



Full wwPDB EM Validation Report ⓘ

Sep 28, 2026 – 12:14 PM EDT

PDB ID : 9PBS / pdb_00009pbs
EMDB ID : EMD-71489
Title : Core SWI/SNF of PIC-Med-SWI/SNF-Nucleosome
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-26
Resolution : 3.50 Å (reported)
Based on initial models : 7c4j, 7egp

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:

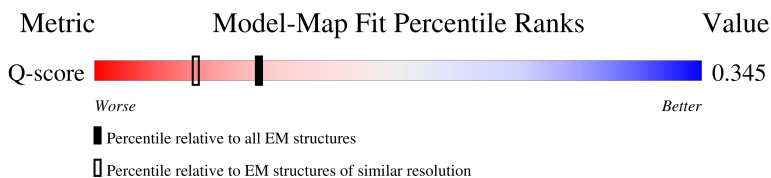
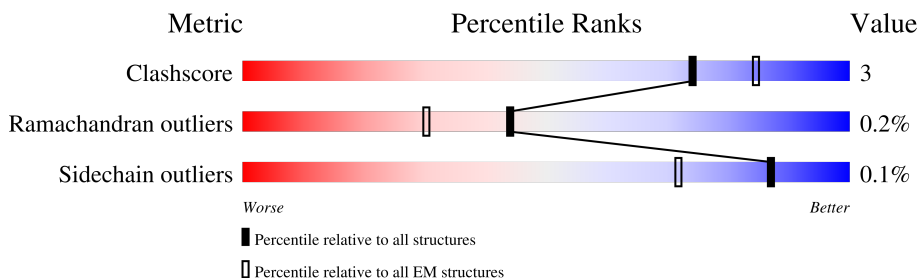
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	566	
2	B	825	
2	D	825	
3	C	332	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	623	18%60%5%34%
5	F	905	39%5%55%
6	G	82	56%.43%
7	H	1703	10%.90%
8	I	1314	38%.58%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24359 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 Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	442	Total	C	N	O	S	0	0
			3552	2231	608	698	15		

- Molecule 2 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	395	Total	C	N	O	S	0	0
			3250	2082	560	597	11		
2	D	421	Total	C	N	O	S	0	0
			3445	2203	592	638	12		

- Molecule 3 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	154	Total	C	N	O	S	0	0
			1266	793	232	236	5		

- Molecule 4 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	411	Total	C	N	O	S	0	0
			3333	2142	569	617	5		

- Molecule 5 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	408	Total	C	N	O	S	0	0
			3349	2116	567	656	10		

- Molecule 6 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	47	Total	C	N	O	0	0
			271	166	56	49		

- Molecule 7 is a protein called Transcription regulatory protein SNF2.

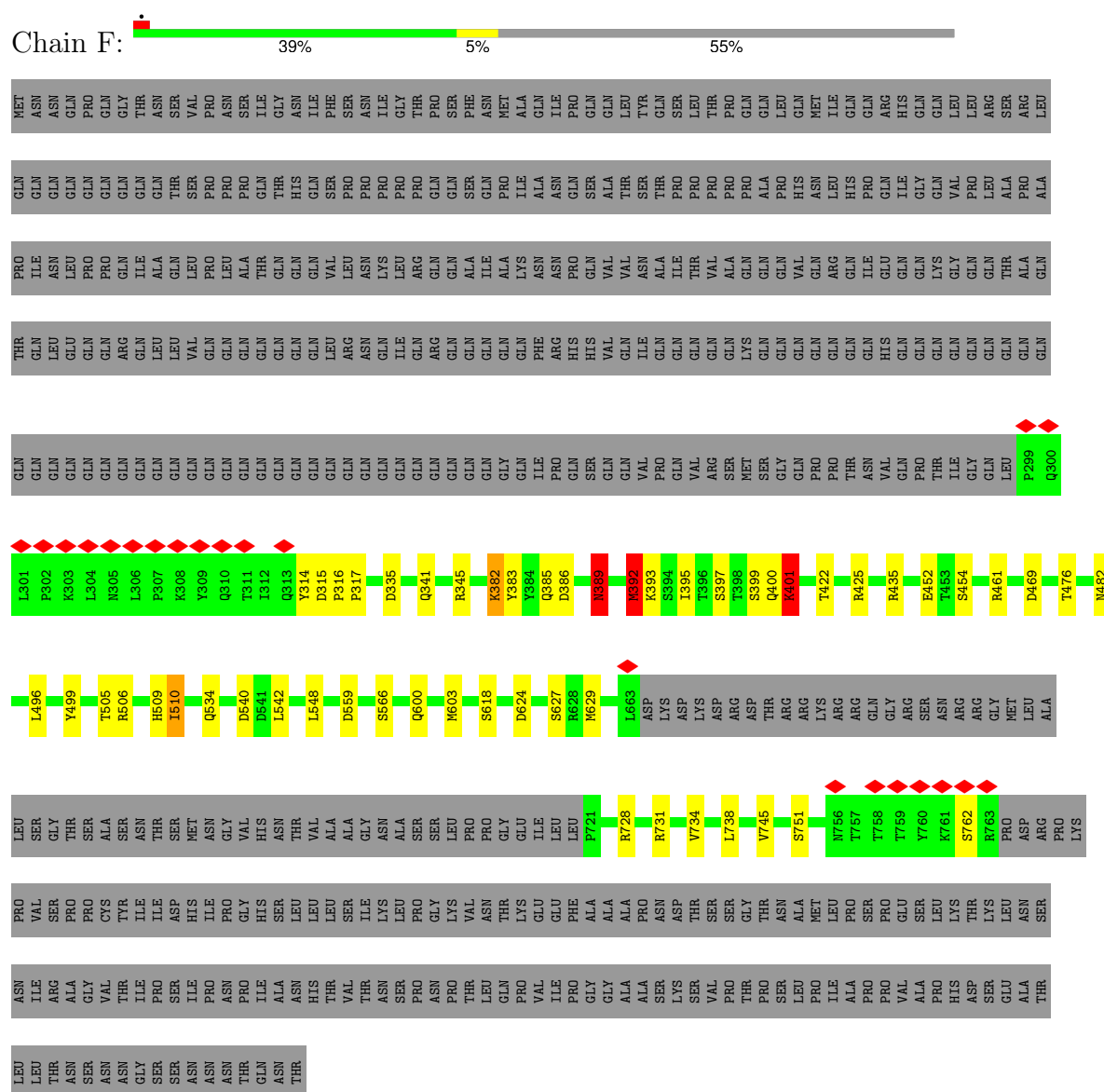
Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	177	Total	C	N	O	S	0	0
			1419	900	237	277	5		

- Molecule 8 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	552	Total	C	N	O	S	0	0
			4474	2894	749	820	11		

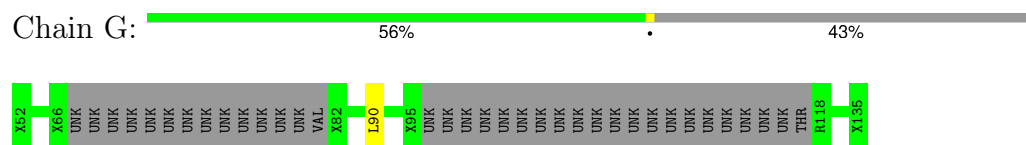
- Molecule 5: SWI/SNF chromatin-remodeling complex subunit SNF5

Chain F:



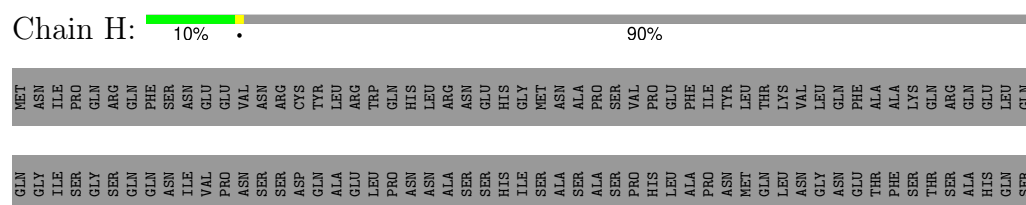
- Molecule 6: Unknown

Chain G:

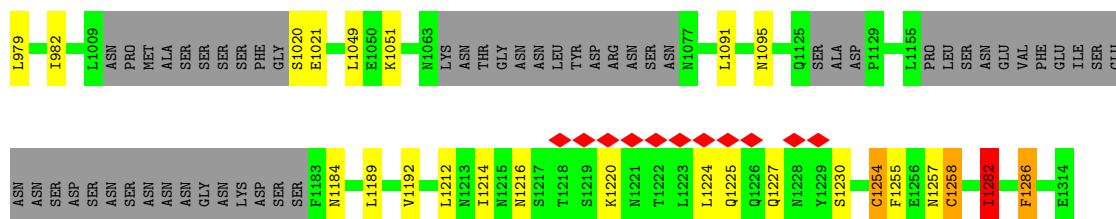


- Molecule 7: Transcription regulatory protein SNF2

Chain H:







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121711	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	3.272	Depositor
Minimum map value	-1.855	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.402	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	A	0.40	6/3616 (0.2%)	0.65	11/4892 (0.2%)
2	B	0.32	1/3318 (0.0%)	0.57	0/4465
2	D	0.40	3/3517 (0.1%)	0.66	4/4735 (0.1%)
3	C	0.38	0/1287	0.65	2/1729 (0.1%)
4	E	0.36	3/3399 (0.1%)	0.54	0/4584
5	F	0.63	13/3422 (0.4%)	0.97	24/4638 (0.5%)
6	G	0.24	0/101	0.36	0/123
7	H	0.67	3/1449 (0.2%)	1.47	7/1979 (0.4%)
8	I	0.36	3/4553 (0.1%)	0.59	6/6166 (0.1%)
All	All	0.44	32/24662 (0.1%)	0.74	54/33311 (0.2%)

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
5	F	0	3
7	H	0	1
8	I	0	2
All	All	0	8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	590	GLU	CB-CG	-15.46	1.06	1.52
5	F	392	MET	N-CA	14.55	1.65	1.46
7	H	590	GLU	CA-C	8.75	1.64	1.52
5	F	392	MET	CB-CG	-8.59	1.26	1.52
5	F	392	MET	SD-CE	-8.38	1.58	1.79
5	F	393	LYS	CB-CG	-8.34	1.27	1.52
5	F	392	MET	CA-C	-7.83	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1282	ILE	CB-CG2	-7.82	1.26	1.52
2	D	344	MET	SD-CE	-7.71	1.60	1.79
8	I	1286	PHE	CG-CD2	-7.41	1.23	1.38
1	A	270	TYR	CA-CB	-7.38	1.41	1.53
2	D	567	GLN	CD-NE2	-7.34	1.17	1.33
7	H	590	GLU	N-CA	-7.09	1.37	1.46
5	F	382	LYS	CG-CD	-7.03	1.31	1.52
5	F	389	ASN	CG-OD1	-6.85	1.10	1.23
1	A	458	GLU	CD-OE1	-6.73	1.12	1.25
4	E	550	ASN	CG-ND2	-6.72	1.19	1.33
5	F	393	LYS	CD-CE	-6.69	1.32	1.52
1	A	270	TYR	CB-CG	-6.27	1.37	1.51
5	F	392	MET	CG-SD	-6.16	1.65	1.80
5	F	382	LYS	CE-NZ	-6.10	1.31	1.49
5	F	401	LYS	CB-CG	-6.07	1.34	1.52
2	B	437	MET	SD-CE	-5.86	1.65	1.79
1	A	303	PRO	CB-CG	-5.86	1.20	1.49
4	E	550	ASN	CG-OD1	-5.69	1.12	1.23
1	A	457	ARG	CG-CD	-5.69	1.35	1.52
5	F	510	ILE	CB-CG2	-5.52	1.34	1.52
8	I	1286	PHE	CE2-CZ	-5.49	1.22	1.38
1	A	271	ASP	C-N	5.30	1.46	1.33
4	E	43	LEU	CG-CD2	-5.24	1.35	1.52
5	F	400	GLN	C-O	-5.10	1.17	1.24
2	D	304	GLU	CG-CD	-5.01	1.39	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	590	GLU	CB-CG-CD	39.63	179.96	112.60
7	H	590	GLU	CA-CB-CG	30.07	174.25	114.10
7	H	590	GLU	N-CA-CB	18.10	137.17	110.20
5	F	392	MET	N-CA-CB	-17.28	83.68	110.30
5	F	389	ASN	OD1-CG-ND2	-16.21	106.39	122.60
5	F	393	LYS	CA-CB-CG	15.12	144.34	114.10
5	F	401	LYS	CB-CA-C	13.12	136.52	110.42
5	F	389	ASN	CB-CG-ND2	-12.98	96.93	116.40
7	H	590	GLU	N-CA-C	-12.63	96.15	111.69
5	F	393	LYS	CD-CE-NZ	11.79	149.64	111.90
7	H	590	GLU	CG-CD-OE1	-11.34	92.31	118.40
5	F	392	MET	CB-CA-C	11.23	133.29	110.38
5	F	401	LYS	N-CA-CB	-11.12	91.70	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	382	LYS	CG-CD-CE	11.05	136.71	111.30
1	A	270	TYR	CB-CG-CD2	-11.01	104.28	120.80
1	A	270	TYR	CA-CB-CG	10.24	132.34	113.90
7	H	590	GLU	CB-CA-C	-9.94	92.51	110.70
1	A	270	TYR	CB-CG-CD1	9.86	135.59	120.80
1	A	270	TYR	CB-CA-C	-9.23	92.04	110.42
5	F	382	LYS	CD-CE-NZ	8.89	140.36	111.90
5	F	392	MET	CB-CG-SD	8.83	139.19	112.70
5	F	392	MET	N-CA-C	-8.63	101.36	112.23
7	H	590	GLU	CG-CD-OE2	8.28	137.44	118.40
8	I	1282	ILE	CA-CB-CG2	8.23	124.49	110.50
5	F	400	GLN	CA-C-N	8.04	136.89	121.54
5	F	400	GLN	C-N-CA	8.04	136.89	121.54
3	C	186	MET	CB-CG-SD	7.98	136.64	112.70
3	C	186	MET	CG-SD-CE	7.94	118.38	100.90
2	D	711	GLU	CG-CD-OE2	-7.93	100.15	118.40
5	F	401	LYS	CA-CB-CG	7.72	129.53	114.10
5	F	389	ASN	CA-CB-CG	7.68	120.28	112.60
8	I	1258	CYS	CA-CB-SG	7.45	131.52	114.40
1	A	271	ASP	CA-C-N	6.61	128.10	119.84
1	A	271	ASP	C-N-CA	6.61	128.10	119.84
2	D	304	GLU	CG-CD-OE2	-6.54	103.35	118.40
5	F	389	ASN	CB-CG-OD1	6.19	133.18	120.80
2	D	631	ILE	CB-CG1-CD1	6.19	126.79	113.80
1	A	270	TYR	N-CA-C	-6.04	97.93	110.80
5	F	392	MET	CA-C-O	-5.82	112.92	119.79
1	A	62	PRO	CA-C-N	5.66	132.35	121.54
1	A	62	PRO	C-N-CA	5.66	132.35	121.54
5	F	392	MET	CG-SD-CE	5.62	113.25	100.90
5	F	618	SER	CA-C-N	5.49	130.20	122.46
5	F	618	SER	C-N-CA	5.49	130.20	122.46
8	I	938	MET	CG-SD-CE	-5.39	89.03	100.90
2	D	437	MET	CG-SD-CE	-5.34	89.16	100.90
5	F	534	GLN	CA-C-N	5.33	129.98	122.46
5	F	534	GLN	C-N-CA	5.33	129.98	122.46
1	A	304	GLU	CA-C-N	5.14	134.33	121.80
1	A	304	GLU	C-N-CA	5.14	134.33	121.80
5	F	392	MET	CA-CB-CG	5.06	124.23	114.10
8	I	698	PHE	CA-C-N	5.04	126.06	120.06
8	I	698	PHE	C-N-CA	5.04	126.06	120.06
8	I	1254	CYS	CA-CB-SG	-5.04	102.80	114.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	TYR	Mainchain
1	A	305	GLU	Peptide
5	F	389	ASN	Sidechain
5	F	397	SER	Mainchain
5	F	469	ASP	Peptide
7	H	589	HIS	Mainchain
8	I	1282	ILE	Mainchain
8	I	866	GLU	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	A	3552	0	3508	27	0
2	B	3250	0	3302	23	0
2	D	3445	0	3505	33	0
3	C	1266	0	1264	7	0
4	E	3333	0	3375	23	0
5	F	3349	0	3271	29	0
6	G	271	0	134	0	0
7	H	1419	0	1405	9	0
8	I	4474	0	4634	32	0
All	All	24359	0	24398	155	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 3.

All (155) 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)
4:E:43:LEU:HD11	7:H:513:LEU:HD21	1.70	0.73
3:C:173:ILE:HG23	2:D:726:ARG:HH12	1.62	0.65
5:F:600:GLN:HA	5:F:603:MET:HE3	1.82	0.61
8:I:929:SER:HB3	8:I:938:MET:HE1	1.82	0.61
5:F:392:MET:HA	5:F:395:ILE:HG22	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:327:ASN:HB3	4:E:330:GLN:HE21	1.68	0.58
2:B:453:LEU:HD13	2:D:437:MET:HE1	1.85	0.58
1:A:181:PHE:HB3	1:A:444:VAL:HG21	1.86	0.58
2:D:676:GLU:HA	2:D:679:MET:HE2	1.85	0.58
1:A:127:ILE:HD12	1:A:442:ILE:HD12	1.86	0.57
2:B:307:ILE:HG23	2:B:390:LEU:HD21	1.87	0.57
1:A:308:MET:HG2	1:A:415:LEU:HB3	1.88	0.56
1:A:115:PRO:HG3	2:D:721:ASN:HB2	1.89	0.55
2:B:557:SER:OG	2:B:559:GLU:OE1	2.24	0.55
2:D:589:LEU:HD12	2:D:592:LEU:HB3	1.88	0.55
8:I:749:LEU:HD21	8:I:938:MET:HG2	1.88	0.55
8:I:951:LEU:HD23	8:I:975:LEU:HD21	1.89	0.55
2:D:728:ASN:O	2:D:732:ASN:ND2	2.39	0.55
4:E:41:VAL:O	4:E:45:GLN:NE2	2.40	0.54
5:F:454:SER:OG	5:F:482:ASN:ND2	2.41	0.54
1:A:69:ILE:HG21	2:D:683:THR:HG21	1.90	0.53
1:A:121:ASN:HB2	1:A:446:ASP:HB3	1.91	0.53
2:D:433:GLN:HG3	2:D:435:PRO:HD2	1.90	0.53
2:D:361:TYR:OH	5:F:435:ARG:NH1	2.42	0.53
2:D:714:THR:O	2:D:718:GLN:NE2	2.41	0.53
5:F:315:ASP:HA	8:I:658:ARG:HH12	1.74	0.53
2:B:459:GLU:HG2	2:B:462:ARG:HH21	1.75	0.52
8:I:699:ALA:HA	8:I:702:LEU:HD23	1.91	0.52
8:I:1227:GLN:HB3	8:I:1230:SER:HB3	1.91	0.52
5:F:314:TYR:O	8:I:658:ARG:NH1	2.43	0.52
5:F:461:ARG:NH2	5:F:728:ARG:O	2.43	0.52
2:B:667:ARG:HB3	2:B:670:ILE:HD13	1.92	0.52
5:F:548:LEU:HD21	5:F:559:ASP:HB3	1.91	0.52
8:I:1091:LEU:O	8:I:1095:ASN:ND2	2.42	0.52
2:B:611:ILE:HA	2:B:614:LEU:HG	1.92	0.52
1:A:399:ASP:OD1	1:A:399:ASP:N	2.43	0.51
8:I:1254:CYS:O	8:I:1257:ASN:N	2.43	0.51
2:B:557:SER:HB3	2:B:560:GLN:HG3	1.91	0.51
1:A:550:GLU:OE1	2:B:567:GLN:NE2	2.44	0.51
2:B:313:TRP:HE1	2:B:388:TRP:HE1	1.59	0.51
2:D:632:GLN:HE22	2:D:640:GLN:HE21	1.57	0.51
1:A:55:HIS:ND1	3:C:97:GLU:OE1	2.44	0.51
1:A:59:MET:N	1:A:59:MET:SD	2.85	0.50
2:B:619:ASN:ND2	2:B:622:THR:OG1	2.42	0.50
2:D:420:ARG:NH2	2:D:425:PHE:O	2.44	0.50
4:E:43:LEU:HA	4:E:46:ILE:HG22	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:527:TRP:HE1	2:D:556:LYS:HD3	1.76	0.50
4:E:116:THR:HB	4:E:126:LEU:HD11	1.92	0.50
7:H:455:MET:HE3	7:H:456:PRO:HD2	1.94	0.49
4:E:99:LYS:NZ	4:E:209:ASP:O	2.44	0.49
4:E:290:ILE:HG21	5:F:745:VAL:HG11	1.94	0.49
5:F:389:ASN:O	5:F:392:MET:N	2.45	0.49
7:H:475:ALA:O	8:I:670:ARG:NH1	2.45	0.49
1:A:381:LEU:HG	1:A:385:LEU:HD22	1.94	0.49
2:B:440:LEU:HD12	2:B:444:MET:HE1	1.95	0.49
8:I:1254:CYS:O	8:I:1258:CYS:N	2.46	0.49
8:I:1020:SER:OG	8:I:1021:GLU:N	2.45	0.49
3:C:97:GLU:N	3:C:97:GLU:OE2	2.46	0.48
2:D:304:GLU:OE2	4:E:552:ASN:HA	2.13	0.48
8:I:1220:LYS:HA	8:I:1225:GLN:HG2	1.95	0.48
2:D:305:ILE:HA	2:D:394:GLN:HE22	1.78	0.48
8:I:932:ASP:N	8:I:932:ASP:OD1	2.45	0.48
4:E:48:GLN:OE1	4:E:49:ILE:HG23	2.12	0.48
5:F:505:THR:O	5:F:509:HIS:ND1	2.47	0.48
8:I:707:LEU:HA	8:I:710:LEU:HD12	1.96	0.48
4:E:68:LEU:HD21	4:E:211:TRP:HB2	1.96	0.48
8:I:979:LEU:HA	8:I:982:ILE:HG22	1.94	0.48
1:A:544:ASN:ND2	2:B:578:ASP:O	2.47	0.47
4:E:276:ILE:HG13	4:E:277:VAL:HG23	1.95	0.47
4:E:61:ASP:O	4:E:228:LYS:NZ	2.42	0.47
2:B:436:ASP:C	2:B:437:MET:HE2	2.40	0.47
4:E:101:GLY:O	4:E:189:ARG:NH1	2.45	0.47
8:I:759:LEU:HD12	8:I:914:ILE:HG23	1.96	0.47
2:B:440:LEU:O	2:B:444:MET:HE3	2.15	0.47
3:C:129:ASP:N	3:C:129:ASP:OD1	2.46	0.47
1:A:298:LEU:HB2	1:A:420:PRO:HB3	1.96	0.46
2:B:685:GLU:HA	2:B:688:ARG:HG2	1.97	0.46
2:D:356:LEU:HD12	5:F:738:LEU:HD21	1.98	0.46
4:E:550:ASN:HD22	5:F:751:SER:C	2.24	0.46
8:I:1212:LEU:O	8:I:1216:ASN:ND2	2.47	0.46
2:D:320:HIS:HD2	2:D:322:ILE:HG12	1.81	0.46
2:B:524:ASP:OD1	2:B:524:ASP:N	2.46	0.46
5:F:316:PRO:HA	5:F:317:PRO:HD3	1.82	0.46
8:I:716:SER:OG	8:I:721:GLU:OE2	2.31	0.46
1:A:470:ALA:HA	1:A:473:LEU:HG	1.97	0.46
4:E:539:THR:HG22	5:F:762:SER:HA	1.97	0.46
1:A:186:VAL:HG22	1:A:267:LYS:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:473:ASP:OD1	7:H:473:ASP:N	2.47	0.46
1:A:186:VAL:HB	1:A:296:SER:HB2	1.98	0.45
4:E:280:GLN:NE2	4:E:282:SER:OG	2.49	0.45
2:B:514:LEU:HD23	2:D:446:THR:HG23	1.98	0.45
2:D:566:LEU:HD11	2:D:615:VAL:HG21	1.97	0.45
7:H:441:VAL:HG21	8:I:660:ILE:HD12	1.98	0.45
2:B:578:ASP:OD1	2:B:578:ASP:N	2.46	0.45
4:E:73:TYR:OH	4:E:194:GLU:OE1	2.34	0.45
5:F:496:LEU:HD23	5:F:506:ARG:HG3	1.98	0.44
7:H:443:ILE:HD11	8:I:662:ARG:HD2	1.99	0.44
2:D:383:LYS:HA	2:D:383:LYS:HD3	1.80	0.44
2:B:385:LEU:HD23	2:B:385:LEU:HA	1.90	0.44
8:I:1189:LEU:HA	8:I:1192:VAL:HG22	2.00	0.44
4:E:292:ASN:HD22	4:E:299:ILE:HG22	1.83	0.44
2:D:524:ASP:OD1	2:D:524:ASP:N	2.47	0.44
1:A:63:ASP:OD1	1:A:64:HIS:N	2.51	0.44
1:A:96:MET:HG2	2:D:707:PHE:CE2	2.53	0.44
2:B:352:ASN:HA	2:B:355:ARG:HG2	2.00	0.44
8:I:1184:ASN:OD1	8:I:1184:ASN:N	2.51	0.44
5:F:624:ASP:O	5:F:627:SER:OG	2.34	0.43
2:D:299:ILE:HG23	4:E:503:ILE:HD11	2.00	0.43
5:F:506:ARG:O	5:F:510:ILE:HG12	2.18	0.43
1:A:270:TYR:O	1:A:275:PRO:HB3	2.18	0.43
4:E:456:GLU:O	4:E:460:GLN:NE2	2.51	0.43
5:F:476:THR:OG1	5:F:731:ARG:NH2	2.47	0.43
2:D:443:MET:HE3	7:H:500:LEU:HD22	2.00	0.43
5:F:382:LYS:O	5:F:385:GLN:N	2.52	0.43
2:D:335:ILE:HD11	5:F:452:GLU:HG3	2.01	0.43
4:E:455:LEU:O	4:E:459:LYS:HB2	2.18	0.43
2:D:437:MET:HA	2:D:440:LEU:HB2	2.01	0.42
2:D:773:MET:SD	2:D:779:THR:OG1	2.75	0.42
5:F:540:ASP:O	5:F:566:SER:OG	2.32	0.42
8:I:665:LYS:NZ	8:I:666:PRO:O	2.47	0.42
1:A:512:VAL:O	1:A:516:ASN:ND2	2.51	0.42
5:F:341:GLN:HE21	5:F:345:ARG:HH21	1.65	0.42
8:I:742:LEU:HD13	8:I:749:LEU:HD11	2.01	0.42
2:D:359:ASN:ND2	4:E:552:ASN:OD1	2.49	0.42
2:B:729:PHE:HZ	2:D:736:ILE:HG21	1.84	0.42
8:I:1224:LEU:HB3	8:I:1230:SER:HB2	2.02	0.42
1:A:310:TYR:OH	1:A:324:THR:O	2.32	0.42
1:A:377:SER:HB2	1:A:403:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:698:PHE:CD2	8:I:700:PRO:HD2	2.55	0.42
1:A:388:LEU:O	1:A:414:HIS:NE2	2.40	0.42
5:F:499:TYR:HE1	5:F:734:VAL:HG12	1.85	0.42
2:B:374:ASP:OD2	2:B:377:ALA:N	2.49	0.41
3:C:182:SER:O	3:C:186:MET:HG3	2.20	0.41
2:B:600:PHE:HB2	7:H:490:THR:HG21	2.03	0.41
8:I:1255:PHE:HA	8:I:1258:CYS:HB2	2.02	0.41
7:H:445:ASP:HA	7:H:446:PRO:HD3	1.95	0.41
4:E:563:LYS:HD3	4:E:563:LYS:HA	1.92	0.41
8:I:1282:ILE:CG2	8:I:1286:PHE:HE2	2.33	0.41
5:F:399:SER:C	5:F:401:LYS:H	2.29	0.41
1:A:300:LYS:HA	1:A:300:LYS:HD2	1.86	0.41
2:D:721:ASN:HA	2:D:724:ILE:HG22	2.03	0.41
5:F:335:ASP:OD1	5:F:335:ASP:N	2.48	0.41
5:F:422:THR:OG1	5:F:425:ARG:NH1	2.54	0.41
1:A:185:ILE:HG12	1:A:297:ILE:HG12	2.02	0.41
1:A:443:GLU:H	3:C:204:VAL:HG12	1.85	0.41
2:D:417:ASP:OD1	2:D:417:ASP:N	2.46	0.41
8:I:964:CYS:HB3	8:I:967:LYS:HG2	2.03	0.40
2:D:385:LEU:HD23	2:D:385:LEU:HA	1.96	0.40
5:F:383:TYR:HA	5:F:386:ASP:OD2	2.20	0.40
8:I:1049:LEU:HD23	8:I:1049:LEU:HA	1.98	0.40
8:I:1214:ILE:HD12	8:I:1214:ILE:HA	1.97	0.40
1:A:182:ILE:HG21	1:A:185:ILE:HG13	2.03	0.40
3:C:175:ALA:O	3:C:180:SER:OG	2.32	0.40
2:D:550:ALA:HA	2:D:553:VAL:HG12	2.03	0.40
5:F:542:LEU:HD23	5:F:629:MET:HE1	2.04	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	436/566 (77%)	413 (95%)	20 (5%)	3 (1%)	18	51
2	B	385/825 (47%)	374 (97%)	11 (3%)	0	100	100
2	D	413/825 (50%)	389 (94%)	24 (6%)	0	100	100
3	C	146/332 (44%)	136 (93%)	10 (7%)	0	100	100
4	E	401/623 (64%)	382 (95%)	19 (5%)	0	100	100
5	F	404/905 (45%)	372 (92%)	31 (8%)	1 (0%)	43	74
6	G	13/82 (16%)	11 (85%)	1 (8%)	1 (8%)	1	8
7	H	175/1703 (10%)	165 (94%)	10 (6%)	0	100	100
8	I	538/1314 (41%)	513 (95%)	23 (4%)	2 (0%)	30	62
All	All	2911/7175 (41%)	2755 (95%)	149 (5%)	7 (0%)	44	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
5	F	401	LYS
1	A	302	SER
6	G	90	LEU
8	I	1051	LYS
8	I	867	PRO
1	A	62	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	408/517 (79%)	408 (100%)	0	100	100
2	B	368/751 (49%)	368 (100%)	0	100	100
2	D	392/751 (52%)	392 (100%)	0	100	100
3	C	141/288 (49%)	141 (100%)	0	100	100
4	E	368/558 (66%)	368 (100%)	0	100	100
5	F	376/823 (46%)	375 (100%)	1 (0%)	86	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	7/15 (47%)	7 (100%)	0	100	100
7	H	165/1520 (11%)	164 (99%)	1 (1%)	78	79
8	I	528/1218 (43%)	528 (100%)	0	100	100
All	All	2753/6441 (43%)	2751 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	392	MET
7	H	590	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	274	ASN
1	A	483	GLN
1	A	516	ASN
1	A	544	ASN
1	A	549	ASN
1	A	556	ASN
2	B	315	ASN
2	B	333	ASN
2	B	370	ASN
2	B	394	GLN
2	B	403	ASN
2	B	605	ASN
2	B	619	ASN
2	B	624	GLN
2	B	731	GLN
2	B	738	ASN
3	C	78	GLN
3	C	147	GLN
3	C	150	HIS
3	C	207	HIS
2	D	394	GLN
2	D	552	ASN
2	D	555	ASN
2	D	587	ASN
2	D	624	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	640	GLN
2	D	669	HIS
2	D	718	GLN
2	D	725	GLN
2	D	730	ASN
2	D	732	ASN
4	E	38	HIS
4	E	45	GLN
4	E	115	ASN
4	E	280	GLN
4	E	306	GLN
4	E	330	GLN
4	E	558	ASN
5	F	341	GLN
5	F	480	ASN
5	F	482	ASN
5	F	555	ASN
5	F	581	GLN
5	F	602	HIS
5	F	651	ASN
7	H	498	GLN
7	H	583	ASN
7	H	588	ASN
8	I	675	ASN
8	I	766	ASN
8	I	771	HIS
8	I	805	ASN
8	I	860	GLN
8	I	874	GLN
8	I	915	ASN
8	I	917	GLN
8	I	981	ASN
8	I	1095	ASN
8	I	1142	GLN
8	I	1188	ASN
8	I	1213	ASN
8	I	1215	ASN
8	I	1216	ASN
8	I	1298	GLN
8	I	1300	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	441:GLN	C	442:TYR	N	4.07
1	E	52:GLN	C	53:ASP	N	3.99
1	E	242:PRO	C	243:SER	N	3.85
1	A	110:GLN	C	111:GLU	N	3.20

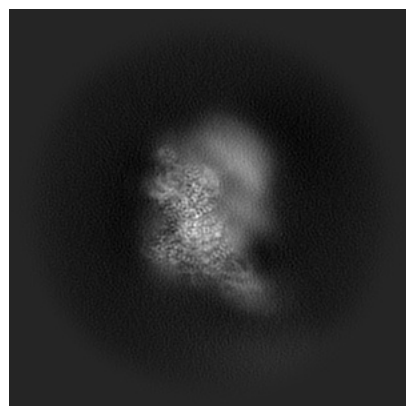
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71489. These allow visual inspection of the internal detail of the map and identification of artifacts.

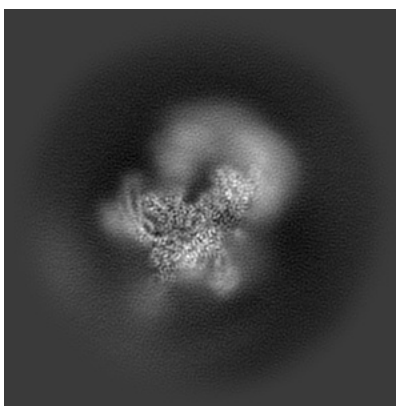
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

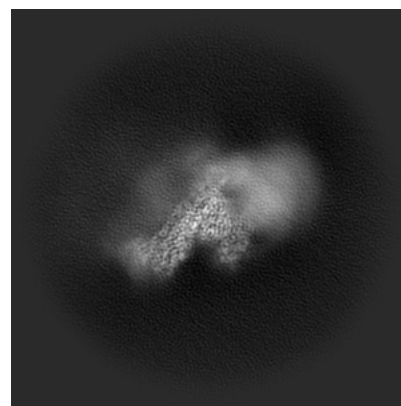
6.1.1 Primary map



X

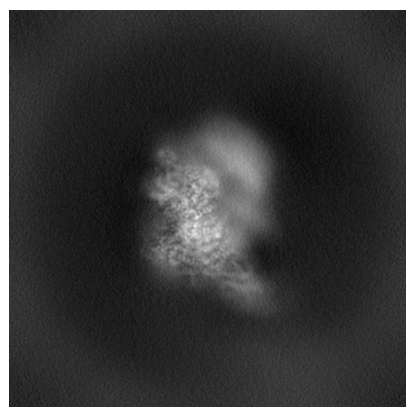


Y

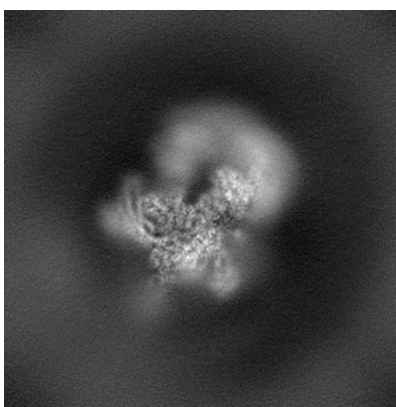


Z

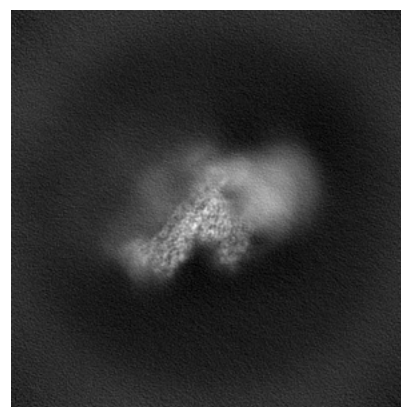
6.1.2 Raw map



X



Y

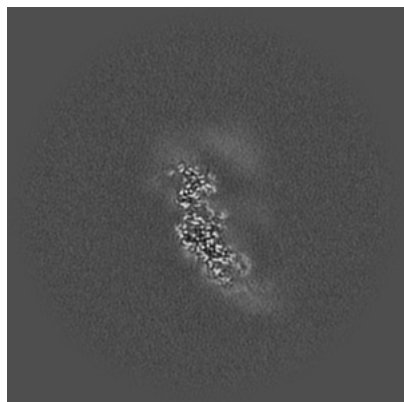


Z

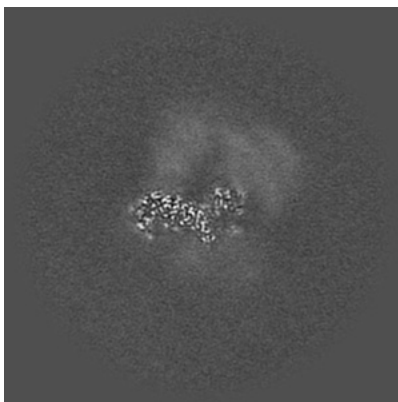
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

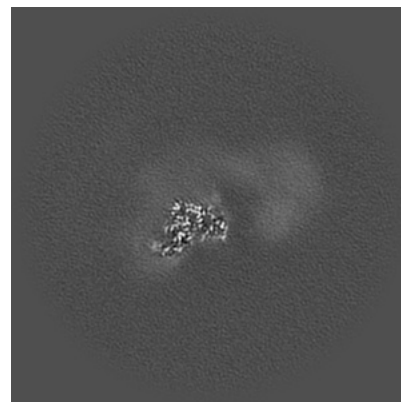
6.2.1 Primary map



X Index: 160

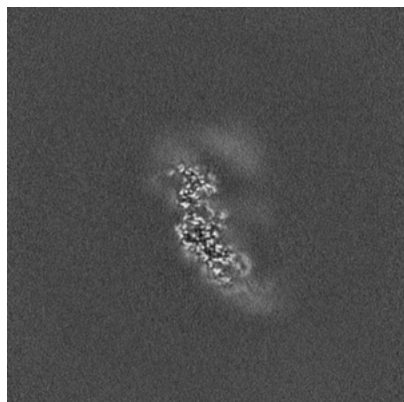


Y Index: 160

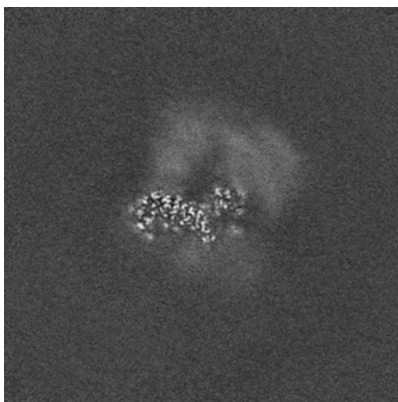


Z Index: 160

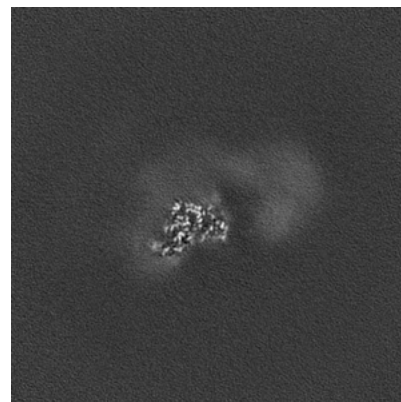
6.2.2 Raw map



X Index: 160



Y Index: 160

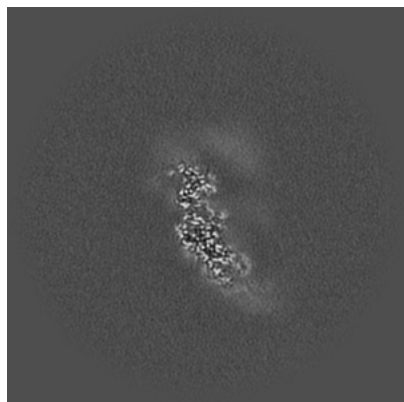


Z Index: 160

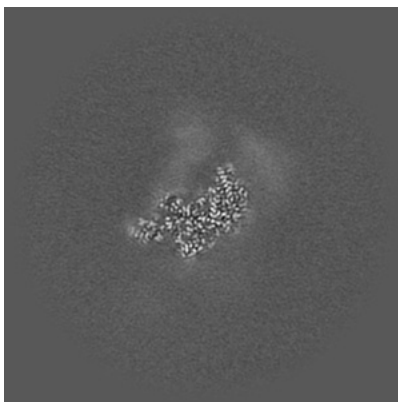
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

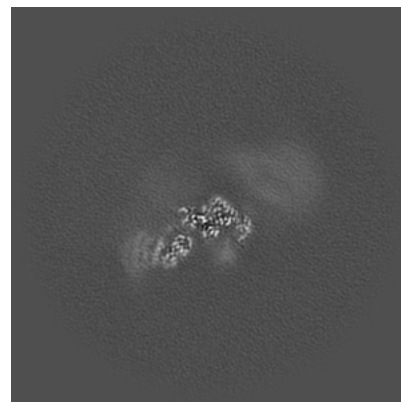
6.3.1 Primary map



X Index: 160

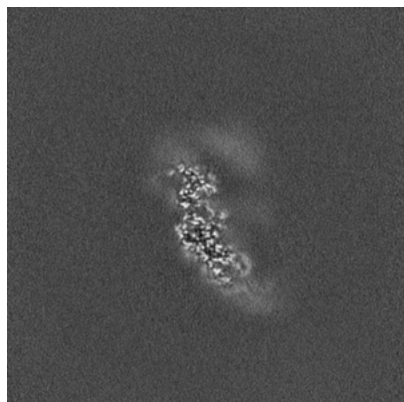


Y Index: 148

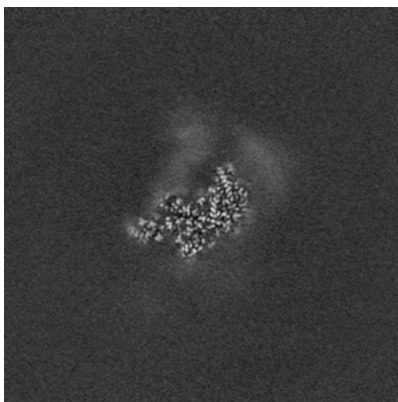


Z Index: 171

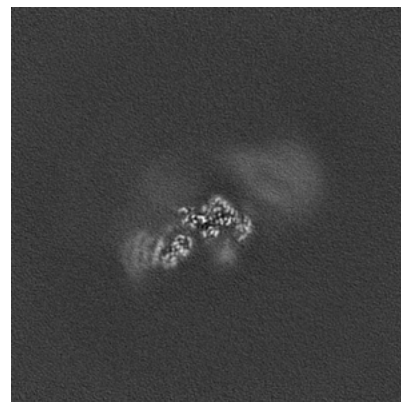
6.3.2 Raw map



X Index: 160



Y Index: 148

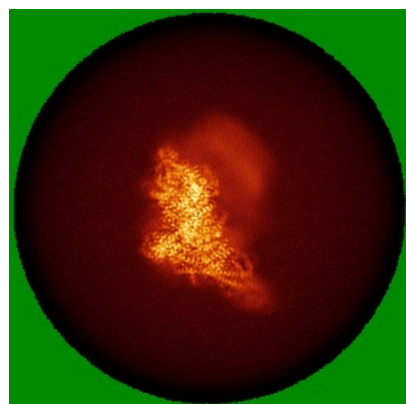


Z Index: 171

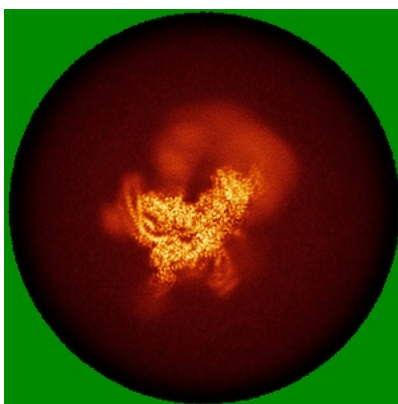
The images above show the largest variance slices of the map in three orthogonal directions.

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

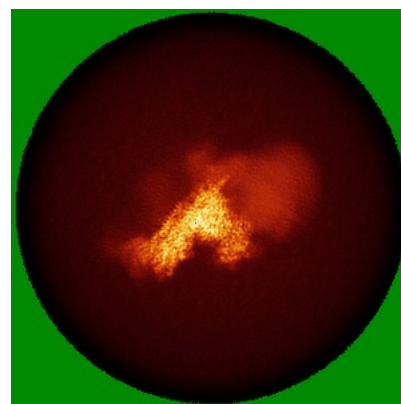
6.4.1 Primary map



X

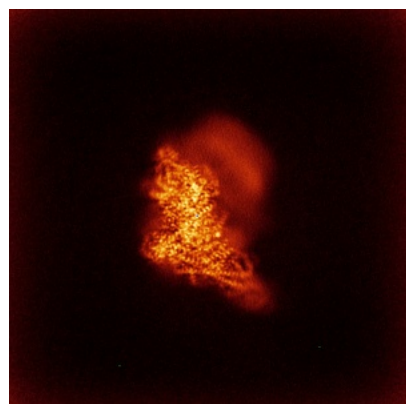


Y

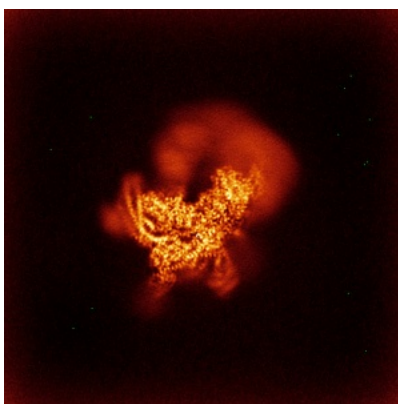


Z

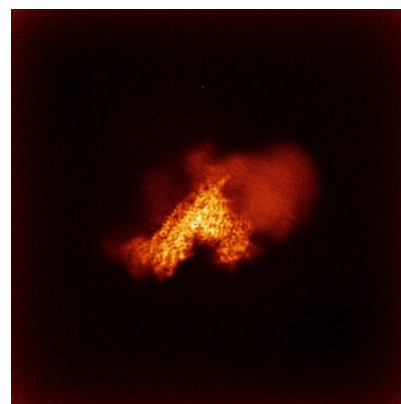
6.4.2 Raw map



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.

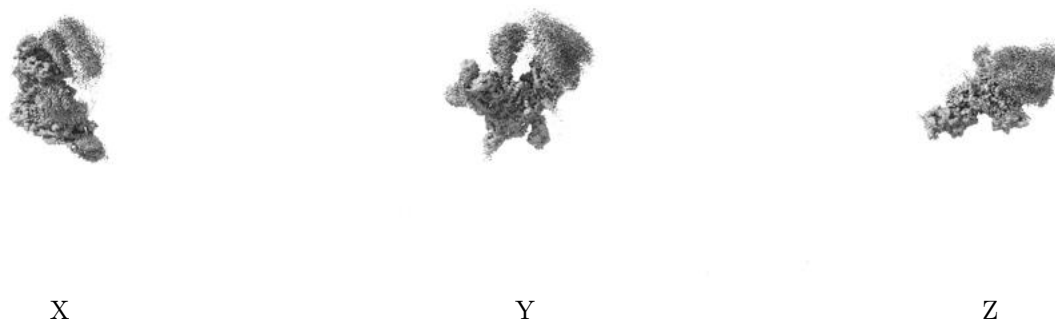
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.402. 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.

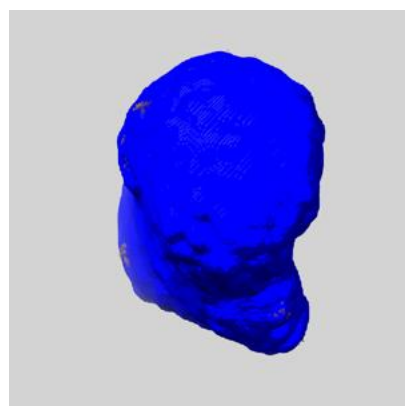
6.6 Mask visualisation [i](#)

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

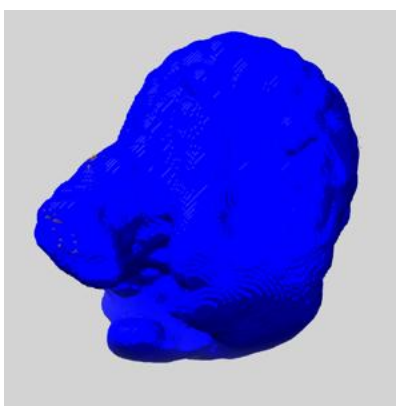
A mask typically either:

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

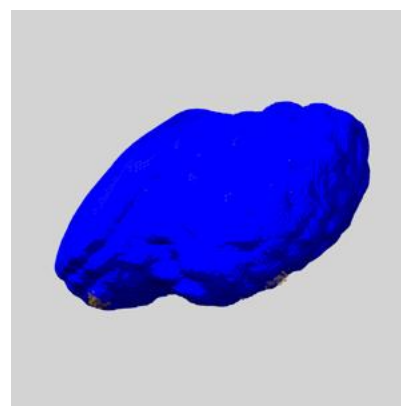
6.6.1 emd_71489_msk_1.map [i](#)



X



Y

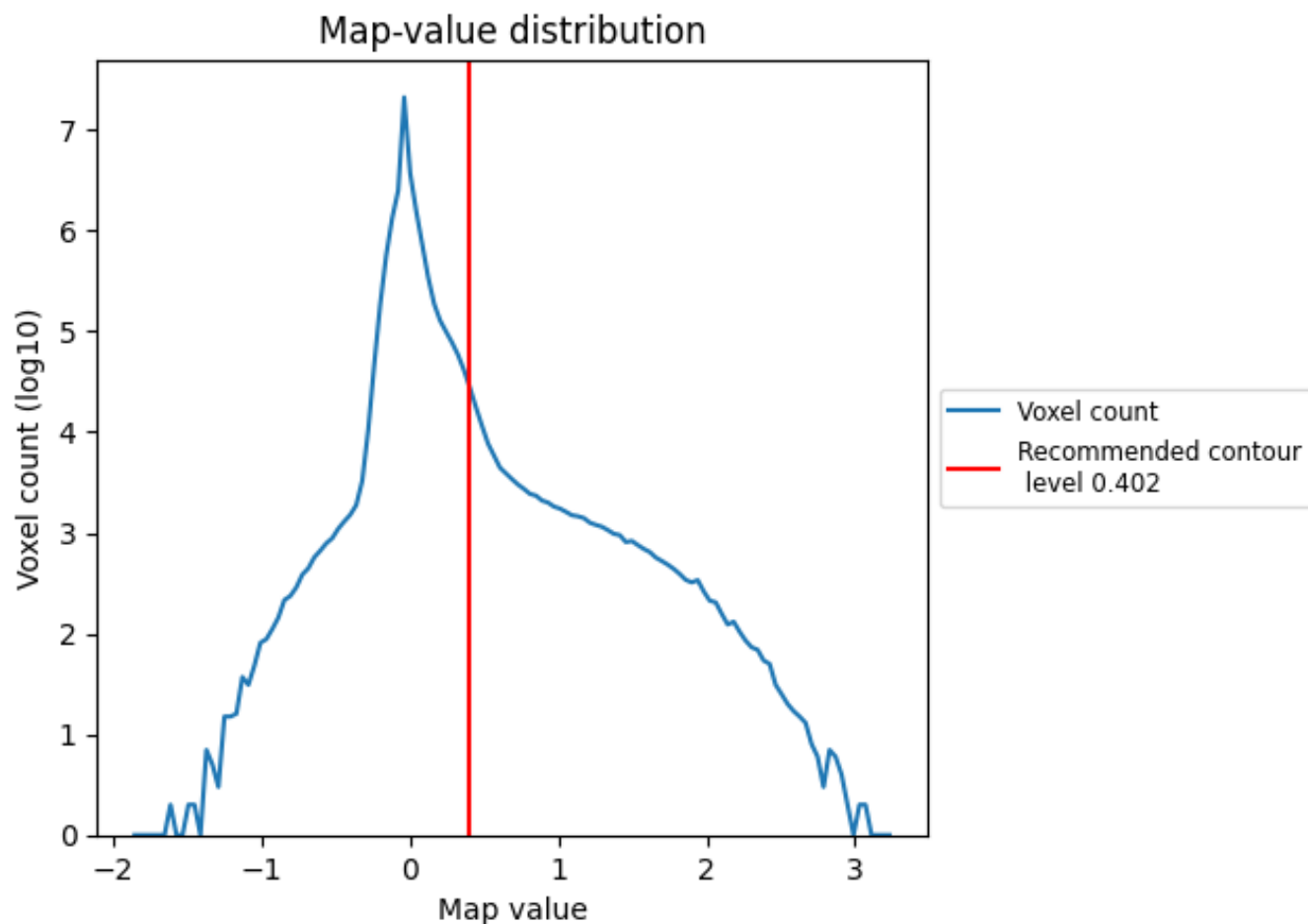


Z

7 Map analysis [i](#)

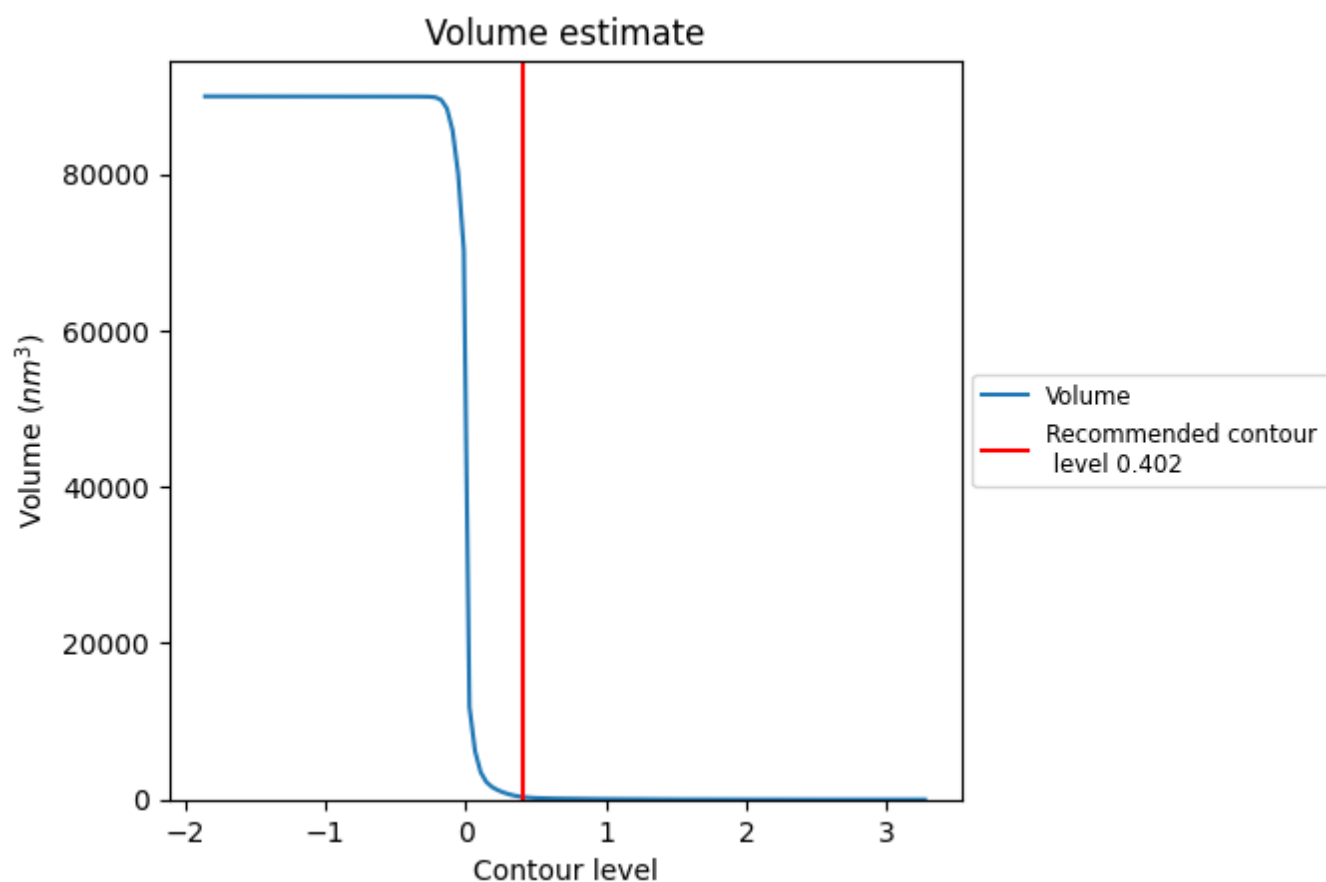
This section contains the results of statistical analysis of the map.

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.

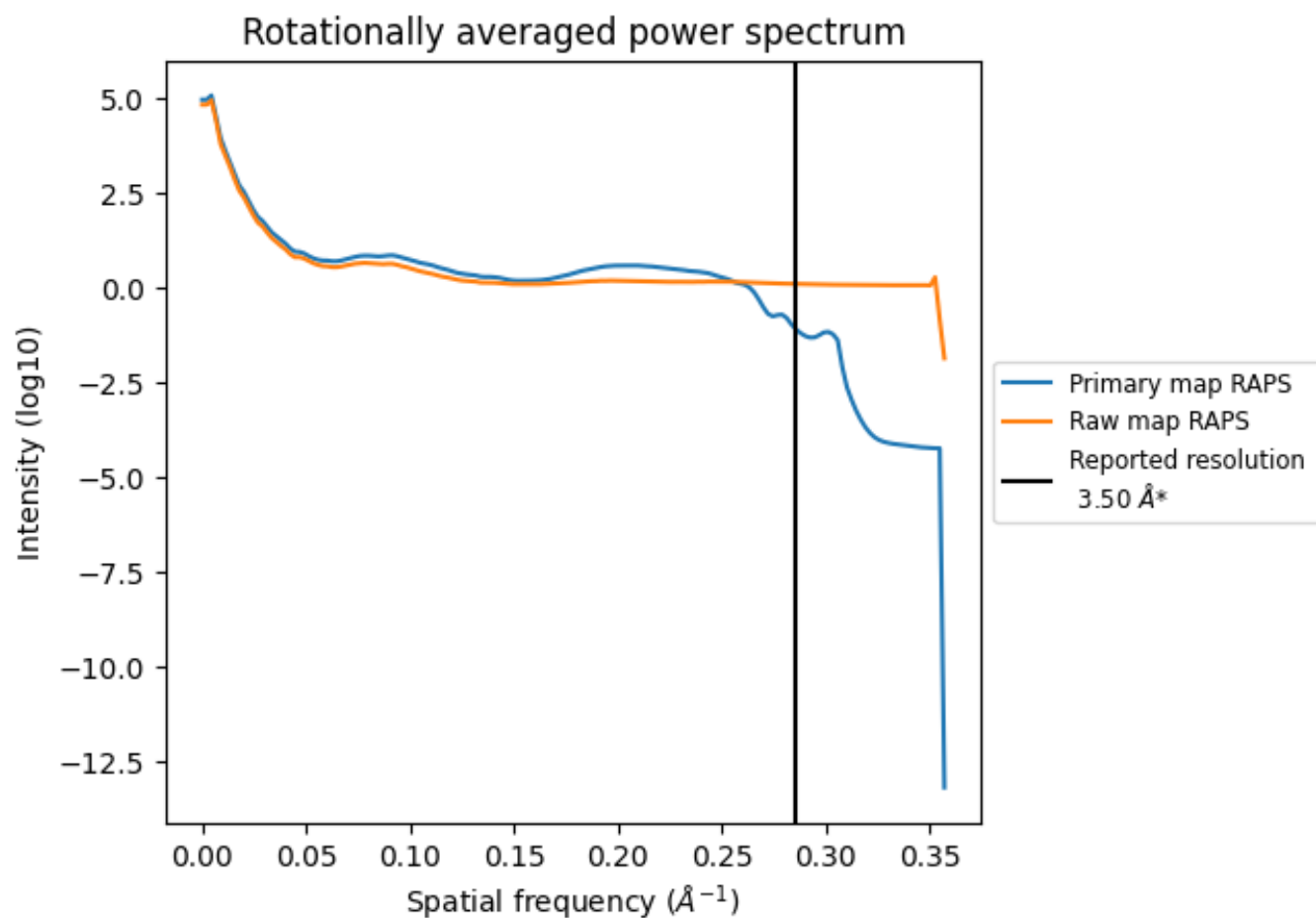
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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 ⓘ

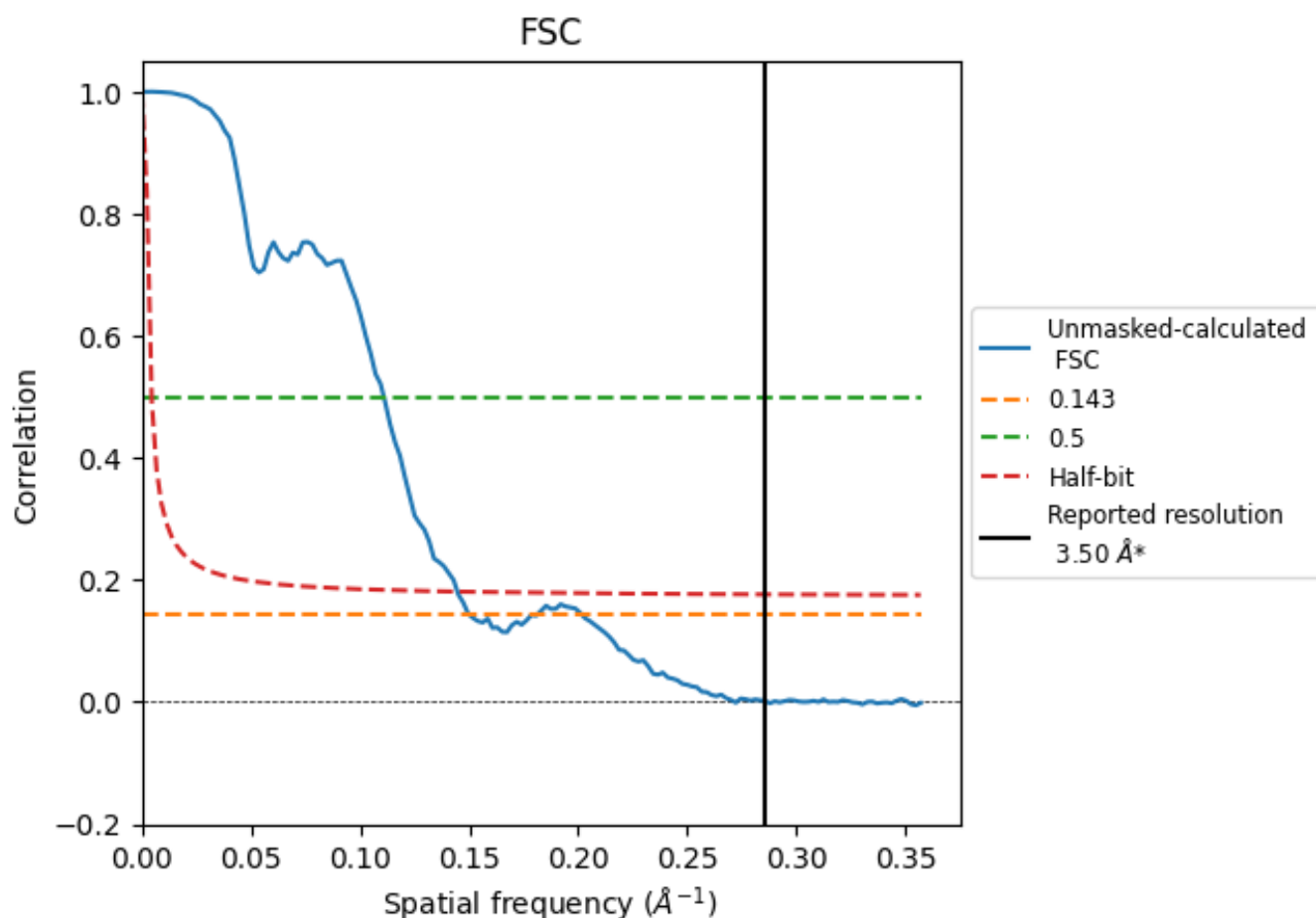


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

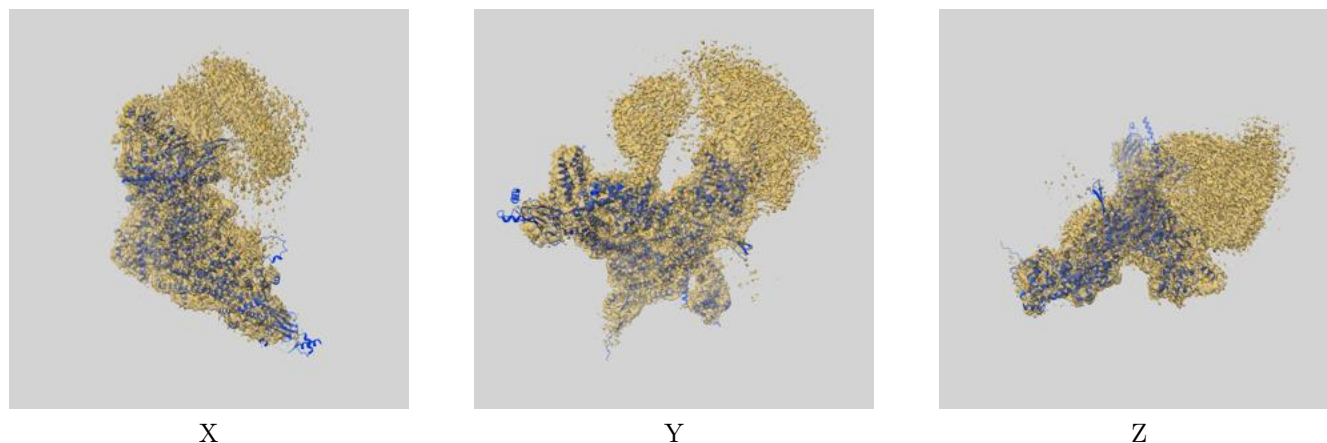
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	9.02	6.92

*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 6.67 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

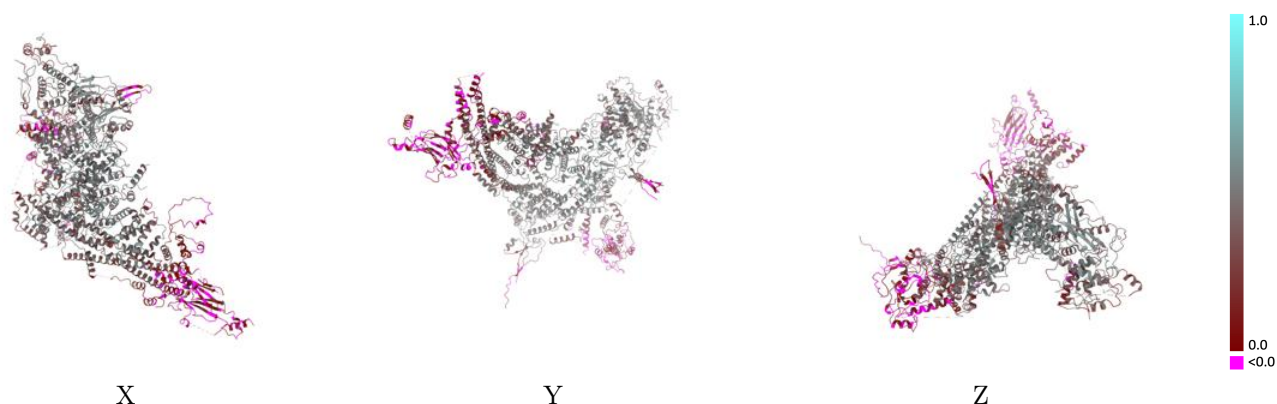
This section contains information regarding the fit between EMDB map EMD-71489 and PDB model 9PBS. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



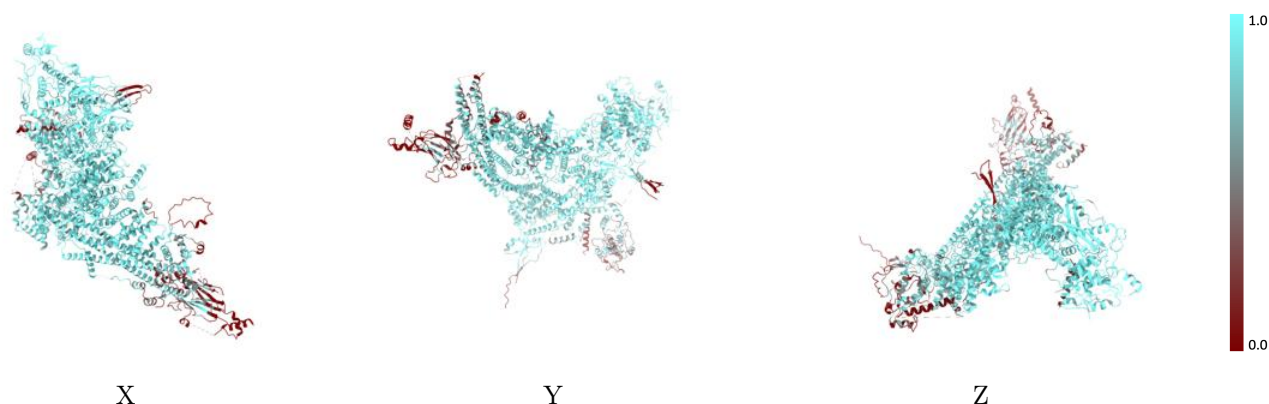
The images above show the 3D surface view of the map at the recommended contour level 0.402 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



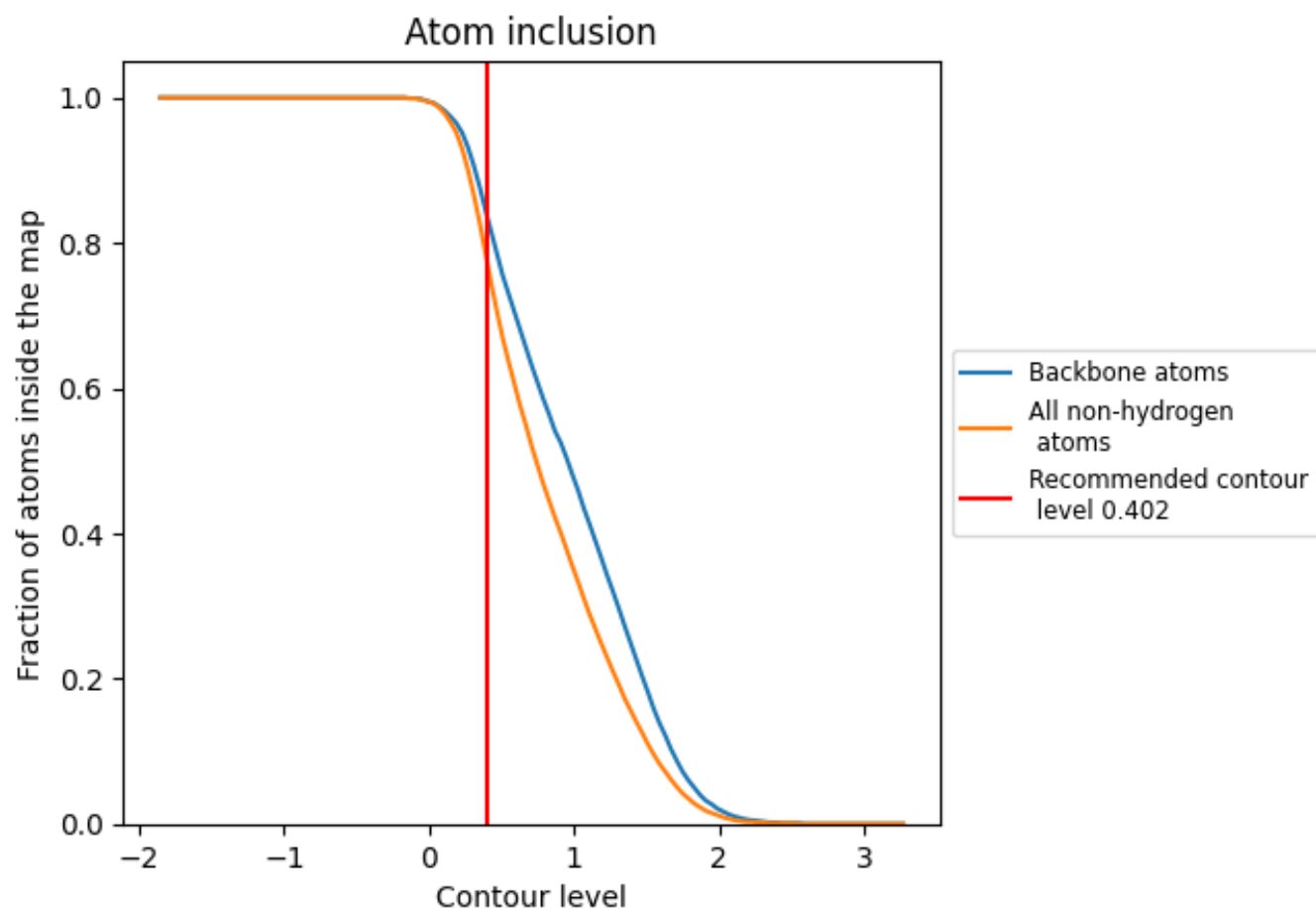
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.402).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.402) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.3450
A	0.5710	0.2120
B	0.8310	0.3680
C	0.6530	0.2950
D	0.8040	0.3700
E	0.6250	0.2330
F	0.8620	0.4160
G	0.9510	0.4340
H	0.9070	0.4270
I	0.8840	0.4300

1.0

0.0

<0.0