



wwPDB EM Validation Summary Report ⓘ

Dec 9, 2024 – 02:58 PM EST

PDB ID : 9EGX
EMDB ID : EMD-48039
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-hexasome, bp +27
Authors : Markert, J.; Farnung, L.
Deposited on : 2024-11-21
Resolution : 2.90 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:

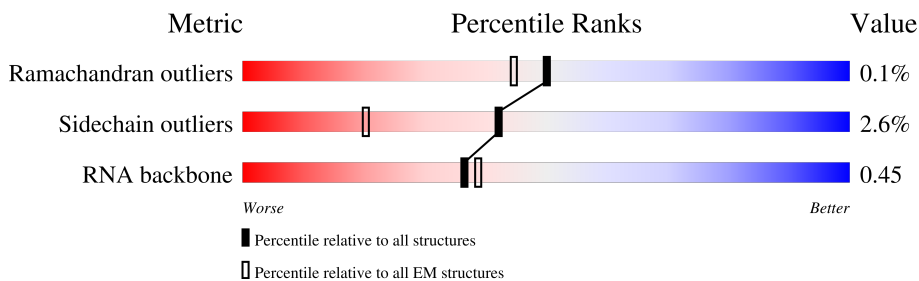
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 2.90 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.




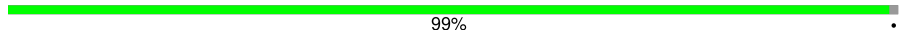
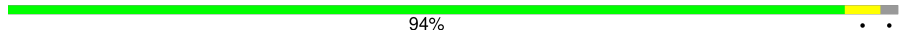











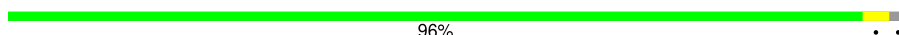

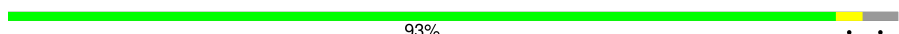







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1984	71% 28%
2	B	1251	88% 10%
3	C	275	92% 6%
4	D	142	87% 11%
5	E	210	100%
6	F	127	58% 39%
7	G	172	97% 5%
8	H	150	94% 5%

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Mol	Chain	Length	Quality of chain
9	I	125	 87% 6% 7%
10	J	67	 99%
11	K	117	 94%
12	L	58	 74% 7% 19%
13	M	1729	 8% 58% 42%
14	N	206	 70% 28%
15	O	821	 16% 84%
16	P	21	 62% 38%
17	Q	1179	 24% 74% 25%
18	R	713	 34% 66%
19	S	304	 53% 47%
20	T	215	 73% 26%
21	U	666	 19% 81%
22	V	531	 9% 46% 54%
23	W	305	 96%
24	X	531	 8% 92%
25	Y	121	 93%
26	Z	1087	 46% 53%
27	a	136	 54% 43%
27	e	136	 68% 29%
28	b	103	 78% 19%
28	f	103	 74% 24%
29	c	130	 77% 21%
30	d	123	 75% 23%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 65003 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	
			Total	C	N	O	P			S
1	A	1426	11210	7040	2013	2086	2	69	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1122	8980	5684	1576	1656	64	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1004	630	170	200	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1333	866	214	245	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1197	759	195	238	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	942	582	168	181	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

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

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

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	47	397	246	77	68	6	0	0

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	1002	4309	2295	1003	1011	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	148	3048	1446	555	899	148	0	0

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	132	656	392	132	132	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	SER	-	expression tag	UNP Q96ST2
O	0	ASN	-	expression tag	UNP Q96ST2
O	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	P	21	432	193	59	159	21	0	0

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	890	6427	4026	1164	1218	19	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	244	1428	866	281	280	1	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	S	161	657	334	161	162	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	T	159	3245	1540	608	939	158	0	0

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	125	617	367	125	125	0	0

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	244	1378	842	267	267	2	0	0

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	300	2333	1483	392	454	4	0	0

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	X	43	353	220	69	64	0	0

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	116	911	570	159	173	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
26	Z	510	4025	2552	709	745	1	18	0	0

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	77	627	397	116	111	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	e	97	801	504	155	139	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	83	662	418	129	114	1	0	0
28	f	78	619	391	120	107	1	0	0

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	c	103	795	501	155	139	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	95	745	469	134	140	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281

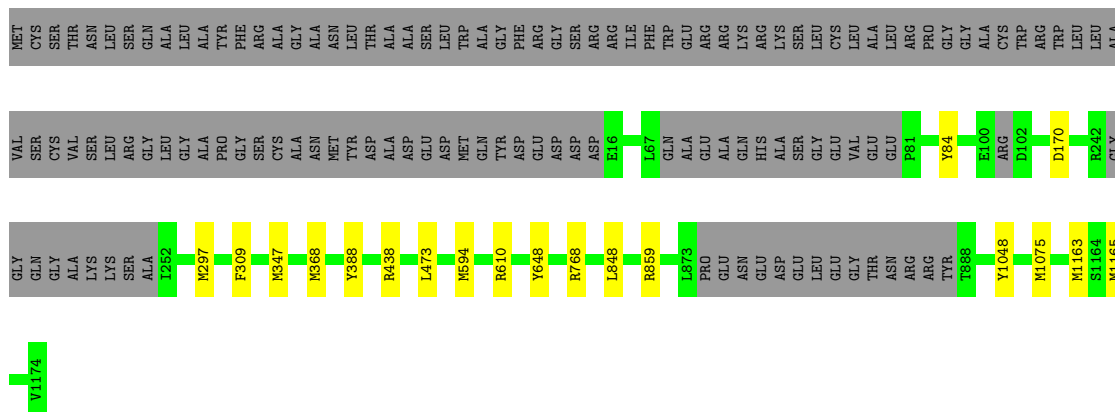
- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

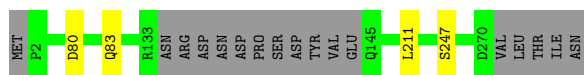
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total 1	Mg 1	0

Chain B: 88% • 10%



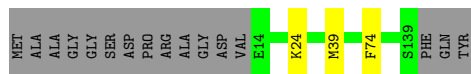
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 92% • 6%



- Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein

Chain D: 87% • 11%



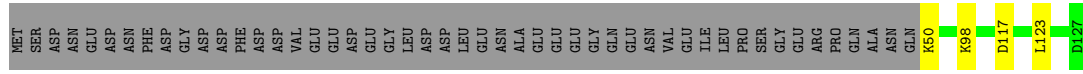
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 100%



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 58% • 39%

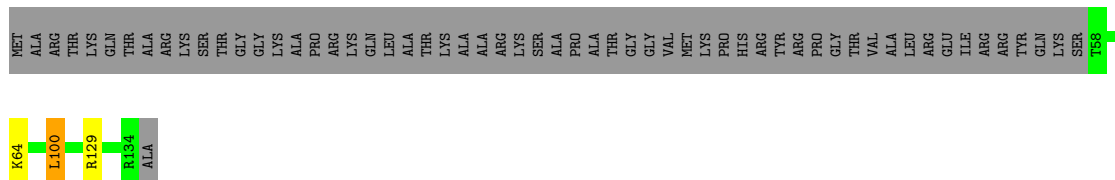


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

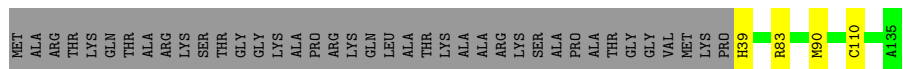
Chain G: 97% ••



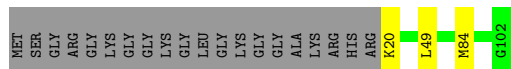
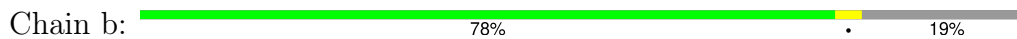
• Molecule 27: Histone H3



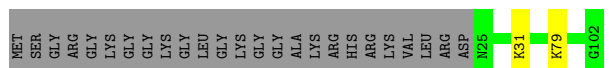
• Molecule 27: Histone H3



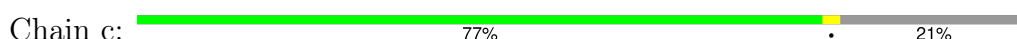
• Molecule 28: Histone H4



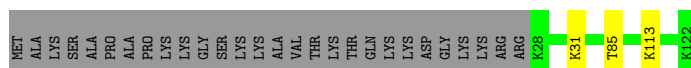
• Molecule 28: Histone H4



• Molecule 29: Histone H2A type 1



• Molecule 30: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1139653	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.708	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	549.46, 549.46, 549.46	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09892, 1.09892, 1.09892	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: ZN, TPO, SEP, 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	0.27	0/11384	0.57	6/15361 (0.0%)
2	B	0.26	0/9158	0.54	1/12360 (0.0%)
3	C	0.26	0/2115	0.54	0/2873
4	D	0.25	0/1017	0.51	0/1368
5	E	0.26	0/1751	0.54	0/2366
6	F	0.29	0/636	0.59	0/859
7	G	0.28	0/1364	0.55	0/1853
8	H	0.30	0/1219	0.61	1/1644 (0.1%)
9	I	0.31	0/964	0.58	0/1305
10	J	0.30	0/533	0.54	0/719
11	K	0.29	0/939	0.51	0/1271
12	L	0.32	0/403	0.70	0/536
13	M	0.22	0/4330	0.42	0/5591
14	N	0.54	0/3417	0.93	4/5275 (0.1%)
15	O	0.23	0/655	0.36	0/913
16	P	0.17	0/477	0.73	0/738
17	Q	0.27	0/6531	0.52	2/8861 (0.0%)
18	R	0.25	0/1437	0.48	0/1972
19	S	0.22	0/659	0.41	0/827
20	T	0.52	0/3642	0.86	2/5614 (0.0%)
21	U	0.24	0/613	0.46	0/847
22	V	0.25	0/1386	0.48	0/1909
23	W	0.32	1/2392 (0.0%)	0.58	3/3257 (0.1%)
24	X	0.30	0/356	0.65	0/478
25	Y	0.25	0/927	0.57	0/1250
26	Z	0.25	0/4084	0.52	0/5498
27	a	0.29	0/634	0.67	1/851 (0.1%)
27	e	0.29	0/812	0.62	0/1088
28	b	0.30	0/669	0.64	1/894 (0.1%)
28	f	0.29	0/626	0.66	0/837
29	c	0.28	0/805	0.58	0/1088
30	d	0.31	0/756	0.60	0/1015

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.31	1/66691 (0.0%)	0.60	21/91318 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	106	PRO	CG-CD	-6.58	1.28	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	106	PRO	CA-N-CD	-13.85	92.11	111.50
1	A	911	PRO	CA-N-CD	-10.19	97.24	111.50
1	A	433	PRO	CA-N-CD	-8.17	100.06	111.50
23	W	106	PRO	N-CD-CG	-7.77	91.55	103.20
14	N	146	DA	OP1-P-OP2	-7.07	109.00	119.60

There are no chirality outliers.

There are no planarity outliers.

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	1408/1984 (71%)	1330 (94%)	76 (5%)	2 (0%)	48	77
2	B	1112/1251 (89%)	1042 (94%)	70 (6%)	0	100	100
3	C	254/275 (92%)	236 (93%)	18 (7%)	0	100	100
4	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	207/210 (99%)	200 (97%)	7 (3%)	0	100	100
6	F	76/127 (60%)	74 (97%)	2 (3%)	0	100	100
7	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
8	H	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	58 (91%)	6 (9%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	45/58 (78%)	39 (87%)	5 (11%)	1 (2%)	5	21
13	M	976/1729 (56%)	935 (96%)	40 (4%)	1 (0%)	48	77
15	O	130/821 (16%)	127 (98%)	3 (2%)	0	100	100
17	Q	888/1179 (75%)	863 (97%)	25 (3%)	0	100	100
18	R	240/713 (34%)	230 (96%)	10 (4%)	0	100	100
19	S	157/304 (52%)	156 (99%)	1 (1%)	0	100	100
21	U	117/666 (18%)	104 (89%)	12 (10%)	1 (1%)	14	43
22	V	234/531 (44%)	220 (94%)	14 (6%)	0	100	100
23	W	298/305 (98%)	282 (95%)	16 (5%)	0	100	100
24	X	41/531 (8%)	40 (98%)	1 (2%)	0	100	100
25	Y	114/121 (94%)	106 (93%)	8 (7%)	0	100	100
26	Z	497/1087 (46%)	477 (96%)	19 (4%)	1 (0%)	44	73
27	a	75/136 (55%)	75 (100%)	0	0	100	100
27	e	95/136 (70%)	95 (100%)	0	0	100	100
28	b	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
28	f	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
29	c	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
30	d	93/123 (76%)	90 (97%)	3 (3%)	0	100	100
All	All	8046/13396 (60%)	7666 (95%)	374 (5%)	6 (0%)	50	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1343	LEU
12	L	39	CYS
13	M	700	HIS

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Mol	Chain	Res	Type
21	U	510	LYS
26	Z	774	GLN

5.3.2 Protein sidechains [i](#)

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	1229/1761 (70%)	1212 (99%)	17 (1%)	62	86
2	B	986/1084 (91%)	968 (98%)	18 (2%)	54	82
3	C	235/252 (93%)	231 (98%)	4 (2%)	56	83
4	D	109/126 (86%)	106 (97%)	3 (3%)	38	73
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	64 (94%)	4 (6%)	16	45
7	G	146/153 (95%)	142 (97%)	4 (3%)	40	73
8	H	130/131 (99%)	123 (95%)	7 (5%)	18	49
9	I	104/112 (93%)	97 (93%)	7 (7%)	13	39
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	99 (95%)	5 (5%)	21	54
12	L	44/55 (80%)	41 (93%)	3 (7%)	13	38
13	M	41/1524 (3%)	41 (100%)	0	100	100
17	Q	533/1011 (53%)	515 (97%)	18 (3%)	32	67
18	R	57/625 (9%)	52 (91%)	5 (9%)	8	26
19	S	4/268 (2%)	4 (100%)	0	100	100
22	V	46/462 (10%)	44 (96%)	2 (4%)	25	57
23	W	255/260 (98%)	249 (98%)	6 (2%)	44	76
24	X	40/467 (9%)	37 (92%)	3 (8%)	11	33
25	Y	102/105 (97%)	98 (96%)	4 (4%)	27	62
26	Z	435/939 (46%)	424 (98%)	11 (2%)	42	75
27	a	67/111 (60%)	64 (96%)	3 (4%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	e	84/111 (76%)	80 (95%)	4 (5%)	21	54
28	b	68/79 (86%)	66 (97%)	2 (3%)	37	72
28	f	63/79 (80%)	61 (97%)	2 (3%)	34	69
29	c	82/102 (80%)	79 (96%)	3 (4%)	29	64
30	d	81/103 (79%)	78 (96%)	3 (4%)	29	64
All	All	5359/10385 (52%)	5221 (97%)	138 (3%)	42	74

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Z	429	CYS
26	Z	635	MET
30	d	85	THR
7	G	104	MET
7	G	8	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1142	ASN
17	Q	311	GLN
28	b	93	GLN
3	C	111	GLN
9	I	91	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	20/21 (95%)	7 (35%)	3 (15%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	8	U
16	P	9	U
16	P	10	U
16	P	11	U
16	P	16	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	8	U
16	P	16	U
16	P	18	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	SEP	A	1547	1	8,9,10	1.62	1 (12%)	7,12,14	1.29	1 (14%)
1	TPO	A	1525	1	8,10,11	1.11	0	10,14,16	2.14	1 (10%)
26	TPO	Z	775	26	8,10,11	1.12	0	10,14,16	1.97	1 (10%)

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
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	0/9/11/13	-
26	TPO	Z	775	26	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.53	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-6.14	106.65	123.33
26	Z	775	TPO	P-OG1-CB	-5.70	107.84	123.33
1	A	1547	SEP	OG-CB-CA	2.81	110.88	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	Z	775	TPO	C-CA-CB-CG2
26	Z	775	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
22	V	1
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	27.06
1	V	299:GLU	C	310:ASN	N	12.67
1	M	1334:ASN	C	1338:ILE	N	5.50

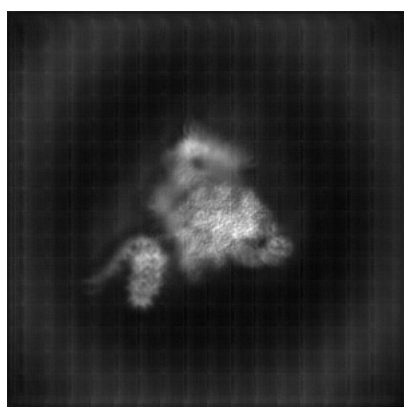
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48039. These allow visual inspection of the internal detail of the map and identification of artifacts.

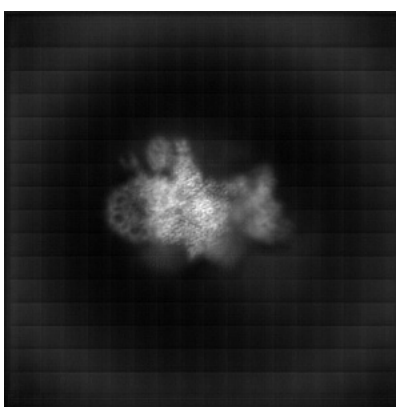
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

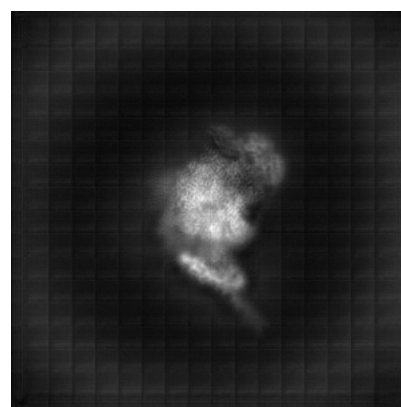
6.1.1 Primary map



X



Y

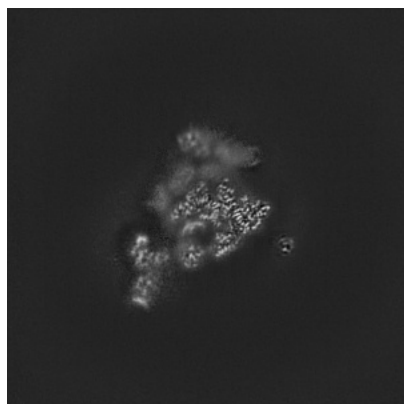


Z

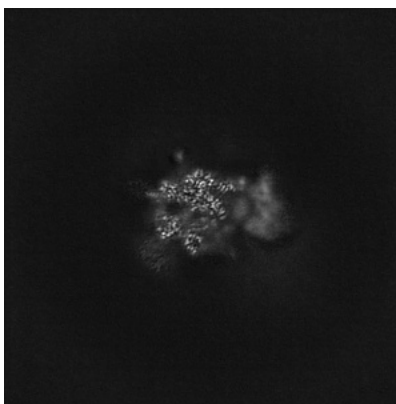
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

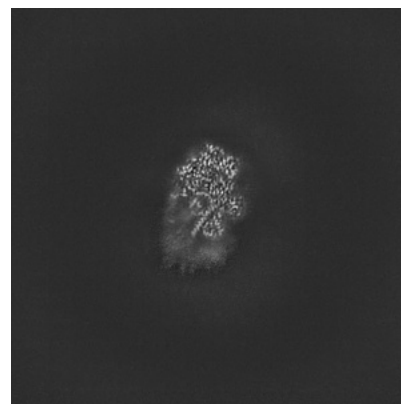
6.2.1 Primary map



X Index: 250



Y Index: 250

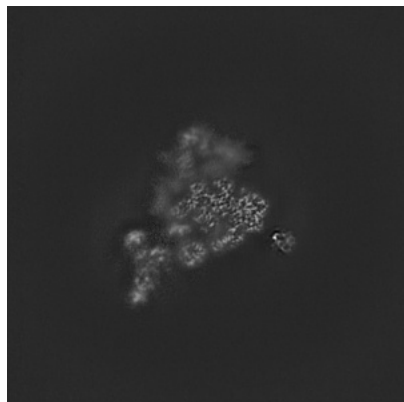


Z Index: 250

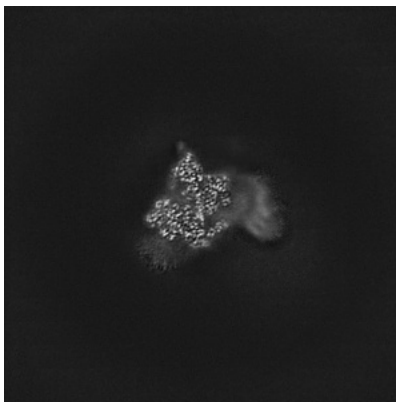
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

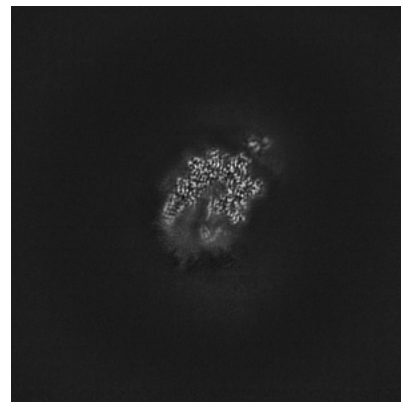
6.3.1 Primary map



X Index: 257



Y Index: 264

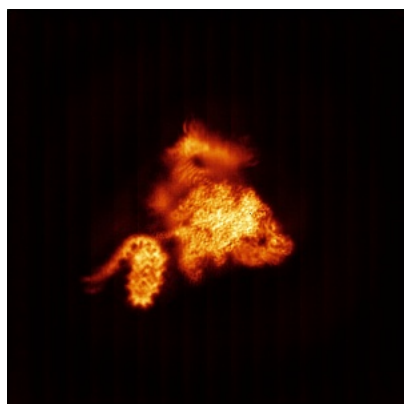


Z Index: 236

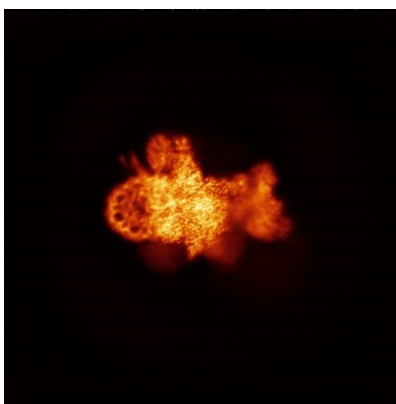
The images above show the largest variance slices of the map in three orthogonal directions.

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

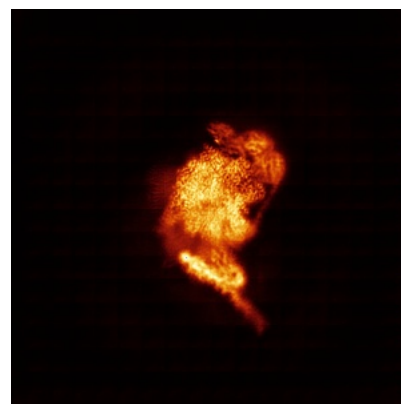
6.4.1 Primary map



X



Y

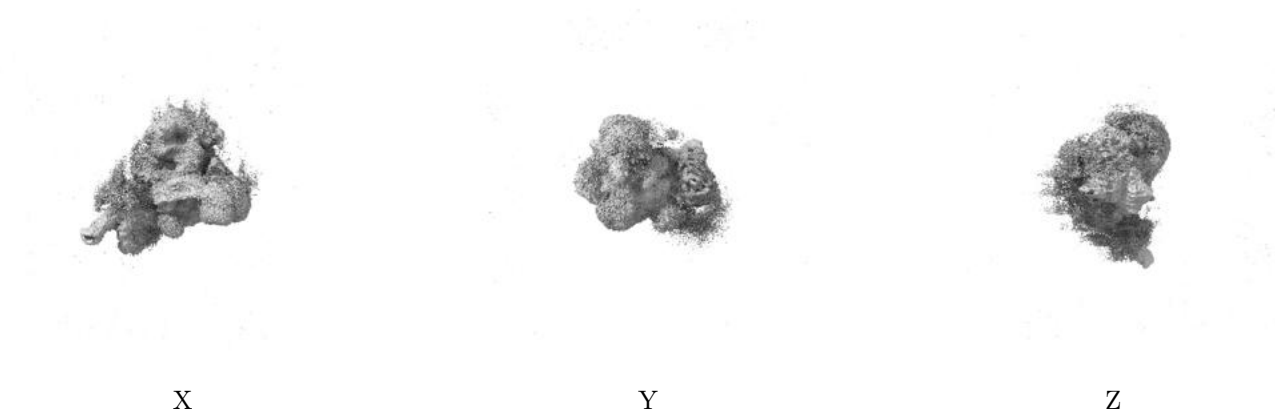


Z

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.

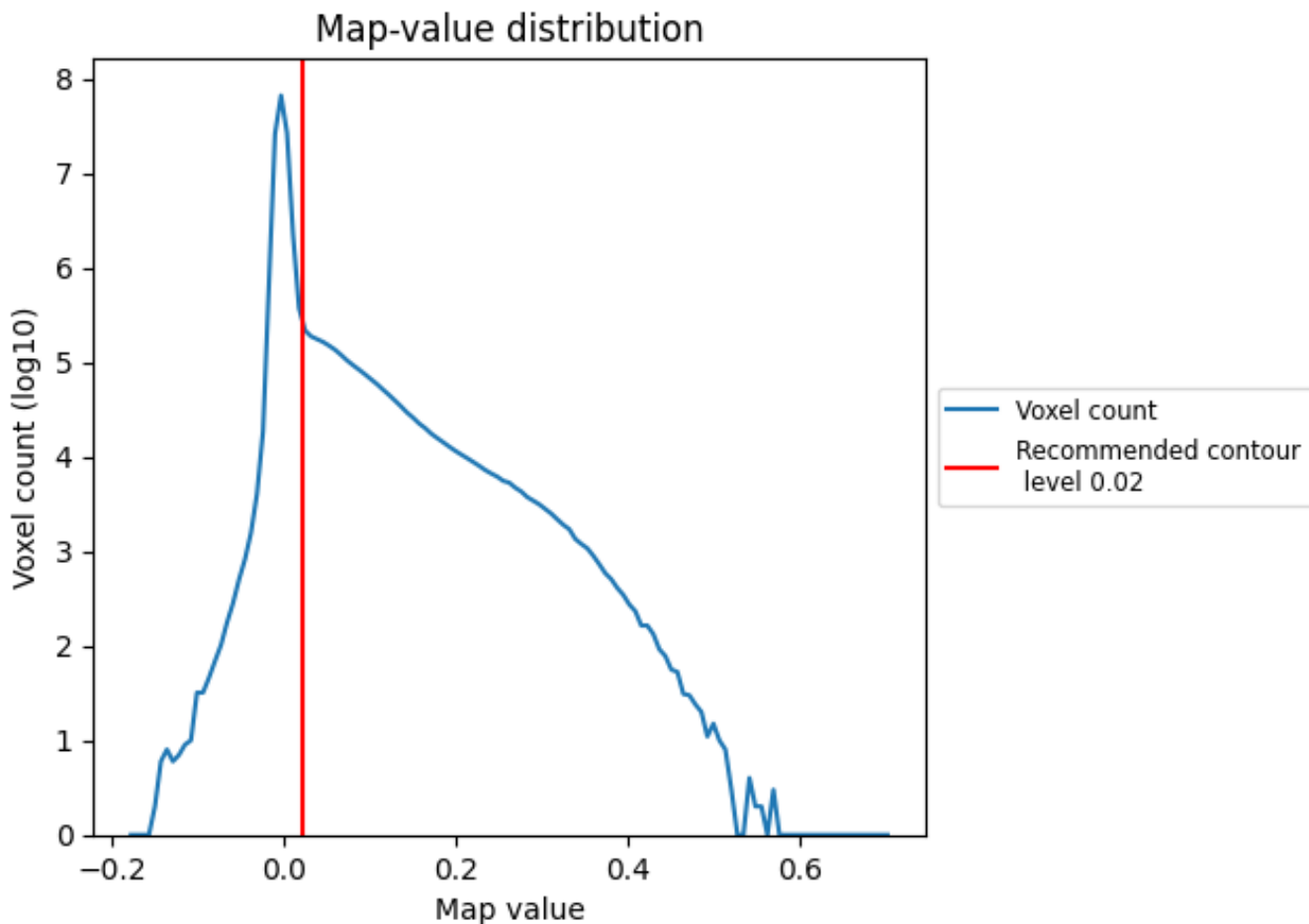
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

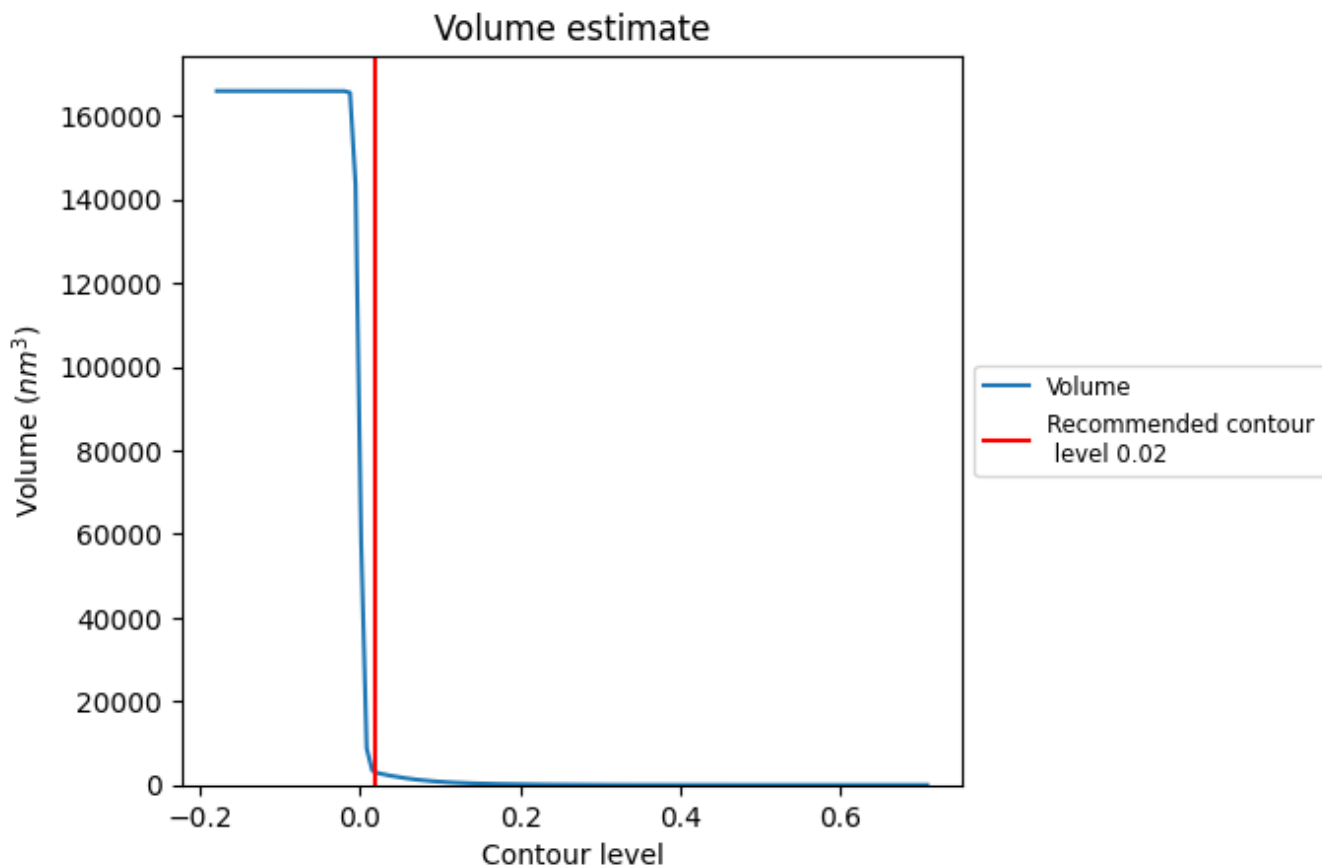
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

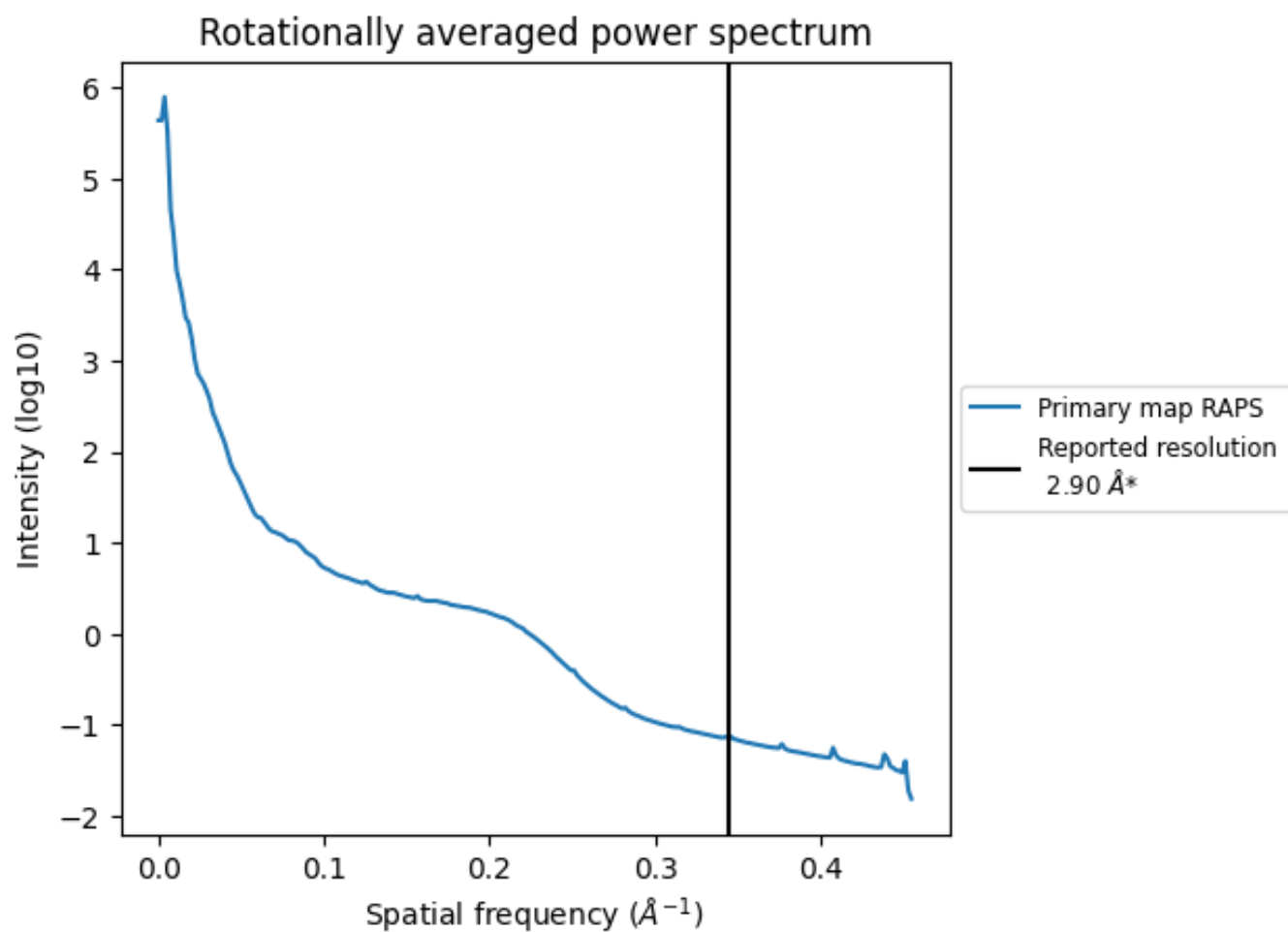
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3060 nm^3 ; this corresponds to an approximate mass of 2764 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

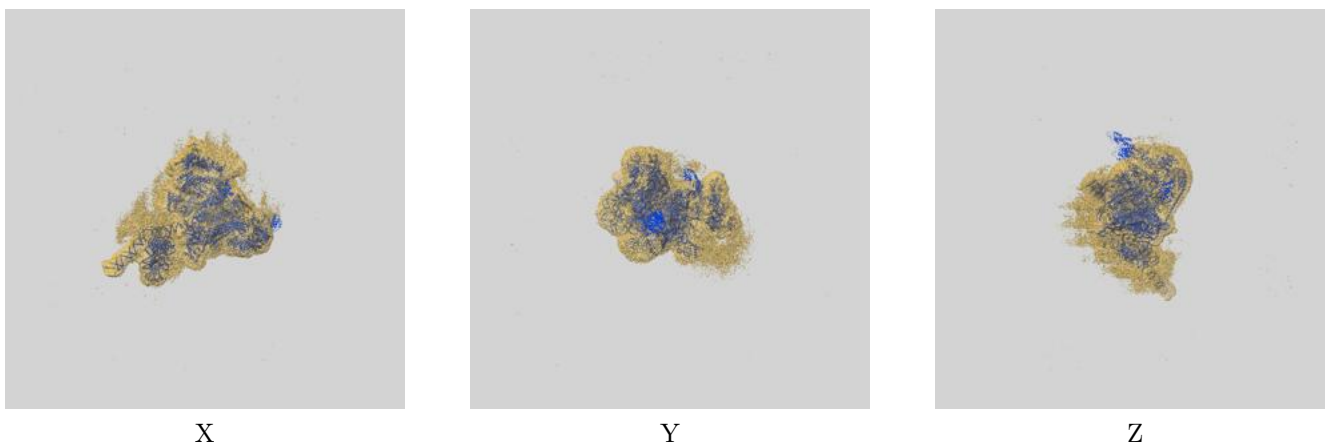
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

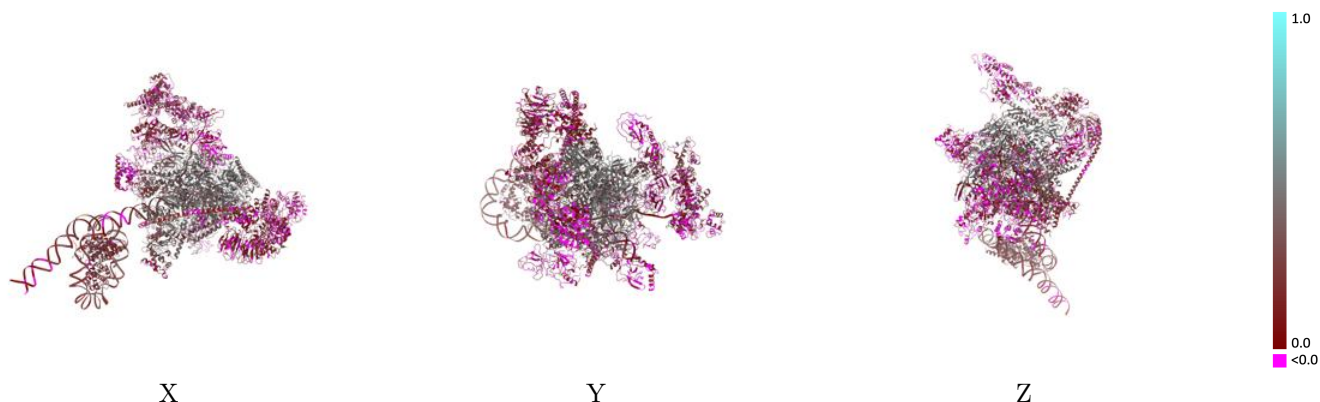
This section contains information regarding the fit between EMDB map EMD-48039 and PDB model 9EGX. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



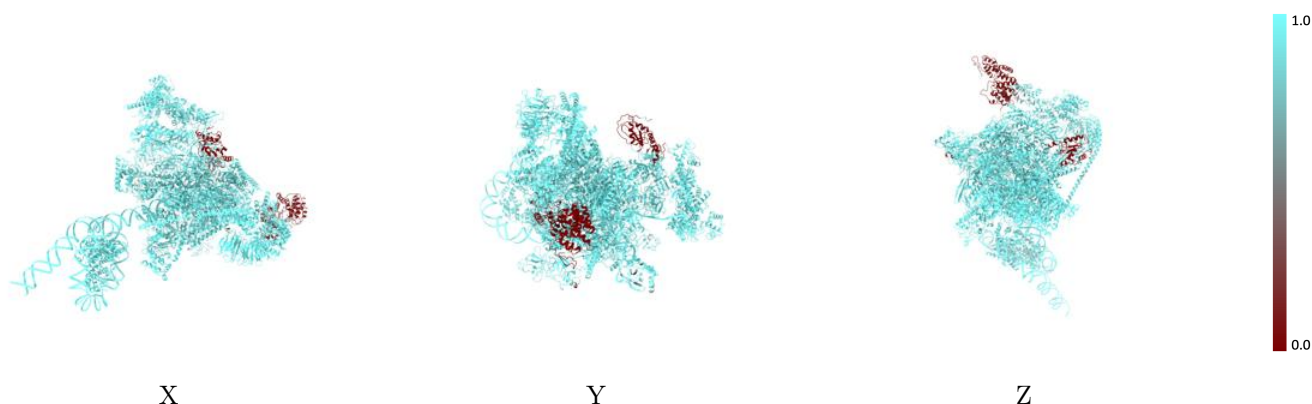
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



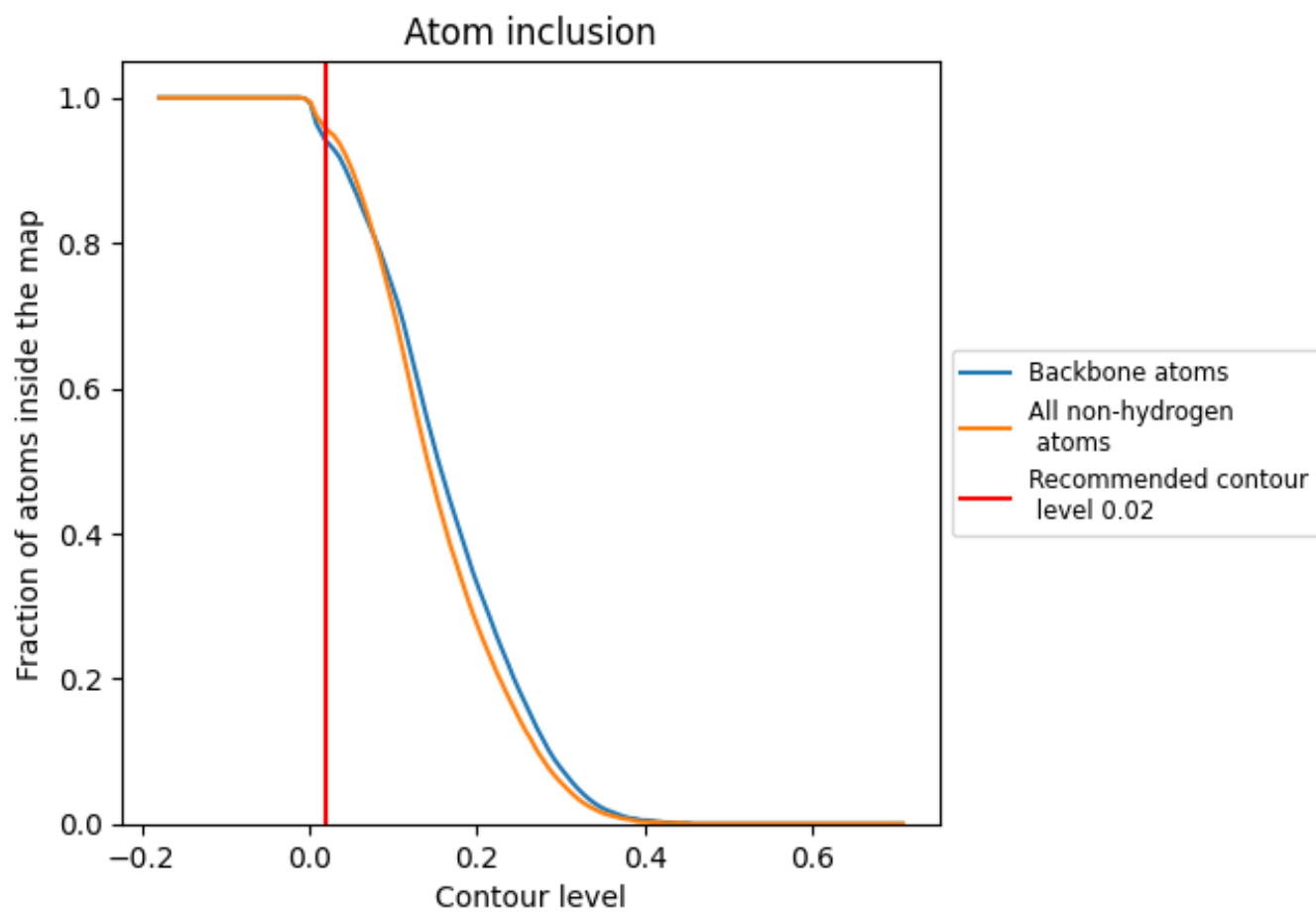
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 96% 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	 0.9570	 0.2500
A	 0.9920	 0.3920
B	 1.0000	 0.4050
C	 1.0000	 0.4320
D	 1.0000	 0.1870
E	 1.0000	 0.3770
F	 1.0000	 0.4380
G	 1.0000	 0.2100
H	 0.9970	 0.4250
I	 1.0000	 0.3720
J	 1.0000	 0.4090
K	 1.0000	 0.4370
L	 1.0000	 0.3950
M	 0.8420	 0.0920
N	 0.9940	 0.1820
O	 1.0000	 -0.0080
P	 1.0000	 0.1930
Q	 0.7640	 0.0960
R	 0.9150	 0.0610
S	 1.0000	 0.1990
T	 0.9910	 0.1850
U	 0.9810	 0.0890
V	 0.7960	 0.0690
W	 1.0000	 0.1390
X	 1.0000	 0.1580
Y	 1.0000	 0.0350
Z	 0.9920	 0.0850
a	 1.0000	 0.2060
b	 1.0000	 0.2210
c	 1.0000	 0.2240
d	 0.9990	 0.2280
e	 1.0000	 0.2110
f	 1.0000	 0.2160

