



Full wwPDB EM Validation Report ⓘ

May 27, 2026 – 12:53 PM EDT

PDB ID : 9YLE / pdb_00009yle
EMDB ID : EMD-73080
Title : State 3 MLL4FC bound to a nucleosome premodified with H2BK120ub and H4K16ac
Authors : Sun, J.; Roeder, R.
Deposited on : 2025-10-08
Resolution : 3.63 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:

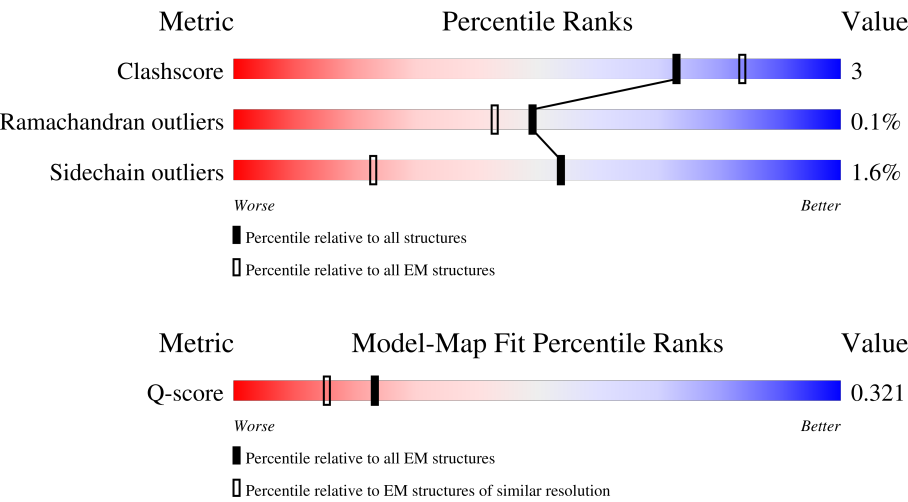
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.63 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.









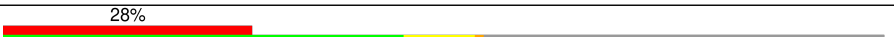
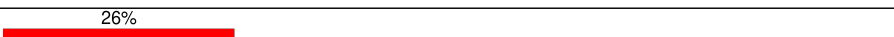
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11696 (3.13 - 4.13)

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	O	76	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>89%11%</div></div>
2	K	1256	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>35%51%45%</div></div>
3	N	538	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>65%6%29%</div></div>
4	T	628	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>13%46%53%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	135	
5	E	135	
6	B	102	
6	F	102	
7	C	129	
7	G	129	
8	D	125	
8	H	125	
9	J	147	
10	R	334	
11	I	147	
12	P	99	
12	Q	99	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 26853 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 Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	76	Total	C	N	O	S	0	0
			603	379	105	117	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	76	CYS	GLY	engineered mutation	UNP P0CG47

- Molecule 2 is a protein called [histone H3]-lysine(4) N-methyltransferase,Histone-lysine N-methyltransferase 2D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	687	Total	C	N	O	S	0	0
			5469	3431	974	994	70		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1348	MET	-	expression tag	UNP A0A6P6IDI8
K	1349	ASP	-	expression tag	UNP A0A6P6IDI8
K	1350	TYR	-	expression tag	UNP A0A6P6IDI8
K	1351	LYS	-	expression tag	UNP A0A6P6IDI8
K	1352	ASP	-	expression tag	UNP A0A6P6IDI8
K	1353	ASP	-	expression tag	UNP A0A6P6IDI8
K	1354	ASP	-	expression tag	UNP A0A6P6IDI8
K	1355	ASP	-	expression tag	UNP A0A6P6IDI8
K	1356	LYS	-	expression tag	UNP A0A6P6IDI8
K	1357	SER	-	expression tag	UNP A0A6P6IDI8

- Molecule 3 is a protein called Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	382	Total	C	N	O	S	0	0
			2977	1876	508	577	16		

- Molecule 4 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	297	Total	C	N	O	S	0	0
			2397	1549	395	445	8		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
5	E	100	Total	C	N	O	S	0	0
			825	520	160	141	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	87	Total	C	N	O	S	0	0
			703	442	142	118	1		
6	F	84	Total	C	N	O	S	0	0
			673	424	133	115	1		

- Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	108	Total	C	N	O		0	0
			835	526	165	144			
7	G	104	Total	C	N	O		0	0
			805	508	157	140			

- Molecule 8 is a protein called Histone H2B type 2-E.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	96	Total	C	N	O	S	0	0
			755	474	138	141	2		
8	H	92	Total	C	N	O	S	0	0
			719	453	129	135	2		

- Molecule 9 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	145	Total	C	N	O	P	0	0
			2988	1414	560	869	145		

- Molecule 10 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	300	Total	C	N	O	S	0	0
			2326	1485	388	444	9		

- Molecule 11 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	145	Total	C	N	O	P	0	0
			2957	1404	537	871	145		

- Molecule 12 is a protein called Protein dpy-30 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	P	54	Total	C	N	O	0	0
			431	279	73	79		
12	Q	54	Total	C	N	O	0	0
			432	279	73	80		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	N	1	Total	O	0
			1	1	
13	A	18	Total	O	0
			18	18	
13	B	14	Total	O	0
			14	14	
13	C	22	Total	O	0
			22	22	
13	D	16	Total	O	0
			16	16	
13	E	28	Total	O	0
			28	28	
13	F	28	Total	O	0
			28	28	
13	G	13	Total	O	0
			13	13	

Continued on next page...


Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
13	H	8	Total 8	O 8	0
13	J	5	Total 5	O 5	0
13	I	4	Total 4	O 4	0

3 Residue-property plots

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

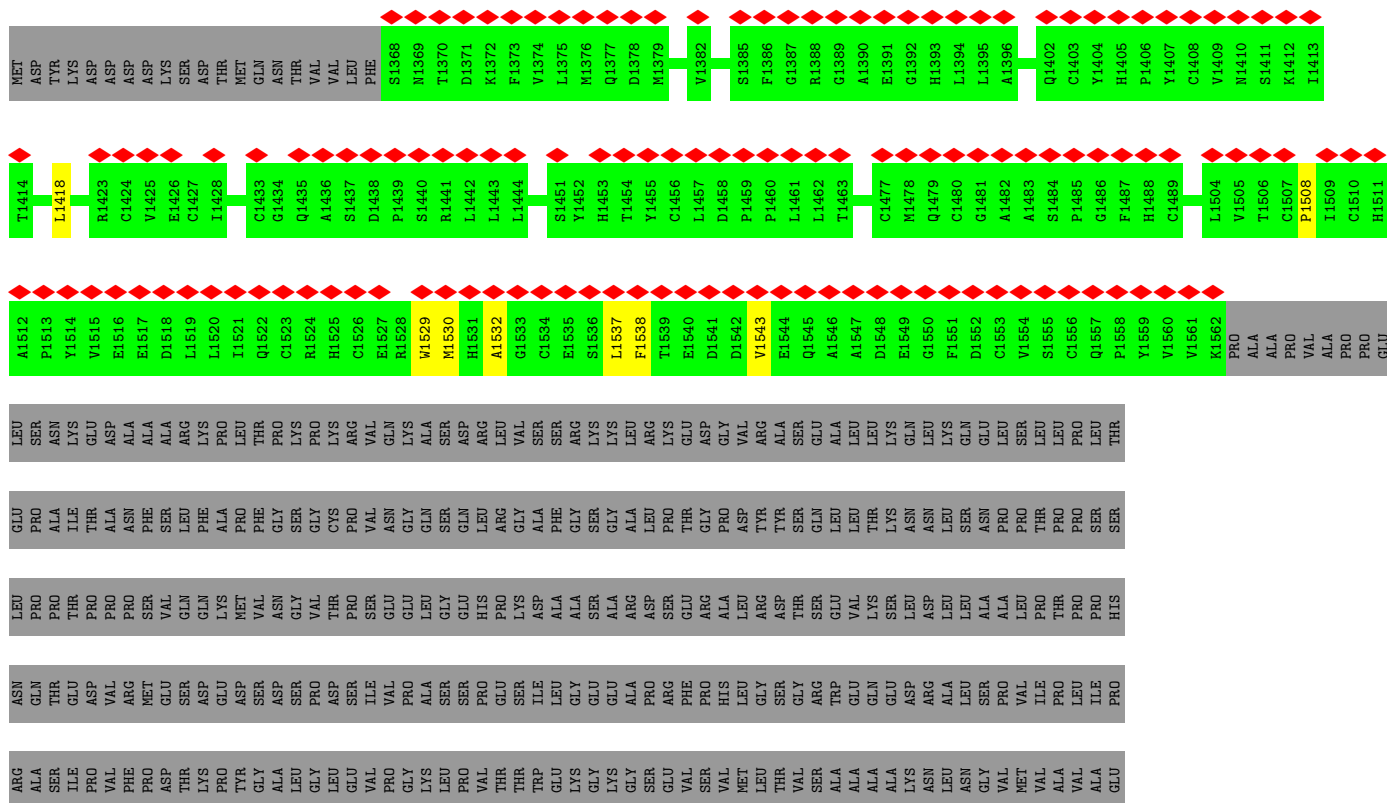
- Molecule 1: Ubiquitin

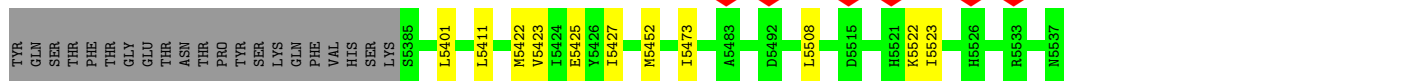
Chain O: 



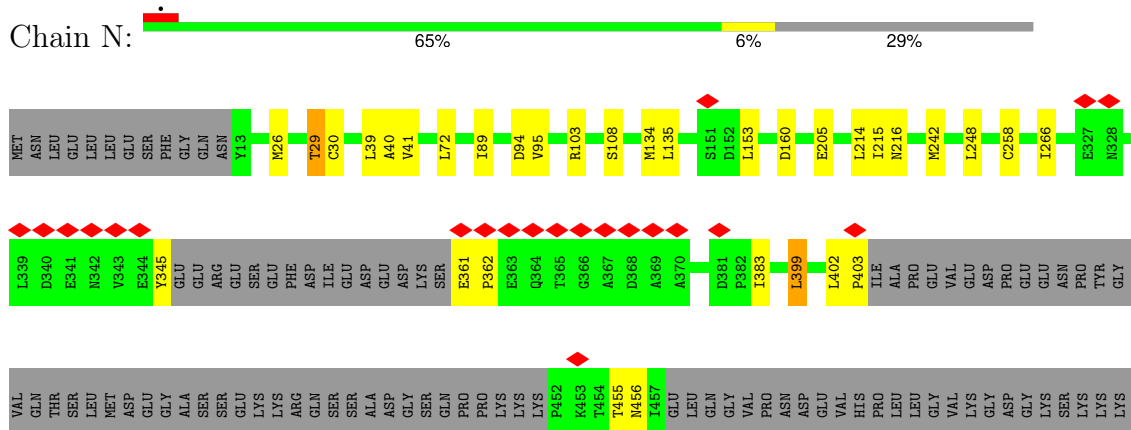
- Molecule 2: [histone H3]-lysine(4) N-methyltransferase,Histone-lysine N-methyltransferase 2D

Chain K: 



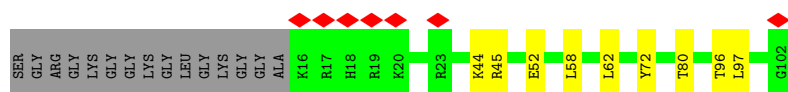


- Molecule 3: Retinoblastoma-binding protein 5

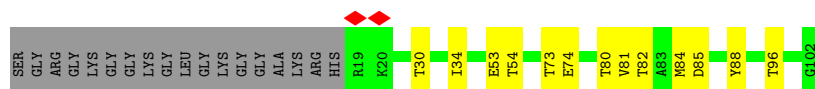


Frequency	Percentage
Often	13%
Sometimes	46%
Never	53%

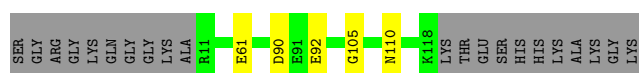
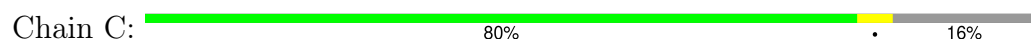




- Molecule 6: Histone H4



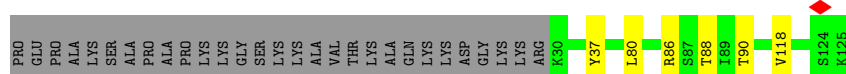
- Molecule 7: Histone H2A type 1-B/E



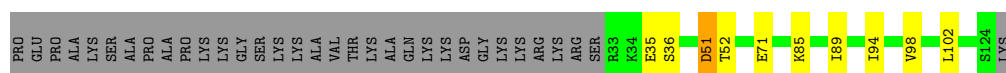
- Molecule 7: Histone H2A type 1-B/E



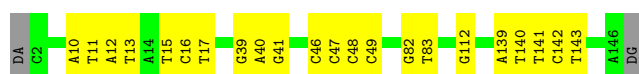
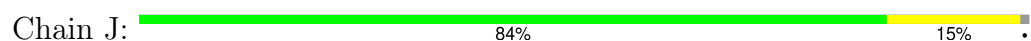
- Molecule 8: Histone H2B type 2-E



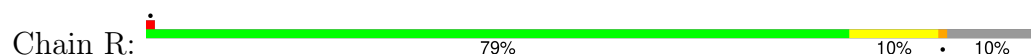
- Molecule 8: Histone H2B type 2-E

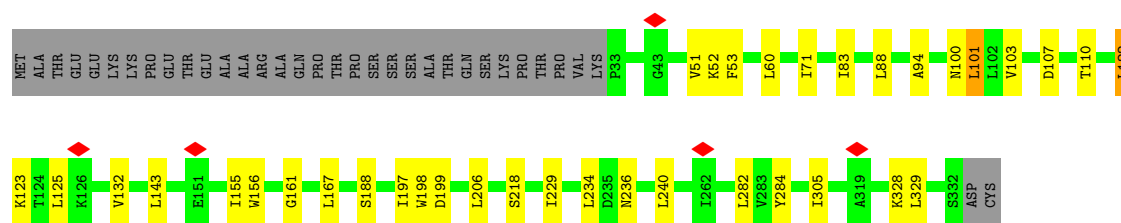


- Molecule 9: DNA (145-MER)

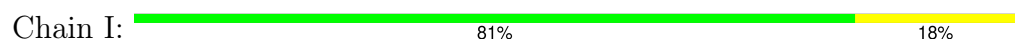


- Molecule 10: WD repeat-containing protein 5

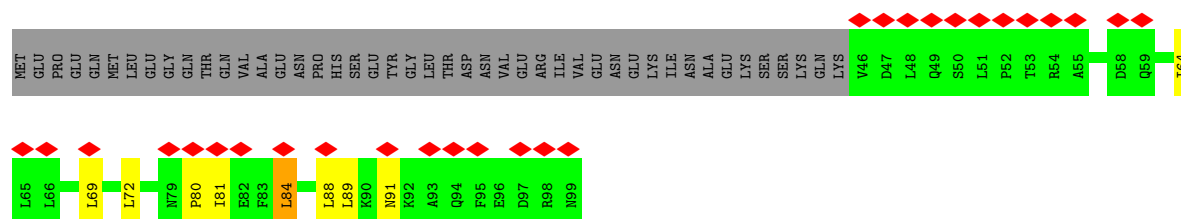




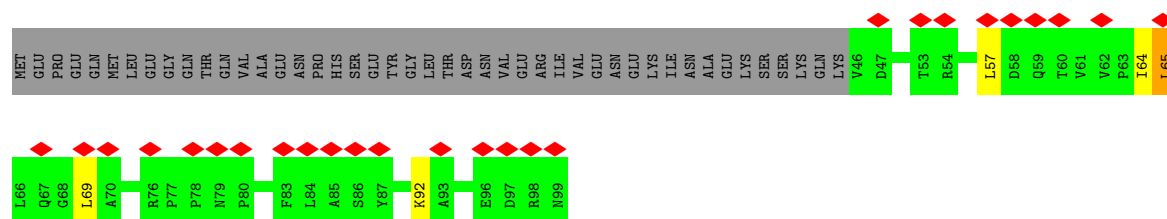
- Molecule 11: DNA (145-MER)



- Molecule 12: Protein dpy-30 homolog



- Molecule 12: Protein dpy-30 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25255	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.528	Depositor
Minimum map value	-0.650	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	O	0.13	0/609	0.28	0/819
2	K	0.09	0/5595	0.25	0/7565
3	N	0.11	0/3039	0.30	0/4131
4	T	0.09	0/2474	0.24	0/3357
5	A	0.11	0/813	0.26	0/1090
5	E	0.12	0/837	0.30	0/1120
6	B	0.12	0/711	0.29	0/948
6	F	0.12	0/680	0.29	0/908
7	C	0.15	0/845	0.37	0/1139
7	G	0.12	0/815	0.28	0/1100
8	D	0.16	0/766	0.30	0/1026
8	H	0.13	0/730	0.30	0/982
9	J	0.19	0/3355	0.43	0/5180
10	R	0.09	0/2382	0.28	0/3231
11	I	0.20	0/3313	0.44	0/5107
12	P	0.12	0/439	0.29	0/598
12	Q	0.13	0/440	0.31	0/598
All	All	0.13	0/27843	0.33	0/38899

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	O	603	0	631	5	0
2	K	5469	0	5335	27	0
3	N	2977	0	2922	23	0
4	T	2397	0	2318	7	0
5	A	801	0	839	9	0
5	E	825	0	869	9	0
6	B	703	0	755	11	0
6	F	673	0	722	8	0
7	C	835	0	897	5	0
7	G	805	0	861	7	0
8	D	755	0	781	4	0
8	H	719	0	737	8	0
9	J	2988	0	1627	18	0
10	R	2326	0	2309	24	0
11	I	2957	0	1628	16	0
12	P	431	0	448	7	0
12	Q	432	0	448	6	0
13	A	18	0	0	0	0
13	B	14	0	0	0	0
13	C	22	0	0	0	0
13	D	16	0	0	0	0
13	E	28	0	0	0	0
13	F	28	0	0	0	0
13	G	13	0	0	0	0
13	H	8	0	0	0	0
13	I	4	0	0	0	0
13	J	5	0	0	0	0
13	N	1	0	0	0	0
All	All	26853	0	24127	167	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 (167) 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)
5:A:92:LEU:HD21	6:B:62:LEU:HD21	1.73	0.70
3:N:205:GLU:HB3	3:N:214:LEU:HD21	1.78	0.65
2:K:5422:MET:HE3	2:K:5422:MET:H	1.63	0.64
2:K:5243:ILE:HD12	2:K:5263:VAL:HG22	1.80	0.64
5:A:96:CYS:SG	6:B:58:LEU:HD11	2.38	0.64
3:N:26:MET:SD	3:N:26:MET:O	2.55	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:399:LEU:HD23	3:N:399:LEU:O	1.99	0.62
10:R:88:LEU:HD23	10:R:107:ASP:O	1.99	0.62
5:E:83:ARG:HB2	6:F:80:THR:HG22	1.81	0.62
10:R:94:ALA:HB3	10:R:103:VAL:HG22	1.82	0.62
4:T:388:ARG:CB	4:T:410:VAL:HG13	2.31	0.61
1:O:56:LEU:HD12	1:O:61:ILE:HD12	1.84	0.60
2:K:5080:VAL:HG21	2:K:5157:ILE:HG23	1.83	0.59
10:R:188:SER:HG	10:R:198:TRP:CD1	2.21	0.58
3:N:214:LEU:CD1	3:N:266:ILE:HD11	2.33	0.58
6:B:96:THR:CG2	7:G:100:VAL:HG12	2.35	0.57
8:D:86:ARG:HH21	8:D:88:THR:HG22	1.69	0.57
2:K:5257:ASP:OD2	2:K:5263:VAL:HG23	2.05	0.57
9:J:15:DT:H3	11:I:133:DA:H61	1.52	0.56
10:R:100:ASN:O	10:R:101:LEU:HD13	2.04	0.56
12:P:69:LEU:HD11	12:Q:57:LEU:HD11	1.86	0.56
2:K:1537:LEU:HD21	2:K:1543:VAL:HG22	1.88	0.55
10:R:71:ILE:HD11	10:R:83:ILE:HG22	1.88	0.55
3:N:160:ASP:OD1	3:N:160:ASP:C	2.50	0.55
9:J:16:DC:C2'	9:J:17:DT:H71	2.37	0.54
5:A:45:THR:HG21	11:I:144:DC:OP1	2.08	0.54
2:K:5425:GLU:OE2	2:K:5427:ILE:HD12	2.08	0.54
4:T:614:VAL:HG11	12:Q:69:LEU:HD21	1.90	0.54
2:K:5401:LEU:HA	2:K:5411:LEU:HD13	1.90	0.53
9:J:142:DC:H2''	9:J:143:DT:H71	1.89	0.53
7:C:90:ASP:OD1	7:C:90:ASP:C	2.50	0.53
2:K:5024:LYS:HA	2:K:5024:LYS:HE2	1.91	0.52
6:B:44:LYS:HB2	7:G:115:LEU:HD12	1.90	0.52
3:N:30:CYS:HB2	3:N:39:LEU:HD21	1.90	0.52
4:T:614:VAL:HB	12:Q:69:LEU:HD11	1.92	0.52
3:N:39:LEU:HD22	3:N:41:VAL:HG22	1.91	0.52
10:R:282:LEU:HD22	10:R:284:TYR:CE1	2.44	0.52
7:C:110:ASN:OD1	7:C:110:ASN:C	2.52	0.52
9:J:16:DC:H2'	9:J:17:DT:H71	1.90	0.52
9:J:142:DC:C2'	9:J:143:DT:H71	2.39	0.52
3:N:361:GLU:N	3:N:362:PRO:CD	2.72	0.52
4:T:388:ARG:HB3	4:T:410:VAL:HG13	1.91	0.52
4:T:432:PRO:O	4:T:434:THR:HG23	2.10	0.52
12:P:80:PRO:O	12:P:84:LEU:HD22	2.09	0.52
11:I:141:DA:H2'	11:I:142:DT:H72	1.92	0.51
2:K:1529:TRP:O	2:K:1530:MET:HE2	2.11	0.51
2:K:5329:LEU:HB2	2:K:5331:LEU:HD23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:39:LEU:HD23	3:N:40:ALA:N	2.26	0.50
8:H:94:ILE:O	8:H:98:VAL:HG23	2.12	0.50
10:R:52:LYS:O	10:R:60:LEU:HD12	2.12	0.50
3:N:214:LEU:HD13	3:N:266:ILE:HD11	1.94	0.49
10:R:51:VAL:HG22	10:R:60:LEU:HD11	1.95	0.49
3:N:214:LEU:HD23	3:N:214:LEU:H	1.77	0.49
5:E:90:MET:HA	5:E:90:MET:HE3	1.95	0.49
2:K:1508:PRO:HD2	2:K:1530:MET:HE1	1.95	0.49
4:T:388:ARG:HB2	4:T:410:VAL:HG13	1.94	0.48
10:R:155:ILE:HD12	10:R:156:TRP:H	1.79	0.48
5:A:60:LEU:HD12	5:A:64:LYS:HE2	1.95	0.48
12:P:88:LEU:HD12	12:P:89:LEU:HD22	1.94	0.48
10:R:143:LEU:HB3	10:R:155:ILE:HD11	1.95	0.48
2:K:1530:MET:HE2	2:K:1530:MET:HA	1.95	0.48
2:K:5183:LEU:HD11	2:K:5212:ALA:HB1	1.95	0.48
1:O:5:VAL:HB	1:O:13:ILE:HG22	1.96	0.48
10:R:122:LEU:HD12	10:R:123:LYS:N	2.29	0.48
2:K:1418:LEU:HD11	2:K:5009:VAL:HG23	1.96	0.47
6:F:73:THR:HG21	6:F:81:VAL:HG12	1.96	0.47
9:J:12:DA:H2'	9:J:13:DT:H71	1.96	0.47
5:E:80:THR:HG23	5:E:81:ASP:OD1	2.14	0.47
11:I:8:DA:H2'	11:I:9:DT:H72	1.96	0.47
3:N:248:LEU:HD21	8:D:118:VAL:CG1	2.45	0.47
10:R:53:PHE:CD1	10:R:60:LEU:HD13	2.49	0.47
10:R:167:LEU:HD11	10:R:198:TRP:CE3	2.50	0.46
5:A:104:PHE:HA	5:A:107:THR:HG22	1.97	0.46
6:B:96:THR:HG23	7:G:100:VAL:HG12	1.96	0.46
1:O:5:VAL:HG11	1:O:69:LEU:HD12	1.98	0.46
8:H:51:ASP:N	8:H:51:ASP:OD1	2.48	0.46
7:C:61:GLU:OE2	7:C:61:GLU:HA	2.15	0.46
10:R:206:LEU:HD12	10:R:206:LEU:H	1.81	0.46
5:A:100:LEU:HD11	6:B:58:LEU:HD13	1.99	0.45
10:R:125:LEU:HD22	10:R:161:GLY:HA3	1.98	0.45
9:J:112:DG:C2	11:I:37:DG:N2	2.84	0.45
9:J:46:DC:H2''	9:J:47:DC:C6	2.51	0.45
3:N:214:LEU:HD12	3:N:266:ILE:HD11	1.97	0.45
5:A:83:ARG:HB2	6:B:80:THR:HG22	1.97	0.45
5:A:118:THR:HG22	6:B:45:ARG:HB3	1.99	0.45
9:J:139:DA:H2'	9:J:140:DT:H72	1.99	0.45
2:K:5427:ILE:HD11	3:N:345:TYR:C	2.41	0.45
10:R:199:ASP:OD1	10:R:206:LEU:HD11	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1532:ALA:HB1	2:K:1537:LEU:HD23	1.99	0.45
12:Q:64:ILE:HG23	12:Q:65:LEU:HD22	1.99	0.45
2:K:5473:ILE:HG23	2:K:5508:LEU:O	2.17	0.45
10:R:282:LEU:HD22	10:R:284:TYR:HE1	1.79	0.45
11:I:104:DT:C6	11:I:105:DT:H72	2.52	0.45
5:E:121:PRO:HB3	6:F:53:GLU:OE1	2.17	0.44
6:F:82:THR:HG23	6:F:85:ASP:H	1.82	0.44
9:J:82:DG:H2'	9:J:83:DT:C6	2.53	0.44
10:R:110:THR:O	10:R:132:VAL:HG21	2.17	0.44
5:E:109:LEU:HD23	5:E:109:LEU:O	2.17	0.44
10:R:197:ILE:HG23	10:R:206:LEU:HB2	2.00	0.44
2:K:5452:MET:SD	2:K:5452:MET:C	3.01	0.44
9:J:47:DC:H2''	9:J:48:DC:C5	2.53	0.44
5:A:92:LEU:HD21	6:B:62:LEU:CD2	2.45	0.44
7:C:105:GLY:O	5:E:58:THR:HG23	2.17	0.44
8:H:89:ILE:HG23	8:H:89:ILE:O	2.17	0.44
9:J:15:DT:H4'	9:J:16:DC:OP1	2.17	0.44
12:P:64:ILE:HD11	12:P:91:ASN:OD1	2.16	0.44
2:K:5219:LEU:HD21	2:K:5267:ILE:HA	2.00	0.43
5:E:97:GLU:OE2	5:E:97:GLU:HA	2.18	0.43
10:R:229:ILE:O	10:R:240:LEU:HD12	2.17	0.43
2:K:5124:MET:C	2:K:5124:MET:SD	3.01	0.43
9:J:10:DA:H2'	9:J:11:DT:H71	1.99	0.43
2:K:5340:ARG:HG2	10:R:305:ILE:HD11	2.01	0.43
1:O:5:VAL:HG13	1:O:67:LEU:HB3	1.99	0.43
6:B:52:GLU:CD	6:B:52:GLU:C	2.85	0.43
7:C:92:GLU:CD	7:C:92:GLU:C	2.87	0.43
10:R:218:SER:HB3	10:R:234:LEU:HD21	2.00	0.43
11:I:85:DG:C2'	11:I:86:DT:H71	2.48	0.43
3:N:29:THR:HG23	3:N:72:LEU:CD1	2.48	0.43
12:P:72:LEU:HD22	12:P:84:LEU:HD21	2.00	0.43
3:N:94:ASP:C	3:N:95:VAL:HG23	2.44	0.43
11:I:68:DT:H2''	11:I:69:DA:N7	2.34	0.43
3:N:402:LEU:N	3:N:403:PRO:CD	2.82	0.43
6:F:34:ILE:HD13	6:F:54:THR:CG2	2.49	0.43
12:P:81:ILE:HG21	12:Q:92:LYS:HE3	2.01	0.42
4:T:469:HIS:O	4:T:472:ILE:HG22	2.17	0.42
5:E:82:LEU:HD22	6:F:81:VAL:HG13	2.01	0.42
11:I:74:DC:C2'	11:I:75:DT:H71	2.49	0.42
5:E:83:ARG:CB	6:F:80:THR:HG22	2.49	0.42
2:K:5299:HIS:O	2:K:5303:ARG:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:455:THR:HG22	3:N:456:ASN:O	2.19	0.42
6:F:84:MET:HE1	6:F:88:TYR:CE2	2.55	0.42
9:J:47:DC:C6	9:J:48:DC:N4	2.88	0.42
2:K:5522:LYS:O	2:K:5523:ILE:HG13	2.19	0.42
7:G:79:ILE:HD12	7:G:79:ILE:HA	1.90	0.42
11:I:104:DT:H2'	11:I:105:DT:H72	2.02	0.42
9:J:39:DG:C6	9:J:40:DA:C6	3.08	0.42
1:O:19:PRO:HA	1:O:56:LEU:HD23	2.02	0.42
11:I:41:DA:C4	11:I:42:DC:C5	3.08	0.42
3:N:39:LEU:HD22	3:N:41:VAL:CG2	2.50	0.41
2:K:5242:VAL:HG23	2:K:5255:PHE:O	2.20	0.41
8:D:37:TYR:N	8:D:37:TYR:CD1	2.88	0.41
10:R:328:LYS:C	10:R:329:LEU:HD22	2.45	0.41
2:K:1532:ALA:CB	2:K:1537:LEU:HD23	2.50	0.41
11:I:42:DC:C2	11:I:43:DA:N7	2.88	0.41
10:R:101:LEU:HD22	10:R:101:LEU:N	2.36	0.41
12:P:81:ILE:HG21	12:Q:92:LYS:CE	2.50	0.41
2:K:5077:LEU:HD23	2:K:5080:VAL:HG22	2.01	0.41
3:N:215:ILE:CG2	3:N:216:ASN:N	2.83	0.41
8:H:35:GLU:OE2	8:H:36:SER:N	2.53	0.41
8:H:71:GLU:HA	8:H:71:GLU:OE1	2.20	0.41
8:H:102:LEU:HD23	8:H:102:LEU:N	2.36	0.41
2:K:5219:LEU:HD23	2:K:5271:VAL:HG13	2.02	0.41
9:J:48:DC:C5	9:J:49:DC:N4	2.88	0.41
11:I:45:DC:C2'	11:I:46:DT:H72	2.50	0.41
7:G:37:GLY:O	7:G:38:ASN:OD1	2.39	0.41
7:G:79:ILE:HG13	7:G:80:PRO:HD2	2.03	0.41
9:J:141:DT:H2''	9:J:142:DC:C5	2.56	0.41
6:B:72:TYR:CE1	8:D:80:LEU:HD13	2.55	0.40
9:J:40:DA:H1'	9:J:41:DG:C8	2.56	0.40
11:I:49:DA:H2''	11:I:50:DG:C8	2.56	0.40
3:N:89:ILE:HG23	3:N:103:ARG:HG2	2.04	0.40
8:H:85:LYS:N	8:H:85:LYS:HD3	2.36	0.40
11:I:3:DG:H2''	11:I:4:DG:C8	2.55	0.40
11:I:110:DC:H2''	11:I:111:DC:C5	2.57	0.40
3:N:134:MET:HE3	3:N:135:LEU:N	2.36	0.40
3:N:215:ILE:HG22	3:N:216:ASN:N	2.35	0.40
7:G:29:ARG:CZ	8:H:35:GLU:OE1	2.70	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	O	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
2	K	681/1256 (54%)	641 (94%)	40 (6%)	0	100	100
3	N	376/538 (70%)	335 (89%)	38 (10%)	3 (1%)	16	45
4	T	295/628 (47%)	286 (97%)	9 (3%)	0	100	100
5	A	95/135 (70%)	93 (98%)	2 (2%)	0	100	100
5	E	98/135 (73%)	93 (95%)	5 (5%)	0	100	100
6	B	85/102 (83%)	80 (94%)	5 (6%)	0	100	100
6	F	82/102 (80%)	80 (98%)	2 (2%)	0	100	100
7	C	106/129 (82%)	104 (98%)	2 (2%)	0	100	100
7	G	102/129 (79%)	99 (97%)	3 (3%)	0	100	100
8	D	94/125 (75%)	86 (92%)	8 (8%)	0	100	100
8	H	90/125 (72%)	88 (98%)	2 (2%)	0	100	100
10	R	298/334 (89%)	274 (92%)	24 (8%)	0	100	100
12	P	52/99 (52%)	52 (100%)	0	0	100	100
12	Q	52/99 (52%)	52 (100%)	0	0	100	100
All	All	2580/4012 (64%)	2432 (94%)	145 (6%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	383	ILE
3	N	153	LEU
3	N	108	SER

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	O	69/69 (100%)	68 (99%)	1 (1%)	59	68
2	K	599/1091 (55%)	591 (99%)	8 (1%)	61	69
3	N	332/462 (72%)	328 (99%)	4 (1%)	63	70
4	T	256/514 (50%)	254 (99%)	2 (1%)	73	74
5	A	85/110 (77%)	82 (96%)	3 (4%)	32	53
5	E	87/110 (79%)	84 (97%)	3 (3%)	32	53
6	B	72/78 (92%)	71 (99%)	1 (1%)	59	68
6	F	69/78 (88%)	66 (96%)	3 (4%)	26	49
7	C	85/99 (86%)	85 (100%)	0	100	100
7	G	83/99 (84%)	80 (96%)	3 (4%)	31	52
8	D	82/105 (78%)	81 (99%)	1 (1%)	63	70
8	H	78/105 (74%)	76 (97%)	2 (3%)	40	58
10	R	262/291 (90%)	259 (99%)	3 (1%)	65	71
12	P	48/89 (54%)	47 (98%)	1 (2%)	47	62
12	Q	48/89 (54%)	47 (98%)	1 (2%)	47	62
All	All	2255/3389 (66%)	2219 (98%)	36 (2%)	54	65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	27	LYS
2	K	1538	PHE
2	K	5020	LEU
2	K	5053	ASP
2	K	5070	TYR
2	K	5132	LEU
2	K	5226	CYS
2	K	5326	LEU
2	K	5423	VAL
3	N	29	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	242	MET
3	N	258	CYS
3	N	399	LEU
4	T	351	HIS
4	T	594	MET
5	A	41	TYR
5	A	65	LEU
5	A	73	GLU
6	B	97	LEU
8	D	90	THR
5	E	73	GLU
5	E	76	GLN
5	E	112	ILE
6	F	30	THR
6	F	74	GLU
6	F	96	THR
7	G	79	ILE
7	G	101	THR
7	G	110	ASN
8	H	51	ASP
8	H	52	THR
10	R	101	LEU
10	R	122	LEU
10	R	236	ASN
12	P	84	LEU
12	Q	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	5200	HIS
2	K	5316	ASN
2	K	5474	ASN
3	N	183	GLN
3	N	273	GLN
4	T	491	ASN
4	T	535	GLN
6	B	75	HIS
7	C	112	GLN
8	H	95	GLN
10	R	44	HIS
10	R	314	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.

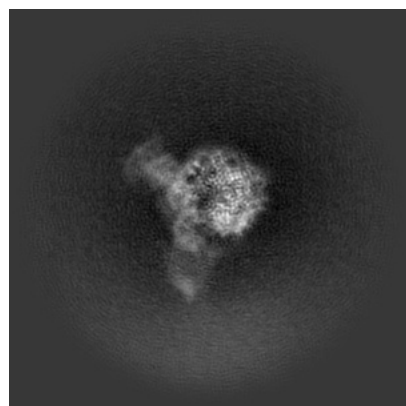
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73080. These allow visual inspection of the internal detail of the map and identification of artifacts.

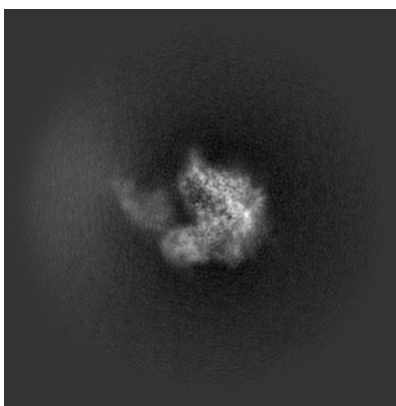
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

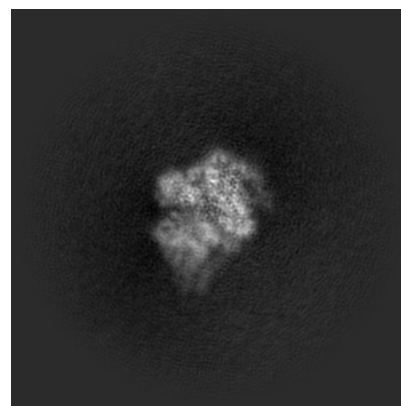
6.1.1 Primary map



X

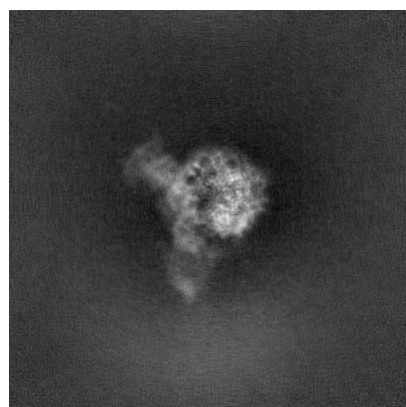


Y

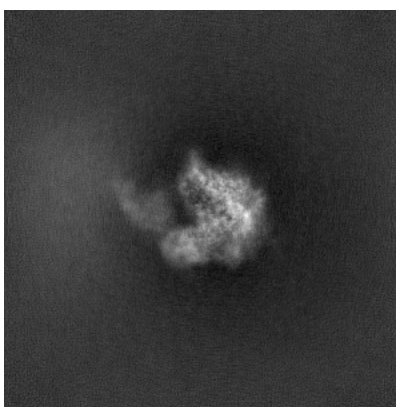


Z

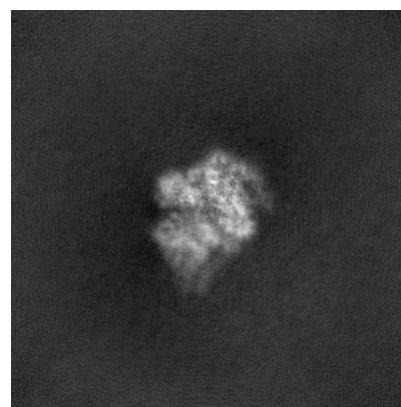
6.1.2 Raw map



X



Y



Z

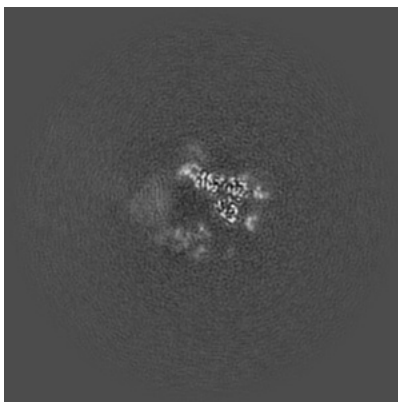
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

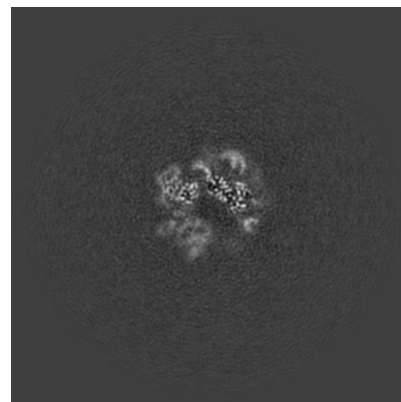
6.2.1 Primary map



X Index: 256



Y Index: 256

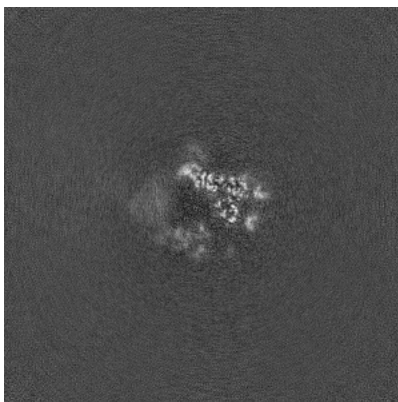


Z Index: 256

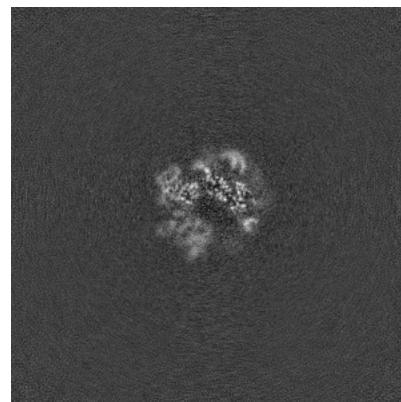
6.2.2 Raw map



X Index: 256



Y Index: 256

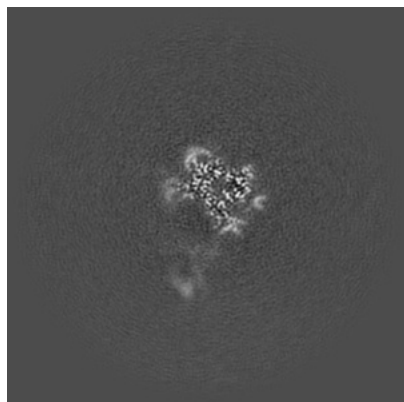


Z Index: 256

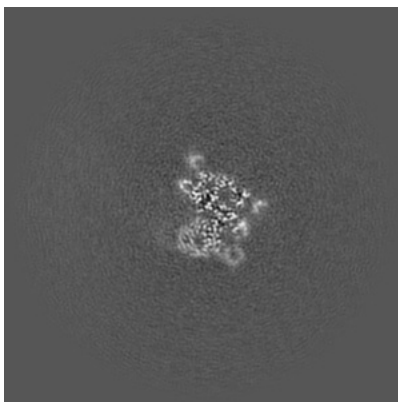
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

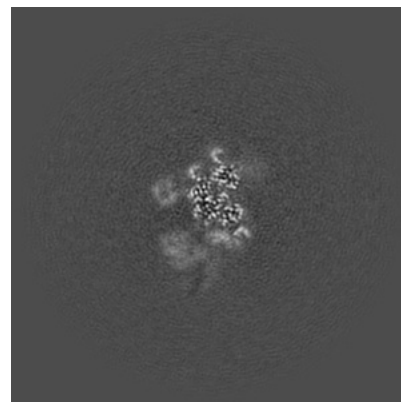
6.3.1 Primary map



X Index: 280



Y Index: 280

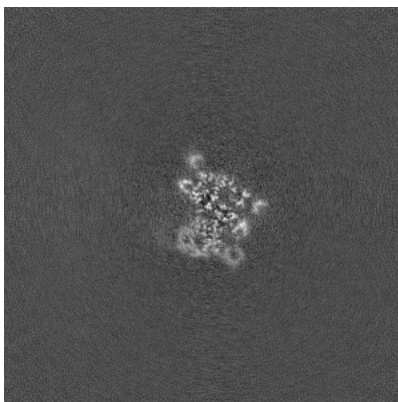


Z Index: 289

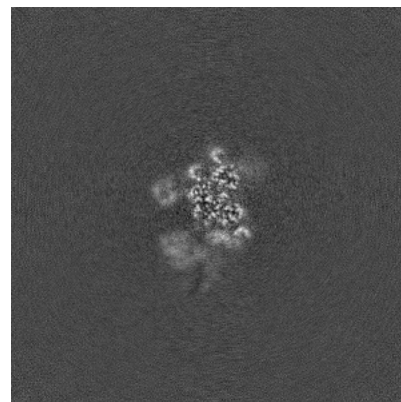
6.3.2 Raw map



X Index: 261



Y Index: 280

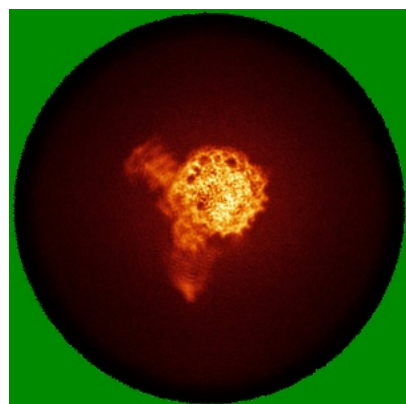


Z Index: 289

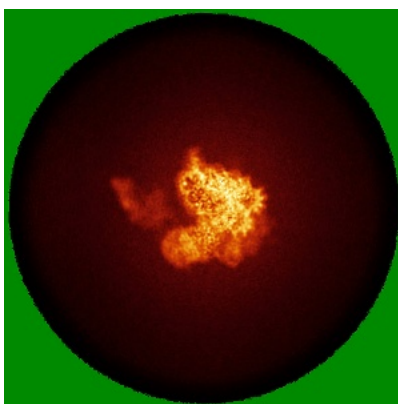
The images above show the largest variance slices of the map in three orthogonal directions.

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

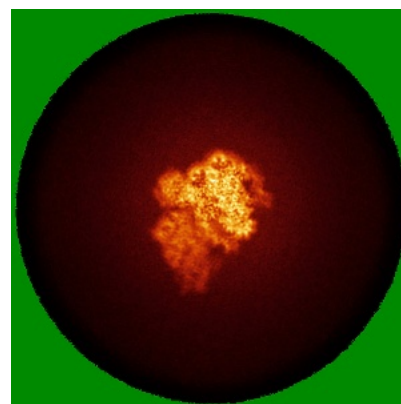
6.4.1 Primary map



X

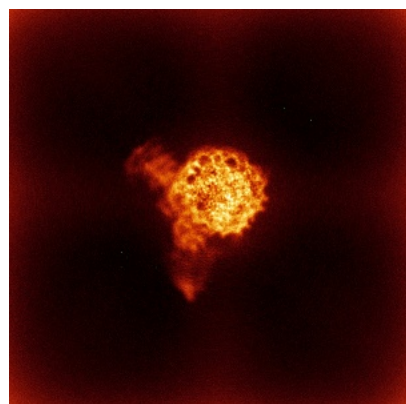


Y

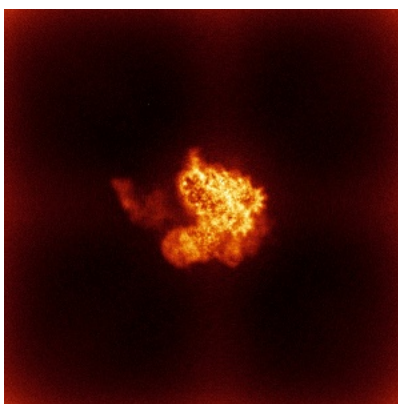


Z

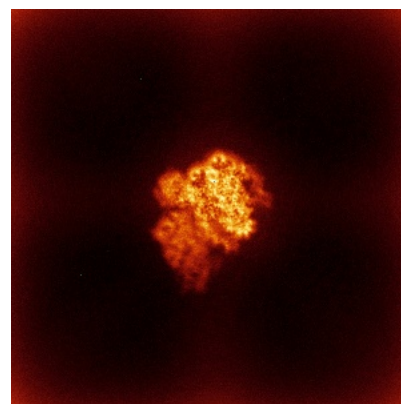
6.4.2 Raw map



X



Y

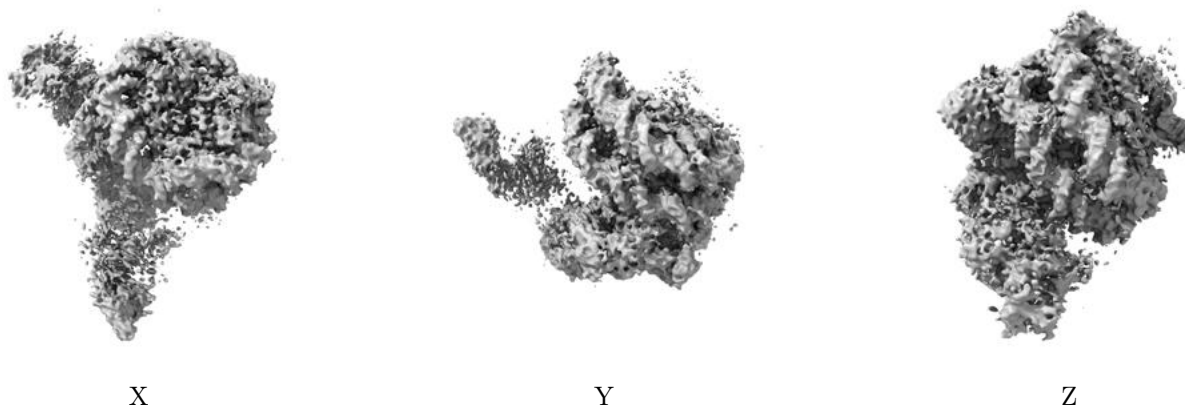


Z

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.

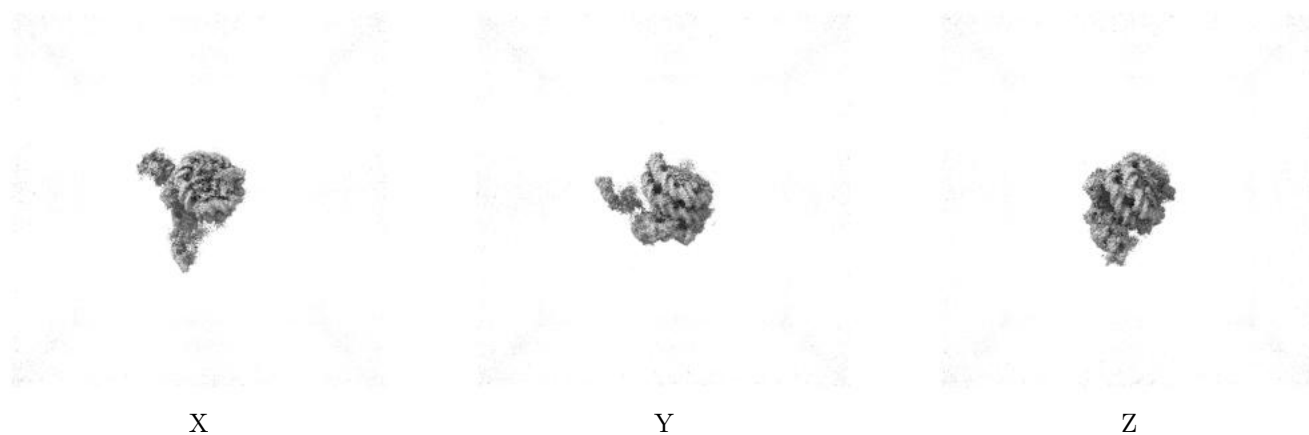
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

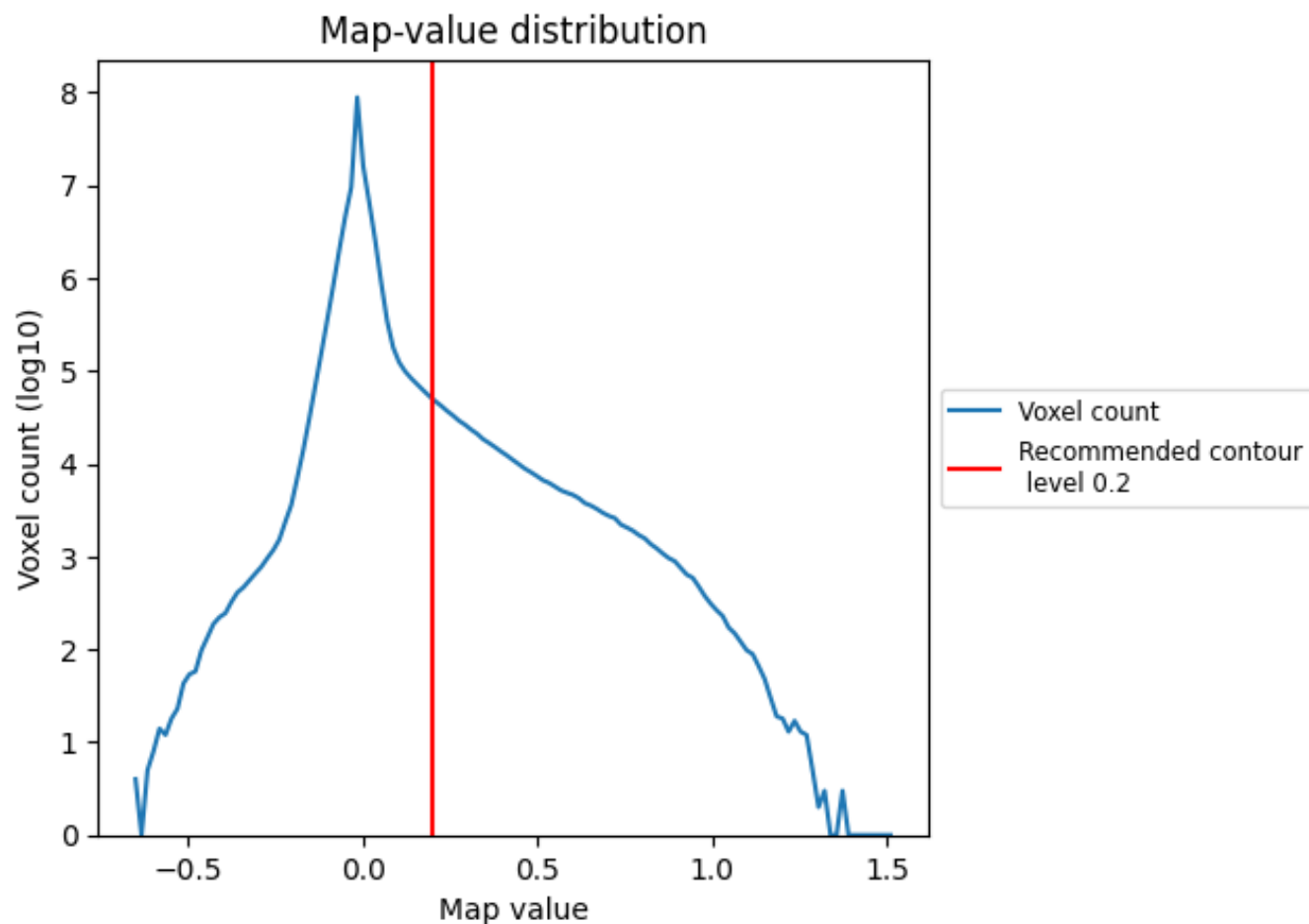
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

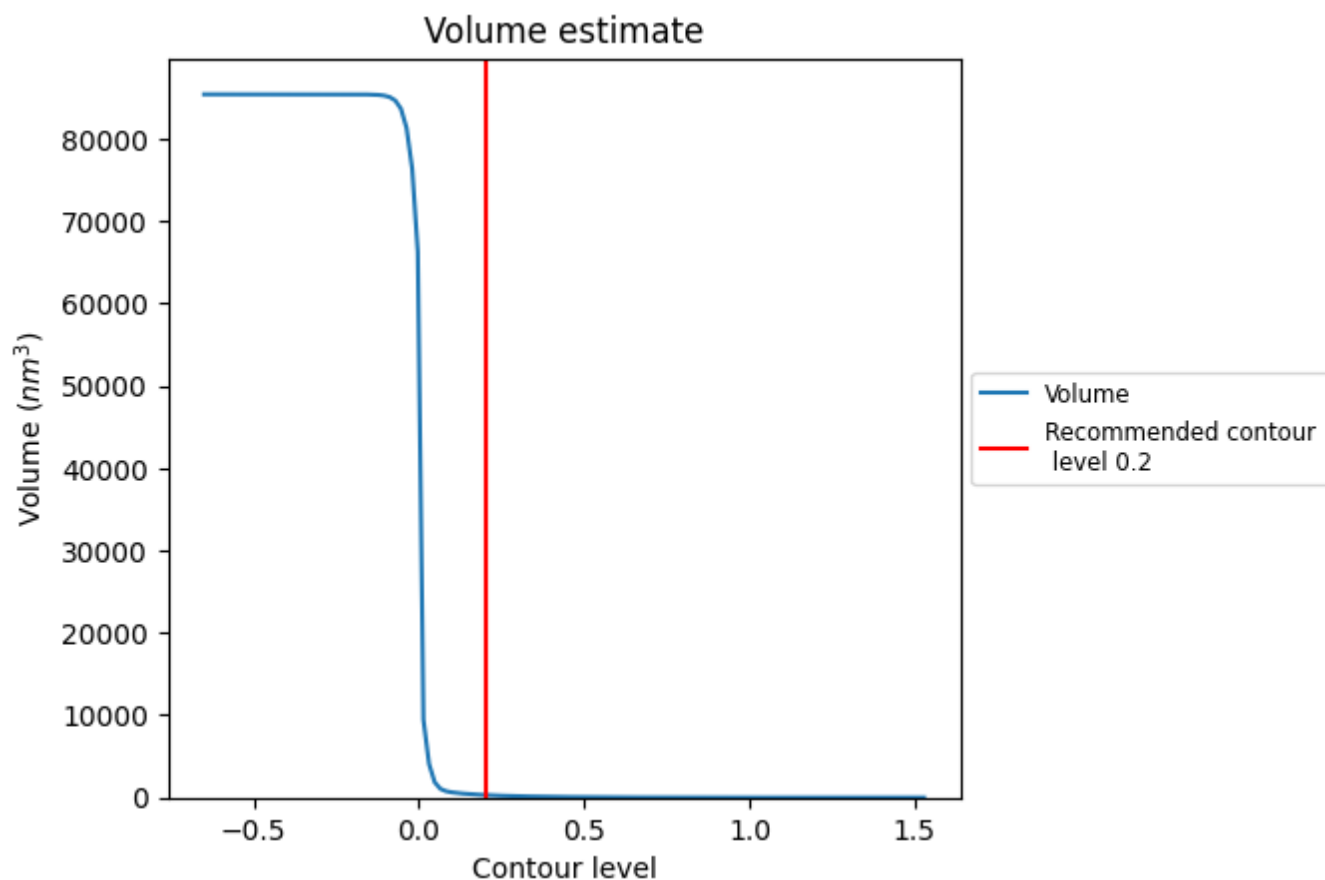
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

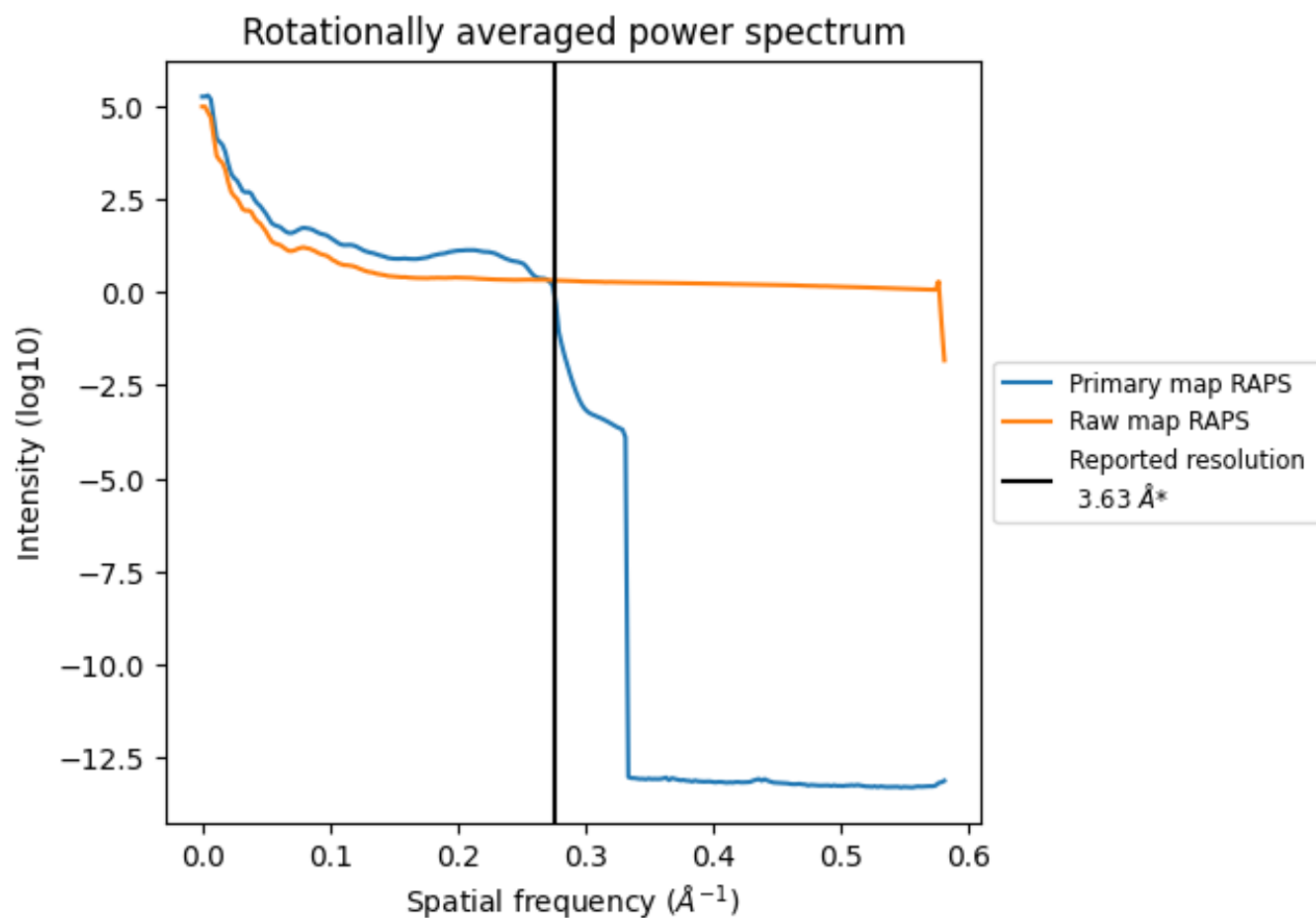
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 276 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 ⓘ

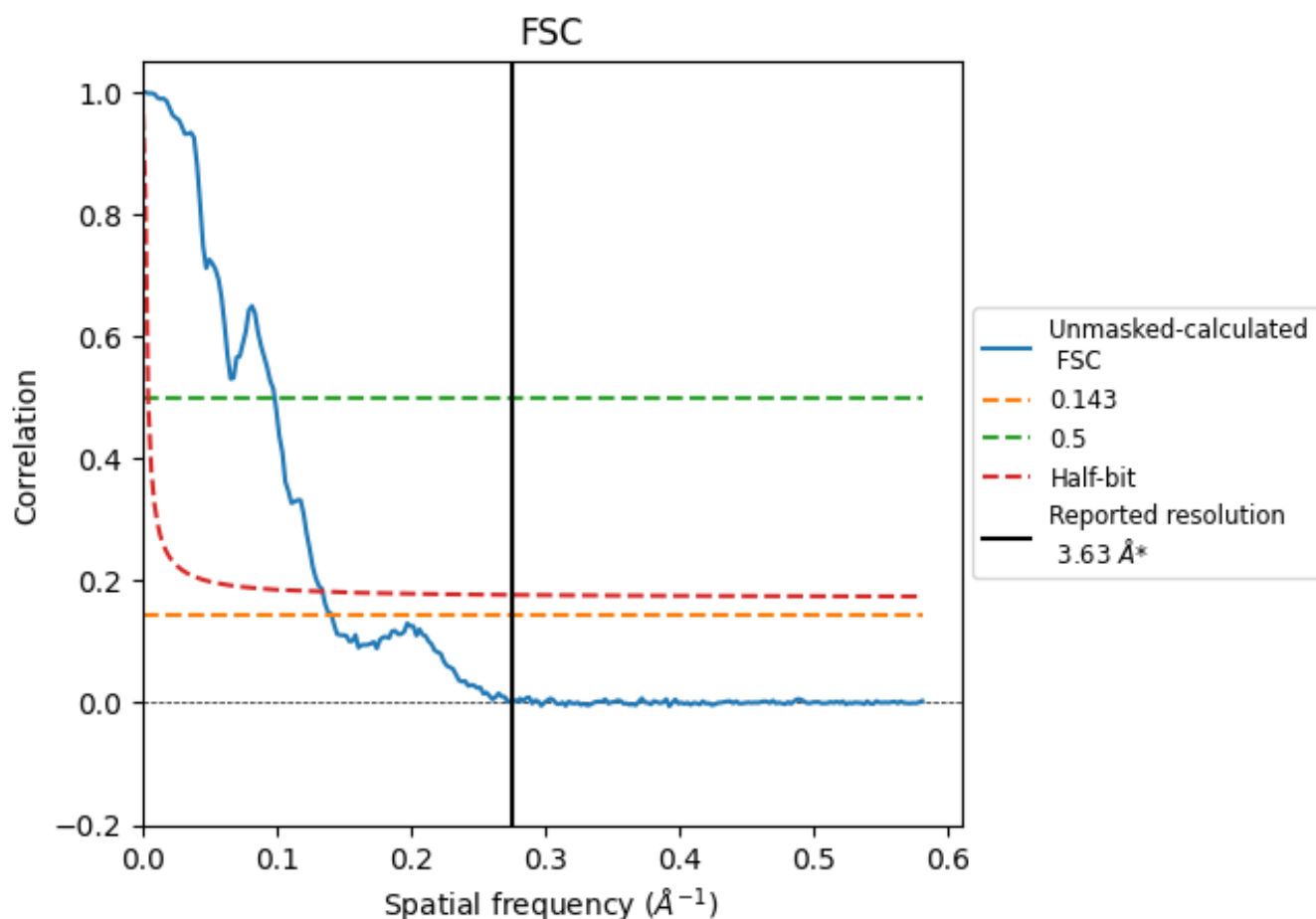


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

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 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

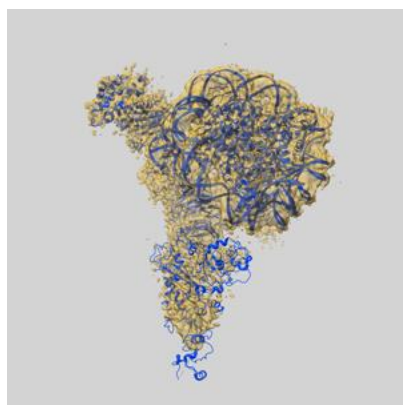
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.09	10.14	7.44

*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 7.09 differs from the reported value 3.63 by more than 10 %

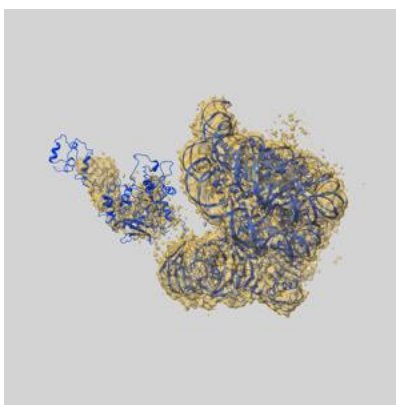
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73080 and PDB model 9YLE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

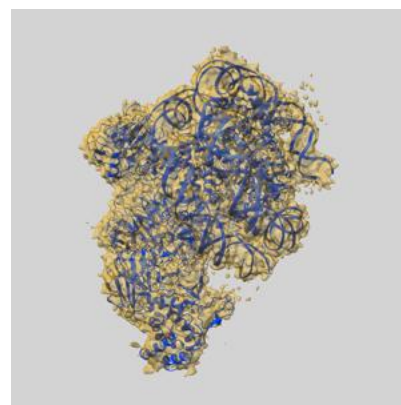
9.1 Map-model overlay [i](#)



X



Y



Z

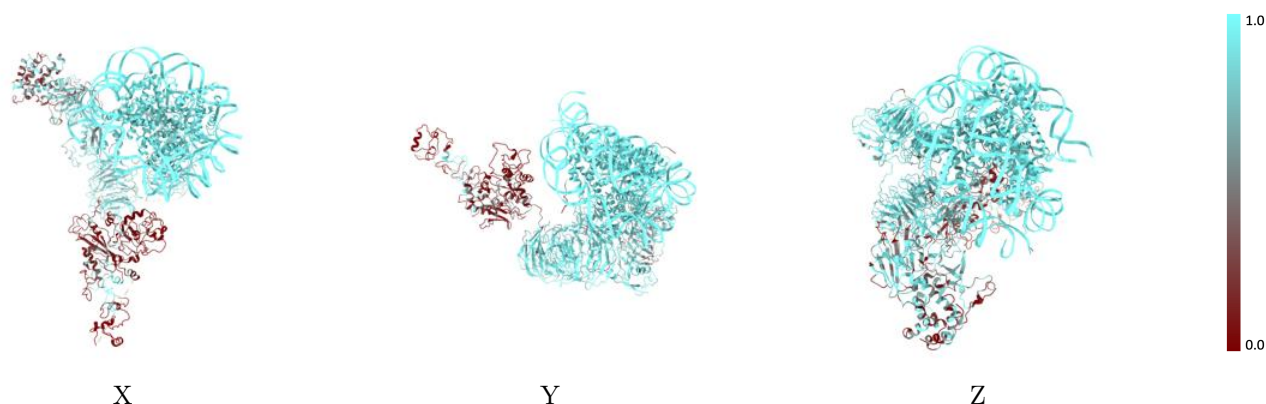
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



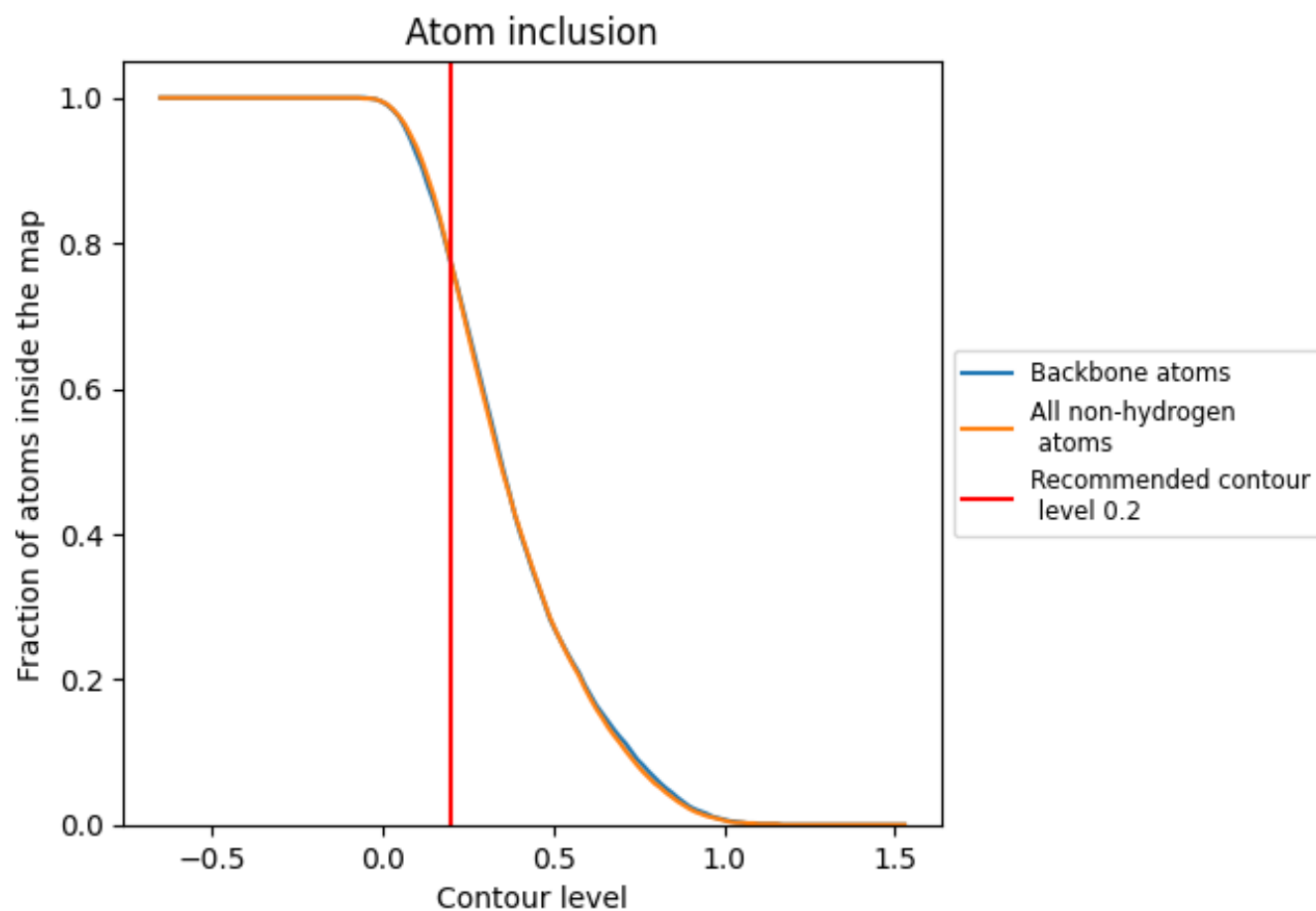
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 78% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.3210
A	 0.9690	 0.5010
B	 0.8910	 0.4870
C	 0.9490	 0.5000
D	 0.9590	 0.4900
E	 0.9570	 0.4910
F	 0.9470	 0.4950
G	 0.9770	 0.5040
H	 0.9830	 0.4980
I	 0.9900	 0.3820
J	 0.9860	 0.3830
K	 0.3580	 0.1520
N	 0.8720	 0.3870
O	 0.8520	 0.2720
P	 0.4160	 0.1220
Q	 0.4410	 0.1360
R	 0.8850	 0.2790
T	 0.6180	 0.1500

