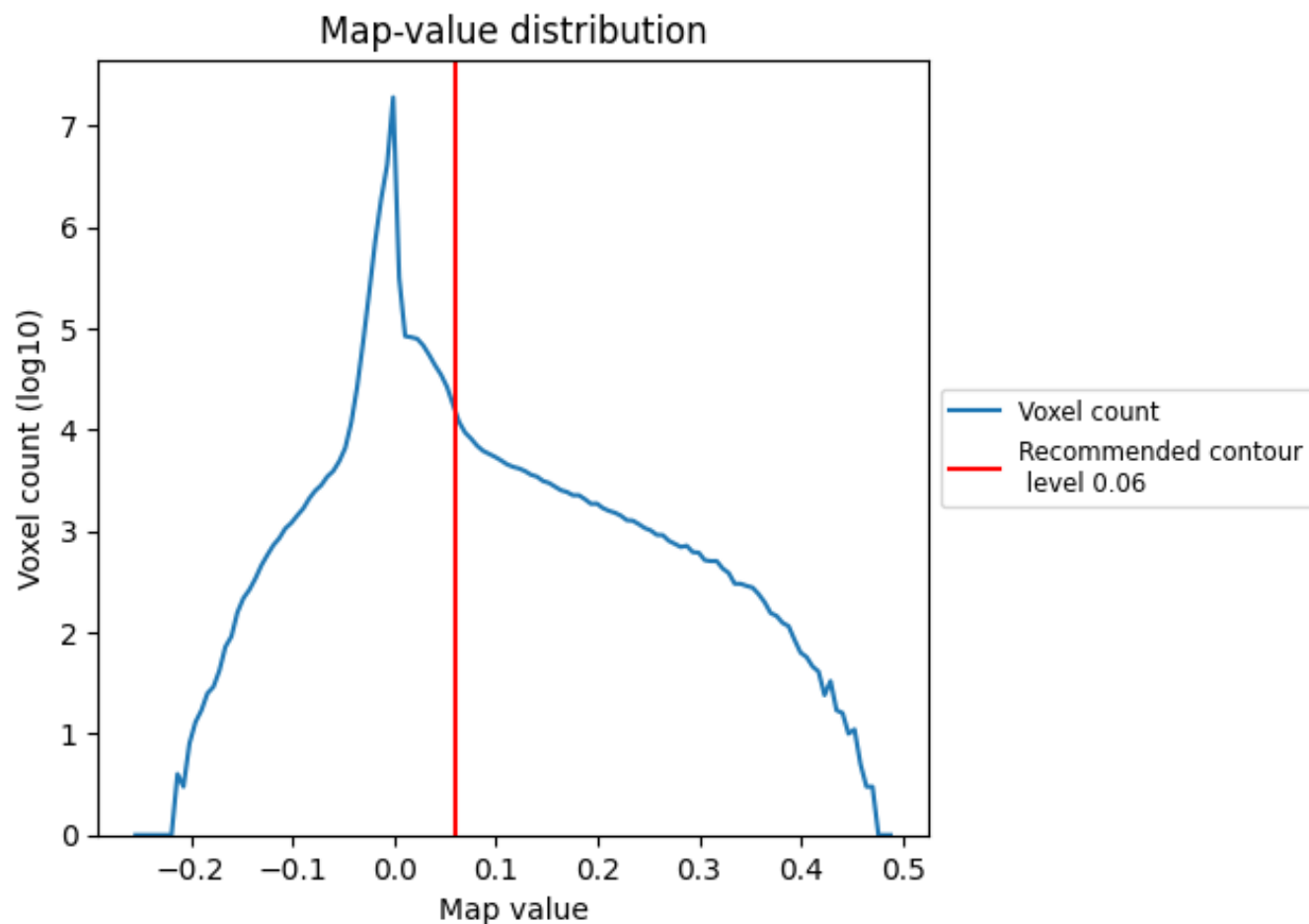


Z

7 Map analysis [i](#)

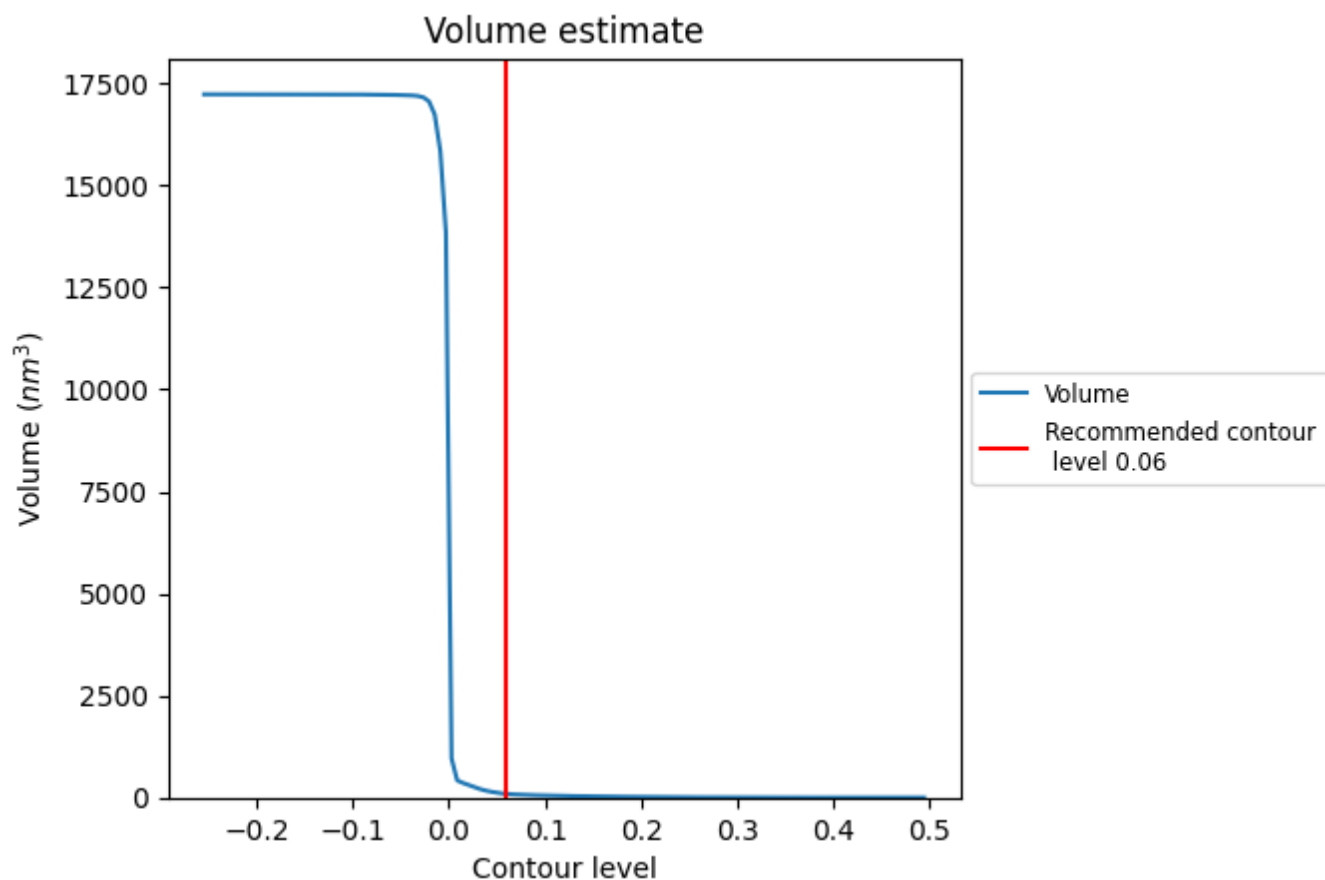
This section contains the results of statistical analysis of the map.

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.

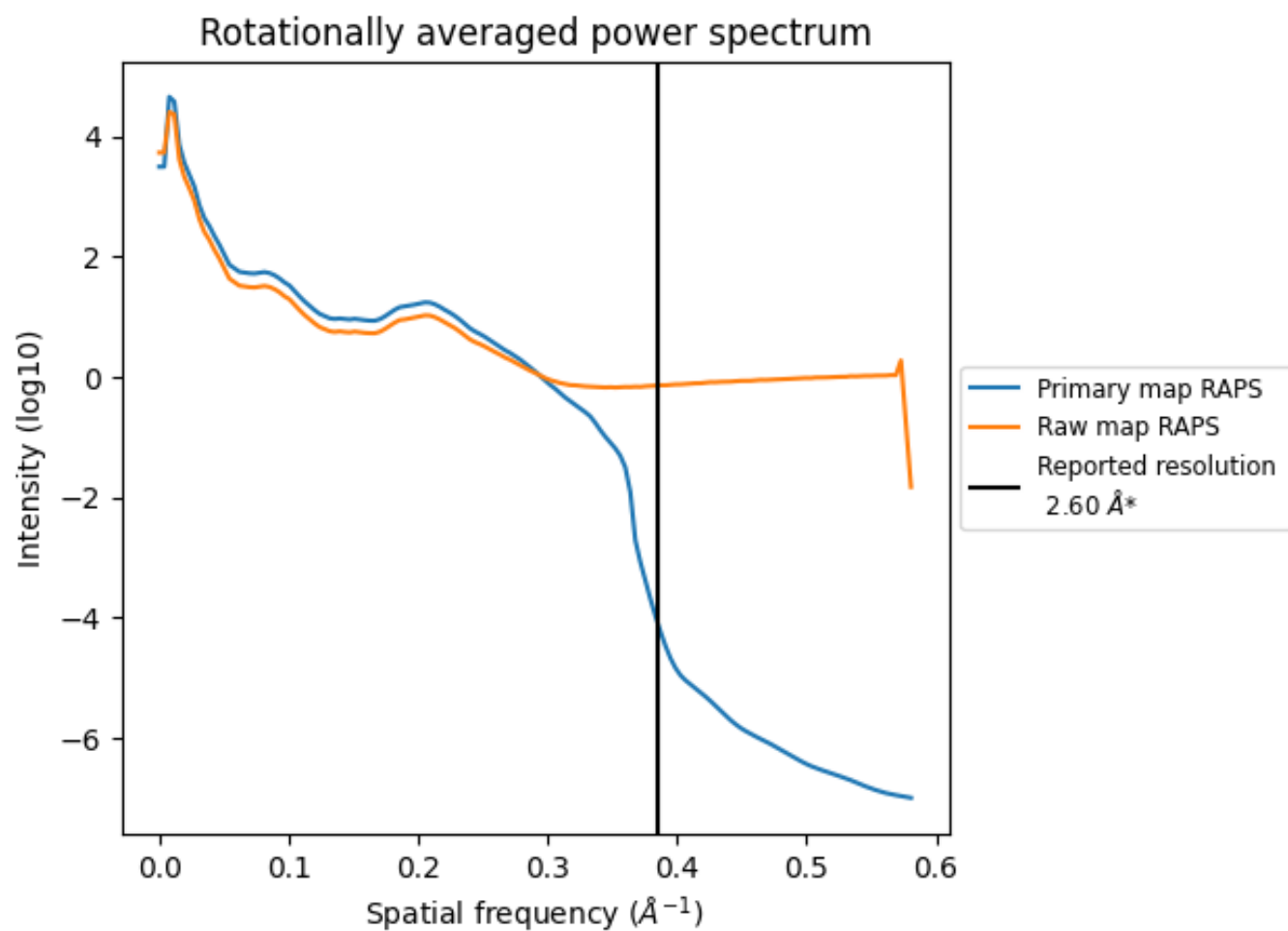
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 81 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 ⓘ

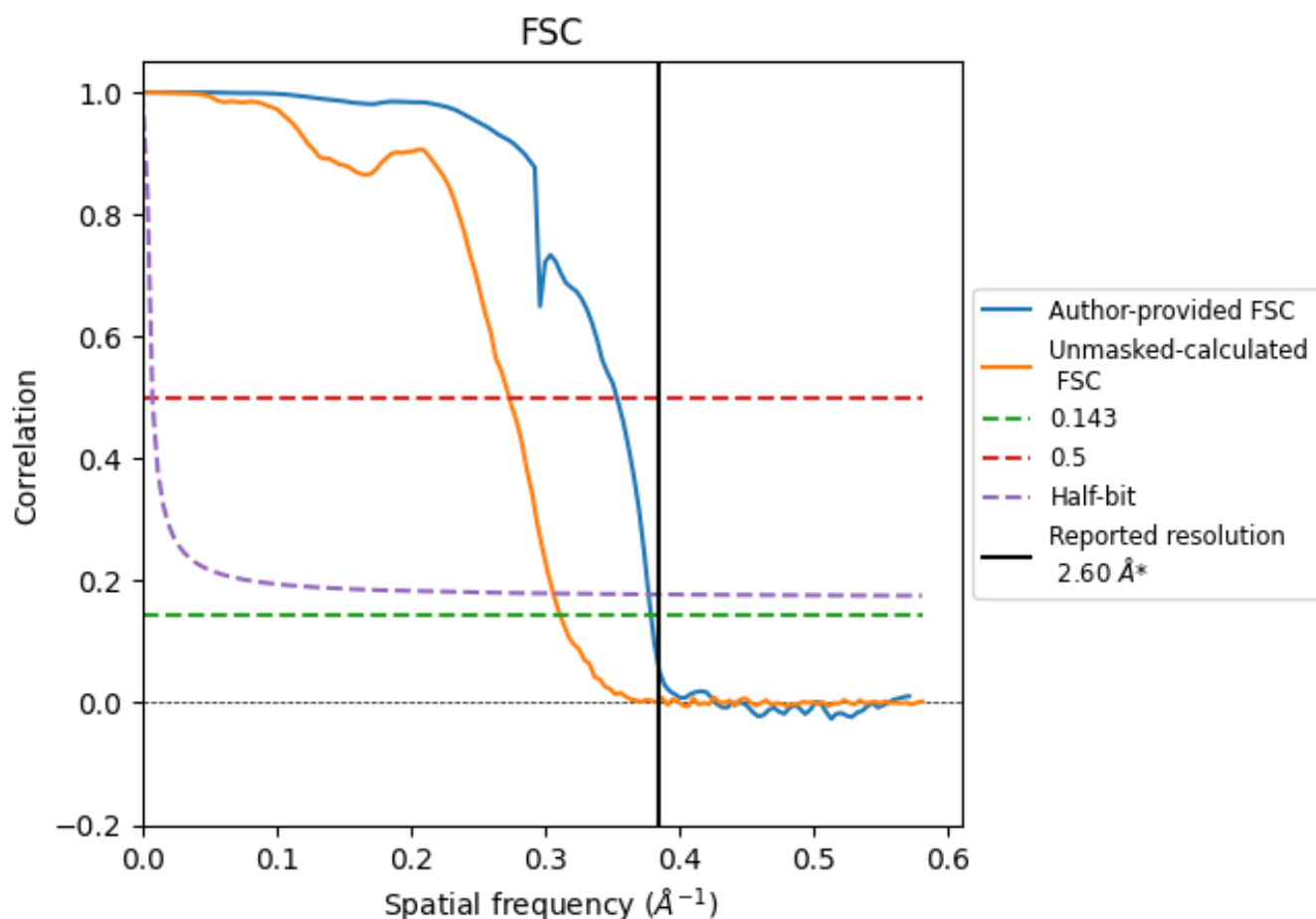


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

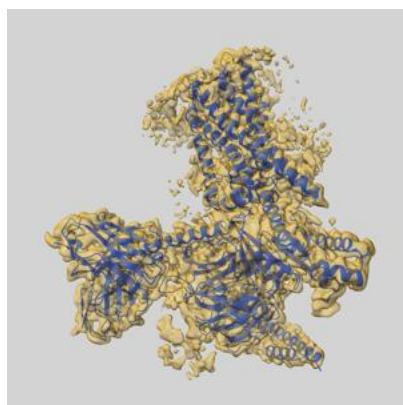
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.64	2.83	2.65
Unmasked-calculated*	3.21	3.66	3.27

*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 3.21 differs from the reported value 2.6 by more than 10 %

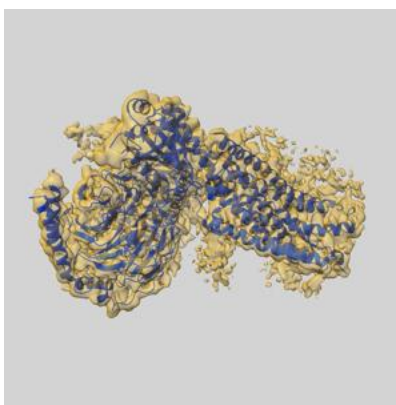
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67426 and PDB model 20ZC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

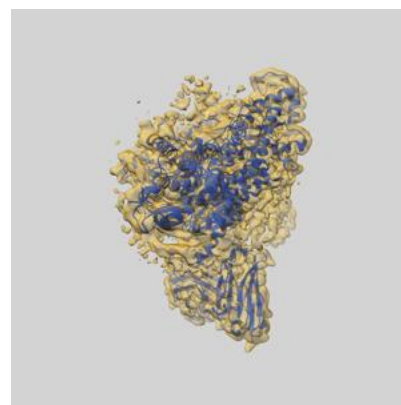
9.1 Map-model overlay [i](#)



X



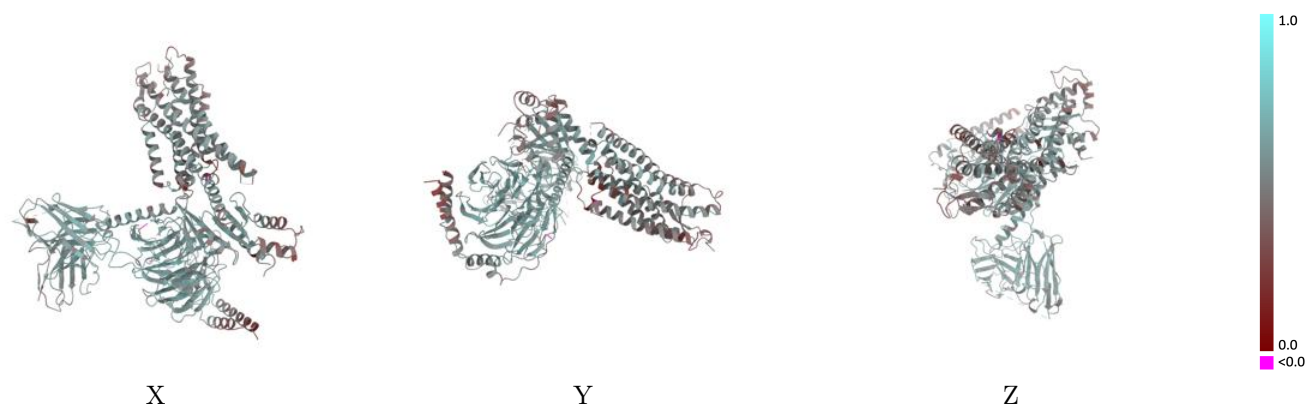
Y



Z

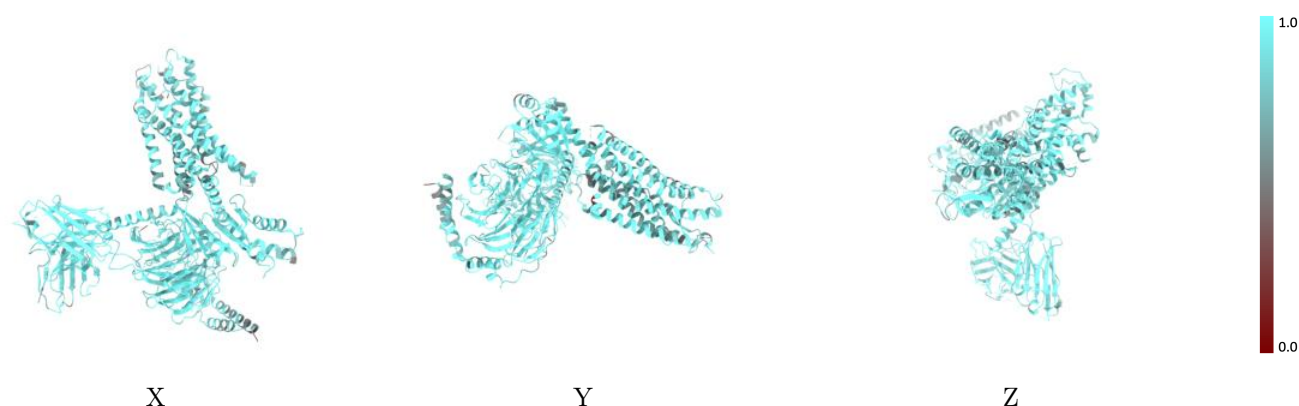
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



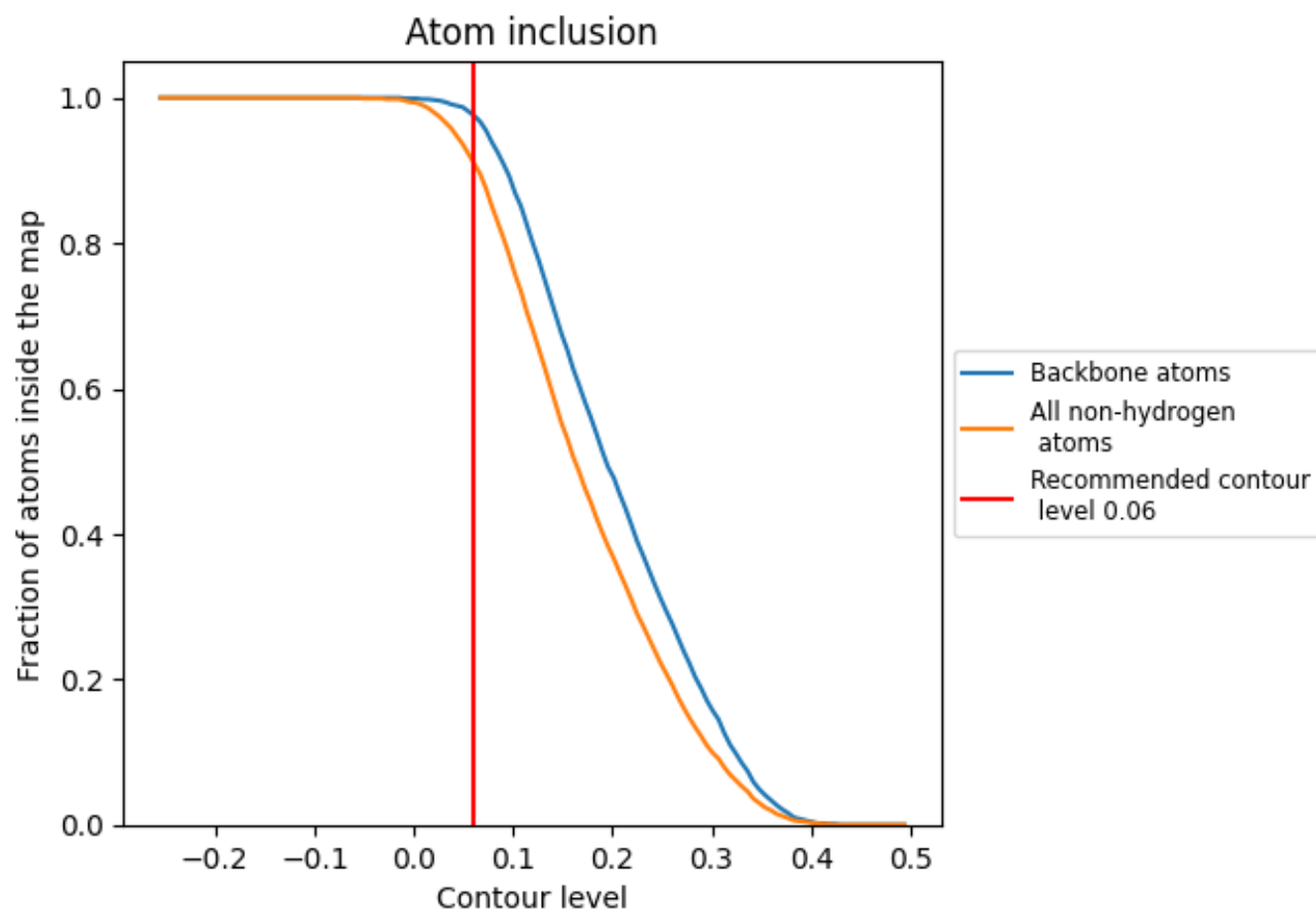
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9120	<div><div></div></div> 0.5200
A	<div><div></div></div> 0.9120	<div><div></div></div> 0.5110
B	<div><div></div></div> 0.9430	<div><div></div></div> 0.5670
C	<div><div></div></div> 0.8350	<div><div></div></div> 0.4540
D	<div><div></div></div> 0.9440	<div><div></div></div> 0.5610
L	<div><div></div></div> 0.8460	<div><div></div></div> 0.4830
R	<div><div></div></div> 0.8690	<div><div></div></div> 0.4580

1.0

0.0

<0.0