



Full wwPDB EM Validation Report ⓘ

Oct 8, 2026 – 02:40 PM EDT

PDB ID : 9PCR / pdb_00009pcr
EMDB ID : EMD-71517
Title : Tail of Mediator of PIC-Med-SWI/SNF
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-29
Resolution : 3.70 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.dev133
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

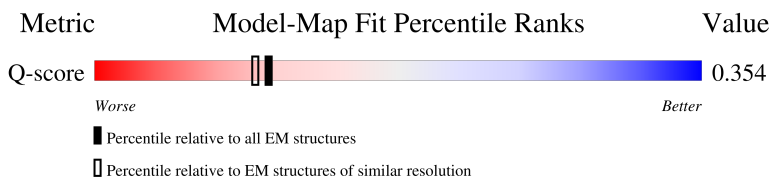
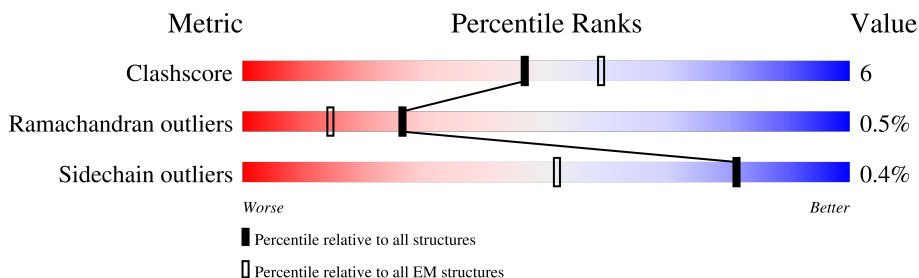
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1	431	
2	2	397	
3	3	1132	
4	4	1082	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	5	1081	7%90%
6	6	974	7%82%13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17805 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 Mediator of RNA polymerase II transcription subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	65	Total	C	N	O	S	0	0
			516	328	82	102	4		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	110	Total	C	N	O	S	0	0
			891	560	155	172	4		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	761	Total	C	N	O	S	0	0
			6173	3979	999	1181	14		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	220	Total	C	N	O	S	0	0
			1780	1136	302	333	9		

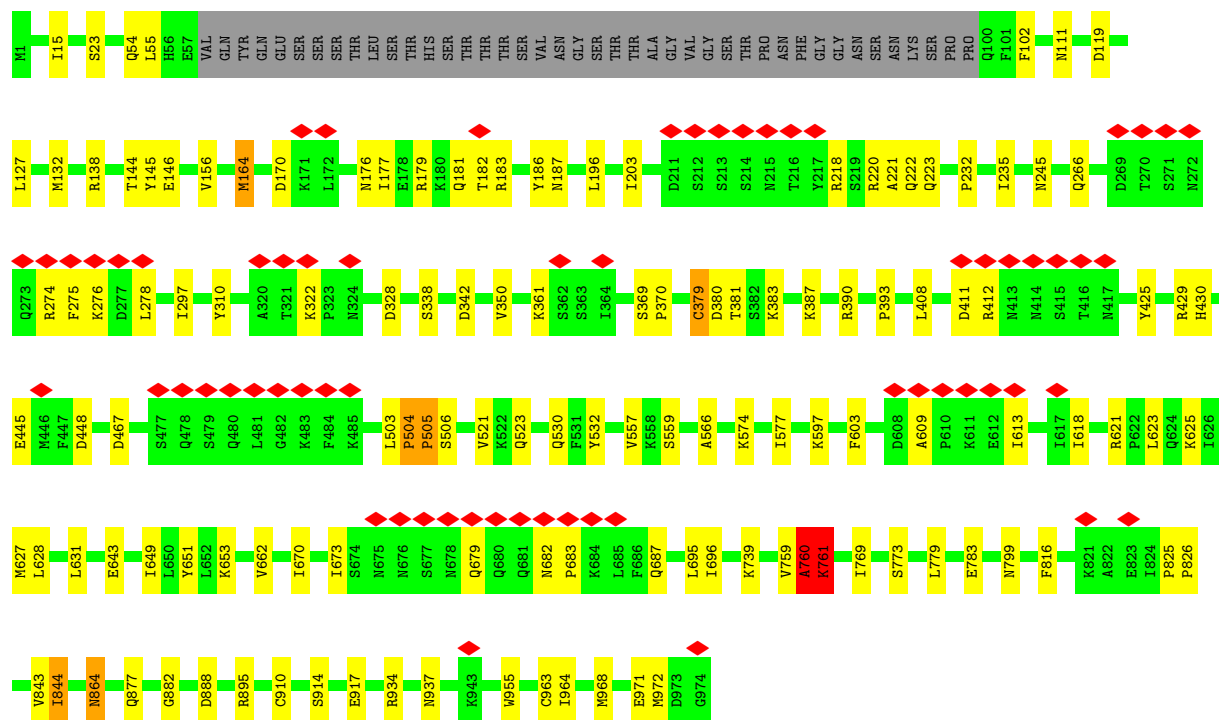
- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	111	Total	C	N	O	S	0	0
			894	558	161	169	6		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	932	Total	C	N	O	S	0	0
			7551	4859	1258	1399	35		

Chain 5: 7% 7% 7% 90%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	678521	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 ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.894	Depositor
Minimum map value	-3.021	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.512	Depositor
Map size ($\text{\AA}$)	448.0, 448.0, 448.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	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	1	0.68	2/520 (0.4%)	0.79	0/693
2	2	0.85	2/902 (0.2%)	1.06	6/1215 (0.5%)
3	3	0.64	17/6293 (0.3%)	0.97	38/8534 (0.4%)
4	4	0.56	5/1817 (0.3%)	0.86	9/2456 (0.4%)
5	5	1.28	16/904 (1.8%)	2.16	31/1202 (2.6%)
6	6	0.46	9/7725 (0.1%)	0.71	9/10461 (0.1%)
All	All	0.63	51/18161 (0.3%)	0.95	93/24561 (0.4%)

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	2	0	1
3	3	1	6
4	4	0	1
5	5	1	2
6	6	0	1
All	All	2	11

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	837	TYR	CG-CD2	19.67	1.80	1.39
5	5	920	LYS	CB-CG	-16.16	1.03	1.52
3	3	289	LYS	CG-CD	-12.14	1.16	1.52
3	3	289	LYS	CB-CG	11.98	1.88	1.52
2	2	34	ASN	CG-OD1	-11.62	1.01	1.23
4	4	1018	MET	CB-CG	-9.04	1.25	1.52
3	3	836	ILE	C-N	8.97	1.46	1.33
3	3	289	LYS	CA-CB	8.88	1.67	1.53
6	6	864	ASN	CG-ND2	-8.64	1.15	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	288	MET	C-N	8.56	1.45	1.33
5	5	943	LEU	CG-CD1	-8.25	1.25	1.52
5	5	919	ARG	NE-CZ	-8.23	1.24	1.33
6	6	132	MET	SD-CE	-8.21	1.59	1.79
3	3	289	LYS	CA-C	-7.63	1.43	1.52
5	5	920	LYS	CA-C	-7.57	1.42	1.52
3	3	290	LEU	N-CA	-7.40	1.37	1.46
5	5	923	LYS	CE-NZ	-7.33	1.27	1.49
4	4	1019	MET	CB-CG	-7.17	1.30	1.52
5	5	920	LYS	CE-NZ	-7.08	1.28	1.49
6	6	972	MET	SD-CE	-6.96	1.62	1.79
2	2	80	GLN	CD-OE1	-6.87	1.10	1.23
1	1	40	LEU	CG-CD1	-6.83	1.30	1.52
3	3	838	SER	CA-C	6.80	1.61	1.52
3	3	919	TYR	CD2-CE2	-6.79	1.18	1.38
6	6	971	GLU	CD-OE1	-6.63	1.12	1.25
3	3	837	TYR	CB-CG	-6.16	1.38	1.51
3	3	837	TYR	N-CA	6.05	1.54	1.46
5	5	923	LYS	CG-CD	-6.03	1.34	1.52
3	3	406	LYS	CA-C	6.02	1.60	1.52
3	3	920	LEU	CG-CD1	-6.00	1.32	1.52
5	5	877	LYS	CD-CE	-5.96	1.34	1.52
4	4	1016	TYR	C-N	5.86	1.41	1.33
1	1	70	GLN	CD-OE1	-5.81	1.12	1.23
5	5	872	ARG	CZ-NH2	-5.78	1.25	1.33
5	5	877	LYS	CA-C	-5.77	1.45	1.52
6	6	955	TRP	C-N	5.77	1.40	1.34
3	3	289	LYS	C-N	-5.70	1.26	1.33
5	5	931	GLN	CB-CG	-5.70	1.35	1.52
6	6	532	TYR	CD1-CE1	-5.66	1.21	1.38
4	4	1000	HIS	C-O	-5.66	1.15	1.23
5	5	877	LYS	CE-NZ	-5.60	1.32	1.49
3	3	633	LEU	CG-CD1	-5.57	1.34	1.52
6	6	761	LYS	CD-CE	-5.53	1.35	1.52
5	5	923	LYS	CB-CG	-5.51	1.35	1.52
5	5	931	GLN	CG-CD	-5.48	1.38	1.52
6	6	54	GLN	CD-NE2	-5.46	1.21	1.33
6	6	164	MET	SD-CE	-5.45	1.66	1.79
4	4	1018	MET	CG-SD	-5.35	1.67	1.80
5	5	931	GLN	CD-NE2	5.30	1.44	1.33
3	3	917	LEU	CG-CD2	-5.29	1.35	1.52
5	5	877	LYS	CG-CD	-5.02	1.37	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	920	LYS	CB-CG-CD	29.85	179.95	111.30
3	3	837	TYR	CB-CG-CD2	-22.98	86.32	120.80
5	5	919	ARG	CD-NE-CZ	21.03	153.85	124.40
5	5	923	LYS	CB-CG-CD	20.42	158.27	111.30
5	5	923	LYS	CG-CD-CE	-18.81	68.03	111.30
4	4	1018	MET	N-CA-CB	17.15	134.95	109.91
5	5	920	LYS	CA-CB-CG	16.43	146.96	114.10
3	3	837	TYR	CD1-CG-CD2	-15.06	95.51	118.10
5	5	877	LYS	CG-CD-CE	14.17	143.89	111.30
5	5	919	ARG	CA-CB-CG	13.27	140.64	114.10
3	3	837	TYR	CG-CD1-CE1	12.82	140.43	121.20
5	5	931	GLN	CB-CG-CD	12.73	134.25	112.60
5	5	920	LYS	CG-CD-CE	-12.51	82.54	111.30
5	5	931	GLN	CG-CD-NE2	-12.49	97.67	116.40
3	3	837	TYR	N-CA-CB	-12.22	91.91	111.22
3	3	837	TYR	CB-CG-CD1	12.08	138.92	120.80
5	5	920	LYS	CB-CA-C	11.53	125.61	109.92
3	3	406	LYS	CA-C-N	11.20	138.99	120.62
3	3	406	LYS	C-N-CA	11.20	138.99	120.62
4	4	1018	MET	CB-CA-C	-10.92	94.14	110.96
5	5	919	ARG	CG-CD-NE	-10.79	88.27	112.00
4	4	1018	MET	CB-CG-SD	10.76	144.98	112.70
6	6	760	ALA	CA-C-N	10.71	141.99	121.54
6	6	760	ALA	C-N-CA	10.71	141.99	121.54
3	3	836	ILE	N-CA-CB	9.66	131.02	110.64
3	3	837	TYR	CA-CB-CG	9.58	131.15	113.90
3	3	409	LYS	N-CA-CB	9.35	126.29	110.49
5	5	920	LYS	CD-CE-NZ	9.01	140.73	111.90
3	3	292	ARG	CD-NE-CZ	8.77	136.67	124.40
3	3	289	LYS	N-CA-CB	8.71	122.88	110.07
6	6	761	LYS	CB-CG-CD	8.56	130.98	111.30
5	5	931	GLN	OE1-CD-NE2	-8.39	114.21	122.60
2	2	107	LYS	O-C-N	-8.35	110.94	122.46
5	5	931	GLN	CG-CD-OE1	8.31	137.43	120.80
4	4	1018	MET	CG-SD-CE	-8.15	82.97	100.90
5	5	919	ARG	CB-CG-CD	7.77	129.17	111.30
5	5	919	ARG	CA-C-N	7.68	136.13	122.08
5	5	919	ARG	C-N-CA	7.68	136.13	122.08
3	3	836	ILE	CB-CG1-CD1	-7.67	97.68	113.80
5	5	919	ARG	N-CA-C	7.64	120.96	109.95
3	3	919	TYR	CZ-CE2-CD2	7.64	133.35	119.60
3	3	838	SER	CB-CA-C	-7.44	98.34	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	877	LYS	CD-CE-NZ	7.42	135.65	111.90
2	2	34	ASN	CB-CG-ND2	7.25	127.27	116.40
3	3	836	ILE	CB-CA-C	-7.03	100.75	111.08
3	3	289	LYS	N-CA-C	-6.98	102.23	111.24
4	4	1018	MET	N-CA-C	6.88	118.47	110.97
5	5	920	LYS	N-CA-CB	6.87	120.32	110.77
2	2	105	TYR	CB-CG-CD2	-6.76	110.66	120.80
3	3	837	TYR	CB-CA-C	6.52	124.79	111.11
6	6	379	CYS	CA-C-N	6.51	133.97	121.54
6	6	379	CYS	C-N-CA	6.51	133.97	121.54
3	3	838	SER	N-CA-C	-6.48	98.62	108.67
5	5	919	ARG	CB-CA-C	6.48	123.86	111.48
3	3	840	ASP	CA-CB-CG	6.26	118.86	112.60
5	5	923	LYS	CA-CB-CG	-6.16	101.79	114.10
5	5	922	THR	CA-C-N	6.14	133.27	121.54
5	5	922	THR	C-N-CA	6.14	133.27	121.54
5	5	877	LYS	N-CA-C	6.11	118.72	111.33
3	3	405	GLU	CA-C-N	-6.02	112.21	120.28
3	3	405	GLU	C-N-CA	-6.02	112.21	120.28
6	6	971	GLU	CG-CD-OE2	5.96	132.11	118.40
2	2	34	ASN	CB-CG-OD1	-5.95	108.90	120.80
3	3	836	ILE	CG1-CB-CG2	5.94	128.53	110.70
5	5	927	ARG	N-CA-CB	5.91	119.77	109.72
5	5	931	GLN	N-CA-CB	-5.89	101.44	110.16
3	3	409	LYS	CB-CA-C	-5.82	98.83	110.42
6	6	504	PRO	N-CA-C	5.72	117.67	110.70
3	3	288	MET	CA-C-N	5.67	130.06	120.88
3	3	288	MET	C-N-CA	5.67	130.06	120.88
2	2	105	TYR	CB-CA-C	-5.49	101.68	110.79
4	4	1052	GLY	CA-C-N	5.45	131.94	121.54
4	4	1052	GLY	C-N-CA	5.45	131.94	121.54
5	5	920	LYS	CA-C-O	-5.44	114.48	119.76
5	5	927	ARG	CB-CG-CD	5.41	123.75	111.30
3	3	412	ARG	CA-C-N	5.37	127.33	120.56
3	3	412	ARG	C-N-CA	5.37	127.33	120.56
3	3	292	ARG	CA-CB-CG	5.33	124.76	114.10
3	3	860	VAL	N-CA-C	5.33	115.95	110.36
4	4	1017	PRO	CA-C-N	-5.27	113.69	120.65
4	4	1017	PRO	C-N-CA	-5.27	113.69	120.65
3	3	843	GLY	CA-C-N	5.24	134.59	121.80
3	3	843	GLY	C-N-CA	5.24	134.59	121.80
3	3	859	ASN	CA-C-N	5.16	127.25	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	859	ASN	C-N-CA	5.16	127.25	120.60
2	2	105	TYR	CB-CG-CD1	5.07	128.41	120.80
6	6	759	VAL	CA-C-N	-5.05	115.98	123.05
6	6	759	VAL	C-N-CA	-5.05	115.98	123.05
5	5	919	ARG	NE-CZ-NH2	-5.04	114.66	119.20
3	3	859	ASN	N-CA-C	5.03	117.49	111.71
3	3	289	LYS	CA-C-O	5.02	126.07	120.80
3	3	841	ALA	CA-C-N	5.00	131.09	121.54
3	3	841	ALA	C-N-CA	5.00	131.09	121.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	3	836	ILE	CB
5	5	920	LYS	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	105	TYR	Sidechain
3	3	288	MET	Mainchain
3	3	292	ARG	Sidechain
3	3	406	LYS	Mainchain
3	3	409	LYS	Mainchain
3	3	837	TYR	Sidechain
3	3	912	SER	Peptide
4	4	1002	HIS	Sidechain
5	5	923	LYS	Mainchain
5	5	931	GLN	Sidechain
6	6	760	ALA	Peptide

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	1	516	0	527	8	0
2	2	891	0	907	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	6173	0	6169	77	0
4	4	1780	0	1765	30	0
5	5	894	0	930	19	0
6	6	7551	0	7605	81	0
All	All	17805	0	17903	219	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 (219) 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)
3:3:837:TYR:CG	3:3:837:TYR:CD2	1.80	1.68
3:3:289:LYS:CG	3:3:289:LYS:CB	1.88	1.50
3:3:837:TYR:CD2	3:3:837:TYR:CB	2.20	1.23
3:3:837:TYR:CD2	3:3:837:TYR:HB3	1.73	1.19
3:3:837:TYR:CD2	3:3:837:TYR:CD1	2.33	0.95
6:6:503:LEU:HG	6:6:505:PRO:HD2	1.62	0.81
5:5:855:LEU:HD22	6:6:769:ILE:HD11	1.68	0.75
5:5:868:ARG:HG2	5:5:872:ARG:HD2	1.72	0.71
4:4:981:THR:HG1	4:4:1004:ALA:N	1.90	0.70
6:6:218:ARG:HH22	6:6:220:ARG:HB2	1.58	0.69
3:3:360:HIS:HD2	3:3:919:TYR:HE2	1.41	0.69
5:5:913:ILE:HD11	5:5:943:LEU:HD13	1.74	0.69
3:3:360:HIS:CD2	3:3:919:TYR:HE2	2.10	0.69
5:5:936:ILE:HG23	5:5:943:LEU:HD11	1.74	0.68
3:3:837:TYR:HB3	3:3:837:TYR:HD2	1.50	0.68
2:2:65:ALA:HA	2:2:68:MET:HE2	1.76	0.67
1:1:46:MET:HE1	1:1:66:SER:H	1.60	0.66
6:6:643:GLU:OE1	6:6:864:ASN:ND2	2.30	0.65
6:6:963:CYS:SG	6:6:964:ILE:N	2.72	0.63
1:1:85:ASP:OD1	2:2:44:ARG:NH2	2.32	0.62
5:5:874:GLU:OE1	5:5:874:GLU:N	2.28	0.61
3:3:406:LYS:O	3:3:409:LYS:N	2.29	0.61
5:5:923:LYS:O	5:5:926:GLN:N	2.34	0.60
6:6:145:TYR:HB2	6:6:968:MET:HE3	1.83	0.60
6:6:503:LEU:HD12	6:6:504:PRO:HD2	1.84	0.60
3:3:289:LYS:CB	3:3:289:LYS:CD	2.67	0.59
6:6:127:LEU:HD21	6:6:182:THR:HG21	1.85	0.59
5:5:909:VAL:HA	5:5:912:HIS:HB2	1.84	0.58
1:1:67:GLN:HA	1:1:70:GLN:OE1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:36:ALA:O	2:2:40:ILE:HG12	2.05	0.56
5:5:934:ILE:HG23	5:5:945:MET:HE1	1.86	0.56
3:3:541:VAL:HG11	3:3:581:PHE:HB2	1.87	0.56
3:3:416:THR:O	3:3:420:ASP:HB2	2.06	0.56
4:4:835:GLN:HG2	4:4:886:THR:HG21	1.89	0.55
2:2:71:TYR:HA	2:2:74:ILE:HG12	1.88	0.55
3:3:301:ASN:ND2	3:3:974:LEU:O	2.38	0.55
4:4:903:PRO:HG3	4:4:936:LYS:HB2	1.87	0.55
6:6:381:THR:HG22	6:6:383:LYS:H	1.72	0.55
4:4:879:ASP:O	4:4:902:ASN:ND2	2.39	0.55
3:3:769:GLN:NE2	6:6:338:SER:O	2.40	0.55
6:6:618:ILE:O	6:6:653:LYS:NZ	2.39	0.54
4:4:971:TYR:HB2	4:4:980:ILE:HB	1.89	0.54
6:6:429:ARG:NH1	6:6:430:HIS:O	2.40	0.54
4:4:1000:HIS:O	4:4:1002:HIS:HD2	1.90	0.54
6:6:23:SER:O	6:6:179:ARG:NH2	2.41	0.54
3:3:888:LEU:HD21	6:6:274:ARG:HD3	1.88	0.54
3:3:1126:MET:HA	3:3:1129:THR:HG22	1.90	0.53
6:6:361:LYS:HB3	6:6:370:PRO:HA	1.91	0.53
5:5:922:THR:OG1	5:5:923:LYS:N	2.41	0.53
6:6:679:GLN:O	6:6:682:ASN:ND2	2.42	0.52
6:6:651:TYR:OH	6:6:910:CYS:SG	2.61	0.52
4:4:881:THR:HB	4:4:897:GLN:HB2	1.92	0.52
4:4:1021:GLN:OE1	4:4:1025:GLN:NE2	2.43	0.52
6:6:683:PRO:O	6:6:687:GLN:NE2	2.43	0.51
3:3:438:ASP:OD1	3:3:441:HIS:ND1	2.44	0.51
3:3:782:ASP:OD1	3:3:783:ILE:N	2.43	0.51
6:6:696:ILE:HG13	6:6:773:SER:HB3	1.92	0.51
6:6:220:ARG:NH1	6:6:221:ALA:O	2.43	0.51
6:6:557:VAL:HG22	6:6:603:PHE:CE1	2.46	0.51
4:4:918:TYR:HA	4:4:921:ILE:HD12	1.93	0.51
6:6:445:GLU:OE1	6:6:448:ASP:HB2	2.10	0.51
6:6:914:SER:OG	6:6:917:GLU:OE1	2.29	0.51
5:5:857:ASP:OD2	5:5:954:ARG:NH2	2.43	0.51
6:6:328:ASP:N	6:6:328:ASP:OD1	2.44	0.51
3:3:360:HIS:CD2	3:3:919:TYR:CE2	2.95	0.50
3:3:981:GLU:OE1	3:3:985:GLN:NE2	2.43	0.50
6:6:369:SER:O	6:6:390:ARG:NH1	2.44	0.50
6:6:877:GLN:NE2	6:6:882:GLY:O	2.44	0.50
6:6:218:ARG:HH12	6:6:220:ARG:HB2	1.76	0.50
4:4:994:ARG:HH12	4:4:996:LYS:HG2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:871:HIS:HA	5:5:874:GLU:OE2	2.11	0.50
3:3:289:LYS:CG	3:3:289:LYS:CA	2.88	0.49
3:3:869:ARG:HH21	3:3:882:LEU:HD23	1.76	0.49
6:6:266:GLN:NE2	6:6:276:LYS:O	2.46	0.49
6:6:888:ASP:O	6:6:895:ARG:NH2	2.45	0.49
6:6:218:ARG:NH2	6:6:220:ARG:HB2	2.26	0.49
2:2:60:GLU:O	2:2:67:ARG:NH2	2.46	0.49
3:3:1114:GLU:HA	3:3:1117:ILE:HG22	1.95	0.49
4:4:909:PRO:O	4:4:913:ASN:ND2	2.46	0.49
6:6:342:ASP:OD2	6:6:387:LYS:NZ	2.46	0.48
2:2:28:LYS:HA	2:2:31:LYS:HE2	1.93	0.48
6:6:55:LEU:O	6:6:164:MET:HE1	2.14	0.48
6:6:934:ARG:HG2	6:6:937:ASN:HD21	1.78	0.48
3:3:405:GLU:O	3:3:406:LYS:C	2.53	0.48
3:3:539:GLU:OE1	3:3:542:LYS:NZ	2.47	0.48
3:3:301:ASN:HD22	3:3:974:LEU:HB3	1.78	0.48
3:3:360:HIS:HD2	3:3:919:TYR:CE2	2.26	0.47
3:3:1087:SER:OG	3:3:1088:PHE:N	2.47	0.47
3:3:1095:ARG:O	3:3:1099:ASN:ND2	2.46	0.47
6:6:467:ASP:OD1	6:6:467:ASP:N	2.46	0.47
6:6:506:SER:OG	6:6:523:GLN:OE1	2.31	0.47
6:6:559:SER:OG	6:6:566:ALA:HB2	2.14	0.47
4:4:1070:HIS:O	4:4:1074:LYS:N	2.46	0.47
6:6:627:MET:SD	6:6:649:ILE:HD11	2.54	0.47
3:3:518:SER:O	3:3:524:GLN:NE2	2.47	0.47
4:4:981:THR:OG1	4:4:1004:ALA:N	2.46	0.47
3:3:371:ARG:O	3:3:375:ILE:HG12	2.14	0.47
6:6:144:THR:OG1	6:6:146:GLU:OE2	2.19	0.47
6:6:609:ALA:HB1	6:6:613:ILE:HD12	1.96	0.47
6:6:779:LEU:O	6:6:783:GLU:HB2	2.14	0.47
1:1:92:SER:HA	2:2:37:ARG:HH22	1.78	0.47
3:3:698:ASP:HA	3:3:702:ASN:HD22	1.79	0.47
3:3:306:TRP:HD1	3:3:580:SER:HA	1.80	0.47
3:3:483:ASN:OD1	3:3:487:ILE:N	2.47	0.47
6:6:297:ILE:HB	6:6:310:TYR:HB2	1.96	0.47
4:4:1001:ILE:HG23	4:4:1055:VAL:HB	1.97	0.47
6:6:670:ILE:HA	6:6:673:ILE:HD12	1.97	0.47
6:6:393:PRO:HA	6:6:425:TYR:HA	1.97	0.46
3:3:830:SER:HB2	3:3:841:ALA:HB1	1.96	0.46
3:3:920:LEU:O	3:3:924:ILE:HG12	2.14	0.46
2:2:77:LYS:HA	2:2:80:GLN:NE2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:1103:LEU:HD22	3:3:1113:ASN:HD22	1.80	0.46
4:4:917:ASP:HB3	4:4:920:PHE:HD2	1.81	0.46
5:5:849:ARG:O	5:5:853:LEU:HD23	2.15	0.46
6:6:170:ASP:OD1	6:6:170:ASP:N	2.48	0.46
6:6:411:ASP:N	6:6:411:ASP:OD1	2.48	0.46
6:6:203:ILE:HA	6:6:223:GLN:HA	1.96	0.46
3:3:364:SER:HB2	3:3:366:LEU:HD13	1.97	0.46
4:4:896:VAL:O	4:4:908:GLN:NE2	2.38	0.46
5:5:896:ASP:OD1	5:5:896:ASP:N	2.48	0.46
5:5:950:ASN:HB3	5:5:954:ARG:HD2	1.98	0.46
3:3:289:LYS:HB3	3:3:290:LEU:HD22	1.97	0.46
3:3:783:ILE:O	3:3:787:ILE:HG12	2.15	0.46
4:4:1023:ARG:NH1	4:4:1027:PHE:O	2.48	0.46
6:6:662:VAL:HB	6:6:695:LEU:HD21	1.98	0.46
3:3:869:ARG:NH2	3:3:882:LEU:HD23	2.31	0.45
4:4:902:ASN:O	4:4:905:HIS:ND1	2.44	0.45
3:3:541:VAL:HG22	3:3:578:ILE:HD13	1.98	0.45
4:4:1058:ASP:OD1	4:4:1061:GLU:HG2	2.17	0.45
3:3:288:MET:HG2	3:3:292:ARG:NH1	2.32	0.45
6:6:408:LEU:O	6:6:412:ARG:NH2	2.48	0.45
5:5:937:SER:O	5:5:943:LEU:HD12	2.17	0.45
5:5:922:THR:HG23	5:5:925:ALA:H	1.82	0.45
6:6:187:ASN:HB3	6:6:245:ASN:HB3	1.99	0.45
6:6:138:ARG:HA	6:6:138:ARG:HD3	1.79	0.45
3:3:789:ASN:OD1	3:3:846:ASN:ND2	2.47	0.44
4:4:1003:PHE:CZ	4:4:1019:MET:HG3	2.52	0.44
2:2:48:ASN:O	2:2:52:GLN:NE2	2.50	0.44
3:3:731:LEU:HD23	3:3:731:LEU:HA	1.86	0.44
4:4:985:GLU:OE1	4:4:1002:HIS:NE2	2.50	0.44
3:3:578:ILE:O	3:3:581:PHE:N	2.50	0.44
3:3:775:LYS:HB2	3:3:826:PHE:HE1	1.81	0.44
6:6:222:GLN:NE2	6:6:223:GLN:O	2.51	0.44
6:6:825:PRO:HA	6:6:826:PRO:HD3	1.85	0.44
6:6:625:LYS:H	6:6:625:LYS:HG2	1.66	0.44
3:3:532:VAL:HB	3:3:537:GLN:HE21	1.82	0.44
6:6:739:LYS:HZ3	6:6:799:ASN:HD21	1.66	0.44
2:2:104:GLU:HA	2:2:107:LYS:HG2	2.00	0.44
6:6:322:LYS:HA	6:6:322:LYS:HD3	1.74	0.44
4:4:1010:THR:O	4:4:1013:SER:OG	2.27	0.43
2:2:77:LYS:HA	2:2:80:GLN:CD	2.42	0.43
6:6:119:ASP:OD1	6:6:119:ASP:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:359:TYR:HE2	3:3:913:THR:HB	1.83	0.43
6:6:102:PHE:HD1	6:6:177:ILE:HG22	1.84	0.43
3:3:824:ARG:NH1	3:3:870:ILE:O	2.42	0.43
3:3:867:ASP:HB3	3:3:870:ILE:HG12	2.00	0.43
3:3:887:PHE:HE1	3:3:919:TYR:HD1	1.67	0.43
6:6:350:VAL:HG23	6:6:379:CYS:HB3	1.99	0.43
3:3:833:ASN:HB2	3:3:834:TYR:H	1.70	0.43
3:3:913:THR:OG1	3:3:914:TYR:N	2.44	0.43
4:4:840:THR:HA	4:4:843:VAL:HG12	2.00	0.43
4:4:1000:HIS:ND1	4:4:1002:HIS:CD2	2.87	0.43
6:6:127:LEU:HD13	6:6:186:TYR:CE2	2.54	0.43
6:6:176:ASN:OD1	6:6:176:ASN:N	2.49	0.43
6:6:181:GLN:HB2	6:6:183:ARG:HH11	1.82	0.43
4:4:1003:PHE:CE1	4:4:1019:MET:HE2	2.53	0.43
3:3:480:PHE:HB3	3:3:488:GLN:HB3	2.01	0.43
3:3:869:ARG:HG2	3:3:876:ASP:OD2	2.19	0.43
3:3:883:GLY:HA2	6:6:275:PHE:HE1	1.84	0.43
6:6:739:LYS:HZ3	6:6:799:ASN:CG	2.26	0.43
3:3:658:ILE:O	3:3:662:ILE:HG12	2.18	0.42
6:6:621:ARG:O	6:6:625:LYS:NZ	2.52	0.42
6:6:628:LEU:HD23	6:6:631:LEU:HD12	2.01	0.42
6:6:111:ASN:HD21	6:6:119:ASP:H	1.67	0.42
4:4:914:SER:HB2	4:4:916:MET:HE2	2.02	0.42
3:3:683:ASP:OD1	3:3:683:ASP:N	2.53	0.42
3:3:958:SER:O	3:3:962:GLU:HB2	2.20	0.42
6:6:218:ARG:HH12	6:6:220:ARG:CB	2.33	0.42
6:6:739:LYS:HZ3	6:6:799:ASN:ND2	2.17	0.42
3:3:378:THR:HG22	3:3:379:LYS:HD3	2.01	0.42
3:3:888:LEU:HA	6:6:278:LEU:HD21	2.00	0.42
6:6:196:LEU:HD23	6:6:196:LEU:HA	1.92	0.42
5:5:913:ILE:HG21	5:5:938:ILE:HB	2.02	0.42
2:2:31:LYS:HA	2:2:34:ASN:HD21	1.85	0.42
3:3:976:ASP:OD2	3:3:1123:TYR:OH	2.38	0.42
4:4:1003:PHE:CE2	4:4:1019:MET:HG3	2.54	0.42
5:5:880:PRO:HA	5:5:883:LEU:HG	2.01	0.42
1:1:31:LYS:HA	1:1:34:VAL:HG12	2.00	0.42
3:3:838:SER:O	3:3:839:SER:C	2.62	0.42
3:3:909:LEU:HG	3:3:967:TYR:HE2	1.84	0.41
4:4:924:TYR:OH	4:4:964:LEU:O	2.33	0.41
3:3:482:ARG:HH22	3:3:517:ASP:HA	1.85	0.41
3:3:732:SER:O	3:3:734:GLU:N	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1023:ARG:HA	4:4:1027:PHE:HB2	2.02	0.41
6:6:843:VAL:HG22	6:6:844:ILE:H	1.83	0.41
6:6:653:LYS:HE2	6:6:653:LYS:HB2	1.81	0.41
1:1:95:SER:OG	2:2:37:ARG:NH2	2.53	0.41
6:6:15:ILE:HD11	6:6:145:TYR:HB3	2.03	0.41
5:5:869:PHE:O	5:5:873:GLN:HG3	2.20	0.41
6:6:597:LYS:HG3	6:6:816:PHE:HE2	1.84	0.41
3:3:1126:MET:HE3	3:3:1126:MET:HB2	1.95	0.41
4:4:859:ALA:HB3	4:4:866:SER:HB2	2.02	0.41
3:3:534:PRO:HA	3:3:537:GLN:HG3	2.02	0.41
3:3:1082:ILE:HD11	6:6:380:ASP:HB3	2.03	0.41
6:6:760:ALA:O	6:6:761:LYS:HG3	2.20	0.41
6:6:769:ILE:HG21	6:6:769:ILE:HD13	1.89	0.41
3:3:352:GLN:HE21	3:3:352:GLN:HB3	1.75	0.41
3:3:356:ASN:O	3:3:360:HIS:ND1	2.52	0.41
1:1:101:LEU:HD12	1:1:102:THR:HG23	2.03	0.40
3:3:593:LYS:O	3:3:597:LEU:HB2	2.22	0.40
3:3:666:PRO:HA	3:3:765:TYR:HB3	2.02	0.40
6:6:521:VAL:HB	6:6:530:GLN:HE21	1.87	0.40
1:1:47:MET:O	1:1:51:GLN:N	2.55	0.40
3:3:413:ILE:O	3:3:417:GLU:HG3	2.22	0.40
6:6:232:PRO:HD2	6:6:235:ILE:HD12	2.04	0.40
6:6:574:LYS:HA	6:6:577:ILE:HG22	2.04	0.40
6:6:623:LEU:HD11	6:6:653:LYS:HE3	2.02	0.40
3:3:443:PHE:O	3:3:447:LEU:HD23	2.22	0.40
3:3:509:SER:O	3:3:513:SER:OG	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1	61/431 (14%)	61 (100%)	0	0	100	100
2	2	108/397 (27%)	105 (97%)	3 (3%)	0	100	100
3	3	749/1132 (66%)	705 (94%)	40 (5%)	4 (0%)	24	56
4	4	214/1082 (20%)	203 (95%)	10 (5%)	1 (0%)	24	56
5	5	109/1081 (10%)	98 (90%)	9 (8%)	2 (2%)	6	34
6	6	928/974 (95%)	889 (96%)	36 (4%)	3 (0%)	36	65
All	All	2169/5097 (43%)	2061 (95%)	98 (4%)	10 (0%)	26	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	844	ASP
4	4	1053	ASN
6	6	761	LYS
3	3	839	SER
6	6	156	VAL
5	5	906	PRO
3	3	362	ALA
6	6	844	ILE
5	5	921	PRO
3	3	928	THR

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	1	60/389 (15%)	60 (100%)	0	100	100
2	2	100/339 (30%)	100 (100%)	0	100	100
3	3	713/1053 (68%)	709 (99%)	4 (1%)	78	79
4	4	205/1001 (20%)	205 (100%)	0	100	100
5	5	103/944 (11%)	99 (96%)	4 (4%)	28	53
6	6	861/897 (96%)	860 (100%)	1 (0%)	88	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2042/4623 (44%)	2033 (100%)	9 (0%)	81	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	833	ASN
3	3	836	ILE
3	3	837	TYR
3	3	838	SER
5	5	877	LYS
5	5	919	ARG
5	5	920	LYS
5	5	931	GLN
6	6	505	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	46	GLN
2	2	52	GLN
2	2	96	GLN
3	3	333	GLN
3	3	352	GLN
3	3	356	ASN
3	3	421	ASN
3	3	485	GLN
3	3	537	GLN
3	3	608	ASN
3	3	632	ASN
3	3	690	ASN
3	3	702	ASN
3	3	769	GLN
3	3	901	ASN
3	3	954	ASN
3	3	1099	ASN
3	3	1105	ASN
3	3	1113	ASN
4	4	893	ASN
4	4	913	ASN
4	4	919	HIS
4	4	1002	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1021	GLN
4	4	1025	GLN
4	4	1070	HIS
5	5	871	HIS
5	5	931	GLN
6	6	6	HIS
6	6	25	ASN
6	6	40	ASN
6	6	44	HIS
6	6	47	GLN
6	6	100	GLN
6	6	109	HIS
6	6	129	ASN
6	6	137	GLN
6	6	162	HIS
6	6	187	ASN
6	6	222	GLN
6	6	266	GLN
6	6	293	GLN
6	6	327	ASN
6	6	530	GLN
6	6	548	ASN
6	6	675	ASN
6	6	687	GLN
6	6	693	GLN
6	6	726	ASN
6	6	771	ASN
6	6	800	ASN
6	6	864	ASN
6	6	894	ASN

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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	3	4
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	1003:PHE	C	1004:ALA	N	4.95
1	3	333:GLN	C	334:ASN	N	3.85
1	3	676:GLU	C	677:SER	N	3.42
1	3	580:SER	C	581:PHE	N	3.27
1	3	667:ASN	C	668:VAL	N	3.25

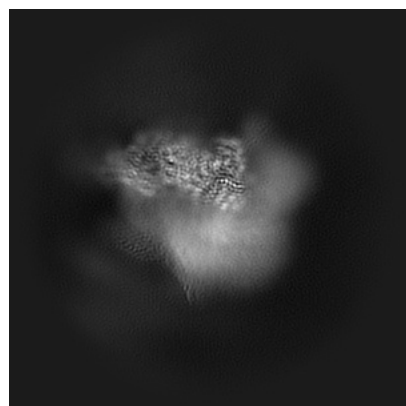
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71517. These allow visual inspection of the internal detail of the map and identification of artifacts.

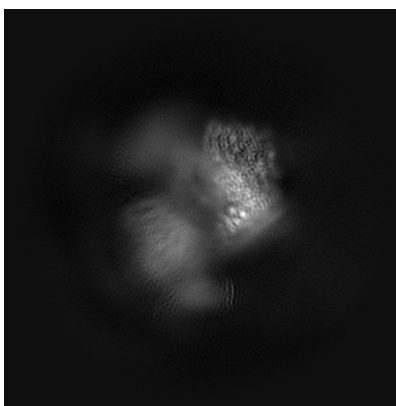
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

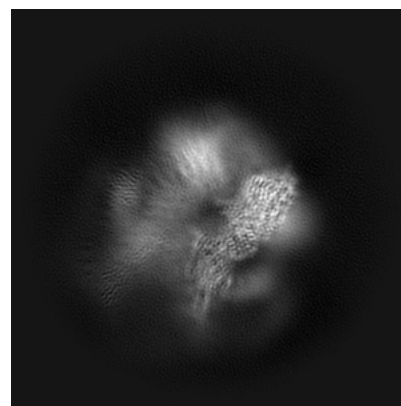
6.1.1 Primary map



X

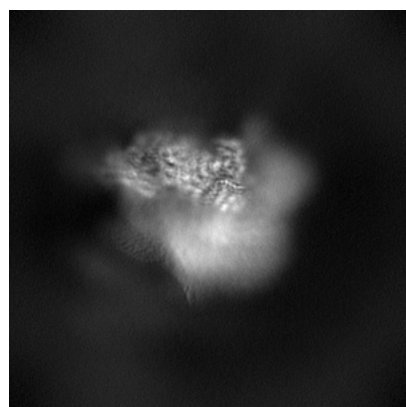


Y

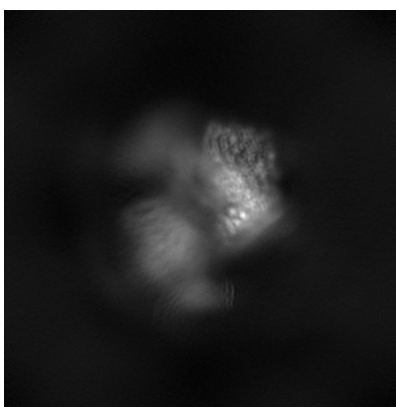


Z

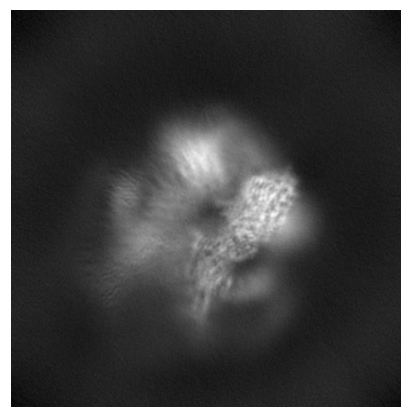
6.1.2 Raw map



X



Y

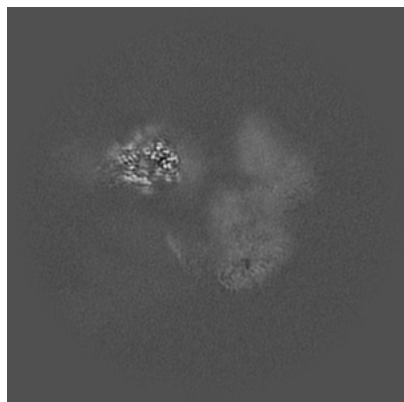


Z

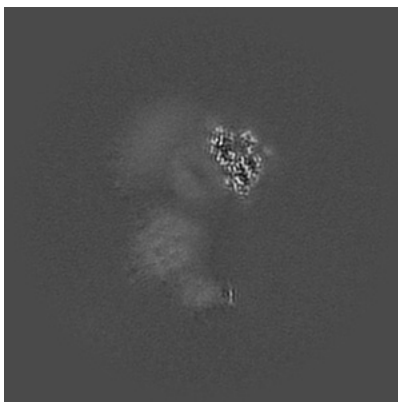
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

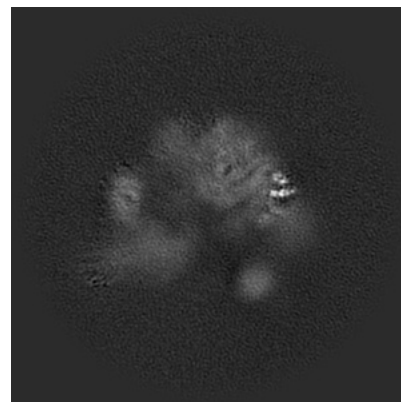
6.2.1 Primary map



X Index: 160

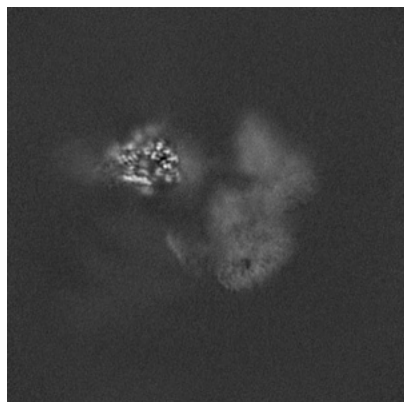


Y Index: 160

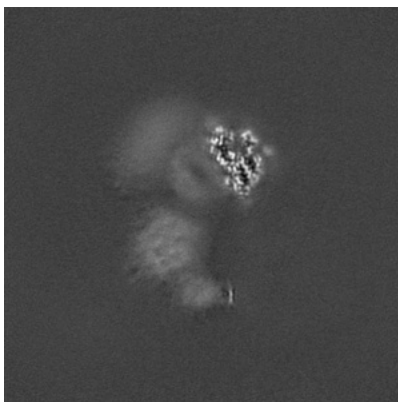


Z Index: 160

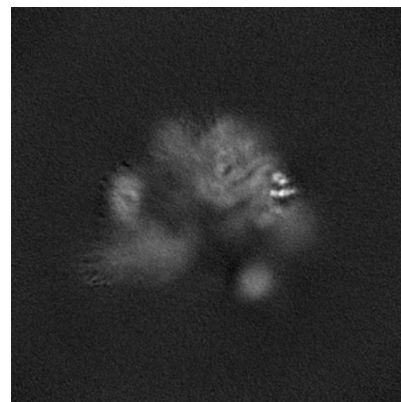
6.2.2 Raw map



X Index: 160



Y Index: 160

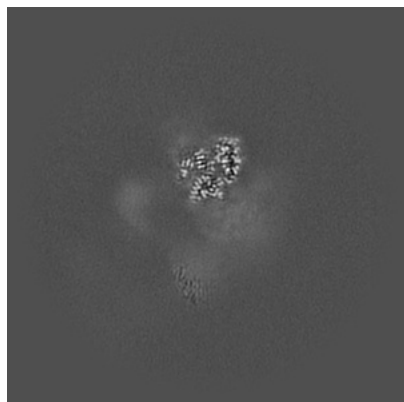


Z Index: 160

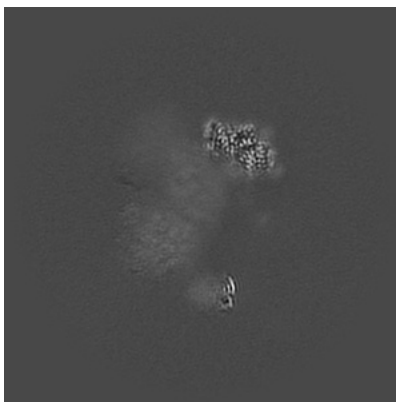
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

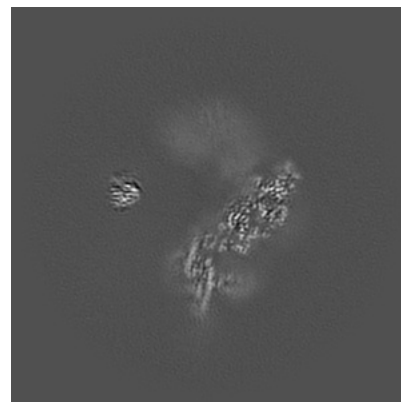
6.3.1 Primary map



X Index: 200

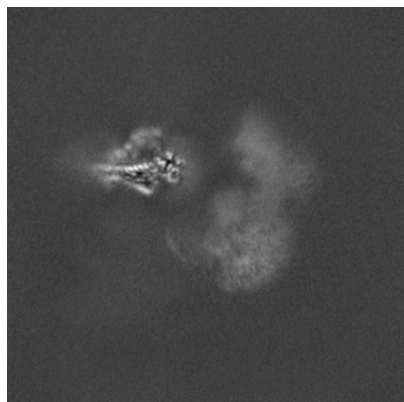


Y Index: 173

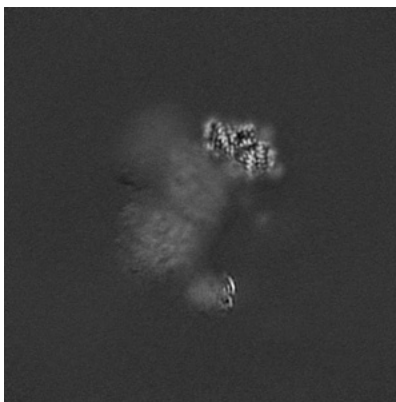


Z Index: 182

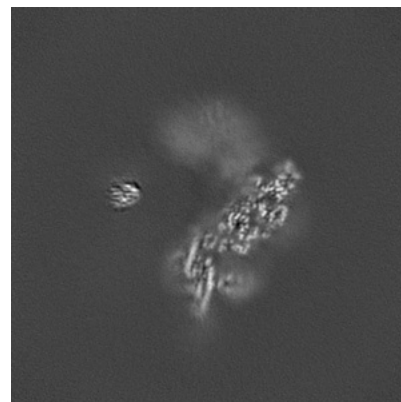
6.3.2 Raw map



X Index: 155



Y Index: 173

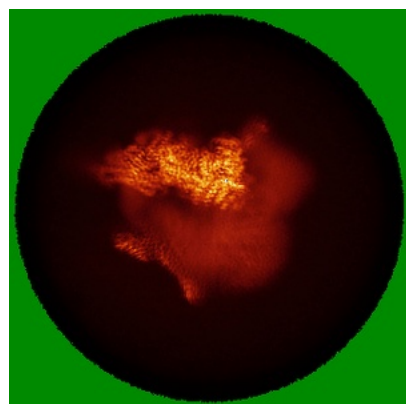


Z Index: 182

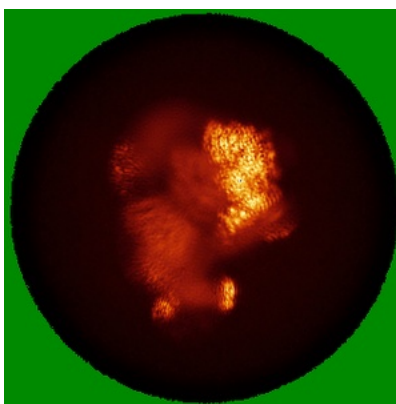
The images above show the largest variance slices of the map in three orthogonal directions.

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

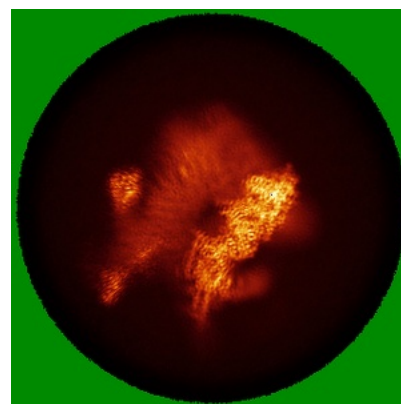
6.4.1 Primary map



X

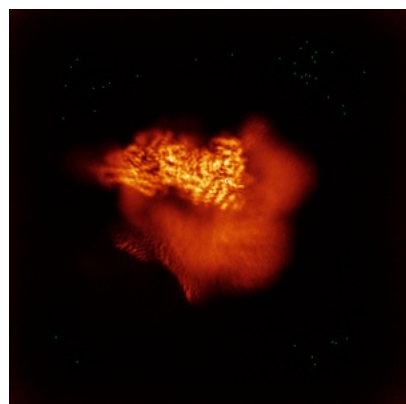


Y

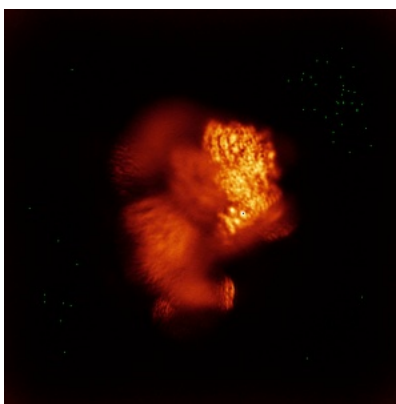


Z

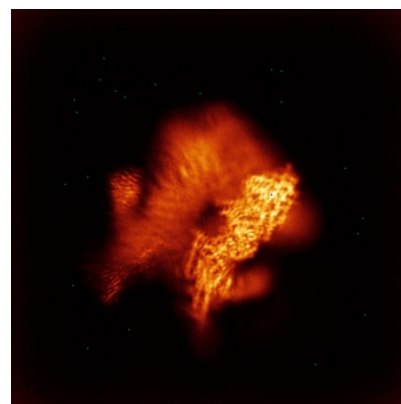
6.4.2 Raw map



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 0.512. 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.

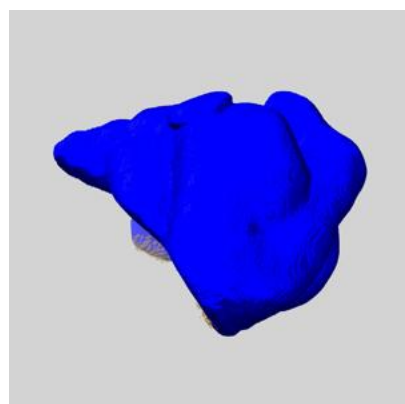
6.6 Mask visualisation [i](#)

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

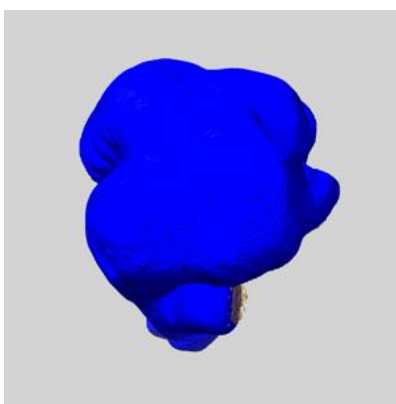
A mask typically either:

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

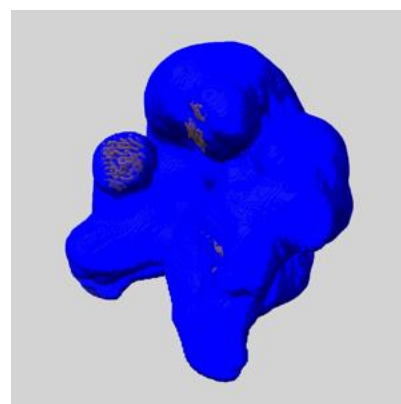
6.6.1 emd_71517_msk_1.map [i](#)



X



Y

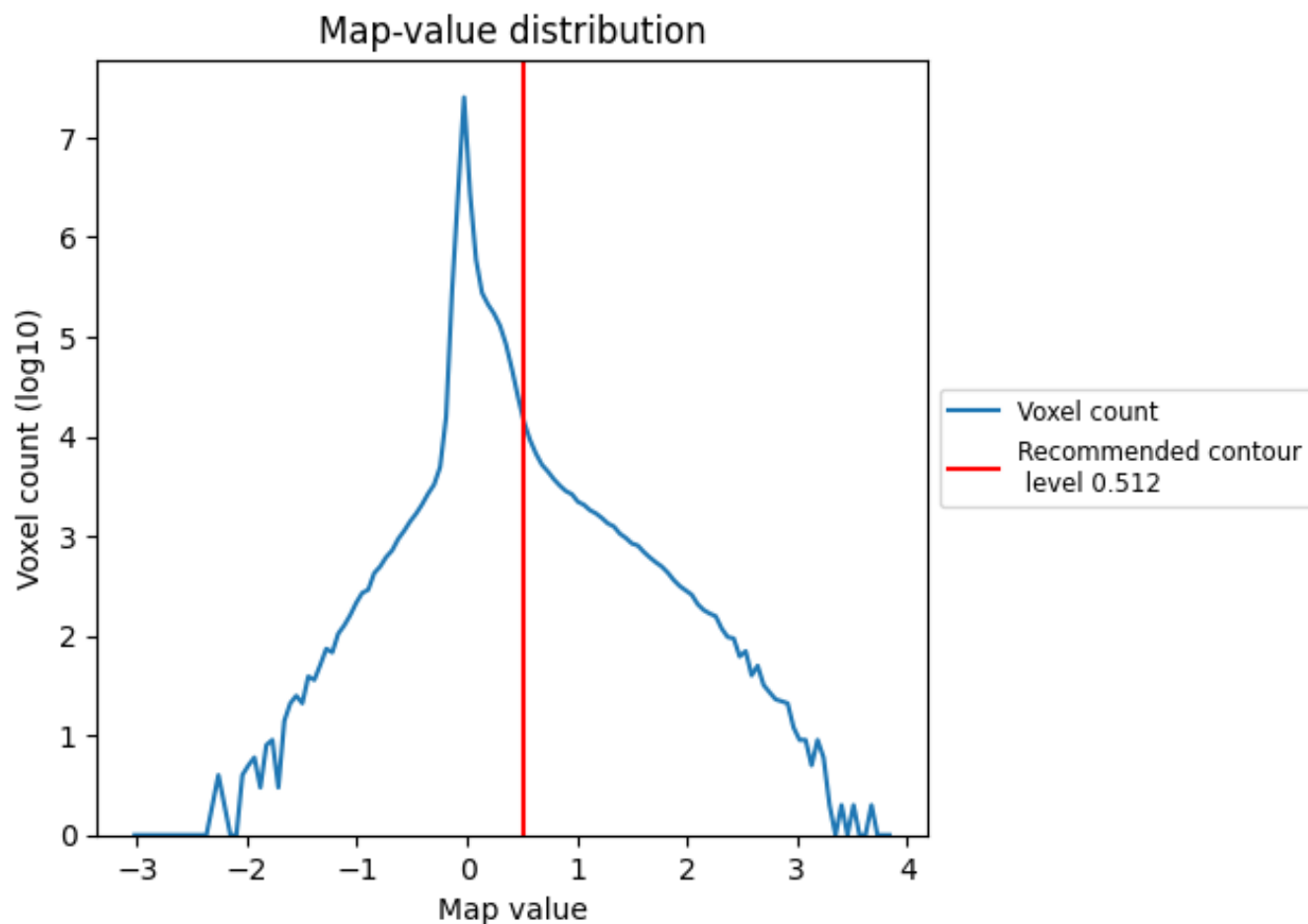


Z

7 Map analysis [i](#)

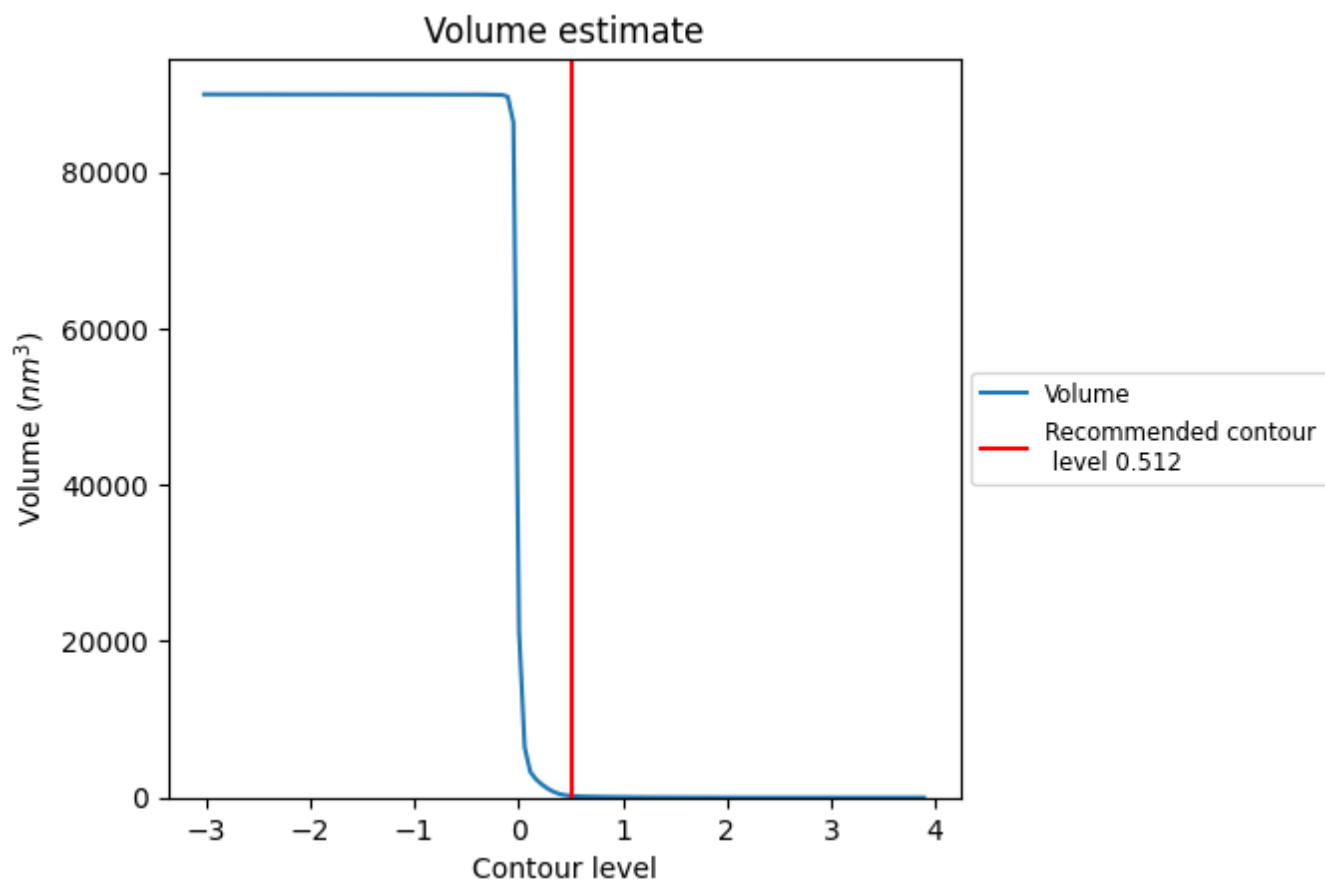
This section contains the results of statistical analysis of the map.

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.

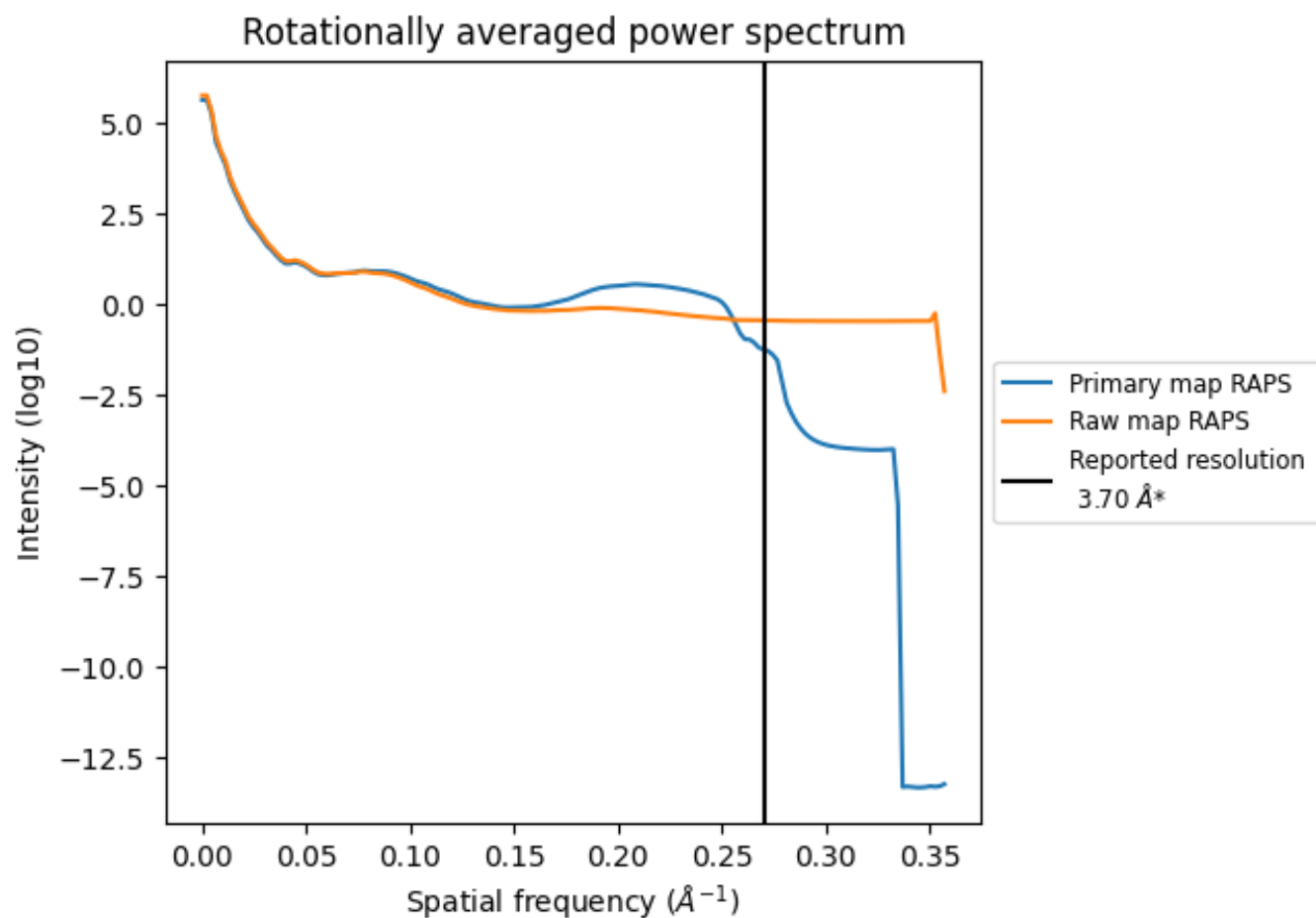
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

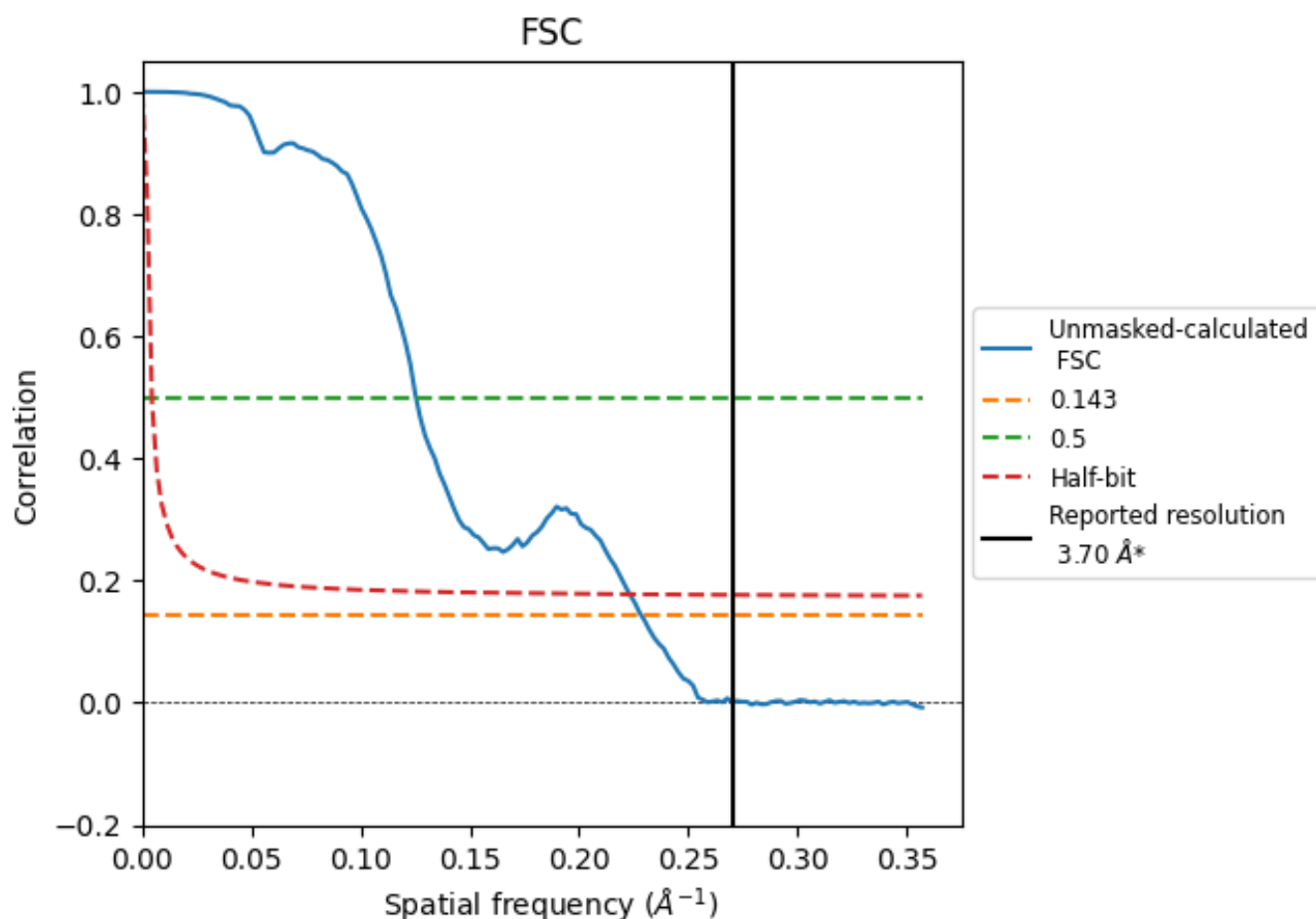


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

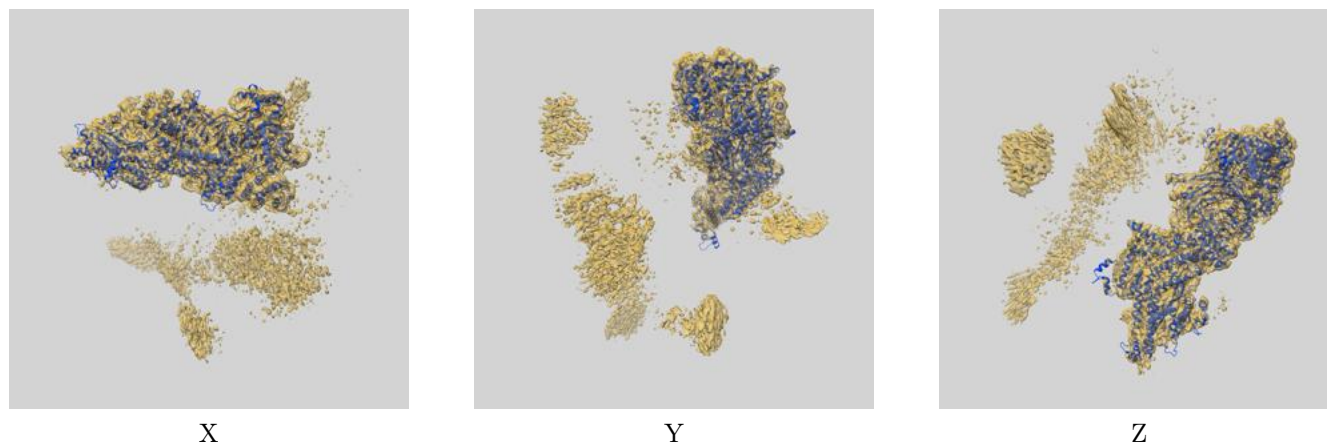
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.38	7.98	4.48

*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 4.38 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

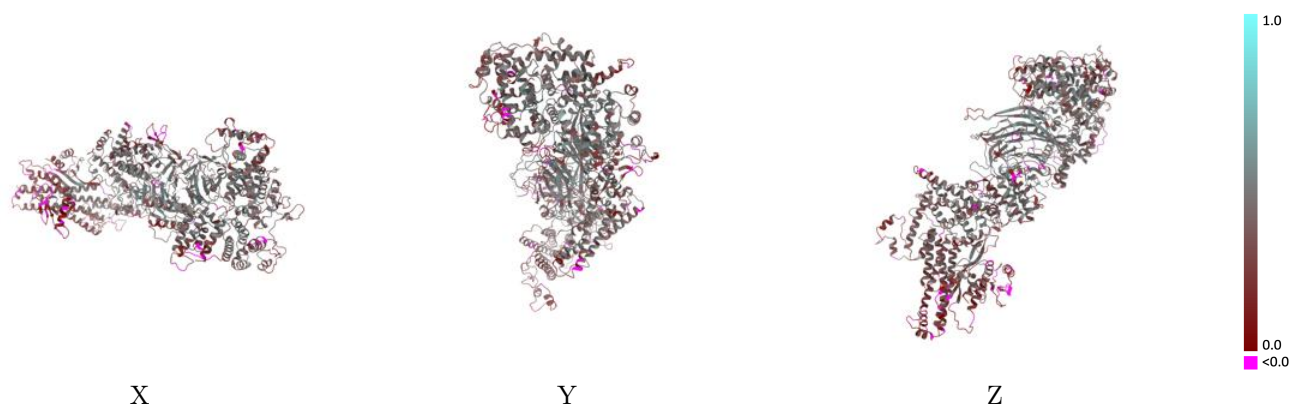
This section contains information regarding the fit between EMDB map EMD-71517 and PDB model 9PCR. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



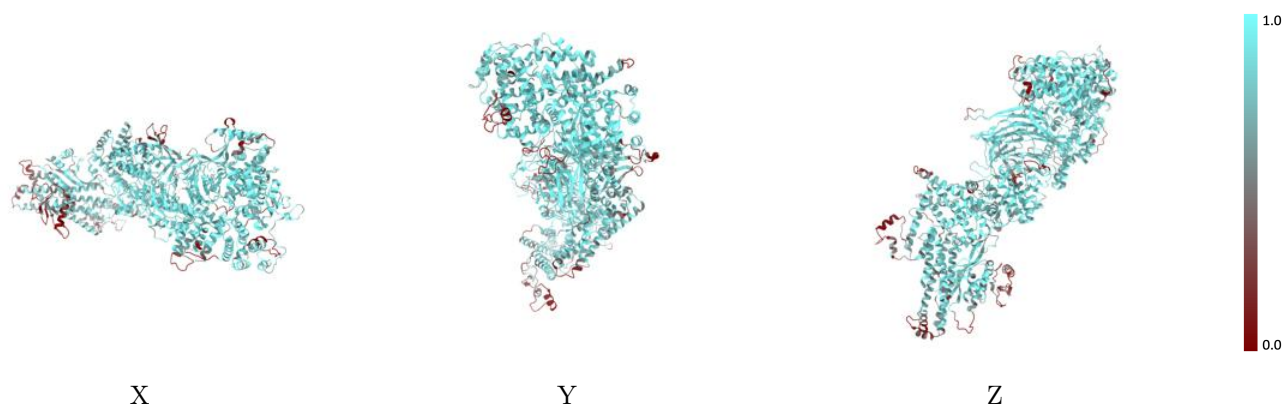
The images above show the 3D surface view of the map at the recommended contour level 0.512 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



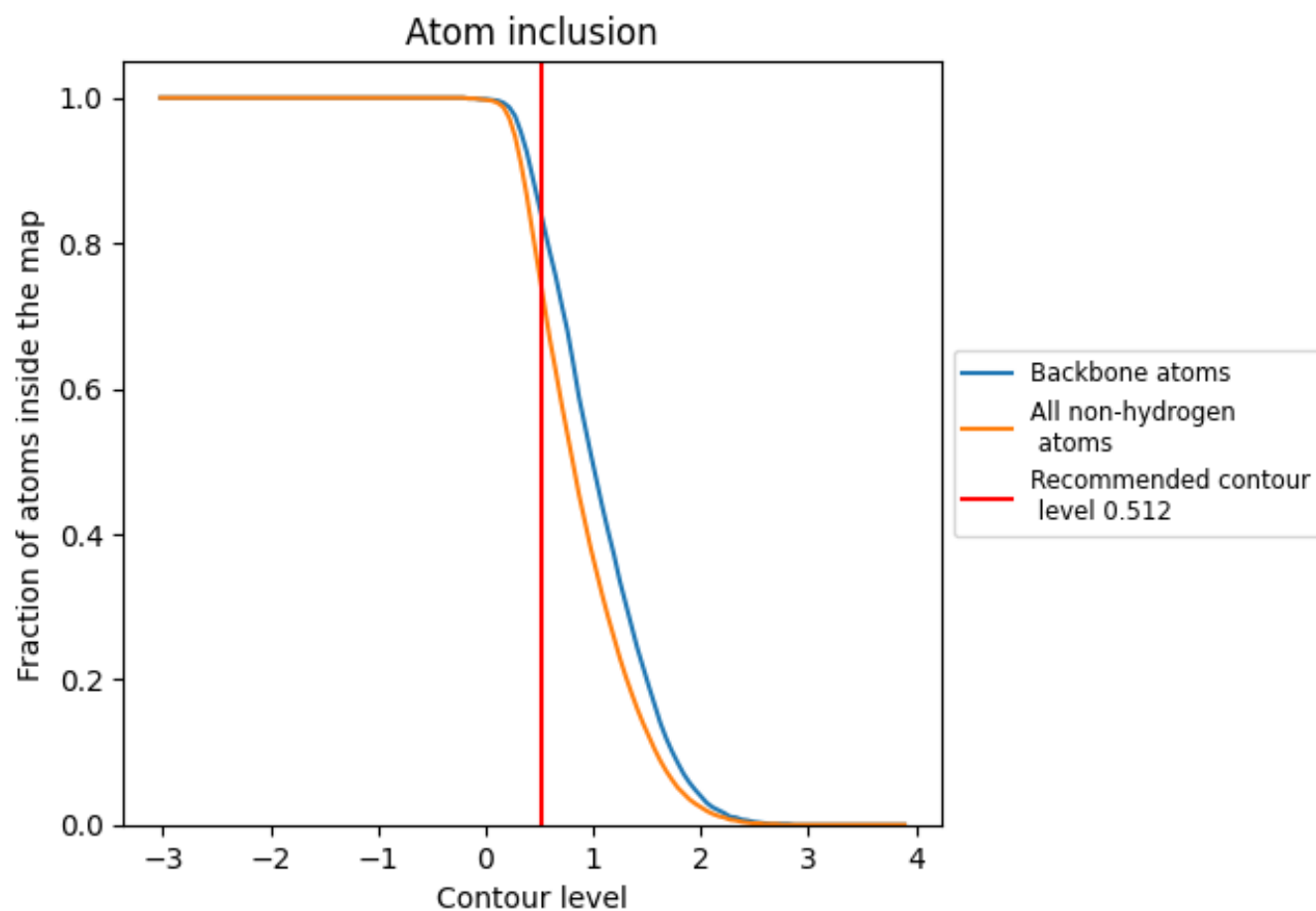
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.512).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.512) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.3540
1	0.7880	0.2750
2	0.6150	0.2200
3	0.7810	0.3780
4	0.5560	0.2160
5	0.5140	0.2540
6	0.8020	0.4010

1.0

0.0

<0.0