



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 06:05 AM JST

PDB ID : 6KIV
EMDB ID : EMD-9999
Title : Cryo-EM structure of human MLL1-ubNCP complex (4.0 angstrom)
Authors : Huang, J.; Xue, H.; Yao, T.
Deposited on : 2019-07-20
Resolution : 4.00 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

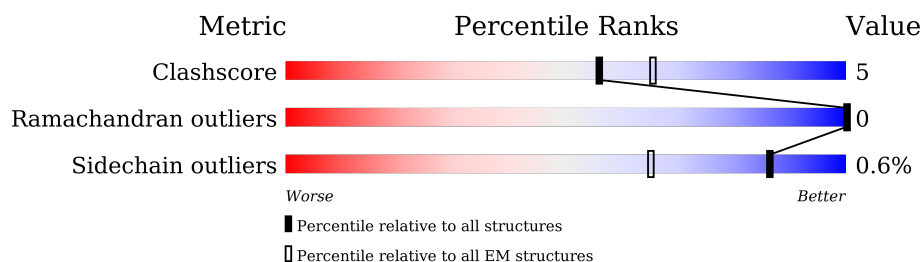
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	145	 88%12%
6	J	145	 90%10%
7	K	216	 10%65%17%17%
8	N	538	 5%56%12%32%
9	O	76	 72%78%22%
10	T	534	 7%24%9%67%
11	R	334	 65%25%10%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20719 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
1	E	97	Total	C	N	O	S	0	0
			802	506	155	138	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	86	Total	C	N	O	S	0	0
			698	440	141	116	1		
2	F	81	Total	C	N	O	S	0	0
			648	410	126	111	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	112	Total	C	N	O		0	0
			865	543	170	152			
3	G	105	Total	C	N	O		0	0
			809	510	158	141			

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			738	463	134	138	3		
4	H	95	Total	C	N	O	S	0	0
			742	466	133	140	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	117	CYS	LYS	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281
H	117	CYS	LYS	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	145	Total	C	N	O	P	0	0
			2955	1403	538	869	145		

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	P	0	0
			2990	1415	559	871	145		

- Molecule 7 is a protein called Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	179	Total	C	N	O	S	0	0
			1434	907	263	250	14		

- Molecule 8 is a protein called Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	366	Total	C	N	O	S	0	0
			2881	1813	494	559	15		

- Molecule 9 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	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 P62979

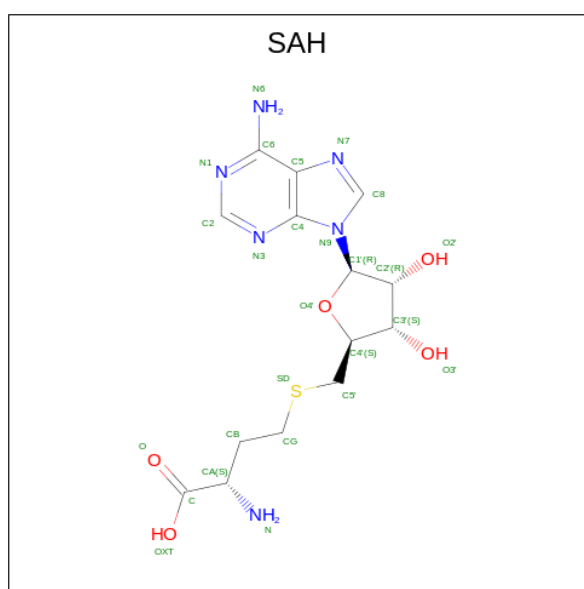
- Molecule 10 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	176	Total	C	N	O	S	0	0
			1399	906	234	253	6		

- Molecule 11 is a protein called WD repeat-containing protein 5.

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

- Molecule 12 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
12	K	1	Total	C	N	O	S	0
			26	14	6	5	1	

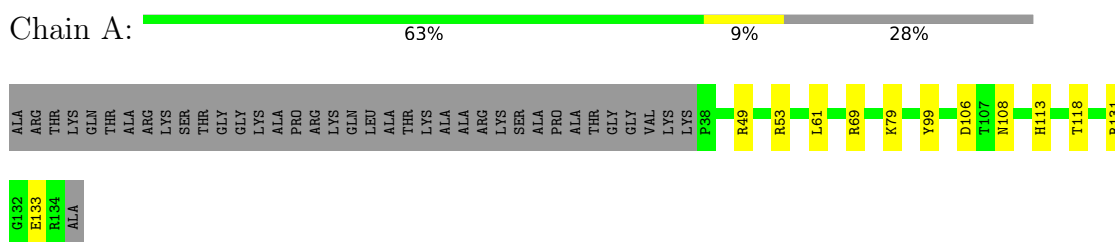
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Zn	0
			1	1	

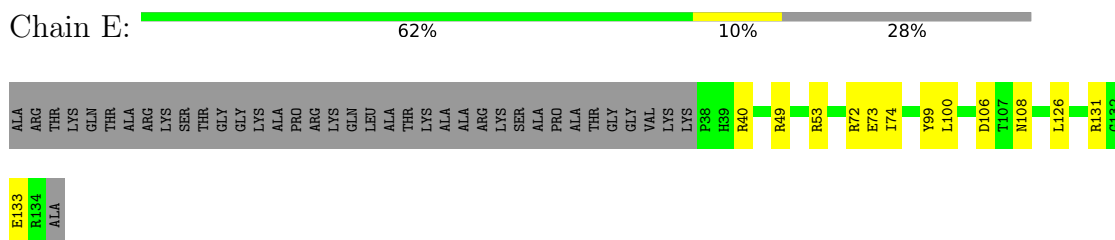
3 Residue-property plots

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.

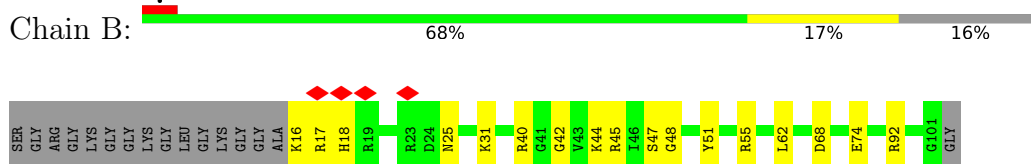
• Molecule 1: Histone H3



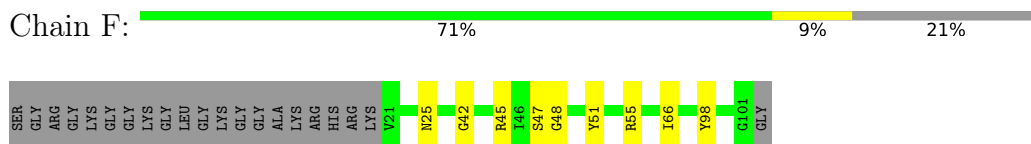
• Molecule 1: Histone H3



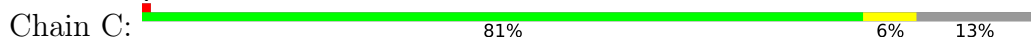
• Molecule 2: Histone H4



• Molecule 2: Histone H4

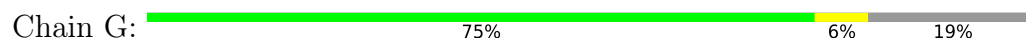


• Molecule 3: Histone H2A

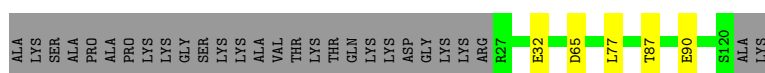




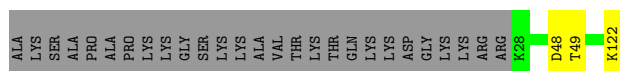
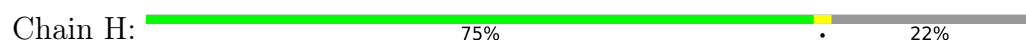
• Molecule 3: Histone H2A



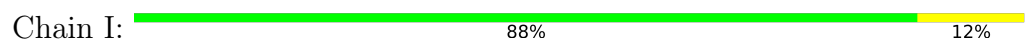
• Molecule 4: Histone H2B 1.1



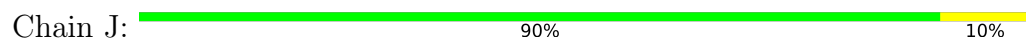
• Molecule 4: Histone H2B 1.1



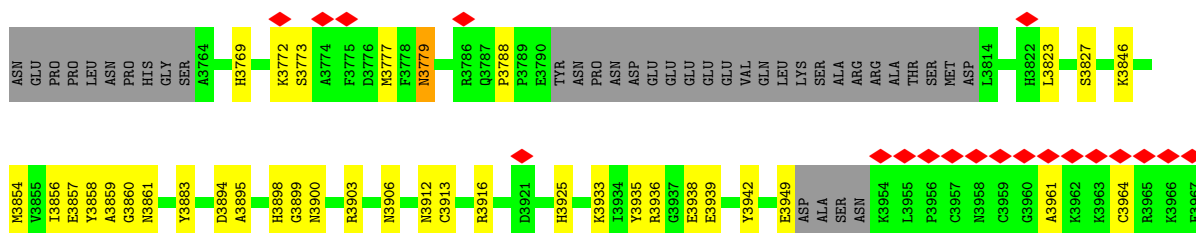
• Molecule 5: DNA (145-MER)



• Molecule 6: DNA (145-MER)



• Molecule 7: Histone-lysine N-methyltransferase 2A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (\AA)	294.30002, 294.30002, 294.30002	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, ZN

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	0.44	0/814	0.57	0/1092
1	E	0.44	0/814	0.57	0/1092
2	B	0.47	0/706	0.64	0/943
2	F	0.51	0/655	0.63	0/878
3	C	0.42	0/875	0.58	0/1179
3	G	0.40	0/819	0.60	0/1106
4	D	0.46	0/749	0.58	1/1008 (0.1%)
4	H	0.40	0/753	0.55	0/1012
5	I	0.87	0/3311	1.03	2/5103 (0.0%)
6	J	0.86	0/3357	1.01	1/5184 (0.0%)
7	K	0.32	0/1462	0.54	0/1954
8	N	0.33	0/2940	0.56	0/3992
9	O	0.26	0/609	0.54	0/819
10	T	0.29	0/1442	0.55	0/1950
11	R	0.29	0/2382	0.54	0/3231
All	All	0.57	0/21688	0.75	4/30543 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
7	K	0	2
8	N	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	48	DT	O4'-C4'-C3'	-5.73	102.21	104.50
5	I	49	DA	O4'-C4'-C3'	-5.55	102.28	104.50
4	D	77	LEU	CB-CG-CD2	-5.20	102.16	111.00
6	J	15	DT	P-O3'-C3'	5.16	125.89	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	31	LYS	Peptide
7	K	3779	ASN	Peptide
7	K	3788	PRO	Peptide
8	N	13	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	841	10	0
1	E	802	0	841	11	0
2	B	698	0	752	11	0
2	F	648	0	693	7	0
3	C	865	0	926	5	0
3	G	809	0	864	5	0
4	D	738	0	760	3	0
4	H	742	0	765	3	0
5	I	2955	0	1627	11	0
6	J	2990	0	1628	11	0
7	K	1434	0	1416	27	0
8	N	2881	0	2814	36	0
9	O	603	0	631	10	0
10	T	1399	0	1363	27	0
11	R	2326	0	2309	55	0
12	K	26	0	17	1	0
13	K	1	0	0	0	0
All	All	20719	0	18247	198	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 5.

All (198) 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)
10:T:297:GLN:HE22	10:T:354:GLN:HE22	1.34	0.76
8:N:300:ASP:HB3	8:N:313:ILE:HD12	1.76	0.67
11:R:283:VAL:HB	11:R:297:LEU:HB2	1.78	0.66
3:C:32:ARG:NH2	4:D:32:GLU:OE2	2.30	0.65
3:C:15:LYS:HB2	3:C:20:ARG:HH21	1.63	0.64
3:G:20:ARG:HH21	4:H:122:LYS:HD2	1.64	0.63
1:E:108:ASN:ND2	2:F:42:GLY:O	2.32	0.63
1:A:106:ASP:OD2	1:A:131:ARG:NH2	2.32	0.62
1:E:49:ARG:NH2	5:I:8:DA:O3'	2.33	0.62
5:I:50:DG:N2	6:J:99:DT:O2	2.32	0.62
7:K:3961:ALA:HB3	7:K:3964:CYS:HB2	1.82	0.62
9:O:6:LYS:O	9:O:68:HIS:ND1	2.32	0.61
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.32	0.60
8:N:238:GLU:O	9:O:42:ARG:NH2	2.33	0.60
1:A:108:ASN:ND2	2:B:42:GLY:O	2.35	0.60
11:R:267:SER:HB3	11:R:273:TRP:HB2	1.84	0.60
11:R:278:SER:H	11:R:304:VAL:HB	1.67	0.59
8:N:26:MET:HB3	8:N:44:ASN:HB2	1.84	0.59
7:K:3779:ASN:HB2	11:R:171:SER:HB3	1.84	0.59
11:R:138:ASN:ND2	11:R:142:ASN:OD1	2.36	0.59
11:R:195:CYS:HB2	11:R:209:LEU:HB3	1.84	0.59
5:I:25:DG:H1	6:J:123:DC:H42	1.51	0.58
8:N:348:ARG:NH1	8:N:350:SER:O	2.37	0.58
8:N:15:GLU:HA	8:N:288:LYS:HE2	1.85	0.58
8:N:30:CYS:HB2	8:N:39:LEU:HD11	1.86	0.58
9:O:36:ILE:HG23	9:O:40:GLN:HE21	1.69	0.57
11:R:63:SER:HA	11:R:69:ILE:HG12	1.87	0.57
7:K:3906:ASN:ND2	7:K:3939:GLU:OE2	2.37	0.57
11:R:286:TRP:HE1	11:R:293:ILE:HA	1.70	0.57
8:N:235:ARG:NH1	8:N:236:ASP:OD2	2.38	0.56
8:N:147:VAL:HG12	8:N:149:ASP:H	1.71	0.56
1:A:61:LEU:HD13	2:B:40:ARG:HH21	1.71	0.56
8:N:334:PRO:HD3	11:R:208:THR:HB	1.88	0.56
2:F:45:ARG:HE	5:I:81:DC:H4'	1.70	0.55
7:K:3857:GLU:OE2	7:K:3925:HIS:ND1	2.39	0.55
9:O:1:MET:HG3	9:O:64:GLU:H	1.71	0.55
1:A:69:ARG:NH1	2:B:25:ASN:OD1	2.40	0.55
11:R:136:ASN:ND2	11:R:177:VAL:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:286:TRP:HD1	11:R:294:VAL:HG22	1.72	0.55
11:R:37:LEU:HD11	11:R:328:LYS:HB3	1.89	0.54
11:R:169:ALA:O	11:R:196:ARG:NH1	2.40	0.54
10:T:366:TRP:HA	10:T:373:LYS:HA	1.89	0.54
11:R:215:PRO:HB2	11:R:233:THR:HB	1.88	0.54
8:N:233:CYS:HA	9:O:44:ILE:HG21	1.90	0.54
11:R:129:SER:OG	11:R:150:ASP:OD2	2.26	0.54
7:K:3857:GLU:O	7:K:3900:ASN:ND2	2.41	0.53
8:N:302:ALA:HB3	8:N:311:ALA:HB3	1.89	0.53
7:K:3883:TYR:OH	12:K:4001:SAH:N	2.41	0.53
7:K:3827:SER:HB2	7:K:3856:ILE:HG13	1.90	0.53
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.26	0.52
5:I:46:DT:H2''	5:I:47:DC:H5'	1.92	0.52
11:R:41:LEU:O	11:R:327:ILE:N	2.42	0.51
11:R:199:ASP:HB2	11:R:206:LEU:HD21	1.93	0.51
11:R:52:LYS:HD3	11:R:308:ALA:HB2	1.93	0.51
8:N:133:VAL:HG22	8:N:144:VAL:HG22	1.92	0.51
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.27	0.51
9:O:27:LYS:HA	9:O:41:GLN:HE22	1.76	0.51
7:K:3949:GLU:HB2	7:K:3969:ASN:HD22	1.76	0.51
11:R:318:SER:OG	11:R:328:LYS:O	2.28	0.50
7:K:3769:HIS:O	7:K:3772:LYS:NZ	2.45	0.50
8:N:222:ILE:HB	8:N:245:LEU:HB2	1.93	0.50
11:R:175:SER:HG	11:R:189:SER:HG	1.58	0.50
8:N:377:VAL:HG13	8:N:378:THR:HG23	1.94	0.50
10:T:365:SER:OG	10:T:374:PHE:O	2.29	0.50
11:R:138:ASN:HD21	11:R:142:ASN:H	1.60	0.50
1:A:118:THR:OG1	2:B:45:ARG:NH1	2.44	0.50
2:F:47:SER:OG	2:F:48:GLY:N	2.44	0.49
6:J:141:DT:OP1	7:K:3916:ARG:NH1	2.42	0.49
2:B:47:SER:OG	2:B:48:GLY:N	2.44	0.49
8:N:156:VAL:O	8:N:169:GLY:N	2.39	0.49
11:R:218:SER:N	11:R:232:ALA:O	2.41	0.49
7:K:3823:LEU:HD13	7:K:3854:MET:HB3	1.93	0.49
8:N:208:ARG:HD2	8:N:261:GLY:HA2	1.95	0.49
11:R:172:ASP:OD2	11:R:190:SER:OG	2.31	0.49
10:T:492:PRO:HB2	10:T:495:LEU:HB3	1.94	0.49
11:R:278:SER:OG	11:R:280:ASP:OD1	2.30	0.49
2:B:16:LYS:O	2:B:18:HIS:ND1	2.44	0.48
11:R:188:SER:HG	11:R:198:TRP:HE1	1.61	0.48
11:R:324:ASP:OD1	11:R:326:THR:OG1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:157:ASP:HB3	11:R:162:LYS:H	1.79	0.48
11:R:41:LEU:N	11:R:327:ILE:O	2.43	0.48
10:T:297:GLN:HG2	10:T:310:GLU:HG3	1.96	0.48
9:O:2:GLN:H	9:O:64:GLU:HG2	1.79	0.48
6:J:94:DG:H2'	6:J:95:DG:C8	2.48	0.47
11:R:155:ILE:O	11:R:164:LEU:N	2.44	0.47
9:O:17:VAL:HG12	9:O:29:LYS:HE3	1.95	0.47
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.41	0.47
10:T:333:VAL:HG13	10:T:480:VAL:HG12	1.97	0.47
11:R:268:VAL:HG23	11:R:269:THR:HG23	1.96	0.47
3:C:17:ARG:NH2	5:I:31:DT:OP2	2.42	0.47
7:K:3846:LYS:HA	7:K:3936:ARG:HG3	1.97	0.47
3:G:26:PRO:HG3	3:G:29:ARG:HD3	1.96	0.47
7:K:3895:ALA:HB1	7:K:3903:ARG:HG2	1.97	0.47
8:N:82:VAL:HG21	8:N:123:VAL:HG21	1.96	0.47
10:T:348:GLN:HB2	10:T:362:PHE:HD1	1.79	0.47
11:R:73:GLY:N	11:R:78:LYS:O	2.48	0.47
11:R:144:ILE:HG13	11:R:158:VAL:HG22	1.97	0.47
11:R:186:ILE:O	11:R:198:TRP:N	2.44	0.47
1:E:40:ARG:HH21	5:I:83:DG:H1'	1.80	0.46
8:N:256:LYS:NZ	8:N:300:ASP:OD1	2.39	0.46
10:T:301:SER:OG	10:T:303:ASP:OD1	2.33	0.46
10:T:336:MET:HB3	10:T:388:GLN:HG3	1.96	0.46
11:R:304:VAL:HA	11:R:320:ALA:HA	1.97	0.46
1:A:49:ARG:HH22	6:J:8:DG:H4'	1.80	0.46
7:K:3861:ASN:HB2	7:K:3894:ASP:HB3	1.97	0.46
11:R:96:SER:OG	11:R:98:ASP:OD1	2.26	0.46
2:B:51:TYR:HB3	2:B:55:ARG:HH12	1.80	0.46
1:E:40:ARG:HG2	5:I:84:DC:H5''	1.97	0.46
6:J:17:DT:H2''	6:J:18:DG:C8	2.50	0.46
7:K:3913:CYS:HB2	7:K:3942:TYR:HB3	1.97	0.46
10:T:298:LEU:HD23	10:T:310:GLU:HG2	1.98	0.46
4:D:65:ASP:OD2	2:F:98:TYR:OH	2.33	0.46
1:A:79:LYS:NZ	2:B:74:GLU:OE2	2.39	0.46
11:R:187:VAL:HG21	11:R:229:ILE:HG21	1.98	0.46
11:R:282:LEU:HD13	11:R:296:LYS:HB3	1.97	0.46
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.49	0.46
11:R:49:SER:H	11:R:64:SER:HA	1.80	0.46
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.51	0.45
3:G:76:THR:O	4:H:49:THR:OG1	2.31	0.45
7:K:3898:HIS:CD2	8:N:337:LYS:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:4:GLU:OE1	11:R:243:TYR:OH	2.32	0.45
5:I:125:DC:H2"	5:I:126:DG:C8	2.52	0.45
8:N:20:THR:OG1	8:N:21:LEU:N	2.49	0.45
10:T:321:GLY:HA3	10:T:469:PHE:HD1	1.81	0.45
10:T:398:LEU:HD21	10:T:463:ILE:HD11	1.98	0.45
11:R:55:PRO:HD3	11:R:95:TRP:HB3	1.98	0.45
10:T:288:LEU:HD13	10:T:304:ARG:HD3	1.98	0.45
1:E:74:ILE:HD11	2:F:66:ILE:HD12	1.98	0.45
11:R:180:ASN:ND2	11:R:184:SER:OG	2.40	0.45
11:R:279:GLU:HA	11:R:303:VAL:HG13	1.99	0.45
10:T:333:VAL:HG12	10:T:389:GLY:HA2	1.99	0.45
5:I:78:DC:H2"	5:I:79:DC:C5	2.52	0.44
7:K:3898:HIS:HB3	8:N:339:LEU:HD23	1.99	0.44
7:K:3860:GLY:HA2	7:K:3899:GLY:HA2	1.98	0.44
7:K:3912:ASN:ND2	7:K:3938:GLU:OE2	2.49	0.44
9:O:7:THR:HG22	9:O:69:LEU:HB3	1.99	0.44
7:K:3883:TYR:HD2	7:K:3903:ARG:HE	1.65	0.44
8:N:149:ASP:OD2	8:N:170:ASN:ND2	2.32	0.44
10:T:291:LEU:HB2	10:T:304:ARG:HH22	1.83	0.44
10:T:449:PHE:HB2	10:T:456:GLN:HB2	2.00	0.44
11:R:157:ASP:HB2	11:R:164:LEU:HD21	1.98	0.44
8:N:158:SER:OG	8:N:159:PHE:N	2.51	0.44
11:R:73:GLY:HA3	11:R:78:LYS:HB3	1.99	0.44
8:N:346:GLU:HG2	10:T:312:GLY:HA2	2.00	0.43
11:R:133:PHE:HB2	11:R:149:PHE:HE1	1.81	0.43
10:T:294:ARG:HA	10:T:316:VAL:HG23	1.98	0.43
7:K:3777:MET:SD	7:K:3777:MET:N	2.87	0.43
11:R:282:LEU:HD13	11:R:296:LYS:HD2	2.00	0.43
8:N:16:GLU:HG3	8:N:324:ASN:HB2	1.99	0.43
8:N:47:ARG:HG2	8:N:63:SER:HA	2.00	0.43
10:T:299:LYS:HD3	10:T:308:VAL:HB	2.01	0.43
8:N:202:LYS:NZ	8:N:254:TRP:O	2.49	0.43
9:O:37:PRO:HA	9:O:38:PRO:HD3	1.81	0.43
8:N:88:ASN:HB2	8:N:105:ARG:HG3	2.01	0.43
11:R:287:ASN:HB3	11:R:290:THR:HG23	2.01	0.43
10:T:395:TYR:HB3	10:T:450:TYR:HE2	1.84	0.42
11:R:41:LEU:HB2	11:R:327:ILE:HB	2.01	0.42
11:R:217:VAL:HG22	11:R:233:THR:HG22	2.01	0.42
7:K:3860:GLY:HA2	8:N:339:LEU:HD11	2.01	0.42
8:N:41:VAL:N	8:N:49:VAL:O	2.51	0.42
5:I:60:DA:H2"	5:I:61:DA:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:343:ARG:HD3	10:T:365:SER:HB2	2.01	0.42
8:N:205:GLU:HB2	8:N:214:LEU:HD21	2.00	0.42
3:C:87:VAL:HG11	3:C:97:LEU:HD12	2.02	0.42
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.87	0.42
7:K:3858:TYR:HE1	7:K:3903:ARG:HA	1.85	0.42
7:K:3933:LYS:HE3	7:K:3935:TYR:HE1	1.85	0.42
11:R:295:GLN:HE21	11:R:297:LEU:HD21	1.85	0.42
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.90	0.42
11:R:149:PHE:CD1	11:R:173:PRO:HB3	2.55	0.42
4:D:87:THR:N	4:D:90:GLU:OE1	2.46	0.41
6:J:3:DC:H2''	6:J:4:DG:C8	2.55	0.41
8:N:290:LEU:HD23	8:N:290:LEU:HA	1.89	0.41
10:T:335:GLU:HB3	10:T:479:THR:HB	2.01	0.41
3:G:34:LEU:HD23	3:G:34:LEU:HA	1.92	0.41
1:E:72:ARG:HH22	6:J:51:DT:P	2.44	0.41
6:J:94:DG:H2'	6:J:95:DG:H8	1.85	0.41
8:N:139:ASP:OD2	8:N:141:LYS:NZ	2.36	0.41
10:T:367:ARG:HH21	10:T:370:LYS:HB2	1.85	0.41
10:T:448:ILE:HG12	10:T:458:VAL:HG22	2.03	0.41
11:R:321:LEU:HB3	11:R:322:GLU:H	1.68	0.41
1:A:61:LEU:HD12	1:A:61:LEU:HA	1.92	0.41
2:F:51:TYR:HB3	2:F:55:ARG:HH12	1.85	0.41
6:J:57:DT:H6	6:J:57:DT:H2'	1.78	0.41
10:T:329:PHE:HB3	10:T:500:MET:HG3	2.02	0.41
10:T:396:ILE:HD11	10:T:463:ILE:HD13	2.02	0.41
7:K:3859:ALA:H	7:K:3900:ASN:ND2	2.19	0.41
4:H:48:ASP:N	4:H:48:ASP:OD1	2.53	0.40
10:T:464:PHE:O	10:T:468:TYR:OH	2.32	0.40
11:R:88:LEU:HD12	11:R:108:ASP:HA	2.03	0.40
6:J:41:DG:H2'	6:J:42:DT:H71	2.02	0.40
7:K:3894:ASP:OD1	7:K:3895:ALA:N	2.54	0.40
3:C:25:PHE:HD1	3:C:25:PHE:HA	1.75	0.40
7:K:3773:SER:OG	11:R:191:TYR:O	2.39	0.40
8:N:240:GLU:HA	8:N:241:PRO:HD3	1.94	0.40
11:R:186:ILE:HB	11:R:198:TRP:HB2	2.04	0.40
2:B:44:LYS:HB2	3:G:115:LEU:HD13	2.03	0.40
8:N:46:GLY:HA2	8:N:69:VAL:HG23	2.03	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	95/135 (70%)	91 (96%)	4 (4%)	0	100	100
1	E	95/135 (70%)	91 (96%)	4 (4%)	0	100	100
2	B	84/102 (82%)	74 (88%)	10 (12%)	0	100	100
2	F	79/102 (78%)	73 (92%)	6 (8%)	0	100	100
3	C	110/129 (85%)	100 (91%)	10 (9%)	0	100	100
3	G	103/129 (80%)	99 (96%)	4 (4%)	0	100	100
4	D	92/122 (75%)	87 (95%)	5 (5%)	0	100	100
4	H	93/122 (76%)	92 (99%)	1 (1%)	0	100	100
7	K	173/216 (80%)	141 (82%)	32 (18%)	0	100	100
8	N	362/538 (67%)	313 (86%)	49 (14%)	0	100	100
9	O	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
10	T	172/534 (32%)	157 (91%)	15 (9%)	0	100	100
11	R	298/334 (89%)	267 (90%)	31 (10%)	0	100	100
All	All	1830/2674 (68%)	1654 (90%)	176 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/110 (77%)	84 (99%)	1 (1%)	71	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	85/110 (77%)	84 (99%)	1 (1%)	71	84
2	B	72/78 (92%)	71 (99%)	1 (1%)	67	81
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	89/101 (88%)	88 (99%)	1 (1%)	73	85
3	G	83/101 (82%)	81 (98%)	2 (2%)	49	69
4	D	81/102 (79%)	81 (100%)	0	100	100
4	H	81/102 (79%)	81 (100%)	0	100	100
7	K	150/189 (79%)	150 (100%)	0	100	100
8	N	322/462 (70%)	319 (99%)	3 (1%)	78	88
9	O	69/69 (100%)	69 (100%)	0	100	100
10	T	149/460 (32%)	149 (100%)	0	100	100
11	R	262/291 (90%)	262 (100%)	0	100	100
All	All	1595/2253 (71%)	1586 (99%)	9 (1%)	86	92

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

Mol	Chain	Res	Type
1	A	53	ARG
2	B	17	ARG
3	C	118	LYS
1	E	53	ARG
3	G	99	ARG
3	G	110	ASN
8	N	34	ARG
8	N	294	ARG
8	N	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	81	ASN
3	G	110	ASN
8	N	79	HIS
8	N	273	GLN
8	N	328	ASN
10	T	297	GLN
10	T	381	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	SAH	K	4001	-	24,28,28	1.18	3 (12%)	25,40,40	1.73	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SAH	K	4001	-	-	5/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	4001	SAH	C2-N3	3.62	1.37	1.32
12	K	4001	SAH	C2-N1	2.36	1.38	1.33
12	K	4001	SAH	OXT-C	-2.20	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	4001	SAH	N3-C2-N1	-5.02	120.83	128.68
12	K	4001	SAH	C5'-SD-CG	-4.22	89.61	102.27
12	K	4001	SAH	C3'-C2'-C1'	2.91	105.36	100.98
12	K	4001	SAH	OXT-C-O	-2.52	118.36	124.09
12	K	4001	SAH	OXT-C-CA	2.03	120.29	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

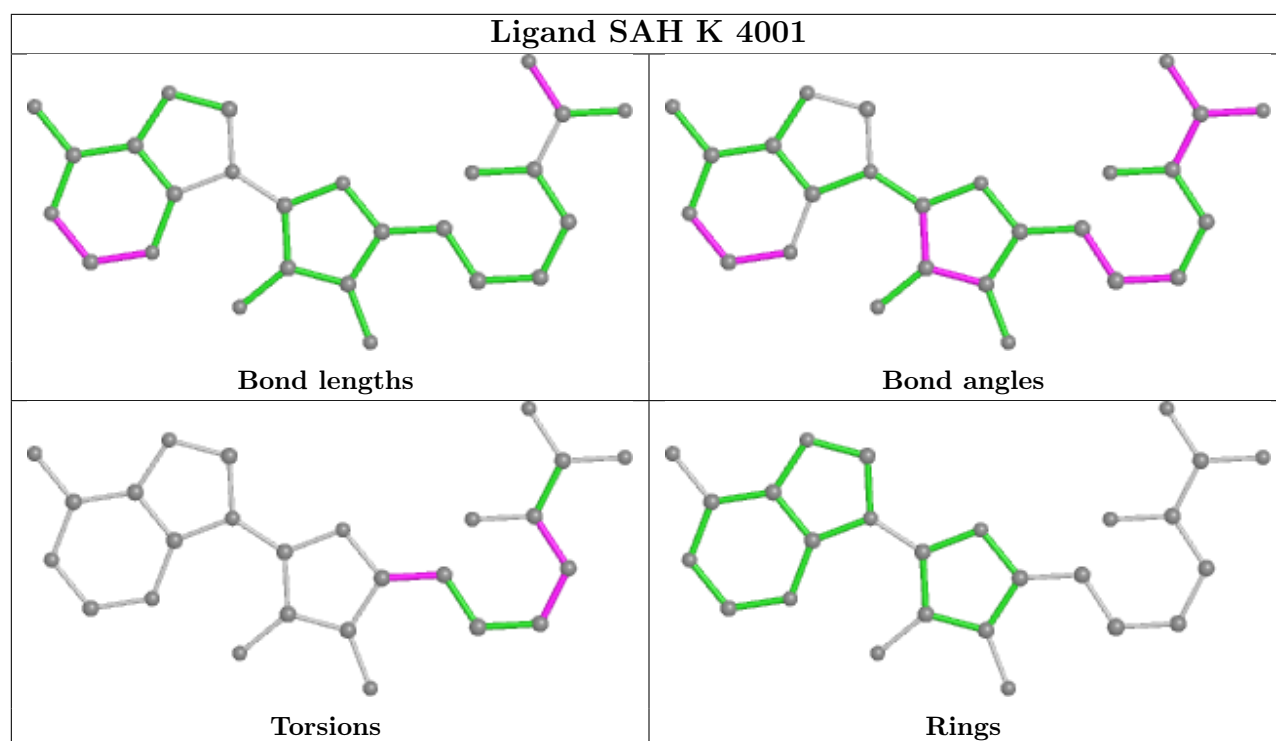
Mol	Chain	Res	Type	Atoms
12	K	4001	SAH	O4'-C4'-C5'-SD
12	K	4001	SAH	C3'-C4'-C5'-SD
12	K	4001	SAH	CA-CB-CG-SD
12	K	4001	SAH	C-CA-CB-CG
12	K	4001	SAH	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	K	4001	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

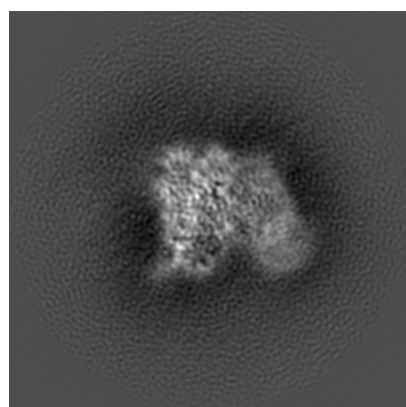
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9999. These allow visual inspection of the internal detail of the map and identification of artifacts.

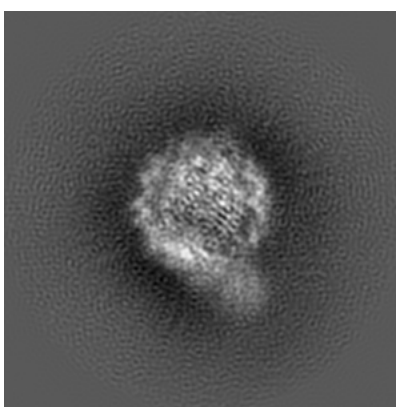
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

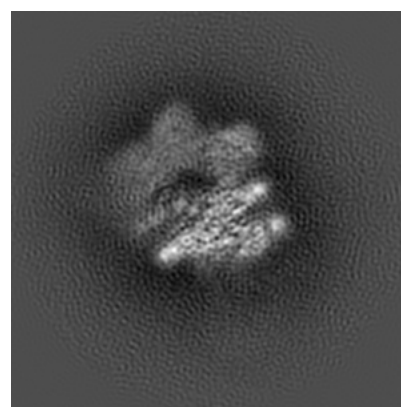
6.1.1 Primary map



X



Y

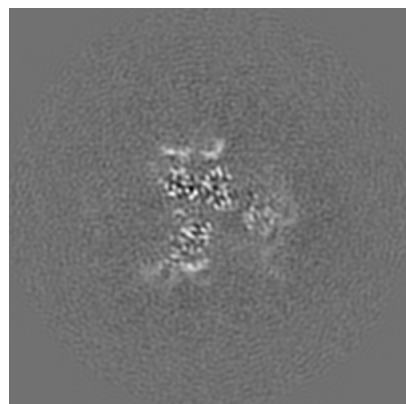


Z

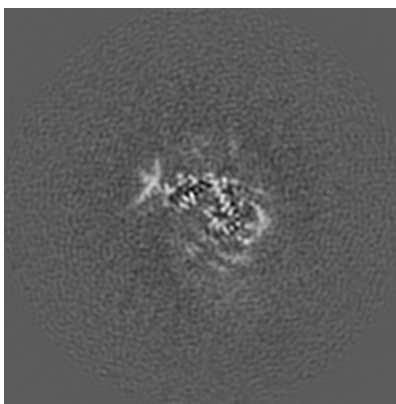
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

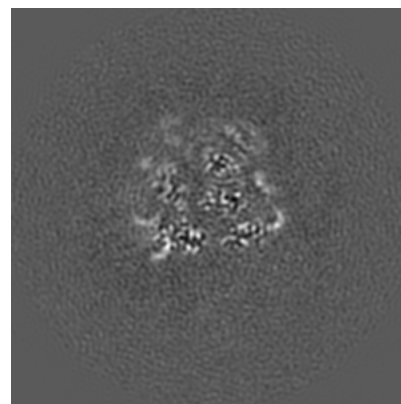
6.2.1 Primary map



X Index: 135



Y Index: 135

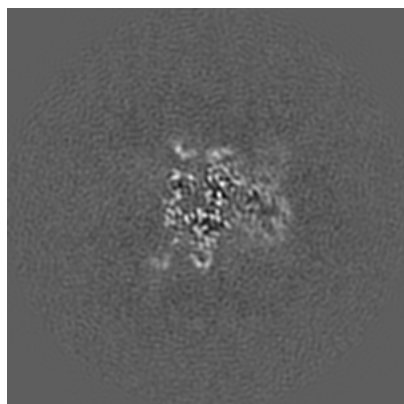


Z Index: 135

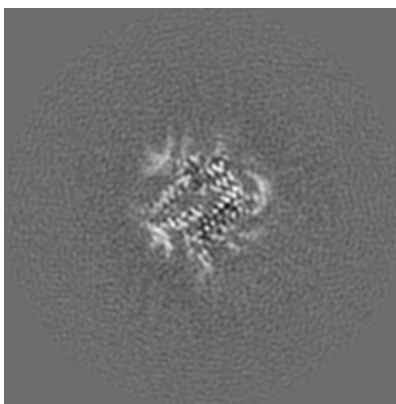
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

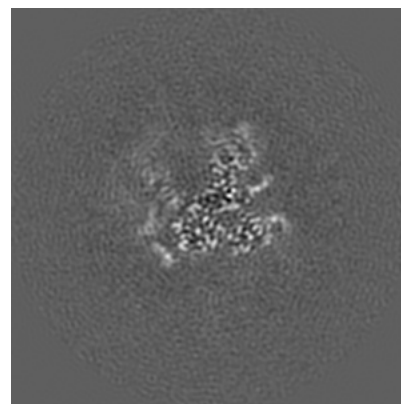
6.3.1 Primary map



X Index: 147



Y Index: 114



Z Index: 143

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

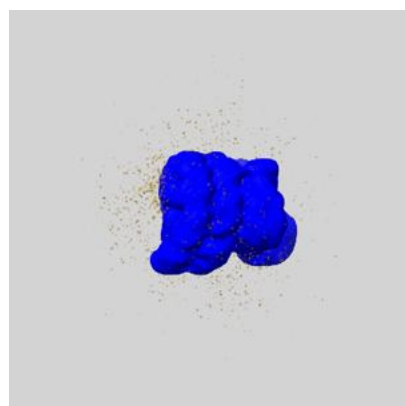
6.5 Mask visualisation [i](#)

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

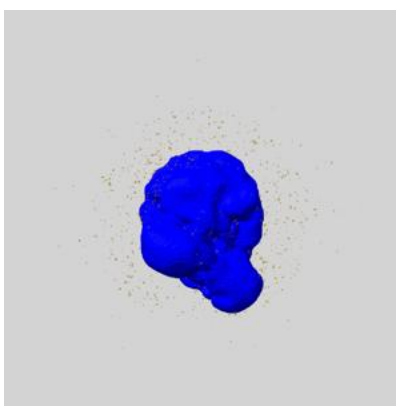
A mask typically either:

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

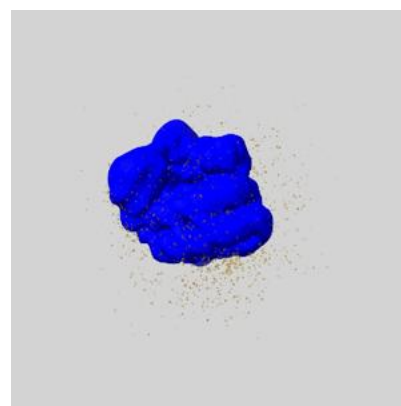
6.5.1 emd_9999_msk_1.map [i](#)



X



Y

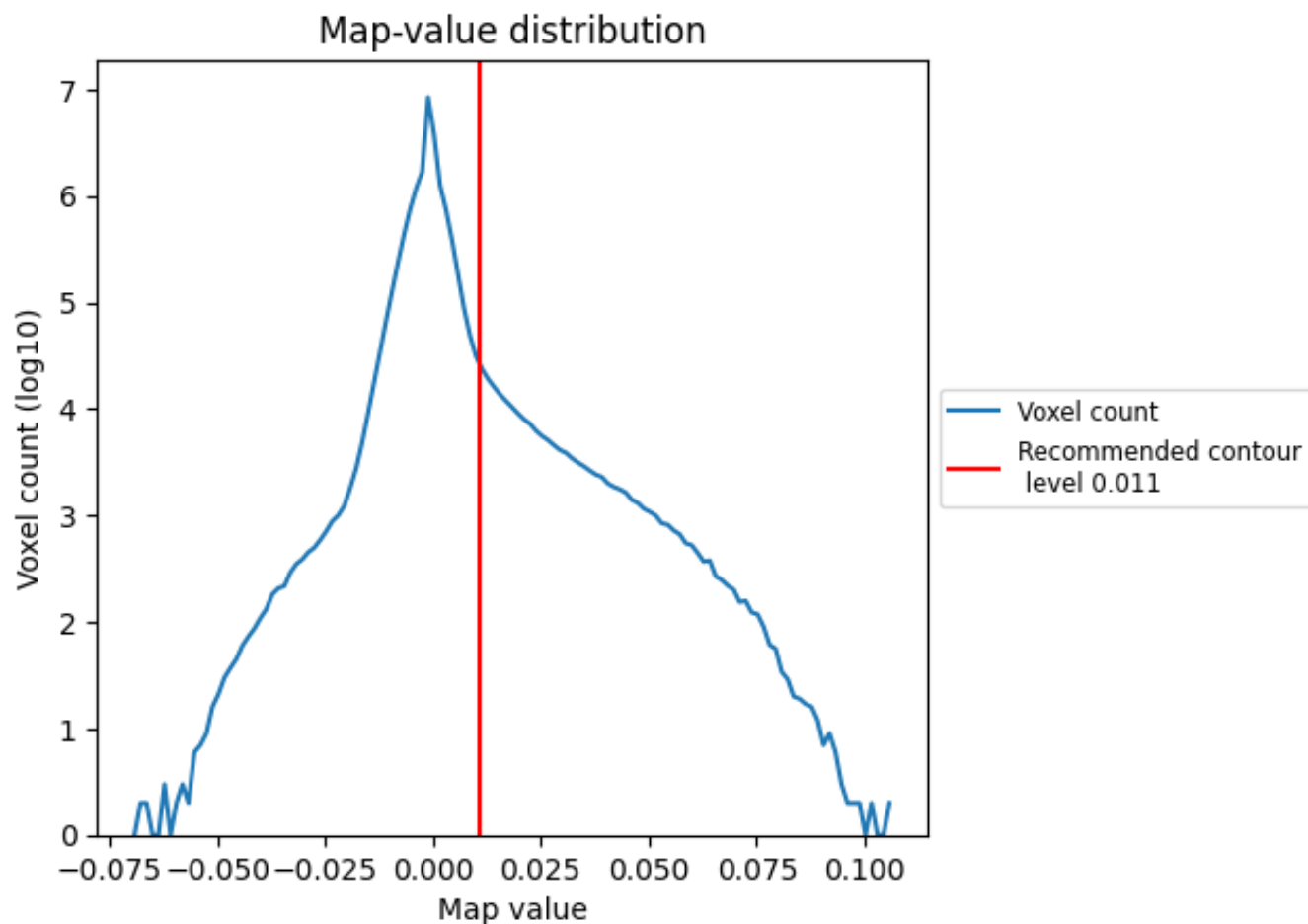


Z

7 Map analysis [i](#)

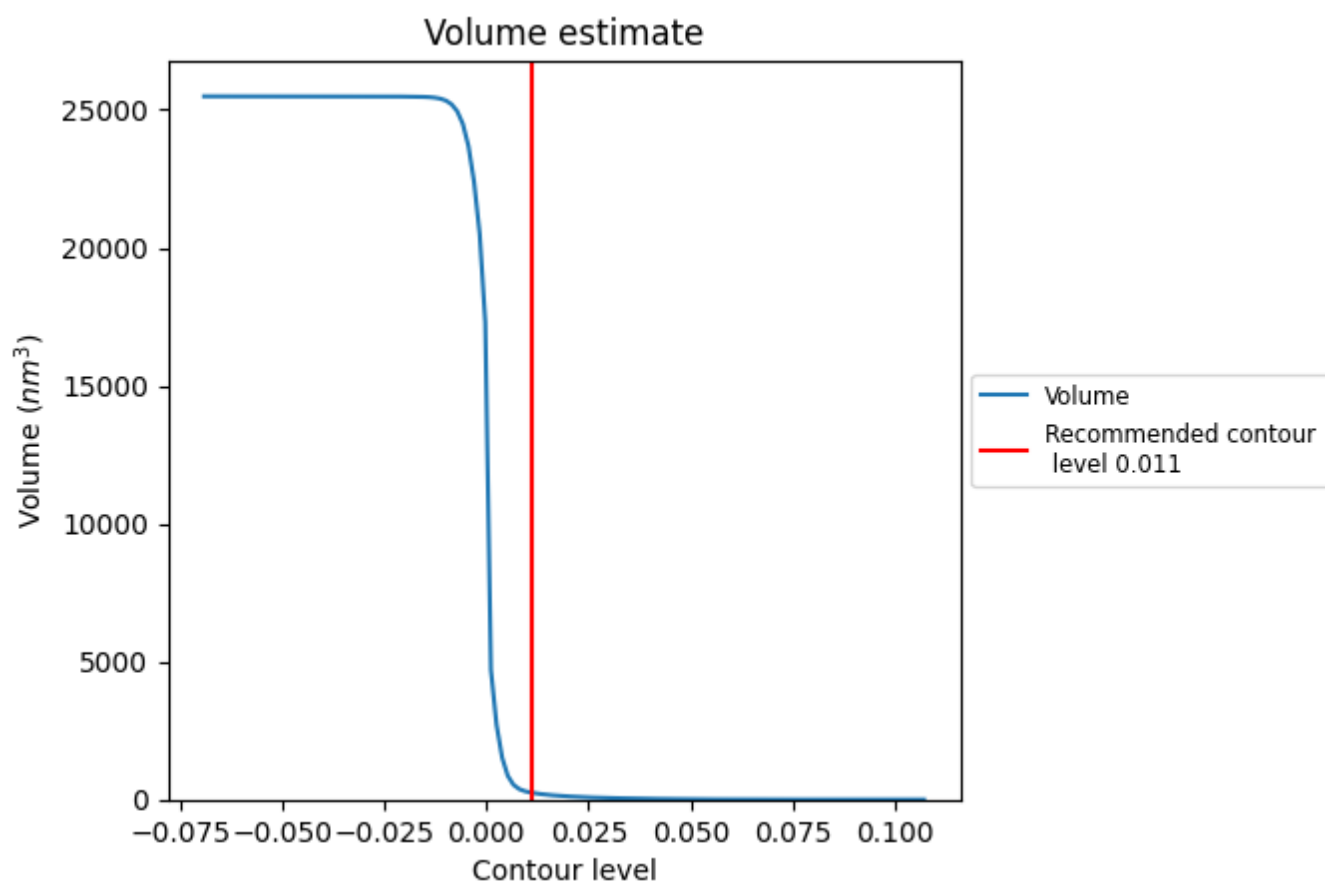
This section contains the results of statistical analysis of the map.

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.

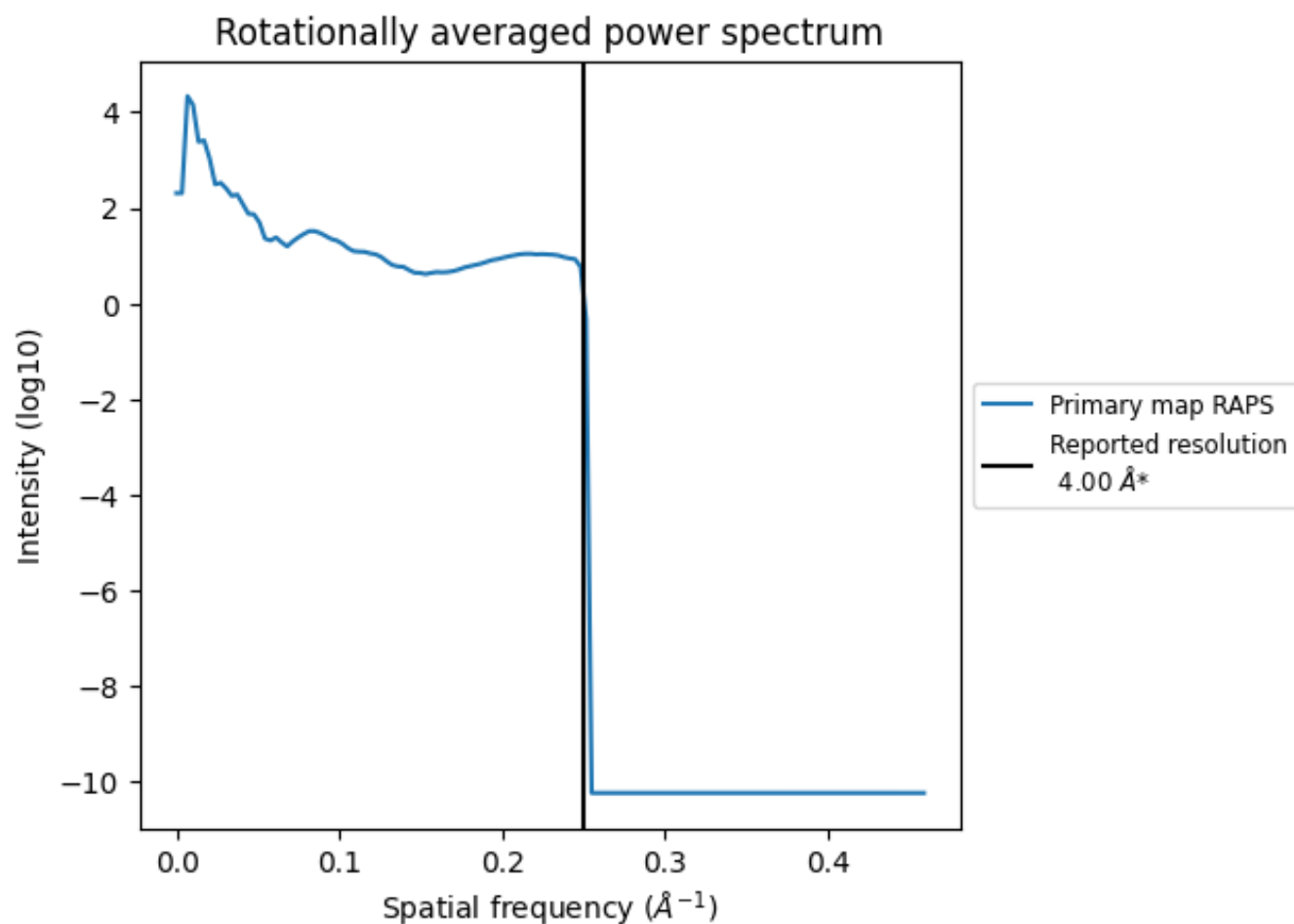
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 227 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 ⓘ

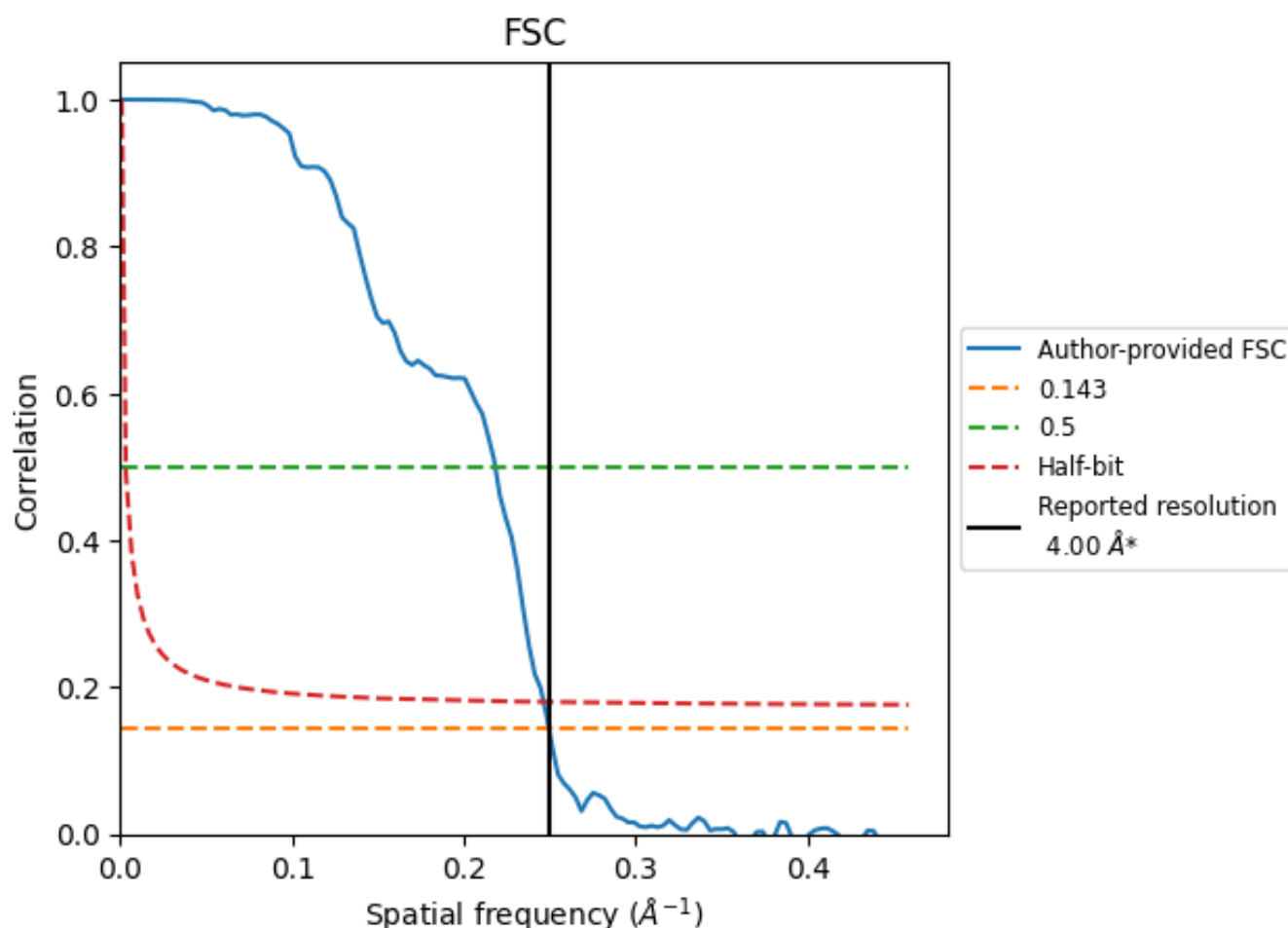


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

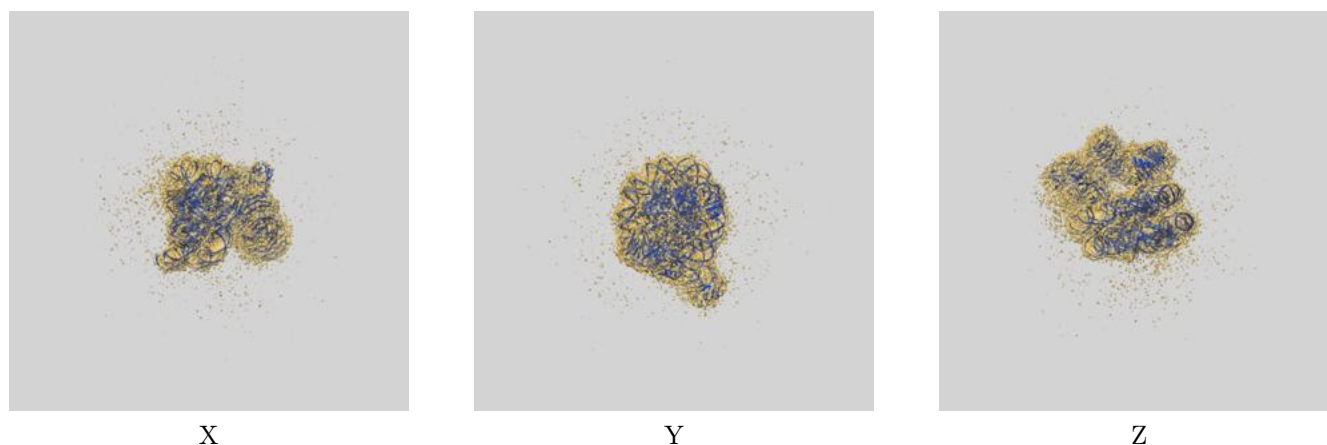
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.01	4.58	4.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

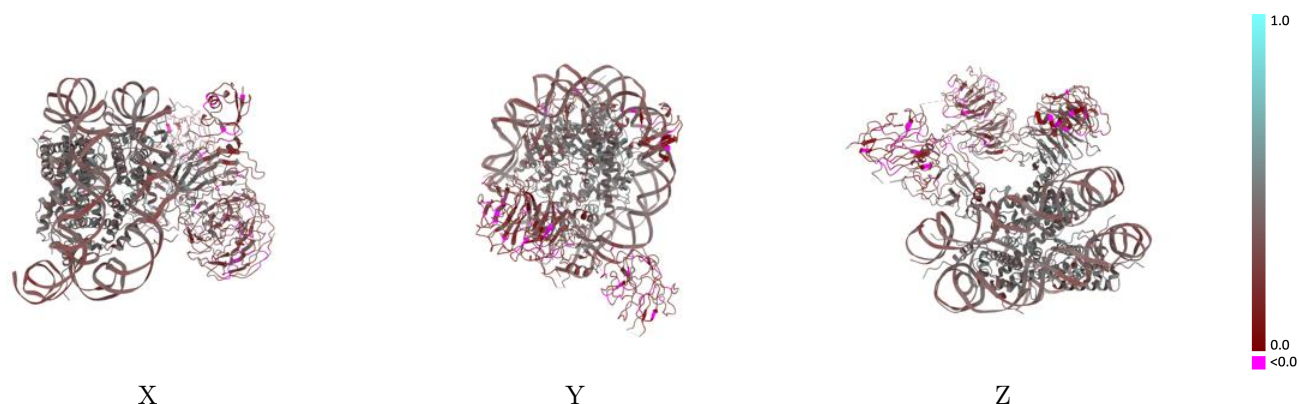
This section contains information regarding the fit between EMDB map EMD-9999 and PDB model 6KIV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



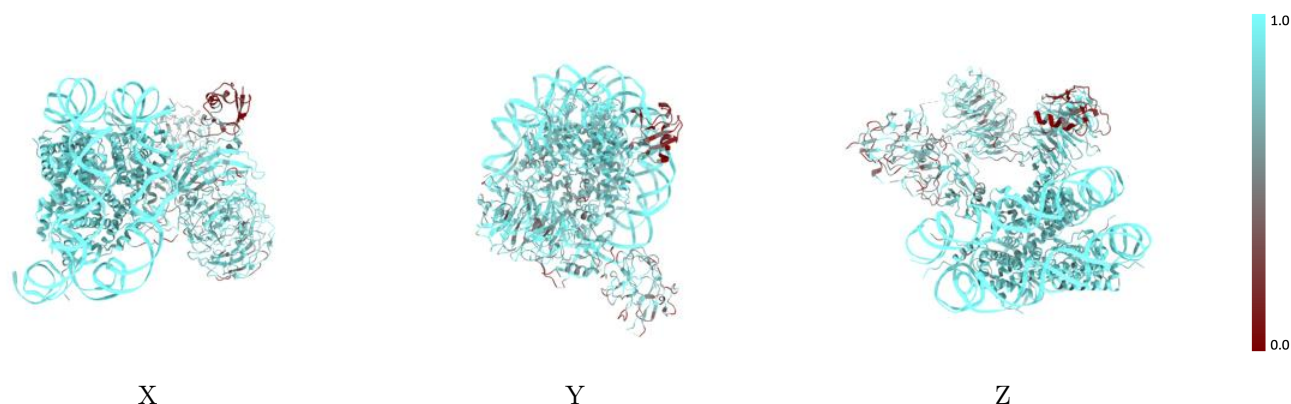
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



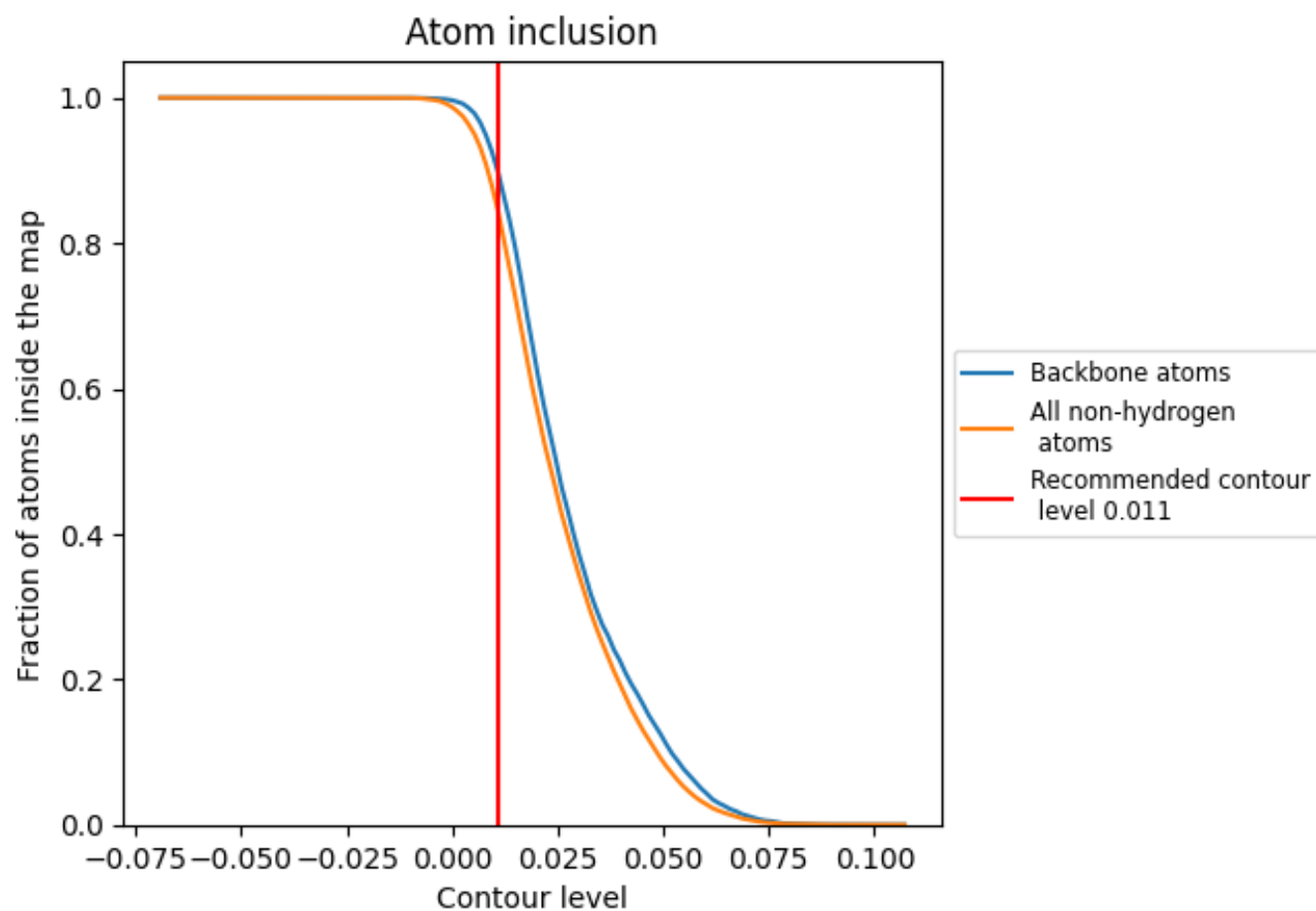
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.3430
A	 0.8599	 0.4210
B	 0.8533	 0.4330
C	 0.8747	 0.4510
D	 0.9082	 0.4470
E	 0.8794	 0.4330
F	 0.9228	 0.4500
G	 0.8967	 0.4470
H	 0.8869	 0.4190
I	 0.9817	 0.3540
J	 0.9813	 0.3530
K	 0.7053	 0.3180
N	 0.7840	 0.3440
O	 0.2795	 0.1930
R	 0.7944	 0.2110
T	 0.6238	 0.1900

