



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2024 – 01:19 AM JST

PDB ID : 8HE5
EMDB ID : EMD-34685
Title : RNA polymerase II elongation complex bound with Rad26 and Elf1, stalled at SHL(-3.5) of the nucleosome
Authors : Osumi, K.; Kujirai, T.; Ehara, H.; Kinoshita, C.; Saotome, M.; Kagawa, W.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2022-11-07
Resolution : 6.95 Å(reported)

This is a wwPDB EM Validation Summary 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

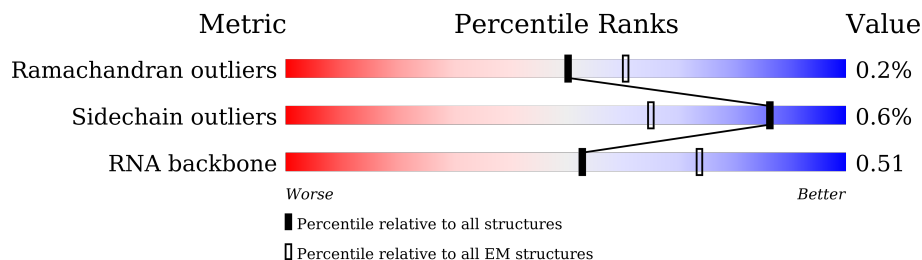
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.95 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1743	
2	B	1227	
3	C	304	
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	

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Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	O	1094	
16	P	16	
17	T	198	
18	a	139	
18	e	139	
19	b	106	
19	f	106	
20	c	133	
20	g	133	
21	d	129	
21	h	129	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48360 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	1412	Total	C	N	O	S	0	0
			11123	7014	1938	2101	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	142	Total	C	N	O	P	0	0
			2922	1385	526	869	142		

- Molecule 15 is a protein called DNA repair protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	516	Total	C	N	O	S	0	0
			4206	2710	739	744	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	GLY	-	expression tag	UNP F2QSG0
O	-4	PRO	-	expression tag	UNP F2QSG0
O	-3	LEU	-	expression tag	UNP F2QSG0
O	-2	GLY	-	expression tag	UNP F2QSG0
O	-1	SER	-	expression tag	UNP F2QSG0
O	0	HIS	-	expression tag	UNP F2QSG0

- Molecule 16 is a RNA chain called RNA (5'-R(P*GP*UP*UP*UP*UP*CP*GP*UP*UP*GP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	16	Total	C	N	O	P	0	0
			329	147	42	124	16		

- Molecule 17 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	154	Total	C	N	O	P	0	0
			3144	1489	605	897	153		

- Molecule 18 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
18	e	97	Total	C	N	O	S	0	0
			800	503	155	138	4		

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
19	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 20 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	c	103	Total	C	N	O	0	0
			796	502	155	139		
20	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 21 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
21	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

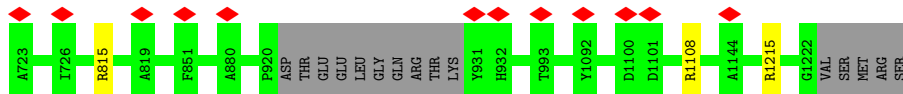
Chain	Residue	Modelled	Actual	Comment	Reference
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899

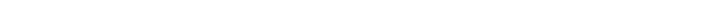
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

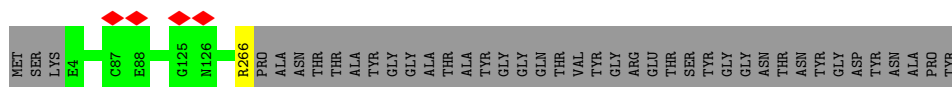
Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	C	1	Total	Zn	0
			1	1	
22	I	2	Total	Zn	0
			2	2	
22	J	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	
22	M	1	Total	Zn	0
			1	1	

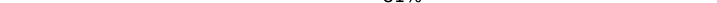
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

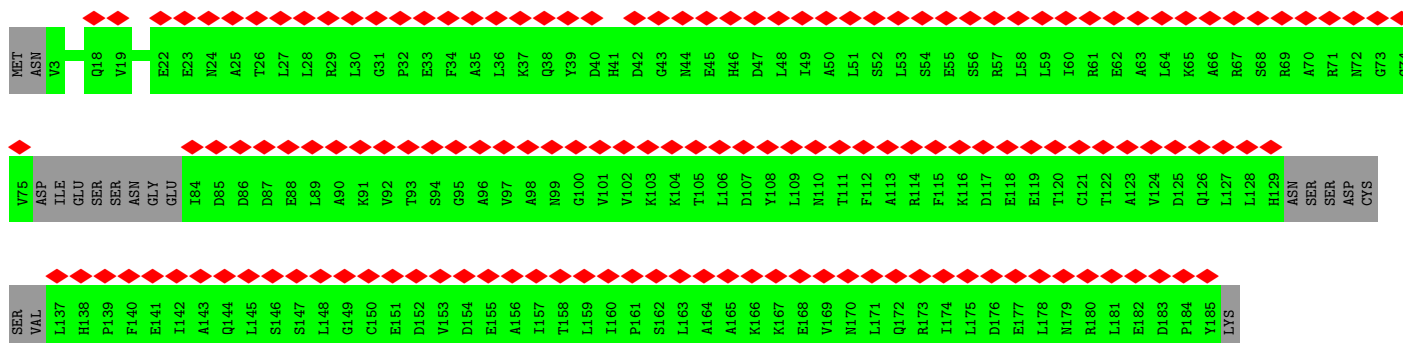
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total 1	Mg 1	0



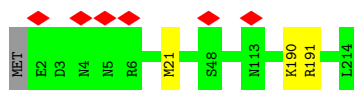
- Chain C:  86% 13%



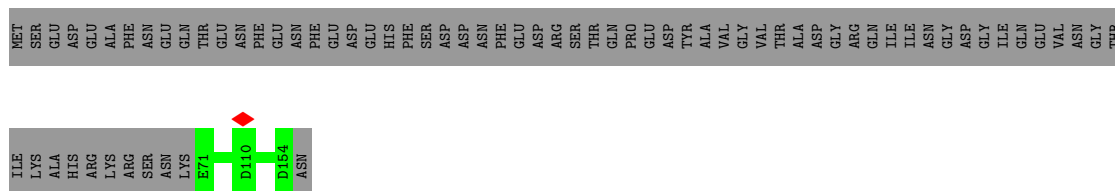
- Chain D:  81% 90% 10%



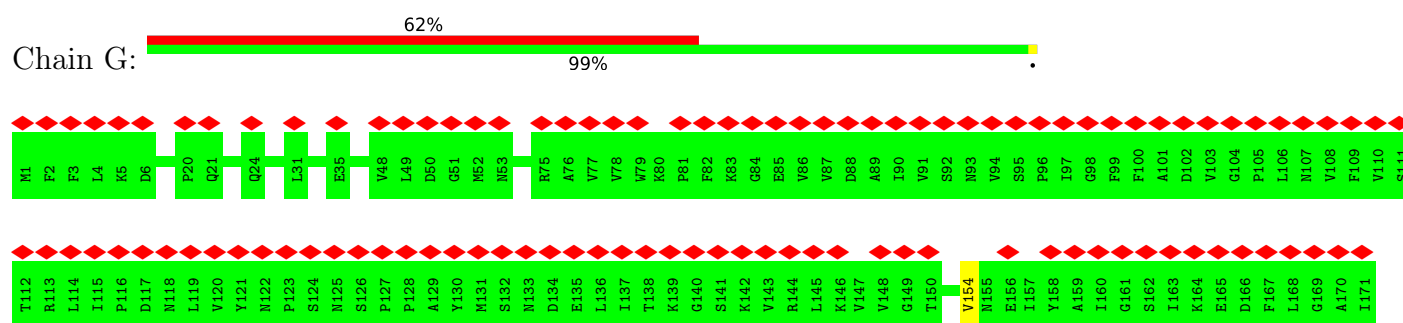
- Chain E:  98%



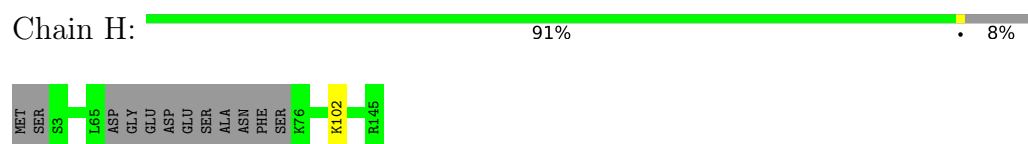
- Chain F:  54% 46%



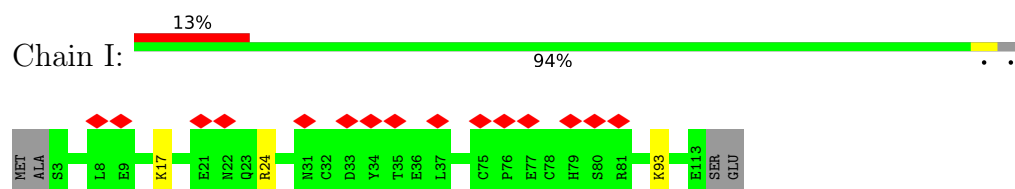
- Molecule 7: RNA polymerase II subunit



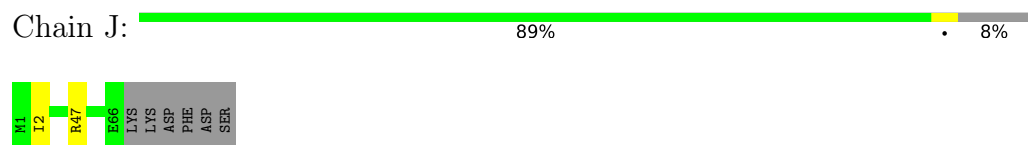
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



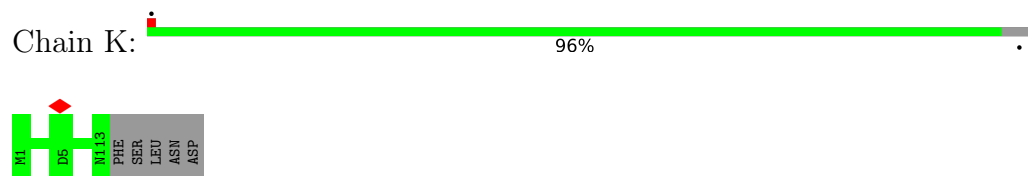
- Molecule 9: DNA-directed RNA polymerase subunit



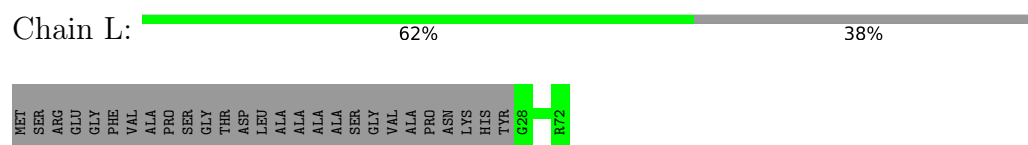
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



- Molecule 11: RNA polymerase II subunit B12.5



- Molecule 12: RNA polymerase subunit ABC10-alpha



- Molecule 13: Transcription elongation factor 1 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29751	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 ($e^-/\text{\AA}^2$)	57.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00519	Depositor
Map size (\AA)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.26	0/11329	0.53	0/15310
2	B	0.26	0/9407	0.55	0/12685
3	C	0.25	0/2139	0.51	0/2895
4	D	0.24	0/1326	0.53	0/1788
5	E	0.29	0/1772	0.58	1/2385 (0.0%)
6	F	0.24	0/687	0.51	0/931
7	G	0.26	0/1353	0.51	0/1837
8	H	0.27	0/1069	0.52	0/1444
9	I	0.26	0/934	0.53	0/1257
10	J	0.25	0/554	0.53	0/742
11	K	0.27	0/953	0.52	0/1291
12	L	0.24	0/365	0.54	0/484
13	M	0.28	0/513	0.55	2/693 (0.3%)
14	N	0.50	0/3273	0.92	0/5053
15	O	0.24	0/4301	0.50	0/5818
16	P	0.17	0/363	0.74	0/561
17	T	0.51	0/3533	0.85	2/5444 (0.0%)
18	a	0.24	0/813	0.53	0/1090
18	e	0.25	0/811	0.55	0/1086
19	b	0.24	0/645	0.54	0/862
19	f	0.25	0/626	0.55	0/837
20	c	0.24	0/806	0.53	0/1089
20	g	0.23	0/820	0.49	0/1107
21	d	0.24	0/757	0.47	0/1015
21	h	0.24	0/736	0.45	0/990
All	All	0.30	0/49885	0.60	5/68694 (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
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	59	DC	OP1-P-OP2	-6.86	109.31	119.60
5	E	21	MET	CA-CB-CG	5.72	123.03	113.30
17	T	58	DG	OP1-P-O3'	5.61	117.53	105.20
13	M	59	PRO	N-CD-CG	-5.56	94.86	103.20
13	M	59	PRO	CA-N-CD	-5.23	104.17	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1228	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1400/1743 (80%)	1313 (94%)	85 (6%)	2 (0%)	51	86
2	B	1145/1227 (93%)	1068 (93%)	75 (7%)	2 (0%)	47	81
3	C	261/304 (86%)	247 (95%)	14 (5%)	0	100	100
4	D	162/186 (87%)	152 (94%)	10 (6%)	0	100	100
5	E	211/214 (99%)	201 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	161 (95%)	7 (4%)	1 (1%)	25	66
8	H	129/145 (89%)	124 (96%)	5 (4%)	0	100	100
9	I	109/115 (95%)	100 (92%)	9 (8%)	0	100	100
10	J	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	9	44
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
12	L	43/72 (60%)	38 (88%)	5 (12%)	0	100	100
13	M	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
15	O	506/1094 (46%)	457 (90%)	45 (9%)	4 (1%)	19	60
18	a	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
18	e	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
19	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
19	f	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
20	c	101/133 (76%)	96 (95%)	5 (5%)	0	100	100
20	g	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
21	d	93/129 (72%)	90 (97%)	3 (3%)	0	100	100
21	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
All	All	5186/6743 (77%)	4876 (94%)	300 (6%)	10 (0%)	50	81

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	62	ALA
15	O	306	ASP
15	O	718	ARG
1	A	255	GLU
7	G	154	VAL

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	1225/1528 (80%)	1213 (99%)	12 (1%)	76	86
2	B	1012/1077 (94%)	1006 (99%)	6 (1%)	86	92
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	94
4	D	143/160 (89%)	143 (100%)	0	100	100
5	E	196/197 (100%)	194 (99%)	2 (1%)	76	86
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	119 (99%)	1 (1%)	81	89
9	I	106/109 (97%)	103 (97%)	3 (3%)	43	65
10	J	60/66 (91%)	59 (98%)	1 (2%)	60	78
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
15	O	463/979 (47%)	463 (100%)	0	100	100
18	a	85/114 (75%)	84 (99%)	1 (1%)	71	83
18	e	84/114 (74%)	84 (100%)	0	100	100
19	b	65/81 (80%)	65 (100%)	0	100	100
19	f	63/81 (78%)	62 (98%)	1 (2%)	62	79
20	c	82/102 (80%)	82 (100%)	0	100	100
20	g	83/102 (81%)	83 (100%)	0	100	100
21	d	81/107 (76%)	81 (100%)	0	100	100
21	h	79/107 (74%)	79 (100%)	0	100	100
All	All	4609/5867 (79%)	4581 (99%)	28 (1%)	86	92

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	598	ARG
19	f	92	ARG
2	B	1215	ARG
9	I	93	LYS
2	B	1108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	669	HIS
20	c	73	ASN
2	B	474	GLN
2	B	359	GLN
20	c	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	5 (33%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-4	U
16	P	-3	U
16	P	0	C
16	P	1	G
16	P	10	U

There are no RNA pucker outliers to report.

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 10 ligands modelled in this entry, 10 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.

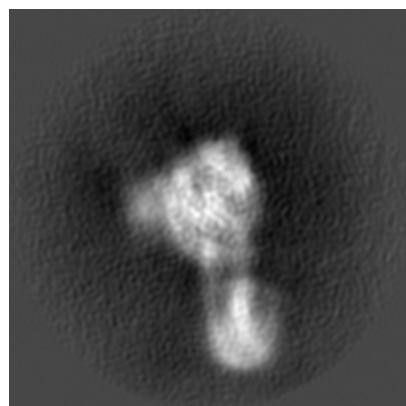
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34685. These allow visual inspection of the internal detail of the map and identification of artifacts.

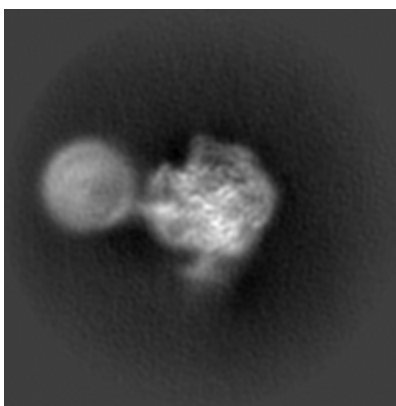
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

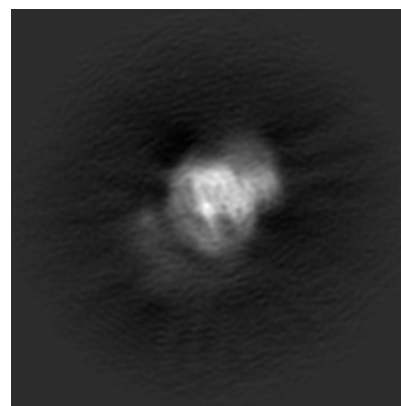
6.1.1 Primary map



X

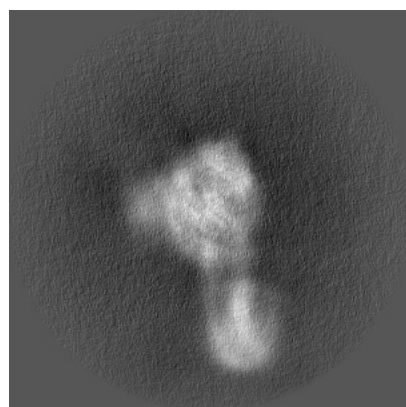


Y

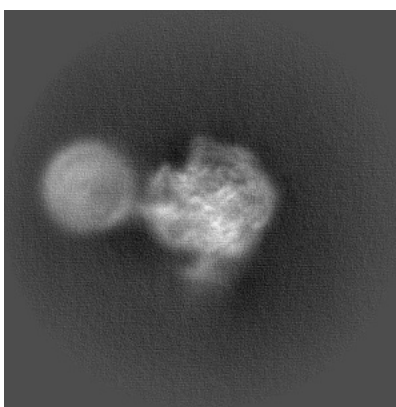


Z

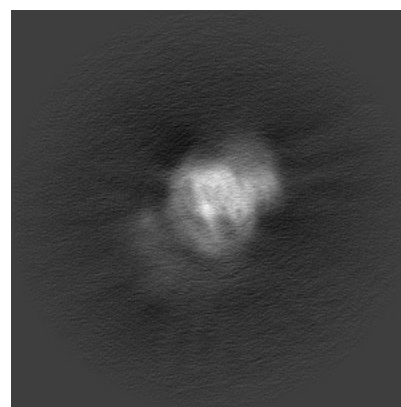
6.1.2 Raw map



X



Y

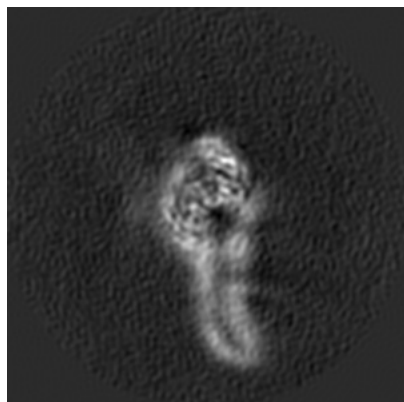


Z

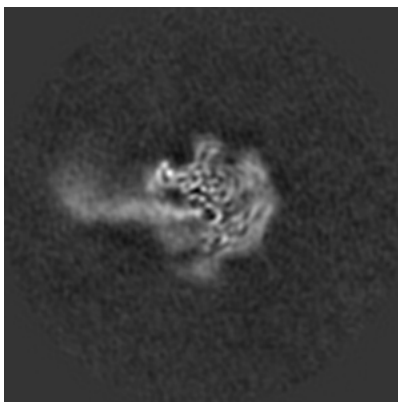
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

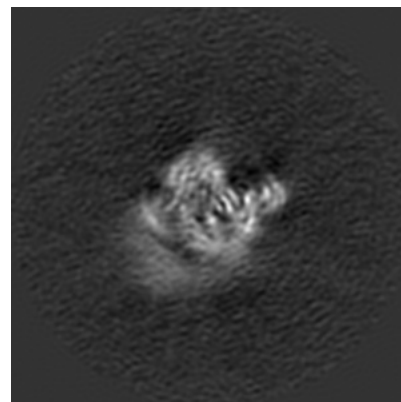
6.2.1 Primary map



X Index: 200

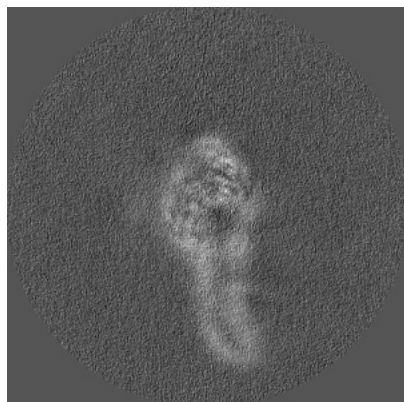


Y Index: 200

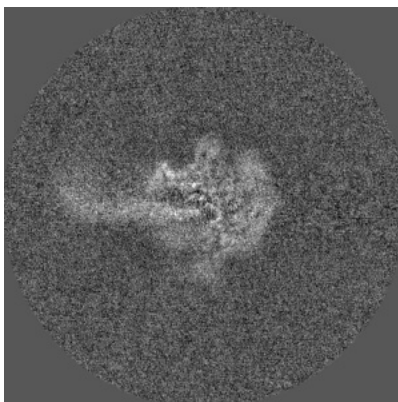


Z Index: 200

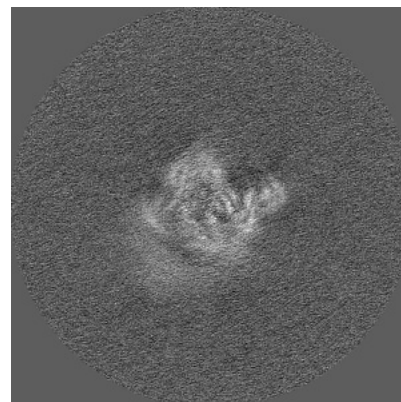
6.2.2 Raw map



X Index: 200



Y Index: 200

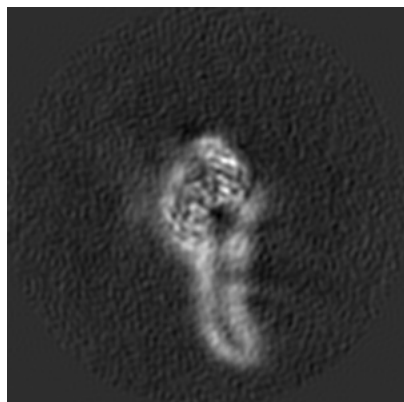


Z Index: 200

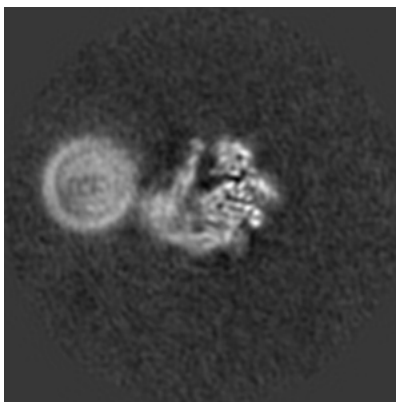
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

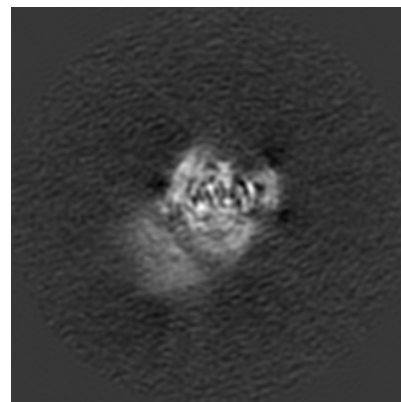
6.3.1 Primary map



X Index: 199

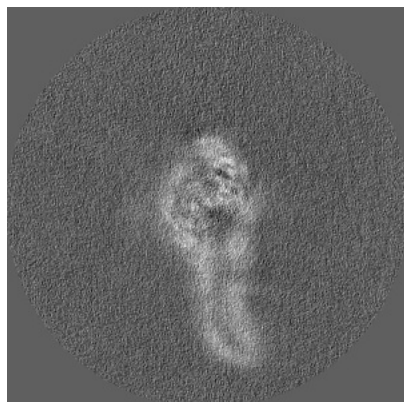


Y Index: 227

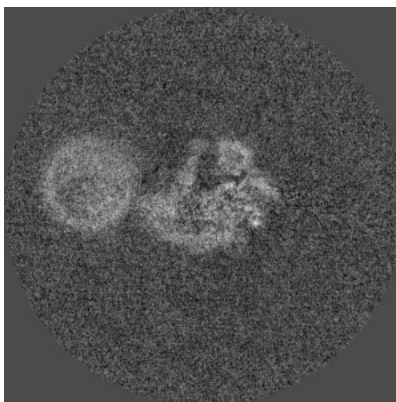


Z Index: 215

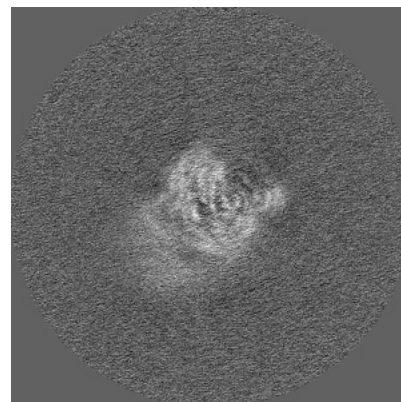
6.3.2 Raw map



X Index: 201



Y Index: 227

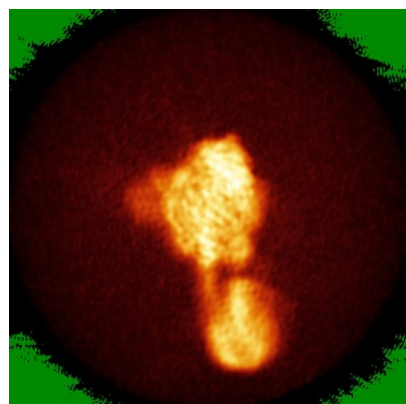


Z Index: 206

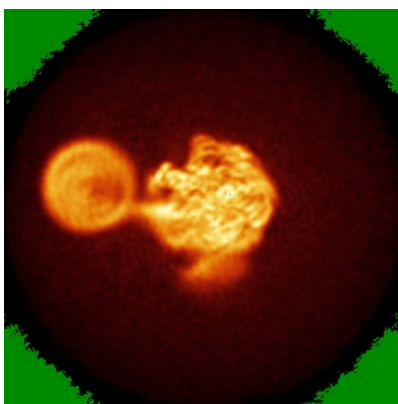
The images above show the largest variance slices of the map in three orthogonal directions.

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

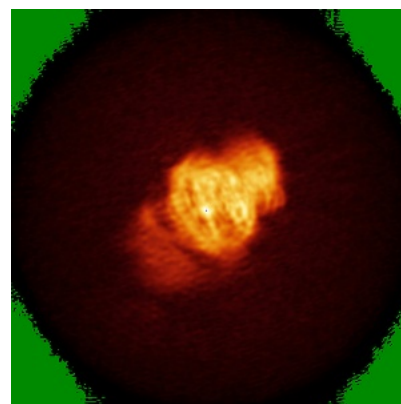
6.4.1 Primary map



X

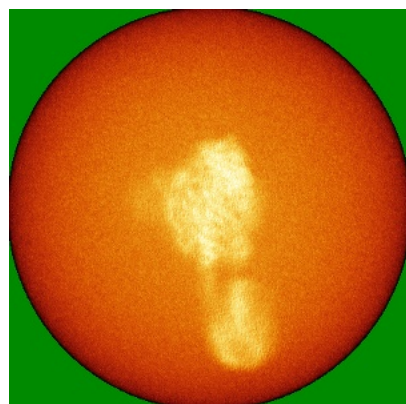


Y

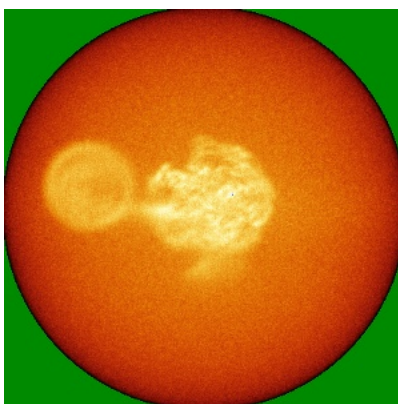


Z

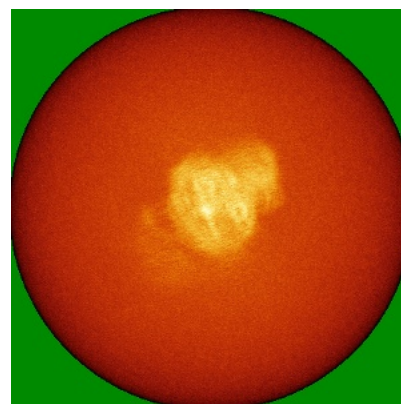
6.4.2 Raw map



X



Y



Z

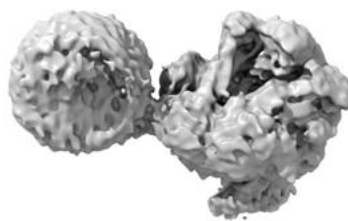
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

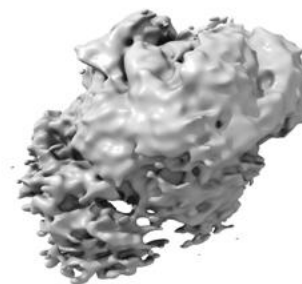
6.5.1 Primary map



X



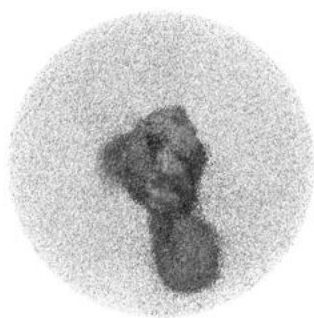
Y



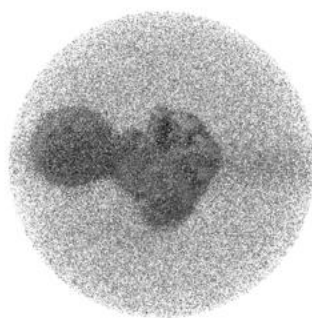
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00519. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

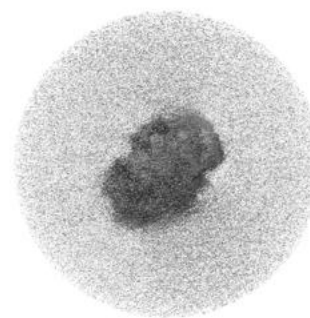
6.5.2 Raw map



X



Y



Z

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.

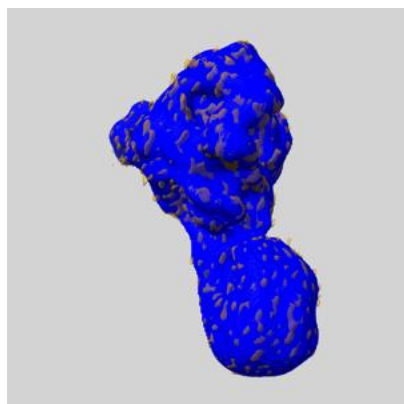
6.6 Mask visualisation [i](#)

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

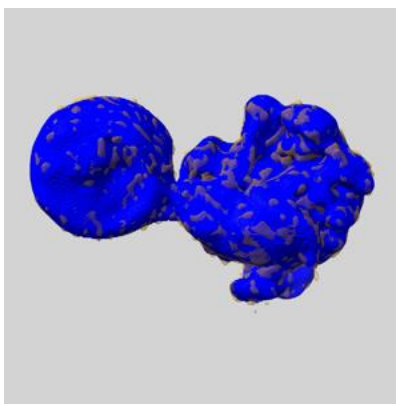
A mask typically either:

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

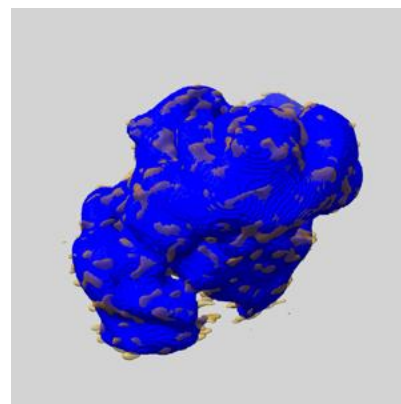
6.6.1 emd_34685_msk_1.map [i](#)



X

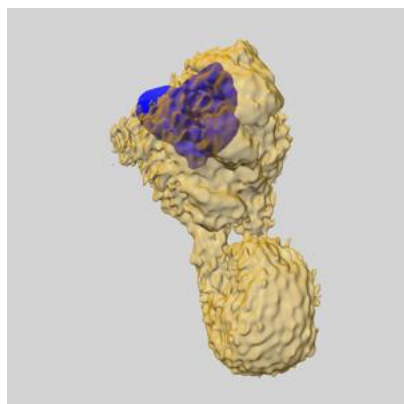


Y

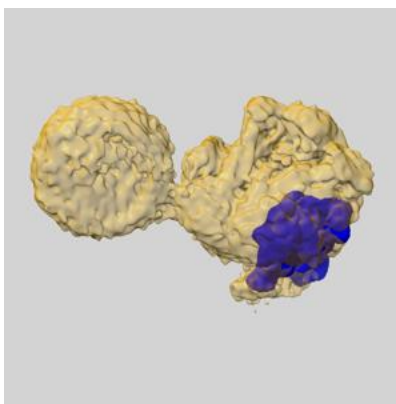


Z

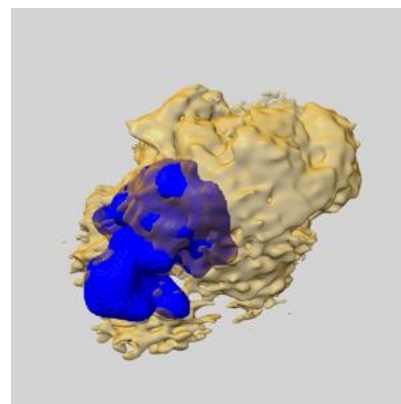
6.6.2 emd_34685_msk_2.map [i](#)



X

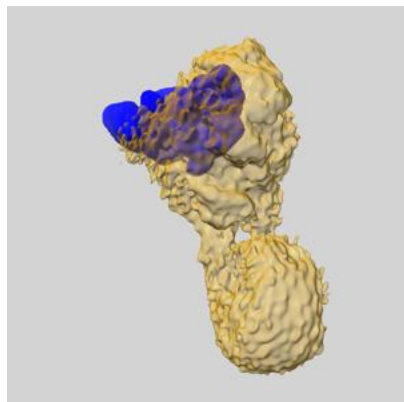


Y

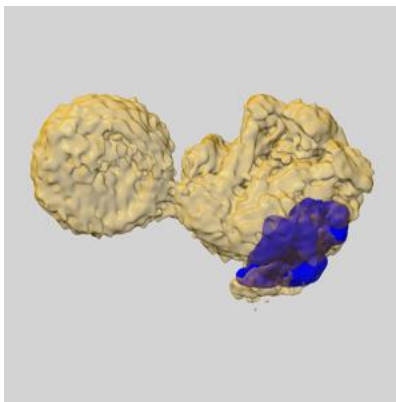


Z

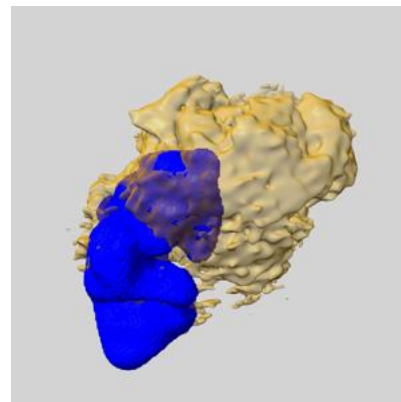
6.6.3 emd_34685_msk_3.map [i](#)



X



Y

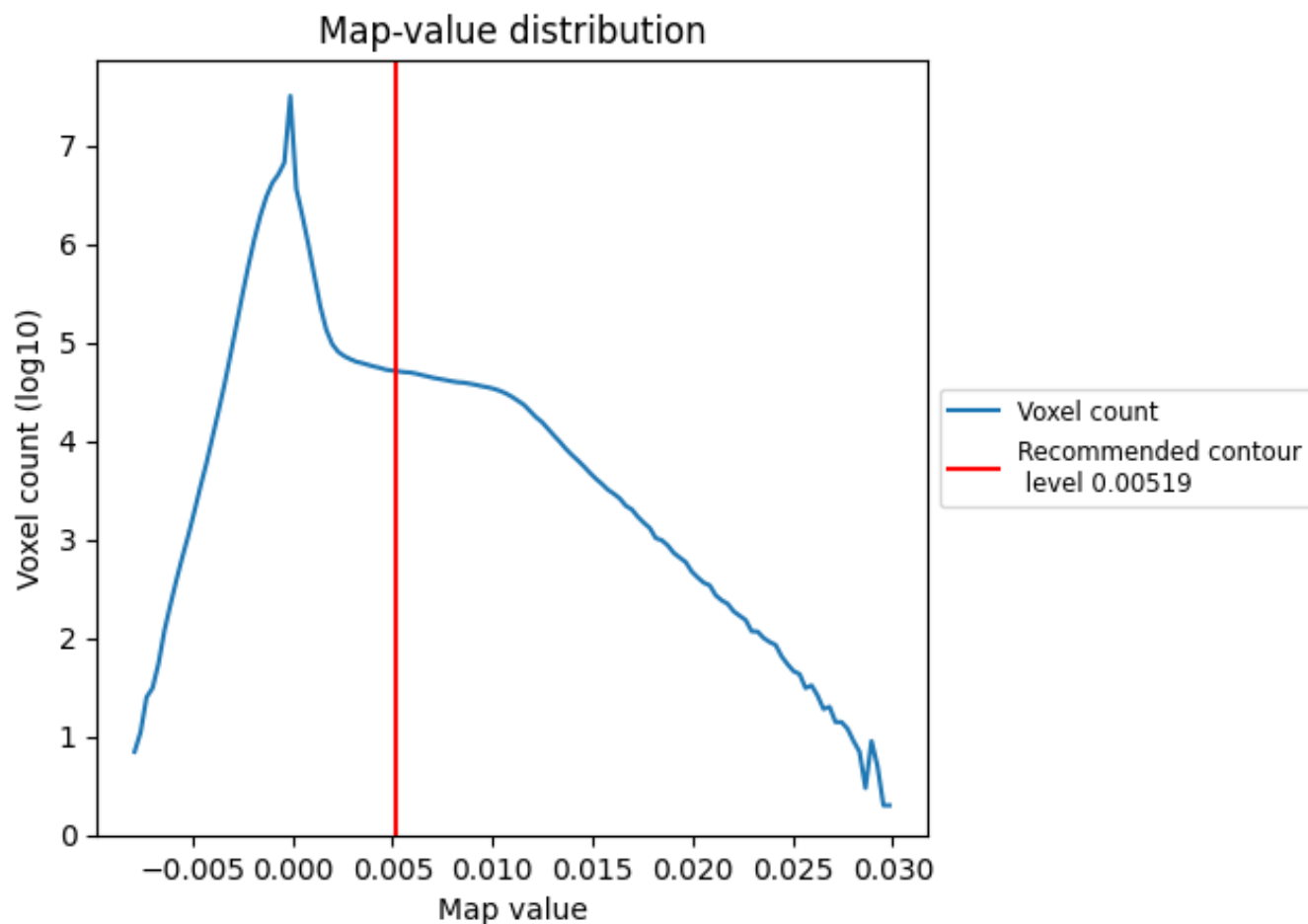


Z

7 Map analysis [i](#)

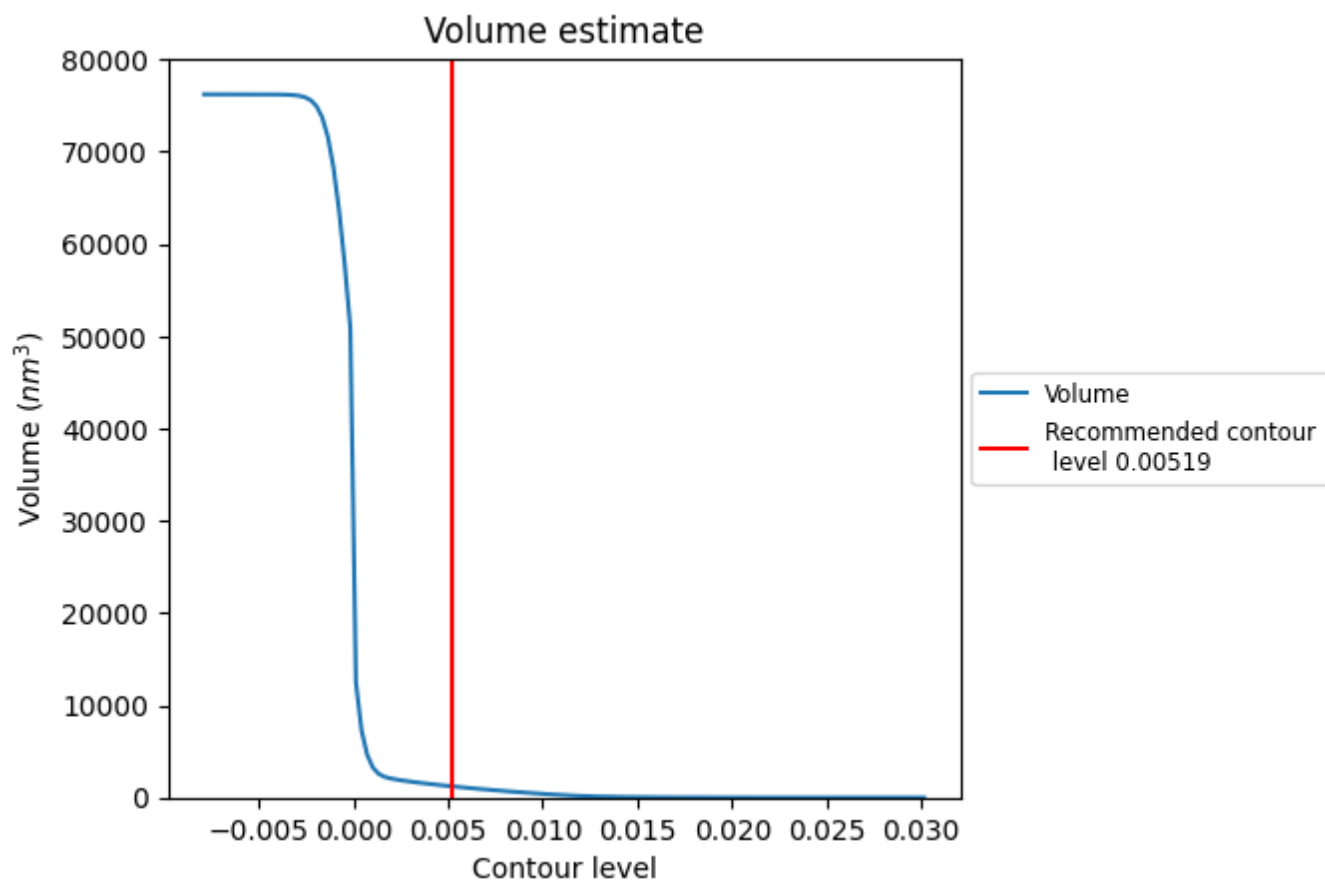
This section contains the results of statistical analysis of the map.

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.

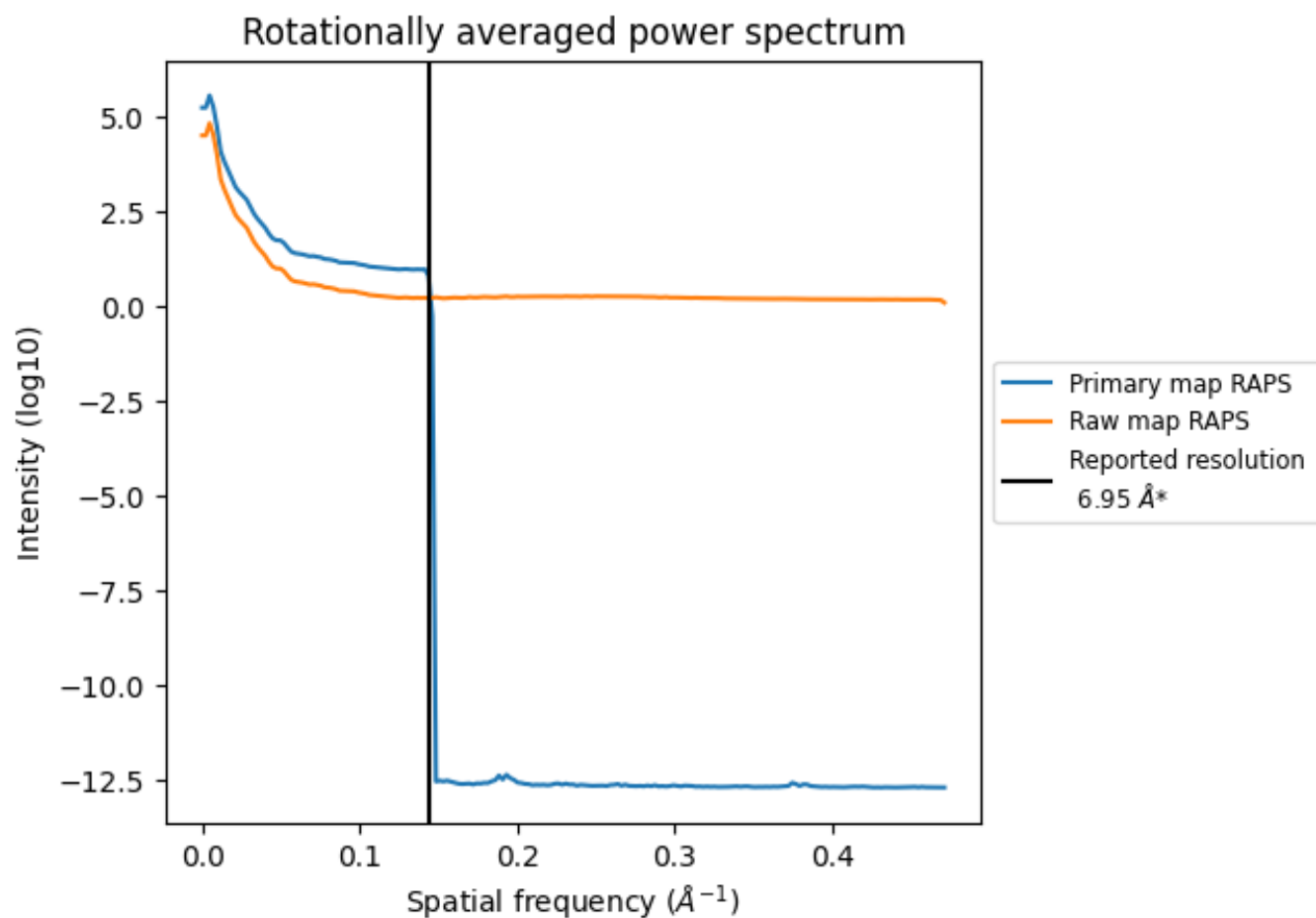
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1220 nm³; this corresponds to an approximate mass of 1102 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 ⓘ

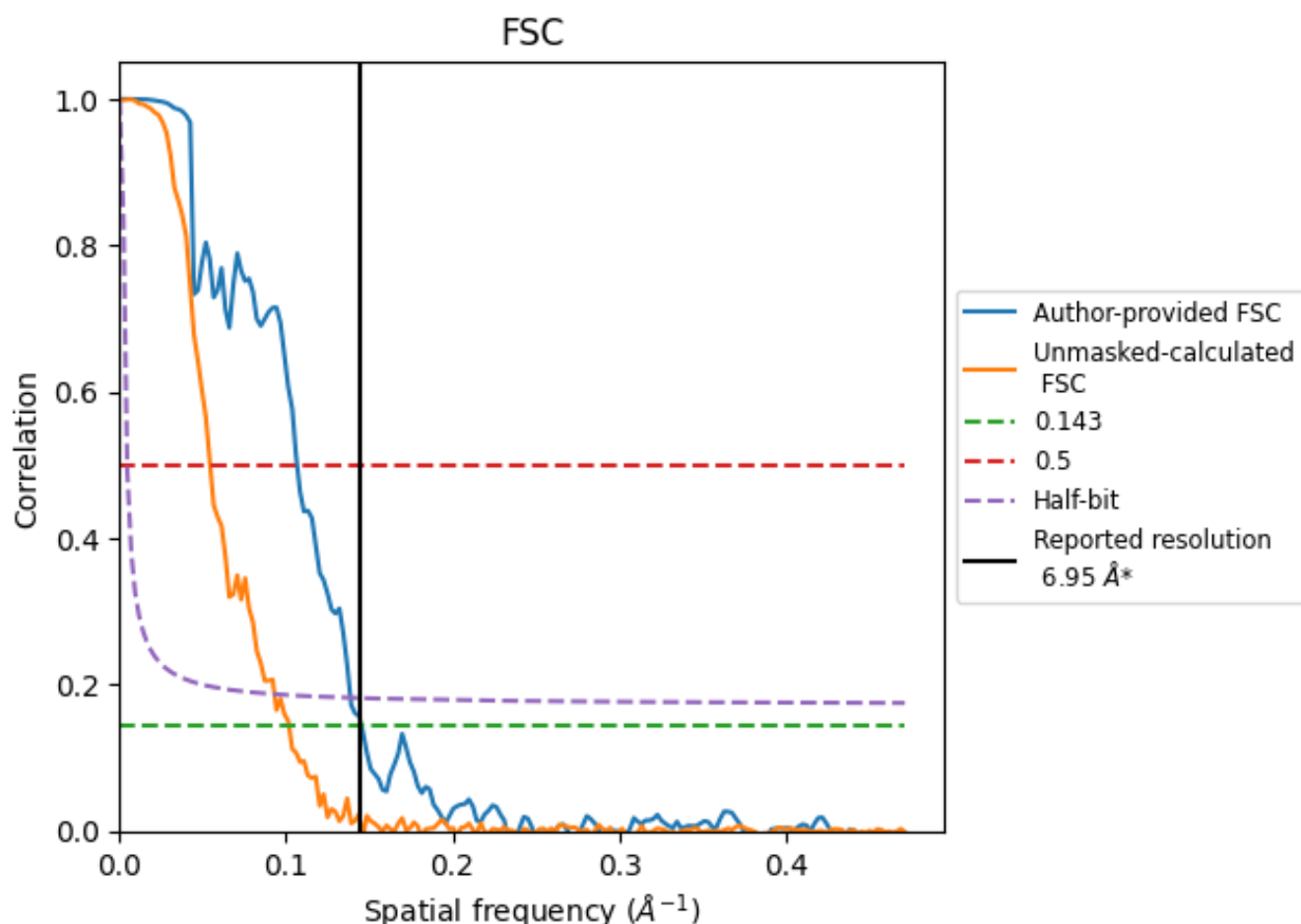


*Reported resolution corresponds to spatial frequency of 0.144 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.144 Å⁻¹

8.2 Resolution estimates [i](#)

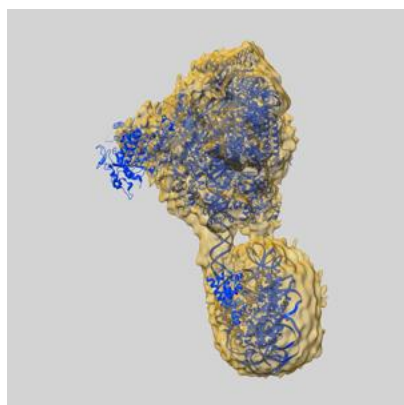
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.95	-	-
Author-provided FSC curve	6.88	9.37	7.21
Unmasked-calculated*	9.82	18.35	10.74

*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 9.82 differs from the reported value 6.95 by more than 10 %

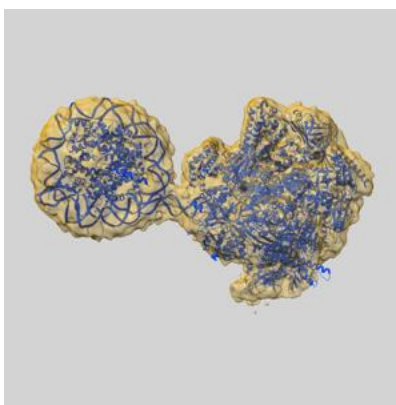
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34685 and PDB model 8HE5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

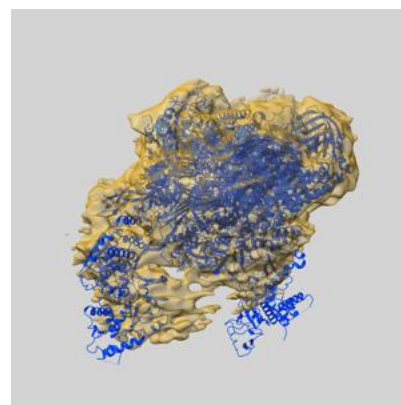
9.1 Map-model overlay [i](#)



X



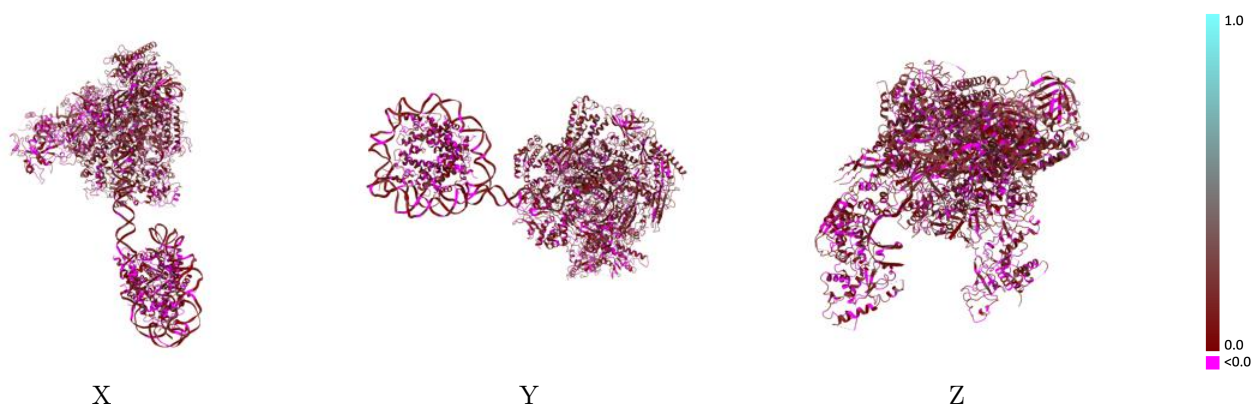
Y



Z

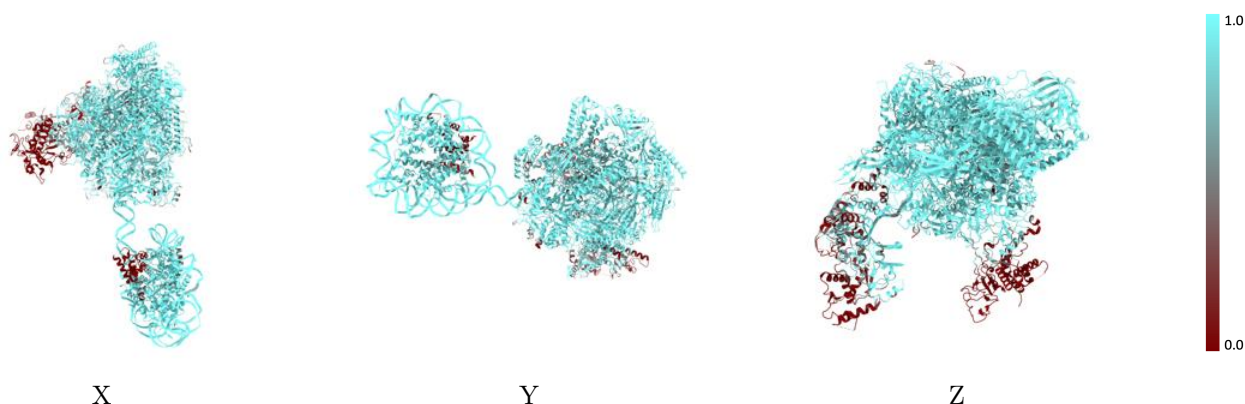
The images above show the 3D surface view of the map at the recommended contour level 0.00519 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



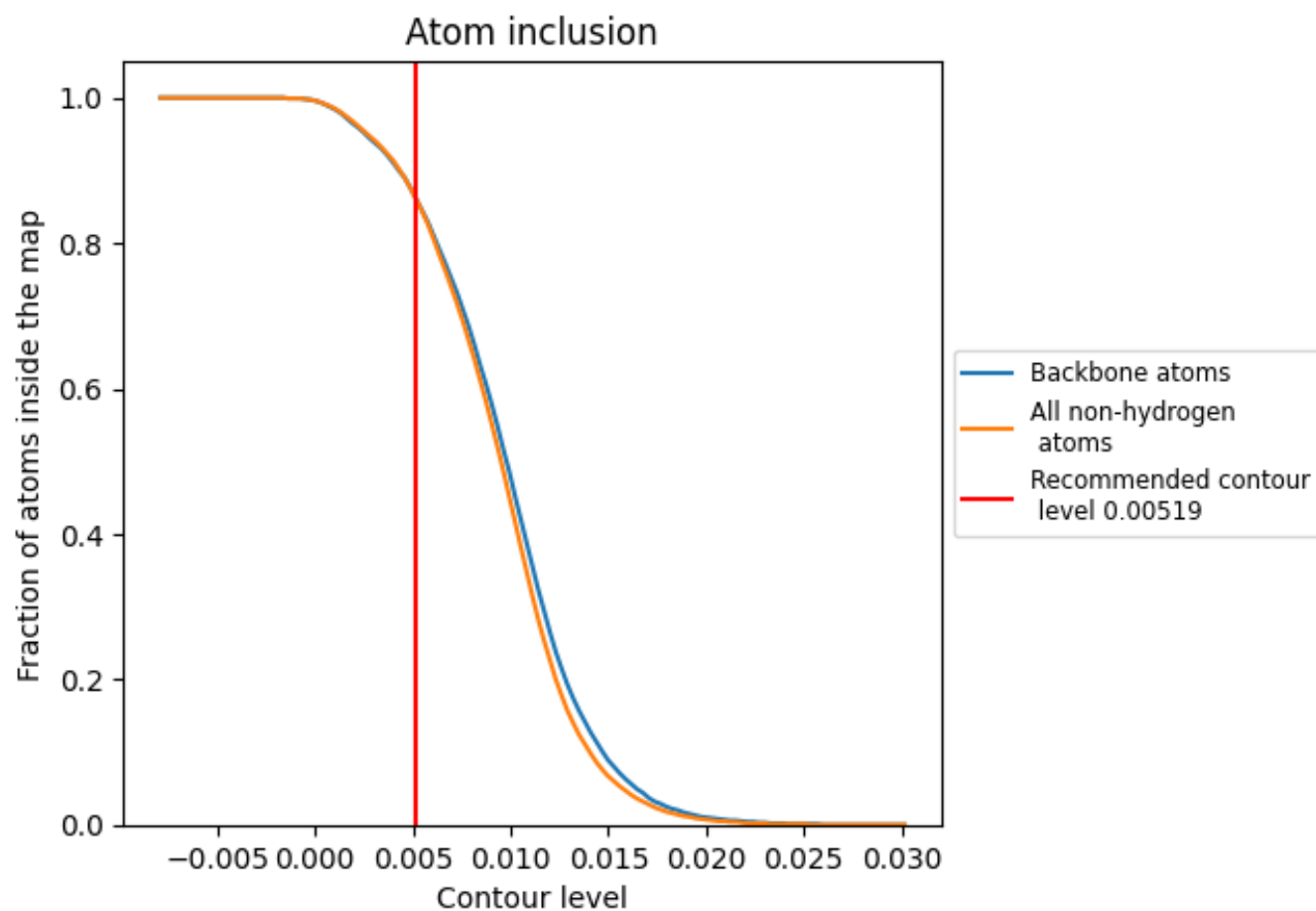
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00519).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.00519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.1050
A	 0.9480	 0.1340
B	 0.9350	 0.1180
C	 0.9860	 0.1240
D	 0.1110	 0.0720
E	 0.9490	 0.1290
F	 0.9770	 0.1000
G	 0.3620	 0.0690
H	 0.9810	 0.1300
I	 0.8580	 0.0740
J	 0.9910	 0.1260
K	 0.9730	 0.1200
L	 1.0000	 0.1140
M	 0.8230	 0.1060
N	 0.9830	 0.1030
O	 0.5070	 0.0620
P	 0.9820	 0.1900
T	 0.9790	 0.1180
a	 0.9880	 0.0550
b	 1.0000	 0.0410
c	 0.9440	 0.0830
d	 0.8780	 0.0370
e	 0.9810	 0.0550
f	 0.9450	 0.0360
g	 0.5460	 0.0480
h	 0.4110	 0.0410

