



Full wwPDB EM Validation Report ⓘ

Dec 5, 2024 – 12:28 pm GMT

PDB ID : 8QEQ
EMDB ID : EMD-18376
Title : RNA polymerase II bound to minimal Alu RNA right arm in the alternative conformation
Authors : Tluckova, K.; Bernecky, C.
Deposited on : 2023-09-01
Resolution : 3.10 Å(reported)
Based on initial model : 5OIK

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:

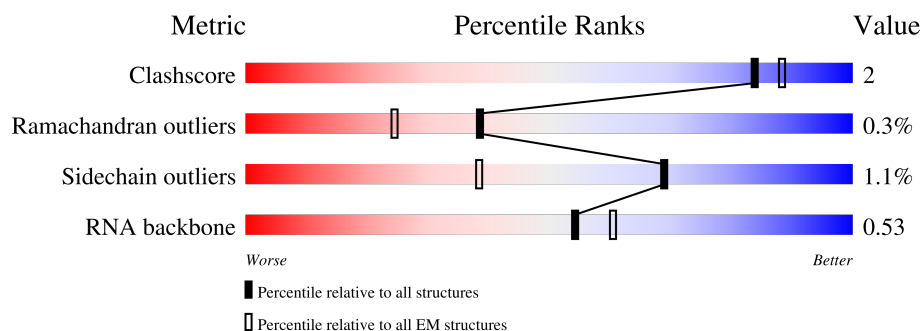
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	<div> <div>12%</div> <div>66%</div> <div>5%</div> <div>28%</div> </div>
2	B	1174	<div> <div>9%</div> <div>89%</div> <div>6%</div> <div>.</div> </div>
3	C	275	<div> <div>7%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
4	E	210	<div> <div>14%</div> <div>93%</div> <div>6%</div> </div>
5	F	127	<div> <div>13%</div> <div>63%</div> <div>35%</div> <div>.</div> </div>
6	H	150	<div> <div>11%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
7	I	125	<div> <div>22%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	67	<div><div></div><div>97%</div><div></div></div>
9	K	117	<div><div>15%</div><div>93%</div><div>5%</div></div>
10	L	58	<div><div>14%</div><div>66%</div><div>12%</div><div>22%</div></div>
11	R	76	<div><div>5%</div><div>24%</div><div>9%</div><div>61%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29242 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11186	7038	2003	2075	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1123	Total	C	N	O	S	0	0
			8980	5685	1577	1654	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	259	Total	C	N	O	S	0	0
			2079	1305	357	411	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	67	Total	C	N	O	S	0	0
			534	345	90	93	6		

- Molecule 9 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 10 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	45	Total	C	N	O	S	0	0
			380	236	73	65	6		

- Molecule 11 is a RNA chain called Alu RNA Minimal Right Arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	30	Total	C	N	O	P	0	0
			640	285	114	211	30		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total	Zn	0
			2	2	
12	B	1	Total	Zn	0
			1	1	
12	I	2	Total	Zn	0
			2	2	
12	J	1	Total	Zn	0
			1	1	
12	L	1	Total	Zn	0
			1	1	

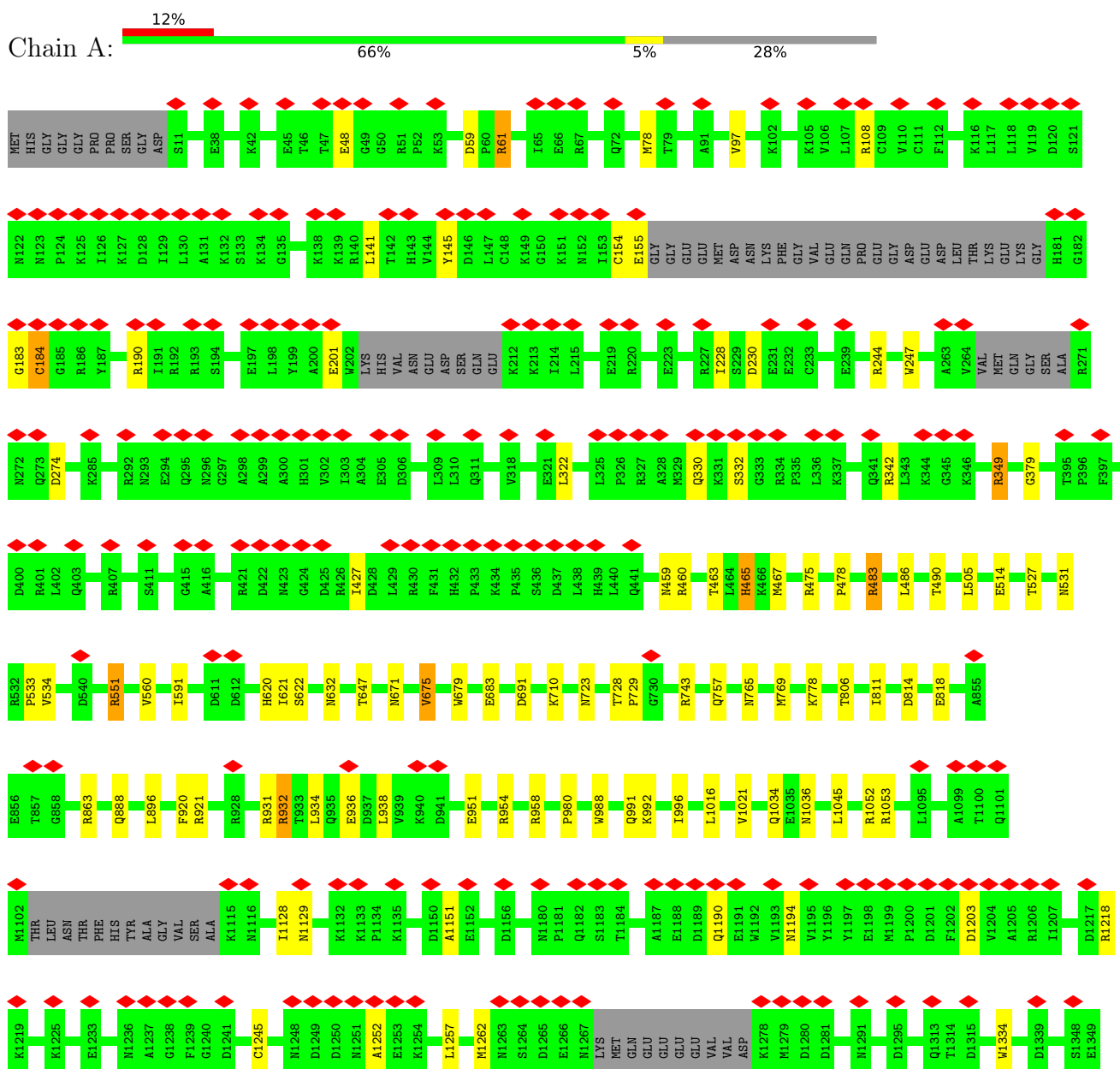
- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	

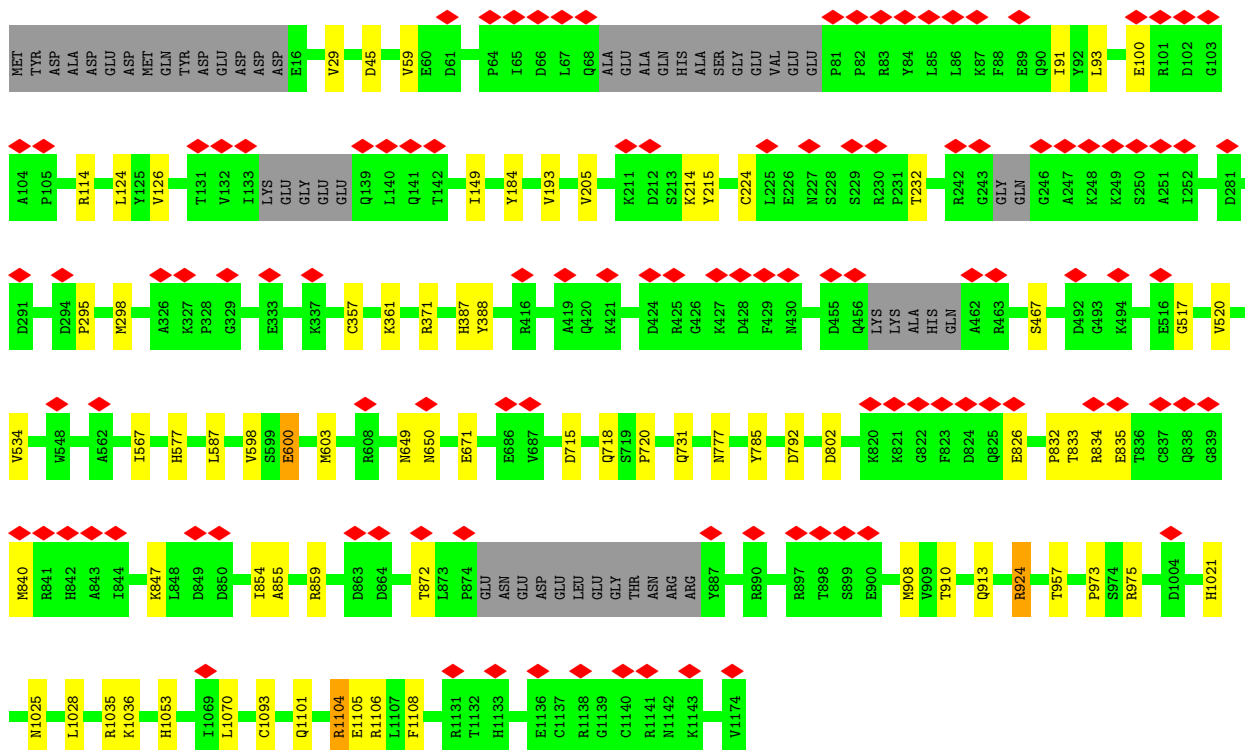
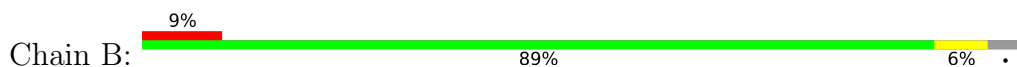
3 Residue-property plots

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.

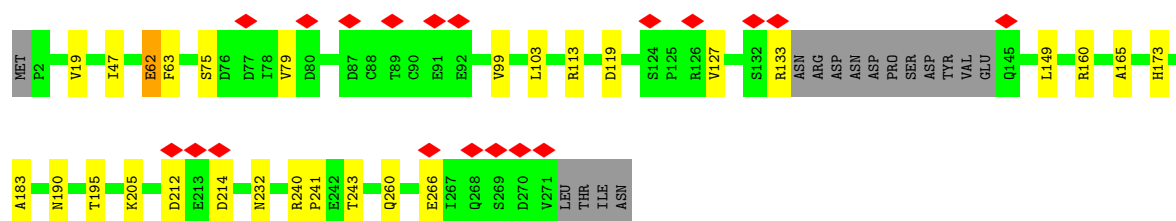
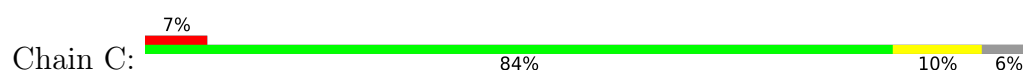
• Molecule 1: DNA-directed RNA polymerase subunit



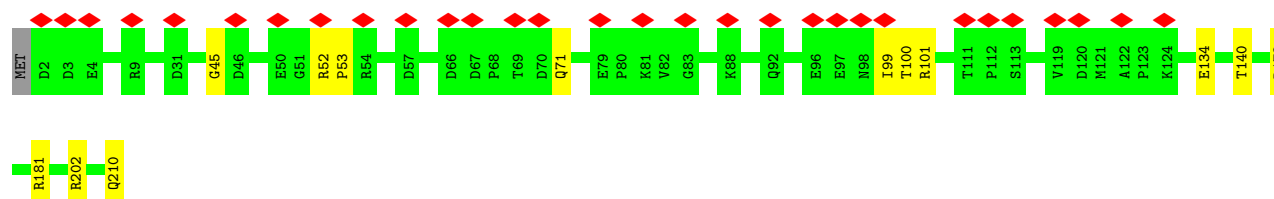
- Molecule 2: DNA-directed RNA polymerase subunit beta



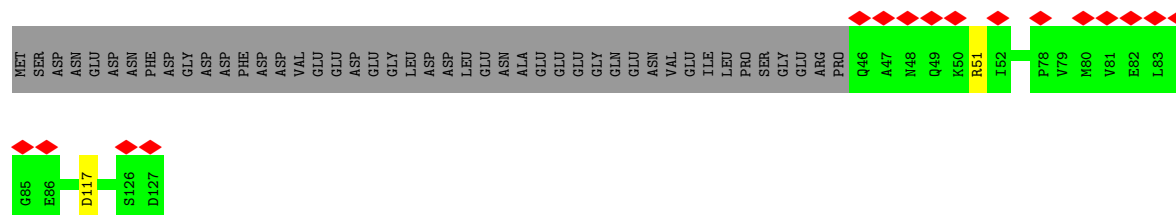
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



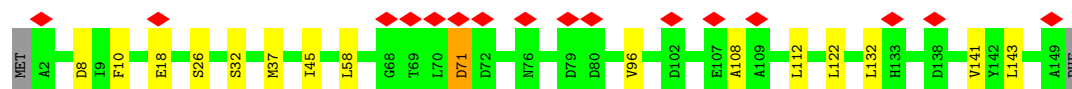
• Molecule 4: DNA-directed RNA polymerase II subunit E



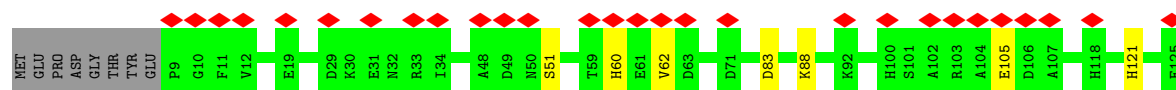
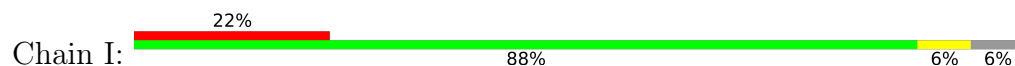
• Molecule 5: DNA-directed RNA polymerase II subunit F



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

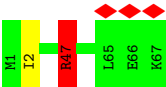


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

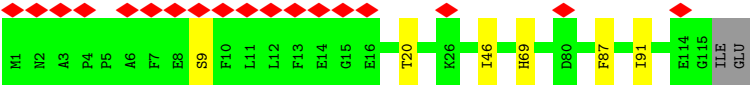
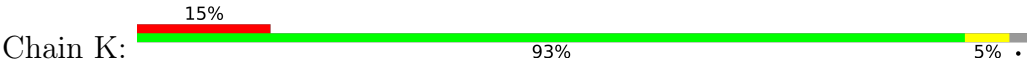


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

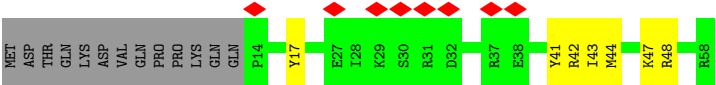




● Molecule 9: RNA_pol_L_2 domain-containing protein



● Molecule 10: RNA polymerase II subunit K



● Molecule 11: Alu RNA Minimal Right Arm



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	428, 428, 428	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9988785, 0.9988785, 0.9988785	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/11390	0.55	0/15374
2	B	0.27	0/9158	0.55	0/12359
3	C	0.29	0/2122	0.57	0/2883
4	E	0.26	0/1752	0.53	0/2366
5	F	0.26	0/668	0.55	0/901
6	H	0.29	0/1207	0.54	0/1628
7	I	0.29	0/973	0.53	0/1316
8	J	0.29	0/543	0.54	0/730
9	K	0.27	0/939	0.50	0/1271
10	L	0.30	0/386	0.69	0/511
11	R	0.40	0/711	1.56	36/1099 (3.3%)
All	All	0.28	0/29849	0.60	36/40438 (0.1%)

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	4
8	J	0	1
All	All	0	5

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	60	G	OP1-P-OP2	-7.58	108.24	119.60
11	R	57	A	OP1-P-OP2	-7.24	108.74	119.60
11	R	75	U	OP1-P-OP2	-7.20	108.80	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	54	G	OP1-P-OP2	-7.12	108.92	119.60
11	R	6	A	OP1-P-OP2	-7.09	108.97	119.60
11	R	56	G	OP1-P-OP2	-7.03	109.06	119.60
11	R	68	C	OP1-P-OP2	-7.03	109.06	119.60
11	R	69	U	OP1-P-OP2	-6.95	109.18	119.60
11	R	63	C	OP1-P-OP2	-6.94	109.19	119.60
11	R	56	G	OP1-P-O3'	6.89	120.36	105.20
11	R	59	A	OP1-P-O3'	6.87	120.32	105.20
11	R	5	C	OP1-P-OP2	-6.86	109.30	119.60
11	R	61	A	OP1-P-OP2	-6.81	109.39	119.60
11	R	70	C	OP1-P-OP2	-6.80	109.41	119.60
11	R	4	G	OP1-P-OP2	-6.79	109.41	119.60
11	R	72	G	OP1-P-OP2	-6.75	109.47	119.60
11	R	53	G	OP1-P-OP2	-6.72	109.51	119.60
11	R	3	G	OP1-P-OP2	-6.63	109.65	119.60
11	R	73	U	OP1-P-OP2	-6.60	109.70	119.60
11	R	59	A	OP1-P-OP2	-6.58	109.73	119.60
11	R	71	U	OP1-P-OP2	-6.55	109.78	119.60
11	R	51	U	OP1-P-OP2	-6.55	109.78	119.60
11	R	58	C	OP1-P-OP2	-6.49	109.86	119.60
11	R	76	C	OP1-P-OP2	-6.47	109.90	119.60
11	R	50	C	OP1-P-OP2	-6.46	109.90	119.60
11	R	55	U	OP1-P-O3'	6.45	119.39	105.20
11	R	68	C	C3'-C2'-C1'	6.29	106.54	101.50
11	R	71	U	O4'-C1'-N1	6.18	113.15	108.20
11	R	74	C	OP1-P-OP2	-6.17	110.34	119.60
11	R	73	U	O4'-C1'-N1	5.79	112.83	108.20
11	R	74	C	OP1-P-O3'	5.54	117.40	105.20
11	R	57	A	OP1-P-O3'	5.50	117.30	105.20
11	R	53	G	OP1-P-O3'	5.49	117.28	105.20
11	R	55	U	OP1-P-OP2	-5.38	111.53	119.60
11	R	4	G	OP1-P-O3'	5.11	116.45	105.20
11	R	71	U	OP1-P-O3'	5.09	116.41	105.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ARG	Sidechain
1	A	483	ARG	Sidechain
1	A	551	ARG	Sidechain
1	A	932	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	J	47	ARG	Sidechain

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	11186	0	11313	54	0
2	B	8980	0	9022	40	0
3	C	2079	0	2032	17	0
4	E	1721	0	1737	7	0
5	F	658	0	684	1	0
6	H	1186	0	1147	9	0
7	I	950	0	879	2	0
8	J	534	0	553	2	0
9	K	920	0	942	4	0
10	L	380	0	386	5	0
11	R	640	0	327	3	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	1	0	0	0	0
All	All	29242	0	29022	128	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 2.

All (128) 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)
6:H:58:LEU:HD11	6:H:143:LEU:HD11	1.75	0.69
1:A:478:PRO:O	1:A:483:ARG:NH2	2.24	0.68
11:R:58:C:H42	11:R:72:G:H1	1.43	0.66
3:C:205:LYS:NZ	3:C:212:ASP:O	2.25	0.66
1:A:931:ARG:NH1	1:A:936:GLU:OE1	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:OD2	1:A:342:ARG:NH2	2.31	0.64
1:A:988:TRP:HE1	1:A:992:LYS:HE2	1.66	0.60
1:A:533:PRO:O	1:A:647:THR:OG1	2.19	0.60
2:B:833:THR:HG22	2:B:835:GLU:H	1.67	0.59
2:B:205:VAL:O	2:B:371:ARG:NH1	2.37	0.58
1:A:1451:MET:HE1	1:A:1460:LEU:HD13	1.86	0.57
3:C:190:ASN:ND2	3:C:195:THR:O	2.30	0.57
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.86	0.56
6:H:32:SER:HB3	6:H:37:MET:H	1.71	0.56
1:A:59:ASP:OD2	1:A:61:ARG:NH1	2.38	0.56
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.88	0.55
2:B:59:VAL:HG21	2:B:91:ILE:HD12	1.89	0.55
1:A:1021:VAL:HA	1:A:1034:GLN:NE2	2.22	0.55
6:H:32:SER:HB3	6:H:37:MET:N	2.22	0.54
2:B:924:ARG:NH1	3:C:62:GLU:OE2	2.40	0.54
1:A:921:ARG:O	1:A:1052:ARG:NH1	2.34	0.53
1:A:1128:ILE:HG23	1:A:1414:ILE:HD12	1.90	0.53
1:A:951:GLU:OE1	1:A:954:ARG:NH1	2.37	0.53
2:B:957:THR:HG22	2:B:1028:LEU:HD22	1.90	0.53
3:C:47:ILE:HA	3:C:165:ALA:HA	1.90	0.53
1:A:551:ARG:NH2	1:A:622:SER:O	2.36	0.53
4:E:45:GLY:HA3	4:E:52:ARG:HD2	1.90	0.52
1:A:710:LYS:NZ	1:A:818:GLU:OE2	2.32	0.52
11:R:49:C:H2'	11:R:50:C:C6	2.45	0.52
1:A:991:GLN:HA	1:A:996:ILE:HD12	1.92	0.51
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.43	0.51
2:B:847:LYS:NZ	2:B:859:ARG:O	2.32	0.51
2:B:224:CYS:HB2	2:B:232:THR:HG22	1.93	0.51
1:A:183:GLY:O	1:A:184:CYS:SG	2.69	0.50
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.45	0.50
2:B:100:GLU:OE1	10:L:42:ARG:NH2	2.43	0.50
5:F:51:ARG:NH2	5:F:117:ASP:O	2.42	0.50
1:A:811:ILE:HD12	1:A:814:ASP:HB2	1.94	0.50
2:B:649:ASN:OD1	2:B:650:ASN:N	2.45	0.50
4:E:71:GLN:HB2	4:E:99:ILE:HD12	1.93	0.50
9:K:9:SER:HA	9:K:69:HIS:CD2	2.47	0.49
1:A:757:GLN:NE2	1:A:778:LYS:O	2.45	0.49
2:B:802:ASP:HB3	3:C:173:HIS:CE1	2.48	0.49
3:C:99:VAL:HG11	3:C:127:VAL:HG21	1.94	0.49
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.47	0.49
1:A:228:ILE:O	1:A:244:ARG:NH2	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ASN:O	1:A:675:VAL:HG13	2.12	0.48
1:A:330:GLN:HG3	1:A:332:SER:H	1.78	0.48
4:E:100:THR:HG23	4:E:101:ARG:HG3	1.95	0.48
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.41	0.48
6:H:112:LEU:HB2	6:H:132:LEU:HD23	1.96	0.48
7:I:88:LYS:HE3	7:I:121:HIS:ND1	2.28	0.48
10:L:17:TYR:HB3	10:L:44:MET:HB3	1.97	0.47
4:E:172:ARG:NH1	4:E:210:GLN:OE1	2.48	0.47
1:A:620:HIS:O	1:A:621:ILE:HG22	2.14	0.47
9:K:46:ILE:HG21	9:K:87:PHE:CE1	2.50	0.47
2:B:587:LEU:HB3	2:B:603:MET:SD	2.55	0.47
2:B:826:GLU:H	2:B:872:THR:HG22	1.81	0.46
3:C:240:ARG:O	3:C:243:THR:HG22	2.16	0.46
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.97	0.46
1:A:888:GLN:NE2	1:A:1403:ASP:OD2	2.32	0.46
3:C:113:ARG:NH2	3:C:119:ASP:OD2	2.42	0.46
2:B:114:ARG:NH2	2:B:184:TYR:OH	2.48	0.46
3:C:149:LEU:HG	8:J:2:ILE:HD11	1.98	0.46
1:A:932:ARG:NH2	6:H:108:ALA:HA	2.31	0.45
1:A:728:THR:HG23	1:A:729:PRO:HD2	1.98	0.45
1:A:1190:GLN:NE2	1:A:1194:ASN:HD21	2.13	0.45
2:B:792:ASP:CG	2:B:975:ARG:HH22	2.20	0.45
1:A:621:ILE:HA	6:H:122:LEU:HD13	1.98	0.45
2:B:832:PRO:HB2	2:B:840:MET:SD	2.56	0.45
1:A:920:PHE:CE1	1:A:1053:ARG:HD2	2.51	0.45
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.99	0.45
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.16	0.45
3:C:75:SER:HB3	3:C:79:VAL:HG21	1.99	0.45
3:C:212:ASP:OD1	3:C:214:ASP:N	2.46	0.44
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.49	0.44
1:A:1151:ALA:HB2	1:A:1334:TRP:CZ2	2.51	0.44
2:B:357:CYS:SG	2:B:361:LYS:HE2	2.57	0.44
10:L:47:LYS:HG2	10:L:48:ARG:H	1.83	0.44
1:A:691:ASP:OD1	1:A:765:ASN:ND2	2.39	0.44
2:B:567:ILE:HD11	2:B:577:HIS:HB2	1.99	0.44
2:B:598:VAL:HG12	2:B:600:GLU:H	1.82	0.43
2:B:777:ASN:O	8:J:47:ARG:NH1	2.46	0.43
4:E:52:ARG:HG2	4:E:53:PRO:HD3	2.00	0.43
1:A:459:ASN:OD1	1:A:460:ARG:N	2.52	0.43
1:A:379:GLY:HA2	1:A:475:ARG:O	2.18	0.43
1:A:505:LEU:O	2:B:1106:ARG:NH2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:LEU:HD13	1:A:980:PRO:HB3	2.01	0.43
1:A:154:CYS:SG	1:A:155:GLU:N	2.91	0.43
7:I:60:HIS:CE1	7:I:62:VAL:HB	2.52	0.43
11:R:69:U:H2'	11:R:70:C:C6	2.54	0.43
2:B:517:GLY:O	2:B:520:VAL:HG23	2.18	0.43
2:B:45:ASP:HB3	2:B:534:VAL:HG21	1.99	0.43
2:B:910:THR:HG22	10:L:43:ILE:HA	1.99	0.43
1:A:863:ARG:NH1	1:A:1129:ASN:OD1	2.49	0.42
2:B:731:GLN:OE1	2:B:1053:HIS:NE2	2.41	0.42
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.50	0.42
2:B:834:ARG:HA	2:B:840:MET:HG3	2.02	0.42
2:B:214:LYS:HE3	2:B:215:TYR:CZ	2.54	0.42
1:A:463:THR:HG22	2:B:1093:CYS:SG	2.60	0.42
1:A:514:GLU:OE1	2:B:1101:GLN:HB2	2.20	0.42
3:C:103:LEU:O	3:C:160:ARG:HA	2.20	0.42
1:A:427:ILE:N	1:A:427:ILE:HD12	2.35	0.42
3:C:75:SER:HB3	3:C:79:VAL:CG2	2.50	0.42
3:C:266:GLU:OE2	9:K:20:THR:HA	2.20	0.42
2:B:715:ASP:OD1	2:B:715:ASP:N	2.52	0.41
1:A:244:ARG:HB3	1:A:247:TRP:CE2	2.55	0.41
1:A:349:ARG:NH2	2:B:1070:LEU:HD21	2.35	0.41
1:A:934:LEU:HD11	1:A:938:LEU:HD23	2.02	0.41
2:B:124:LEU:HD23	2:B:149:ILE:HD11	2.02	0.41
4:E:134:GLU:OE2	4:E:181:ARG:NH2	2.47	0.41
1:A:1245:CYS:HB3	1:A:1257:LEU:HD11	2.01	0.41
6:H:26:SER:HB3	6:H:45:ILE:HG13	2.02	0.41
1:A:769:MET:SD	2:B:973:PRO:HG3	2.61	0.41
10:L:41:TYR:CE2	10:L:43:ILE:HB	2.56	0.41
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	2.03	0.41
2:B:854:ILE:HG22	2:B:855:ALA:N	2.36	0.41
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.56	0.40
2:B:193:VAL:O	2:B:467:SER:HA	2.21	0.40
3:C:260:GLN:HB2	9:K:91:ILE:HG21	2.04	0.40
6:H:71:ASP:N	6:H:71:ASP:OD1	2.54	0.40
1:A:97:VAL:HG21	1:A:322:LEU:HD11	2.03	0.40
1:A:1036:ASN:OD1	4:E:202:ARG:NH1	2.41	0.40
2:B:1021:HIS:CD2	2:B:1025:ASN:HD22	2.39	0.40
2:B:295:PRO:HA	2:B:298:MET:HG2	2.03	0.40
1:A:190:ARG:N	1:A:201:GLU:O	2.53	0.40
1:A:527:THR:HB	1:A:534:VAL:HG13	2.04	0.40
1:A:679:TRP:CH2	1:A:683:GLU:HG3	2.56	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	1398/1970 (71%)	1333 (95%)	58 (4%)	7 (0%)	25	58
2	B	1111/1174 (95%)	1071 (96%)	39 (4%)	1 (0%)	48	79
3	C	255/275 (93%)	246 (96%)	9 (4%)	0	100	100
4	E	207/210 (99%)	195 (94%)	12 (6%)	0	100	100
5	F	80/127 (63%)	74 (92%)	6 (8%)	0	100	100
6	H	146/150 (97%)	139 (95%)	7 (5%)	0	100	100
7	I	115/125 (92%)	104 (90%)	9 (8%)	2 (2%)	7	30
8	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
9	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
10	L	43/58 (74%)	38 (88%)	5 (12%)	0	100	100
All	All	3533/4273 (83%)	3374 (96%)	149 (4%)	10 (0%)	38	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1262	MET
7	I	105	GLU
7	I	51	SER
1	A	48	GLU
1	A	78	MET
1	A	184	CYS
1	A	531	ASN
1	A	1351	ASP
2	B	785	TYR
1	A	1414	ILE

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	1244/1749 (71%)	1230 (99%)	14 (1%)	70	84
2	B	985/1027 (96%)	975 (99%)	10 (1%)	73	86
3	C	236/252 (94%)	233 (99%)	3 (1%)	65	82
4	E	191/192 (100%)	190 (100%)	1 (0%)	86	92
5	F	71/111 (64%)	71 (100%)	0	100	100
6	H	129/131 (98%)	125 (97%)	4 (3%)	35	63
7	I	105/112 (94%)	104 (99%)	1 (1%)	73	86
8	J	56/56 (100%)	55 (98%)	1 (2%)	54	76
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	42/55 (76%)	42 (100%)	0	100	100
All	All	3163/3791 (83%)	3129 (99%)	34 (1%)	69	84

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	141	LEU
1	A	465	HIS
1	A	486	LEU
1	A	490	THR
1	A	632	ASN
1	A	675	VAL
1	A	723	ASN
1	A	743	ARG
1	A	806	THR
1	A	958	ARG
1	A	1203	ASP
1	A	1396	ARG
1	A	1410	HIS
2	B	29	VAL
2	B	93	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	126	VAL
2	B	388	TYR
2	B	600	GLU
2	B	908	MET
2	B	913	GLN
2	B	924	ARG
2	B	1104	ARG
2	B	1105	GLU
3	C	62	GLU
3	C	63	PHE
3	C	133	ARG
4	E	140	THR
6	H	18	GLU
6	H	71	ASP
6	H	96	VAL
6	H	141	VAL
7	I	83	ASP
8	J	47	ARG

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

Mol	Chain	Res	Type
1	A	757	GLN
1	A	861	GLN
1	A	1034	GLN
1	A	1194	ASN
2	B	312	GLN
2	B	749	HIS
2	B	913	GLN
2	B	1025	ASN
6	H	133	HIS
7	I	50	ASN
9	K	69	HIS
10	L	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	27/76 (35%)	3 (11%)	1 (3%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	55	U
11	R	56	G
11	R	69	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	R	68	C

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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

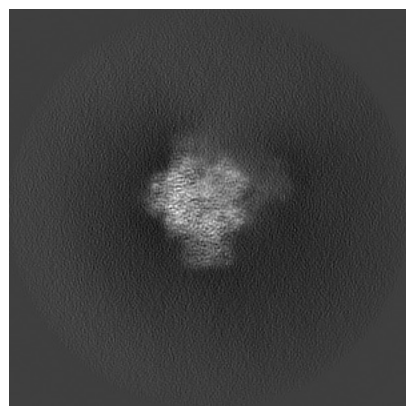
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18376. These allow visual inspection of the internal detail of the map and identification of artifacts.

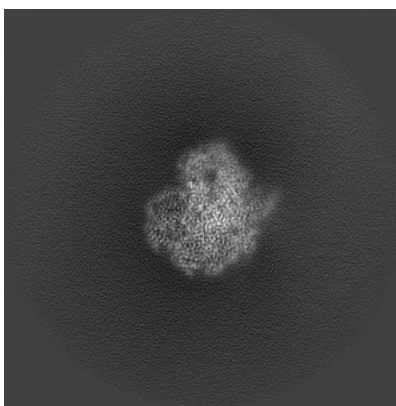
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

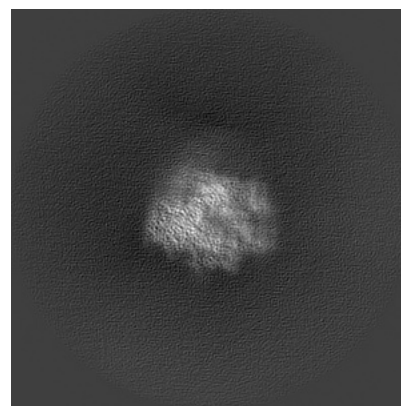
6.1.1 Primary map



X

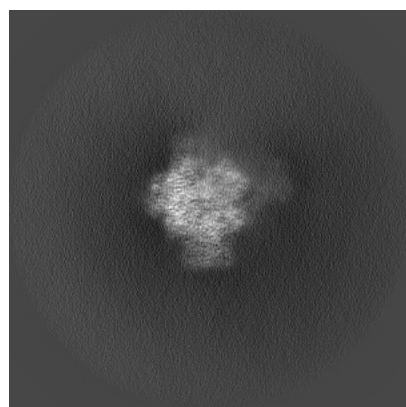


Y

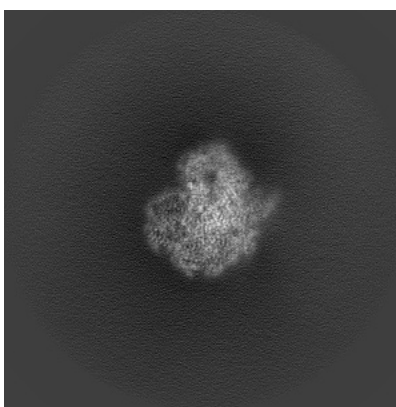


Z

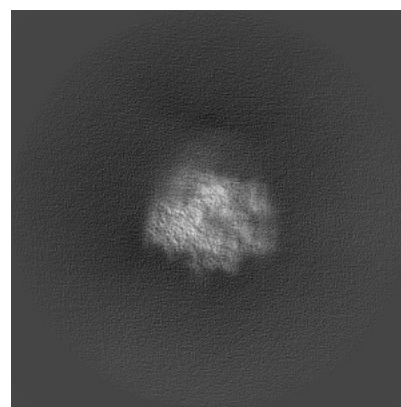
6.1.2 Raw map



X



Y

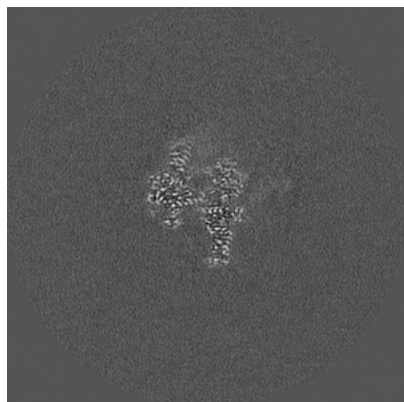


Z

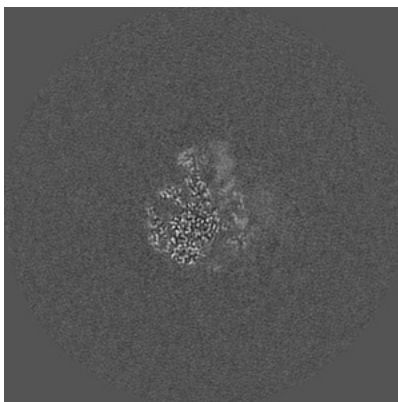
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

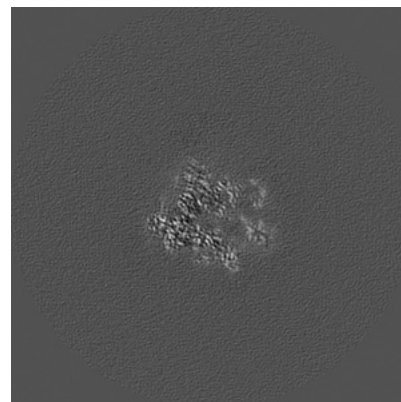
6.2.1 Primary map



X Index: 214

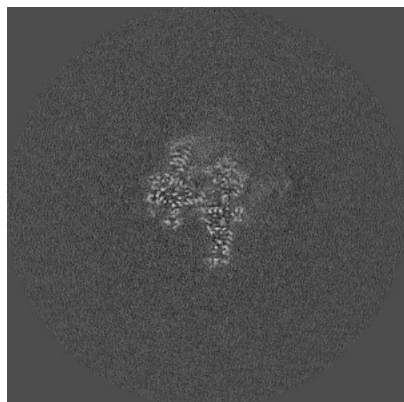


Y Index: 214

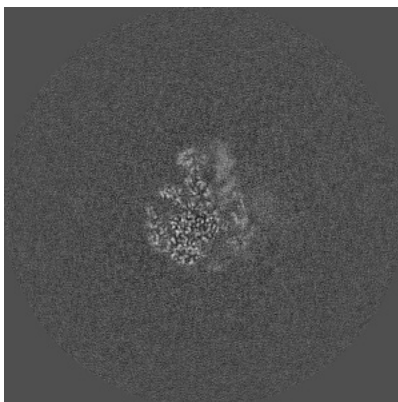


Z Index: 214

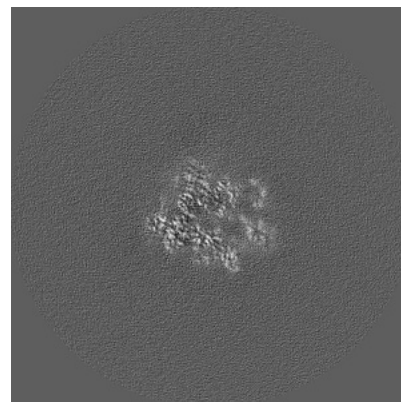
6.2.2 Raw map



X Index: 214



Y Index: 214

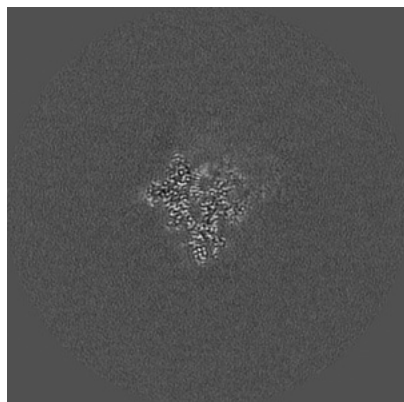


Z Index: 214

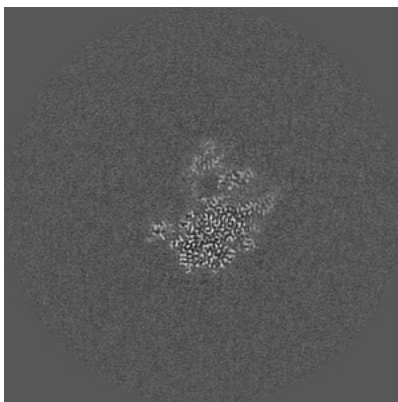
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

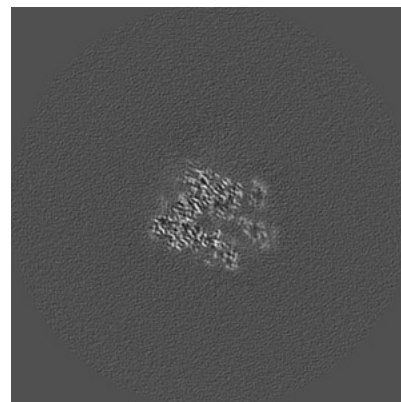
6.3.1 Primary map



X Index: 200

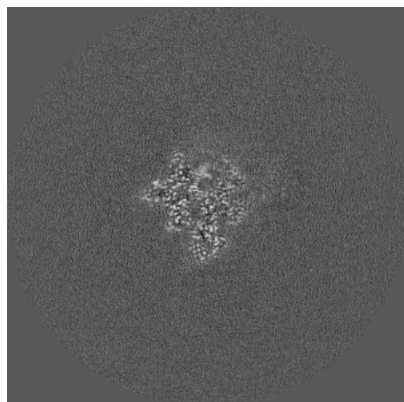


Y Index: 189

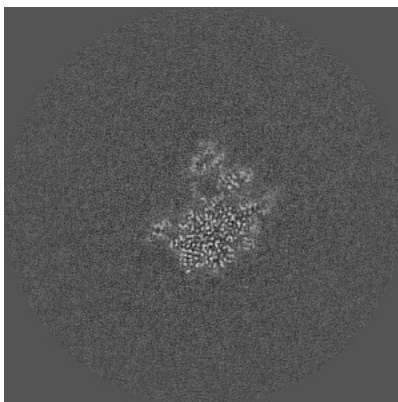


Z Index: 212

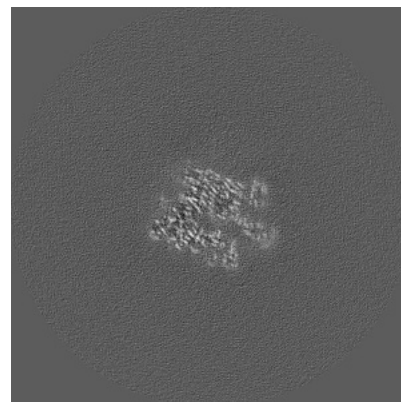
6.3.2 Raw map



X Index: 201



Y Index: 188

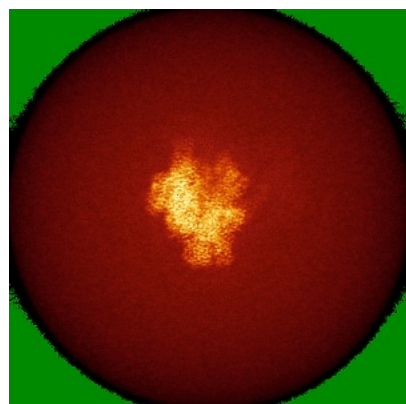


Z Index: 211

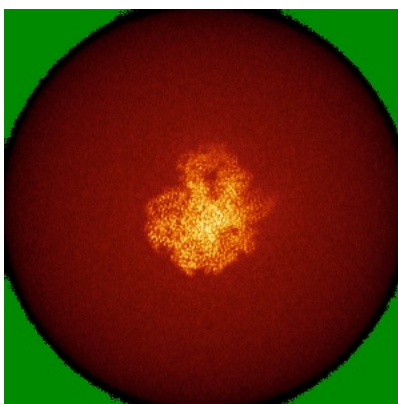
The images above show the largest variance slices of the map in three orthogonal directions.

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

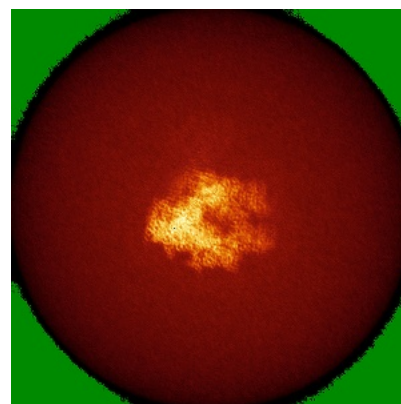
6.4.1 Primary map



X

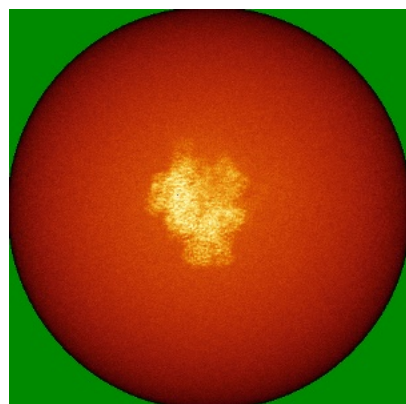


Y

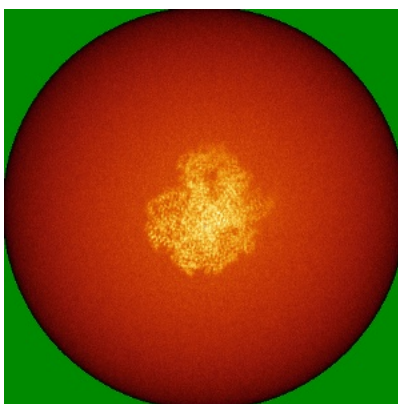


Z

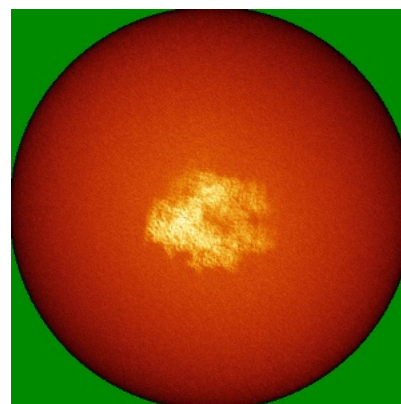
6.4.2 Raw map



X



Y

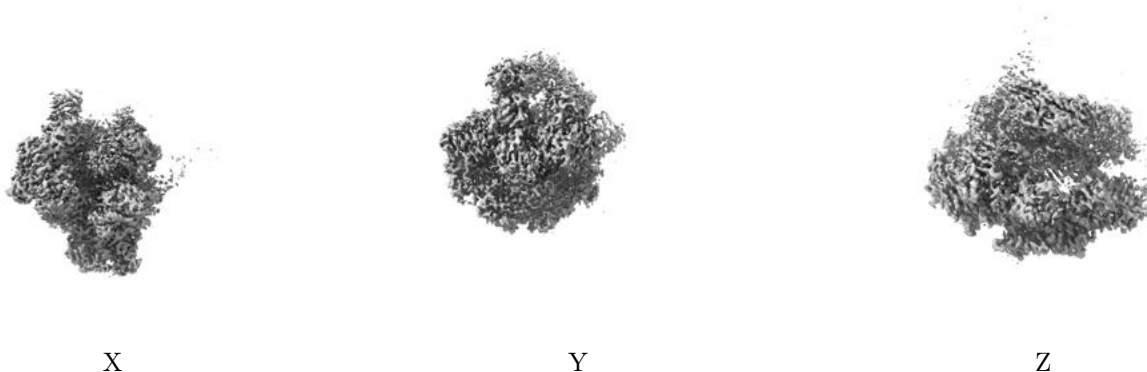


Z

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.

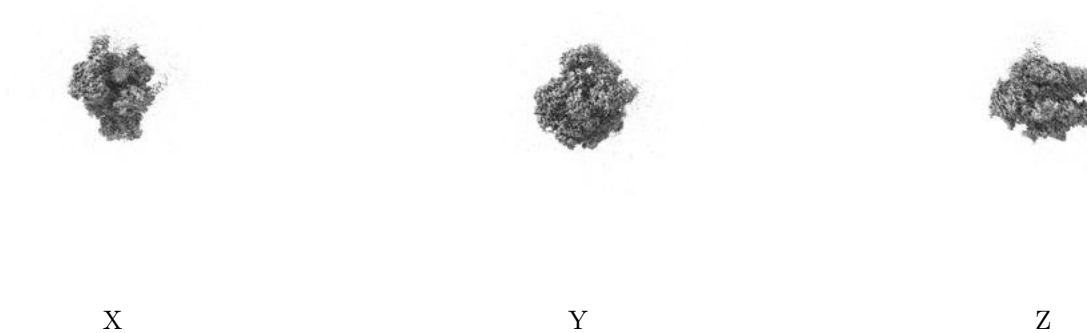
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

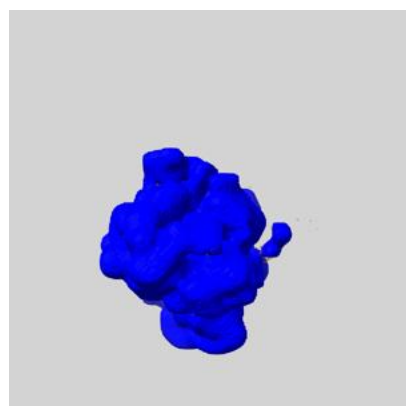
6.6 Mask visualisation [i](#)

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

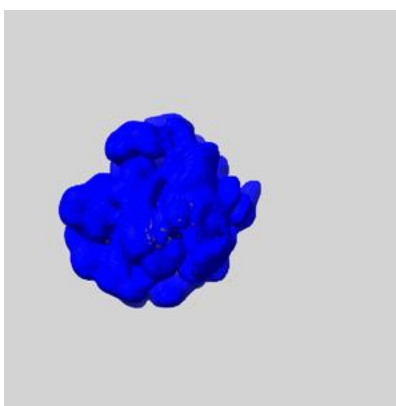
A mask typically either:

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

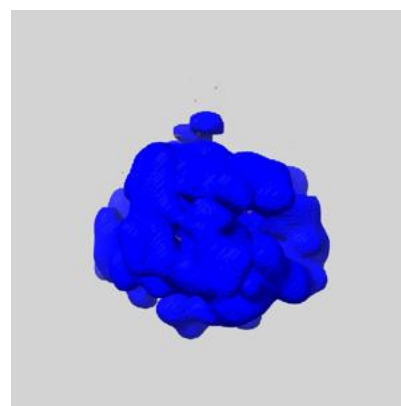
6.6.1 emd_18376_msk_1.map [i](#)



X



Y

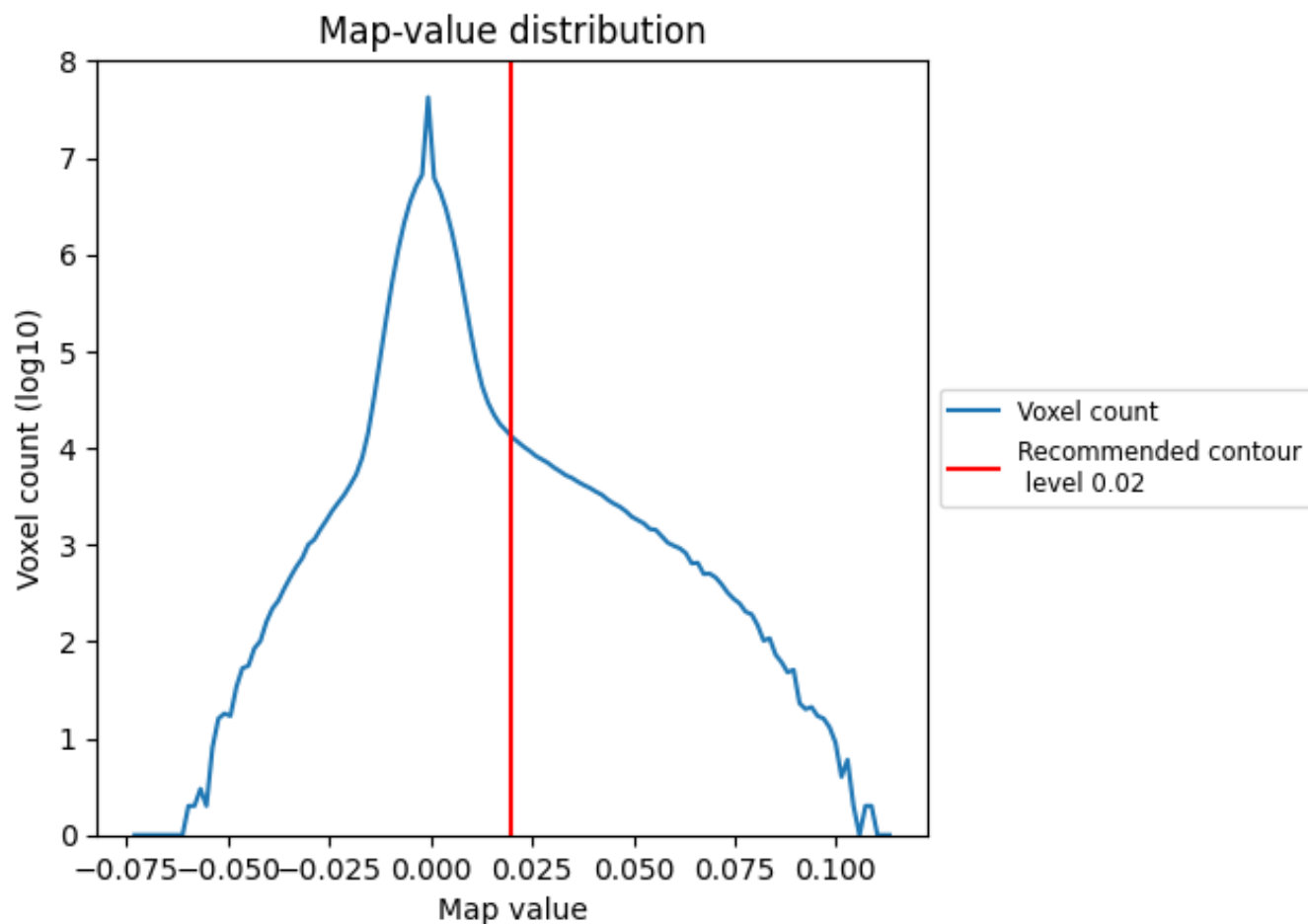


Z

7 Map analysis [i](#)

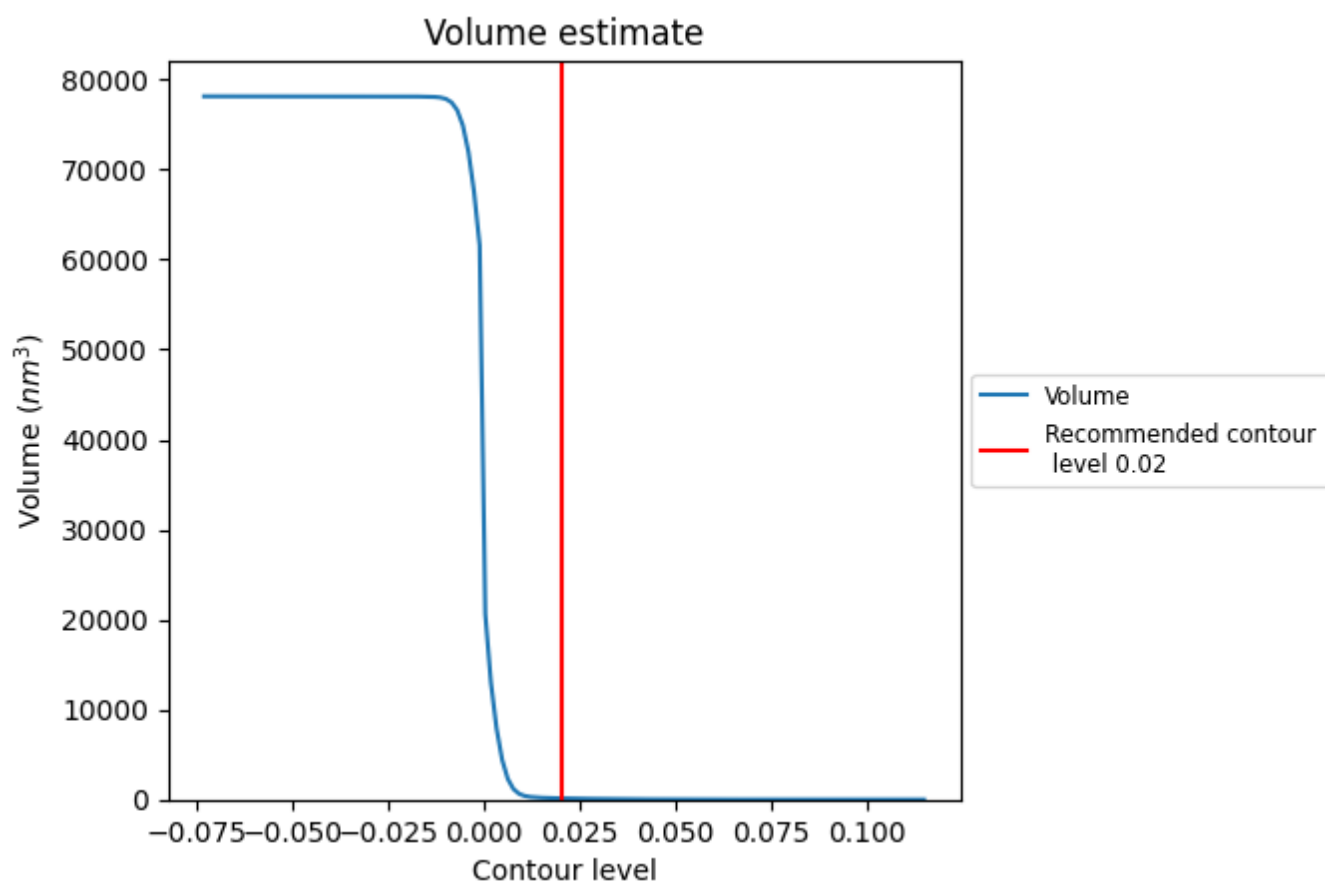
This section contains the results of statistical analysis of the map.

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.

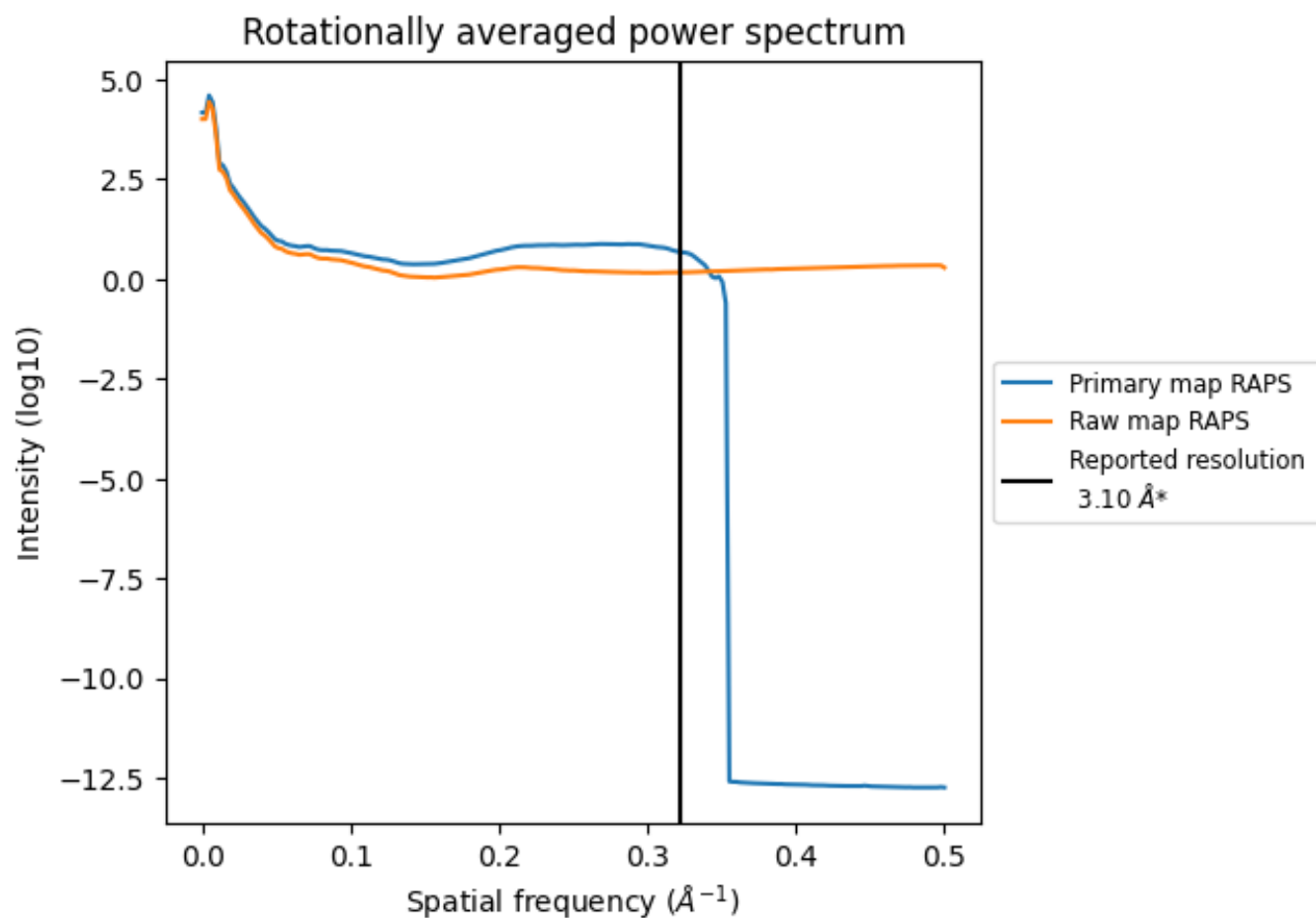
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 ⓘ

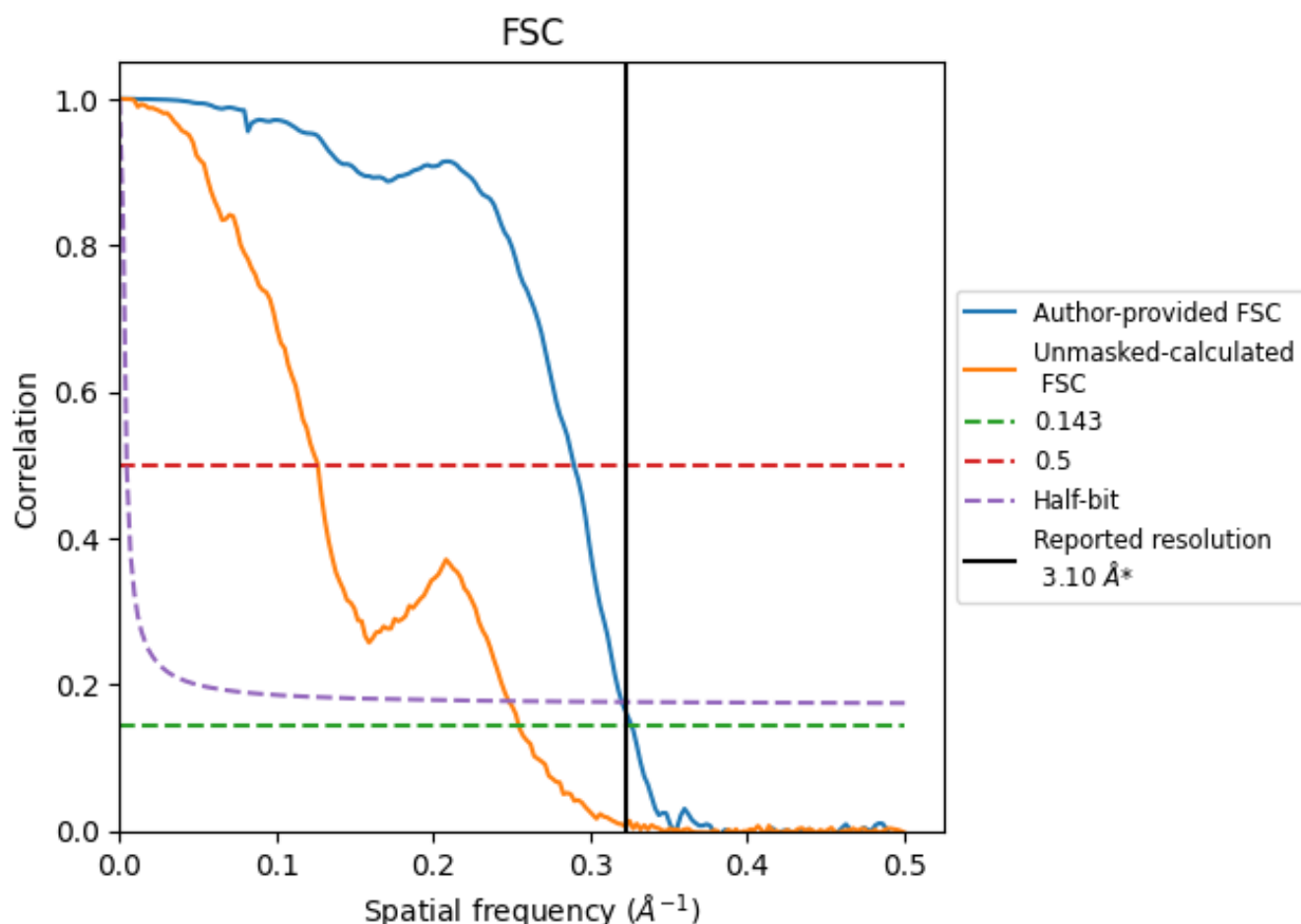


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

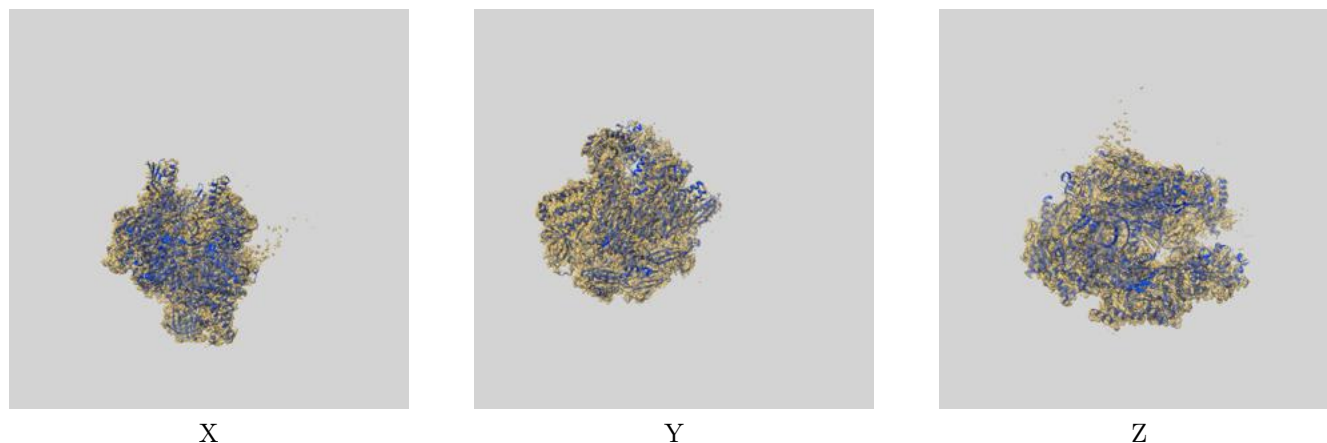
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.45	3.12
Unmasked-calculated*	3.93	7.91	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

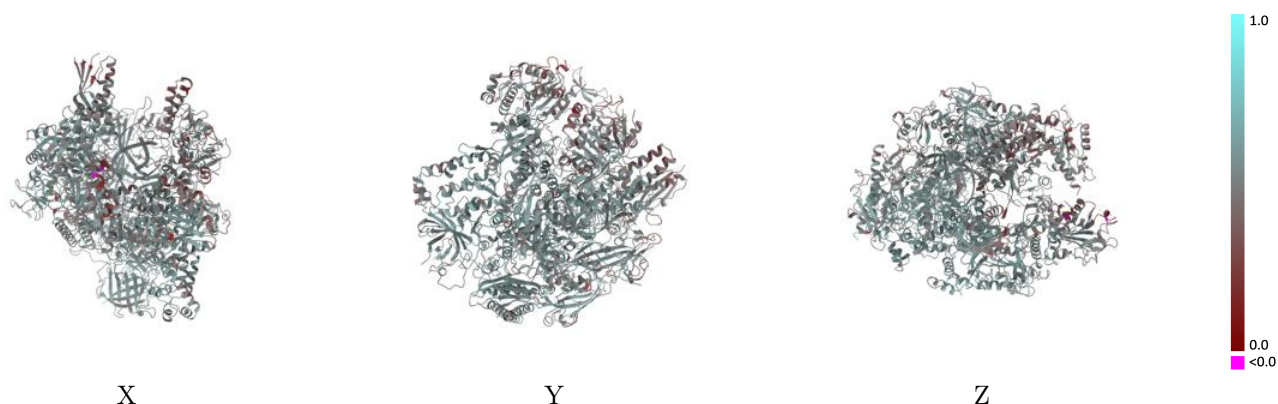
This section contains information regarding the fit between EMDB map EMD-18376 and PDB model 8QEQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



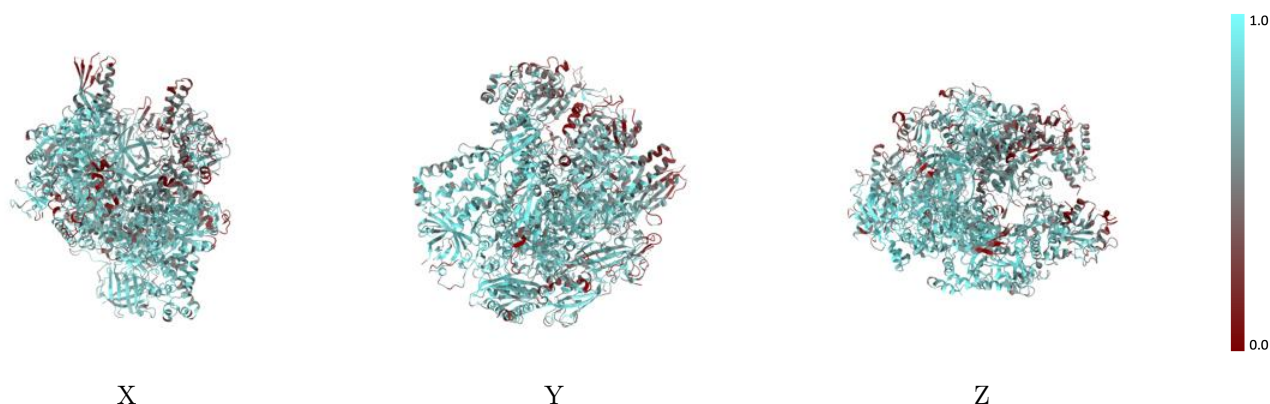
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



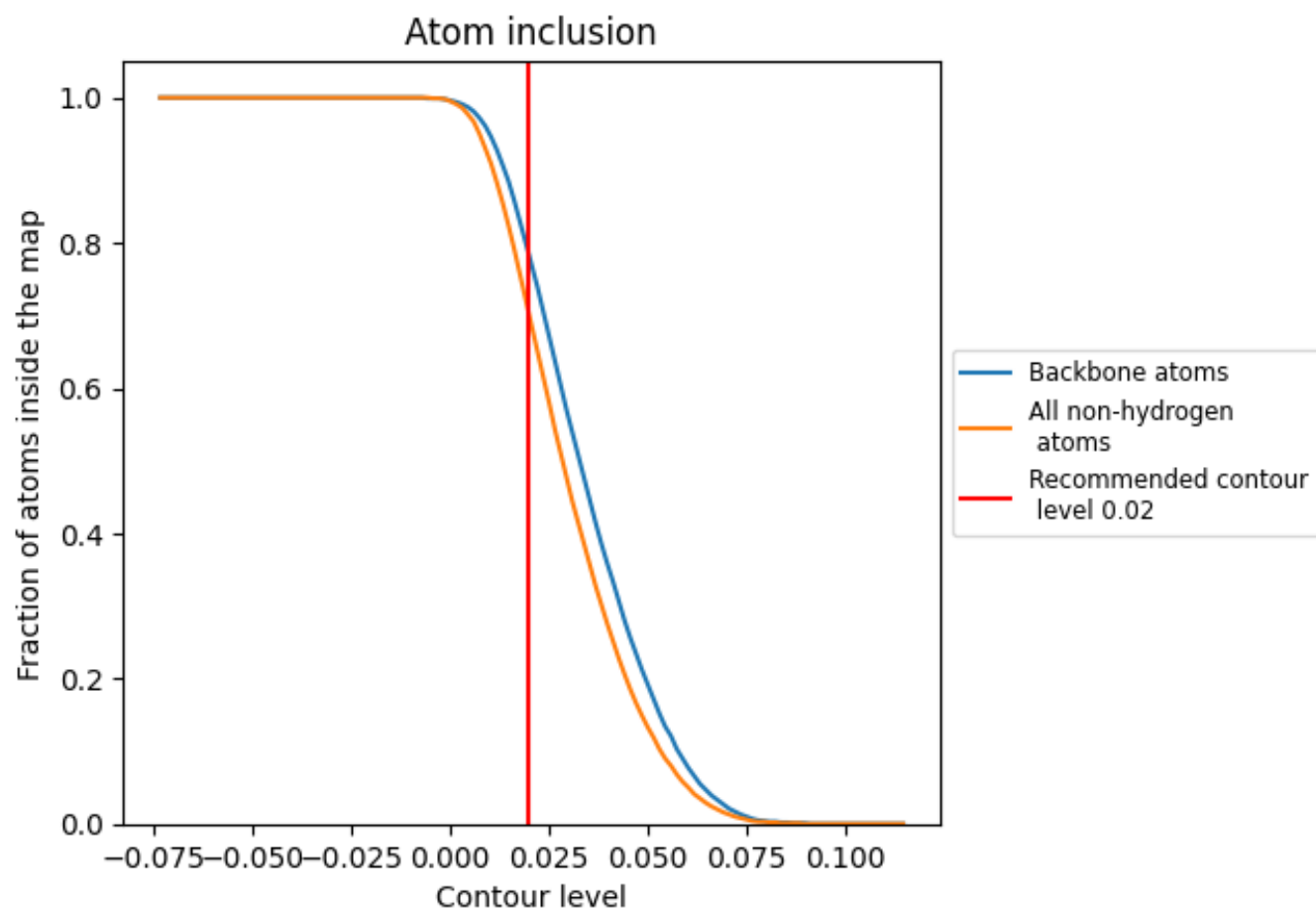
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7060	<div></div> 0.5230
A	<div></div> 0.6680	<div></div> 0.5110
B	<div></div> 0.7400	<div></div> 0.5360
C	<div></div> 0.7700	<div></div> 0.5390
E	<div></div> 0.6650	<div></div> 0.4950
F	<div></div> 0.6590	<div></div> 0.5140
H	<div></div> 0.7540	<div></div> 0.5360
I	<div></div> 0.6200	<div></div> 0.5050
J	<div></div> 0.8370	<div></div> 0.5720
K	<div></div> 0.7130	<div></div> 0.5400
L	<div></div> 0.6730	<div></div> 0.5170
R	<div></div> 0.8030	<div></div> 0.5280

1.0

0.0

<0.0