



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 12:22 PM EDT

PDB ID : 7UI9
EMDB ID : EMD-26542
Title : Core Mediator-PICearly (Copy A)
Authors : Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.
Deposited on : 2022-03-28
Resolution : 3.30 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:

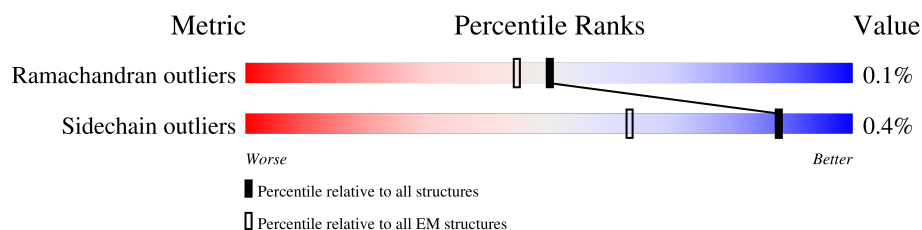
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.30 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.




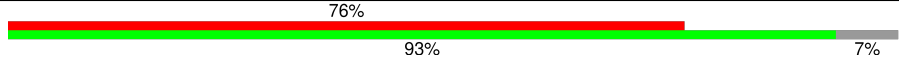
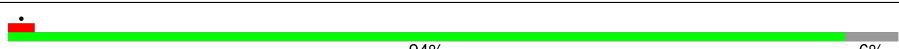
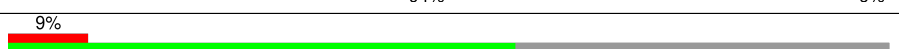
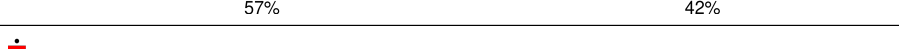



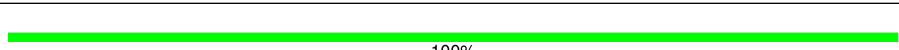
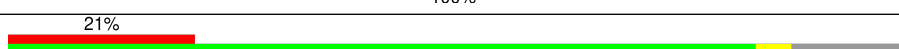
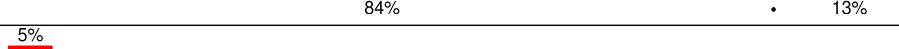
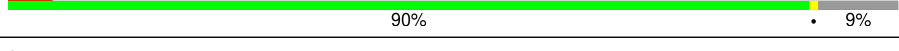

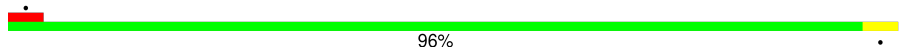
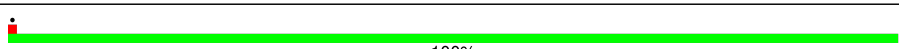
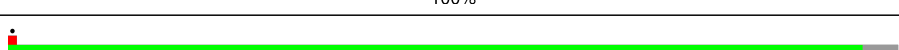
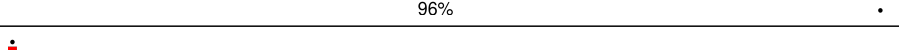



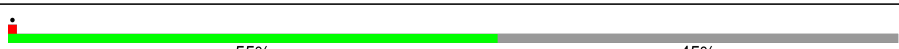

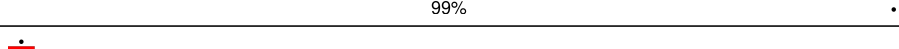
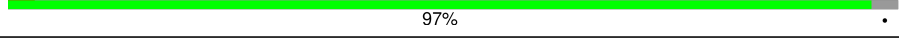
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	M	345	
2	P	735	
3	Q	400	
4	S	309	
5	a	566	
6	d	284	
7	f	295	
8	g	222	
9	h	223	

Continued on next page...

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Mol	Chain	Length	Quality of chain
10	i	149	
11	j	157	
12	k	115	
13	n	1082	
14	q	687	
15	r	307	
16	s	220	
17	t	210	
18	u	140	
19	v	120	
20	w	127	
21	z	25	
22	A	1453	
23	B	1224	
24	C	318	
25	D	221	
26	E	215	
27	F	155	
28	G	171	
29	H	146	
30	I	122	
31	J	70	
32	K	120	
33	L	70	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 63137 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 Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	35	Total	C	N	O	S	0	0
			263	169	41	49	4		

- Molecule 2 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	103	Total	C	N	O	S	0	0
			861	554	142	162	3		

- Molecule 3 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		

- Molecule 4 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	169	Total	C	N	O	S	0	0
			1409	903	238	263	5		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	136	Total	C	N	O	S	0	0
			1126	709	199	215	3		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	83	Total	C	N	O	S	0	0
			709	444	130	134	1		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	146	Total	C	N	O	S	0	0
			1173	725	206	239	3		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	625	Total	C	N	O	S	0	0
			5139	3318	884	913	24		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	81	Total	C	N	O	S	0	0
			657	415	109	132	1		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	122	Total	C	N	O	S	0	0
			978	611	163	199	5		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	109	Total	C	N	O	S	0	0
			869	540	143	180	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	103	Total	C	N	O	S	0	0
			871	575	135	155	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	z	25	Total	C	N	O	0	0
			184	116	25	43		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	1453	Total	C	N	O	S	0	0
			11425	7192	1995	2176	62		

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		

- Molecule 26 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	86	Total	C	N	O	S	0	0
			697	445	118	131	3		

- Molecule 28 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	141	Total	C	N	O	S	0	0
			1126	706	189	226	5		

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	116	Total	C	N	O	S	0	0
			943	580	171	181	11		

- Molecule 31 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 32 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	116	Total	C	N	O	S	0	0
			929	596	158	173	2		

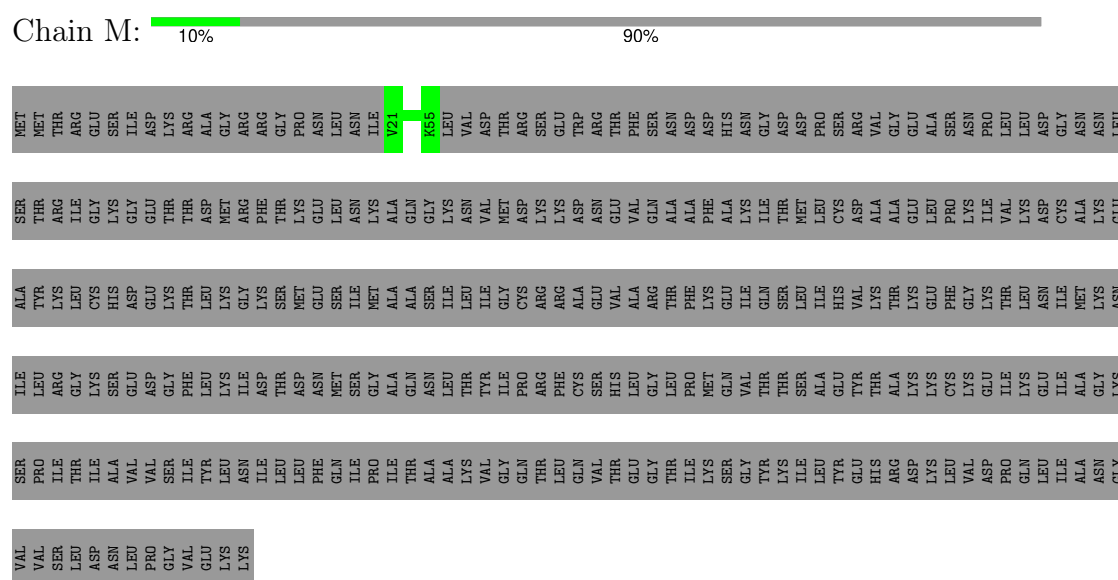
- Molecule 33 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

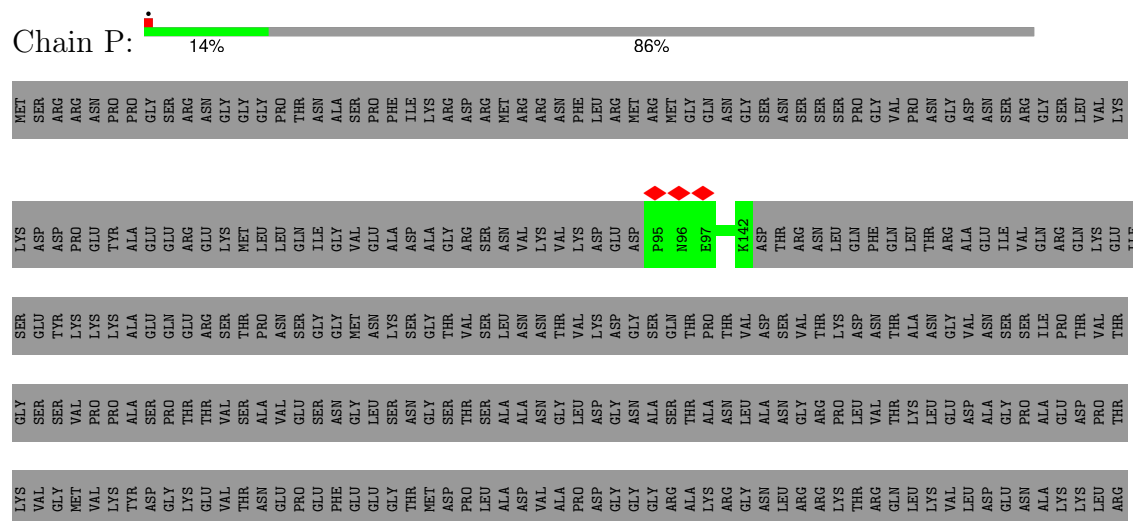
3 Residue-property plots

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.

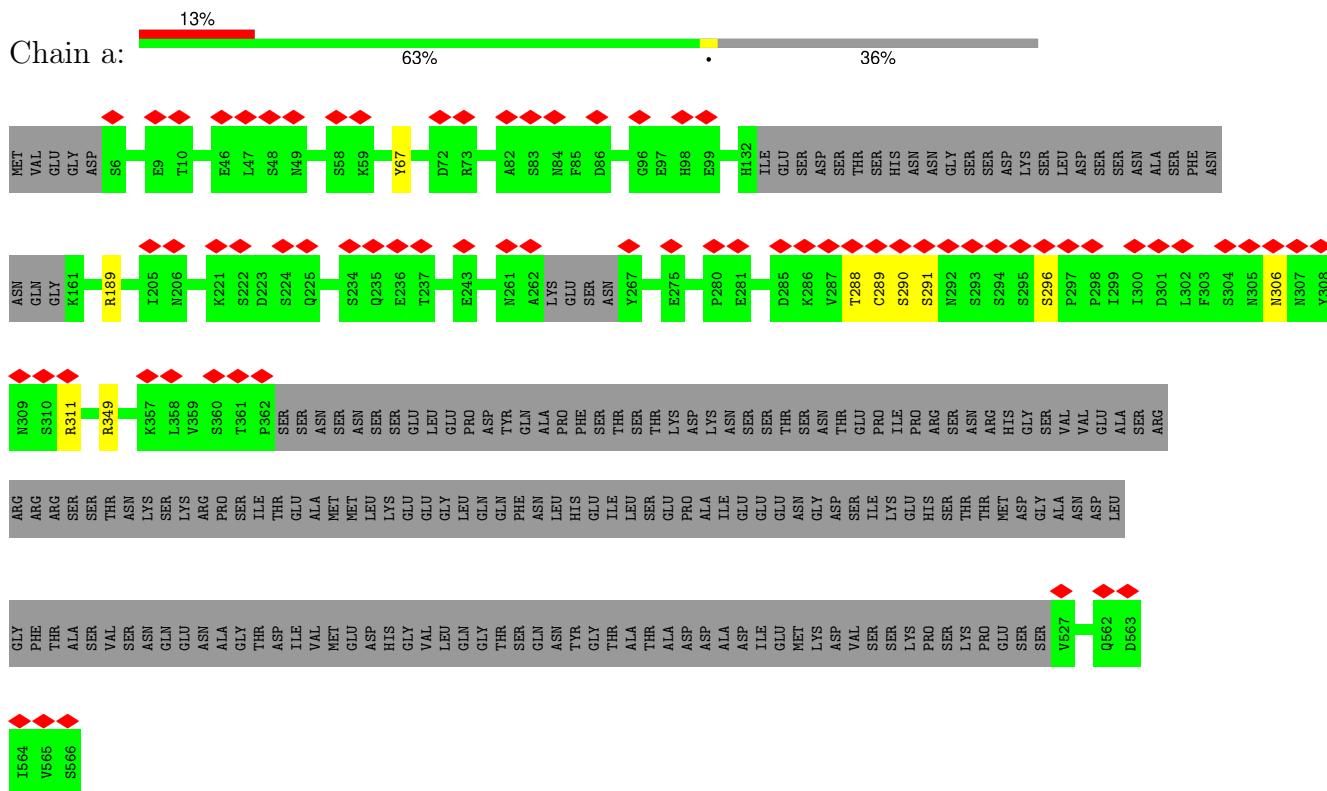
• Molecule 1: Transcription initiation factor IIB



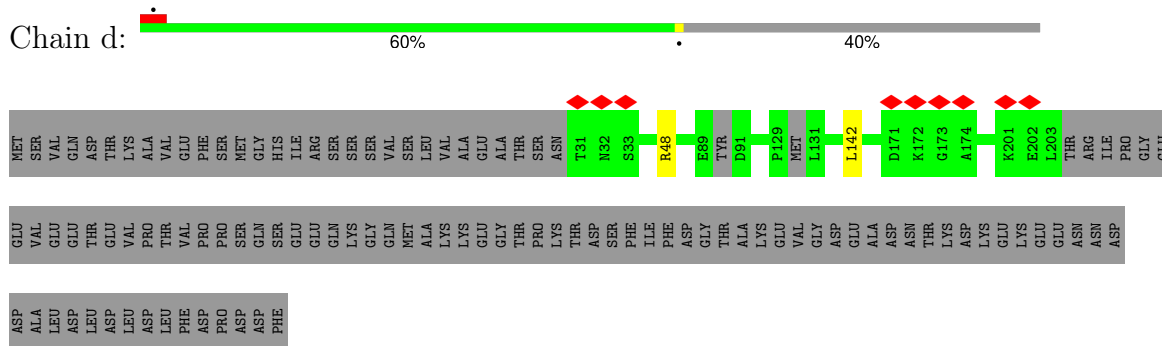
• Molecule 2: Transcription initiation factor IIF subunit alpha



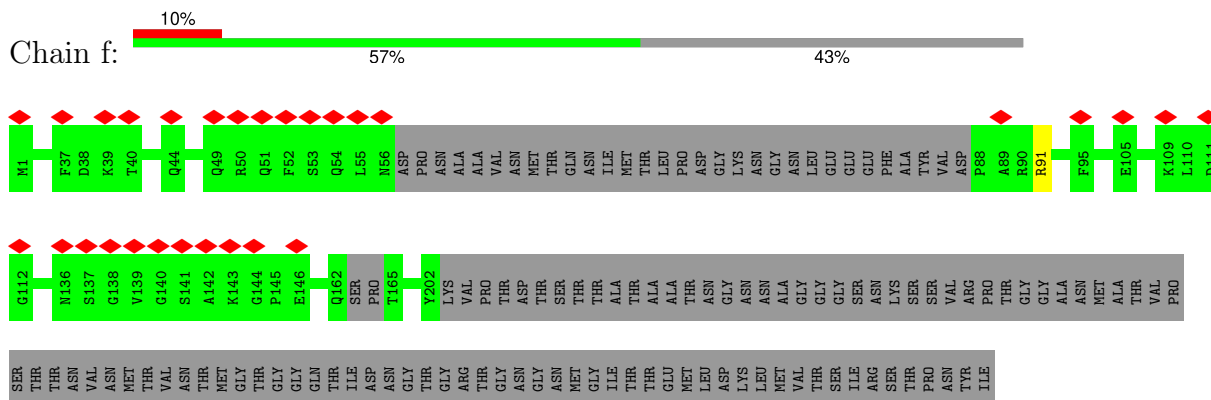
Chain a:



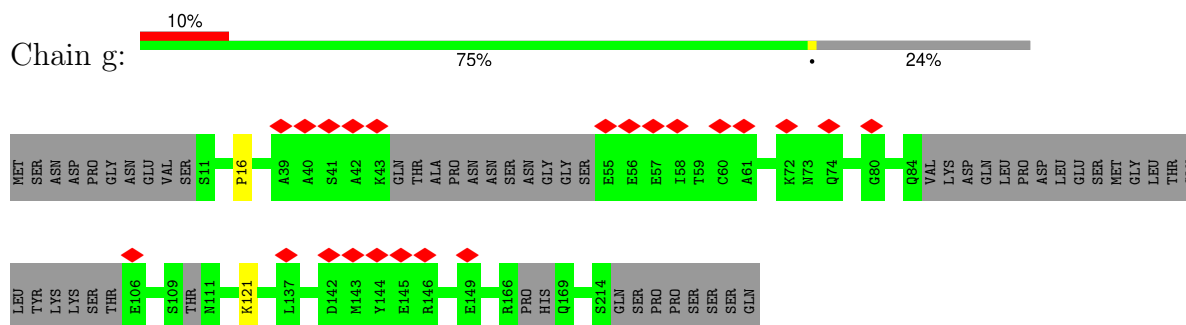
Chain d:



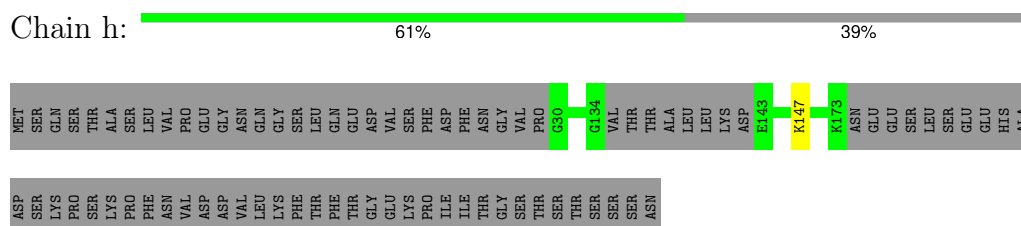
Chain f:



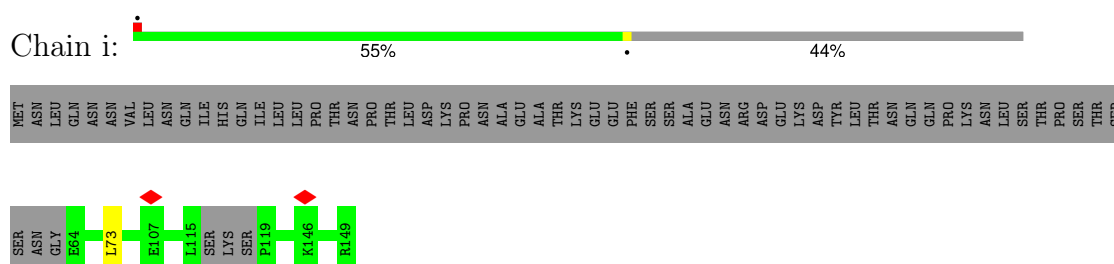
- Molecule 8: Mediator of RNA polymerase II transcription subunit 7



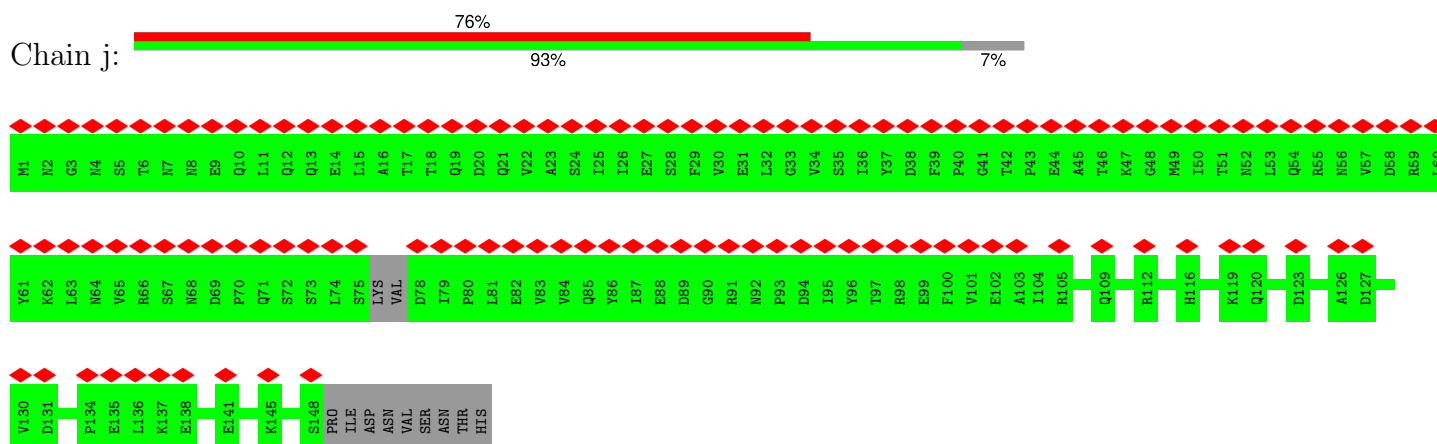
- Molecule 9: Mediator of RNA polymerase II transcription subunit 8



- Molecule 10: Mediator of RNA polymerase II transcription subunit 9

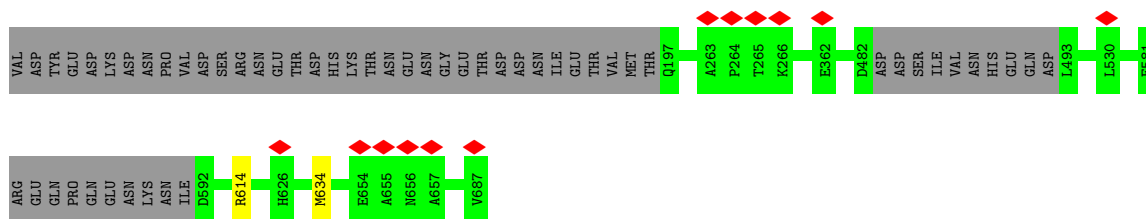


- Molecule 11: Mediator of RNA polymerase II transcription subunit 10



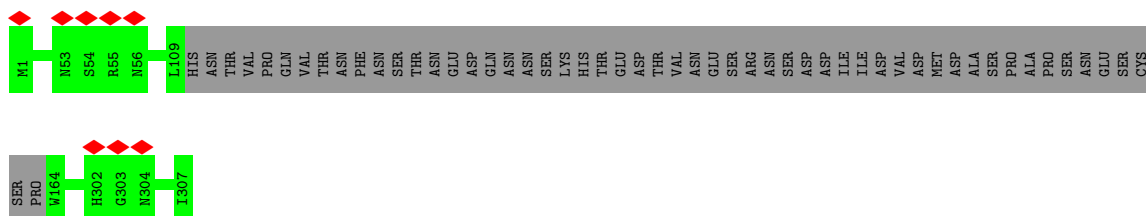
- Molecule 12: Mediator of RNA polymerase II transcription subunit 11





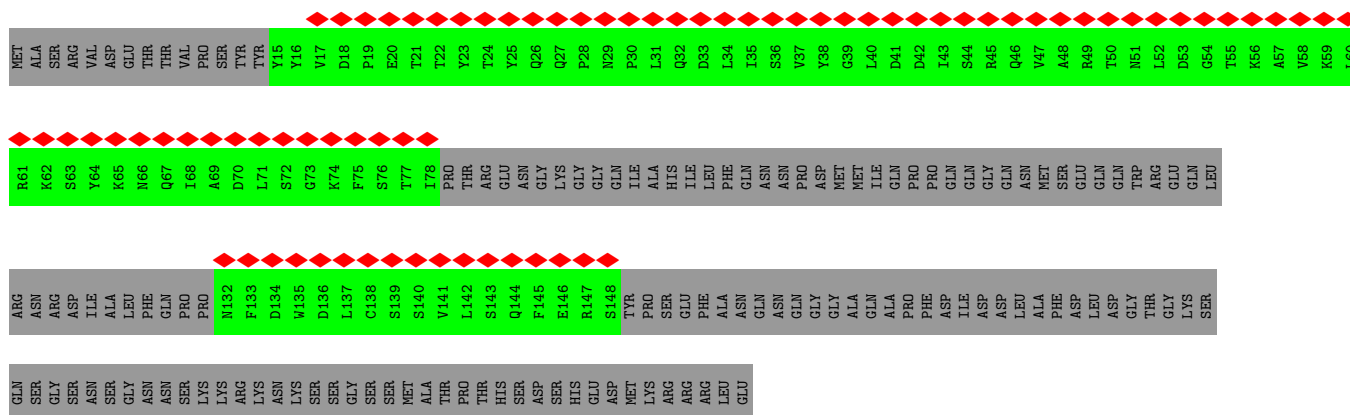
- Molecule 15: Mediator of RNA polymerase II transcription subunit 18

Chain r: 82% 18%



- Molecule 16: Mediator of RNA polymerase II transcription subunit 19

Chain s: 36% 37% 63%



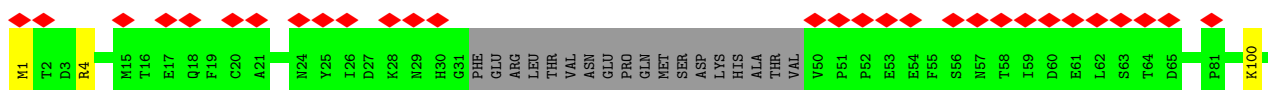
- Molecule 17: Mediator of RNA polymerase II transcription subunit 20

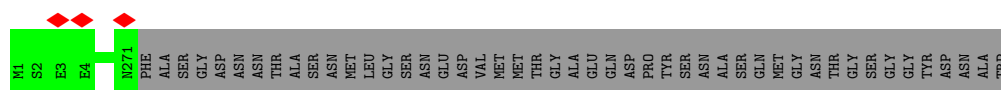
Chain t: 100%

There are no outlier residues recorded for this chain.

- Molecule 18: Mediator of RNA polymerase II transcription subunit 21

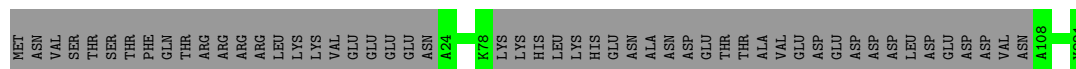
Chain u: 21% 84% 13%





- Molecule 25: DNA-directed RNA polymerase II subunit RPB4

Chain D: 76% 24%



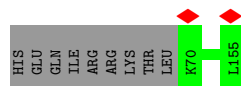
- Molecule 26: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 100%



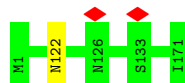
- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 55% 45%



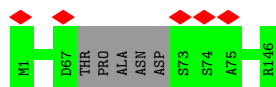
- Molecule 28: DNA-directed RNA polymerase II subunit RPB7

Chain G: 99%



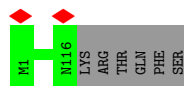
- Molecule 29: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 97%



- Molecule 30: DNA-directed RNA polymerase II subunit RPB9

Chain I: 95% 5%



- Molecule 31: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  100%



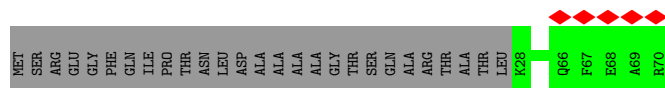
- Molecule 32: DNA-directed RNA polymerase II subunit RPB11

Chain K:  97%



- Molecule 33: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  7% 61% 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1102984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (\AA)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.26	0/267	0.47	0/362
2	P	0.25	0/886	0.47	0/1198
3	Q	0.24	0/1049	0.48	0/1413
4	S	0.25	0/1462	0.48	0/1973
5	a	0.65	0/3067	0.86	4/4148 (0.1%)
6	d	0.27	0/1405	0.58	1/1889 (0.1%)
7	f	0.27	0/1440	0.50	0/1946
8	g	0.28	0/1434	0.50	1/1930 (0.1%)
9	h	0.26	0/1147	0.55	0/1552
10	i	0.26	0/720	0.63	1/965 (0.1%)
11	j	0.24	0/1188	0.45	0/1604
12	k	0.27	0/885	0.49	0/1183
13	n	0.24	0/5226	0.46	0/7051
14	q	0.26	0/4245	0.49	0/5702
15	r	0.26	0/2030	0.50	0/2747
16	s	0.24	0/669	0.43	0/906
17	t	0.26	0/1635	0.50	0/2215
18	u	0.28	0/984	0.58	0/1317
19	v	0.26	0/873	0.51	0/1177
20	w	0.26	0/897	0.42	0/1219
21	z	0.25	0/194	0.40	0/270
22	A	0.28	0/11632	0.51	0/15735
23	B	0.27	0/9520	0.52	0/12839
24	C	0.27	0/2171	0.50	0/2941
25	D	0.24	0/1365	0.44	0/1831
26	E	0.26	0/1796	0.49	0/2416
27	F	0.27	0/709	0.50	0/956
28	G	0.26	0/1368	0.49	0/1844
29	H	0.28	0/1144	0.53	0/1548
30	I	0.25	0/961	0.55	0/1294
31	J	0.29	0/587	0.57	0/786
32	K	0.28	0/947	0.51	0/1279
33	L	0.25	0/346	0.61	0/457
All	All	0.29	0/64249	0.53	7/86693 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	349	ARG	NE-CZ-NH1	7.21	123.91	120.30
5	a	67	TYR	CB-CG-CD2	-6.36	117.19	121.00
5	a	189	ARG	NE-CZ-NH1	6.24	123.42	120.30
10	i	73	LEU	CA-CB-CG	5.85	128.76	115.30
5	a	311	ARG	NE-CZ-NH1	5.45	123.03	120.30

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	M	33/345 (10%)	33 (100%)	0	0	100	100
2	P	99/735 (14%)	98 (99%)	1 (1%)	0	100	100
3	Q	121/400 (30%)	121 (100%)	0	0	100	100
4	S	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
5	a	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	16	46
6	d	165/284 (58%)	164 (99%)	1 (1%)	0	100	100
7	f	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
8	g	159/222 (72%)	159 (100%)	0	0	100	100
9	h	132/223 (59%)	129 (98%)	3 (2%)	0	100	100
10	i	79/149 (53%)	79 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	j	142/157 (90%)	137 (96%)	5 (4%)	0	100	100
12	k	104/115 (90%)	104 (100%)	0	0	100	100
13	n	611/1082 (56%)	607 (99%)	4 (1%)	0	100	100
14	q	505/687 (74%)	500 (99%)	5 (1%)	0	100	100
15	r	249/307 (81%)	244 (98%)	5 (2%)	0	100	100
16	s	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
17	t	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
18	u	116/140 (83%)	115 (99%)	1 (1%)	0	100	100
19	v	105/120 (88%)	105 (100%)	0	0	100	100
20	w	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
21	z	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	14
22	A	1451/1453 (100%)	1407 (97%)	43 (3%)	1 (0%)	48	76
23	B	1164/1224 (95%)	1132 (97%)	32 (3%)	0	100	100
24	C	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
25	D	165/221 (75%)	163 (99%)	2 (1%)	0	100	100
26	E	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
27	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
28	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
29	H	137/146 (94%)	133 (97%)	4 (3%)	0	100	100
30	I	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
31	J	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
32	K	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
33	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	7715/11003 (70%)	7560 (98%)	150 (2%)	5 (0%)	50	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	z	21	SER
5	a	291	SER
5	a	306	ASN
5	a	289	CYS
22	A	958	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	M	32/299 (11%)	32 (100%)	0	100	100
2	P	95/641 (15%)	95 (100%)	0	100	100
3	Q	119/363 (33%)	118 (99%)	1 (1%)	79	87
4	S	158/274 (58%)	157 (99%)	1 (1%)	84	90
5	a	350/528 (66%)	347 (99%)	3 (1%)	75	85
6	d	158/258 (61%)	157 (99%)	1 (1%)	84	90
7	f	158/259 (61%)	157 (99%)	1 (1%)	84	90
8	g	160/208 (77%)	159 (99%)	1 (1%)	84	90
9	h	128/207 (62%)	127 (99%)	1 (1%)	79	87
10	i	82/144 (57%)	82 (100%)	0	100	100
11	j	134/145 (92%)	134 (100%)	0	100	100
12	k	101/108 (94%)	101 (100%)	0	100	100
13	n	591/1001 (59%)	588 (100%)	3 (0%)	86	91
14	q	482/642 (75%)	480 (100%)	2 (0%)	89	93
15	r	228/280 (81%)	228 (100%)	0	100	100
16	s	75/195 (38%)	75 (100%)	0	100	100
17	t	178/178 (100%)	178 (100%)	0	100	100
18	u	115/132 (87%)	110 (96%)	5 (4%)	25	53
19	v	101/112 (90%)	100 (99%)	1 (1%)	73	84
20	w	97/117 (83%)	97 (100%)	0	100	100
21	z	25/25 (100%)	25 (100%)	0	100	100
22	A	1268/1268 (100%)	1265 (100%)	3 (0%)	92	95
23	B	1018/1061 (96%)	1015 (100%)	3 (0%)	91	94
24	C	239/274 (87%)	239 (100%)	0	100	100
25	D	150/200 (75%)	150 (100%)	0	100	100
26	E	197/197 (100%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	F	76/137 (56%)	76 (100%)	0	100	100
28	G	152/152 (100%)	151 (99%)	1 (1%)	81	88
29	H	124/128 (97%)	124 (100%)	0	100	100
30	I	110/116 (95%)	110 (100%)	0	100	100
31	J	65/65 (100%)	65 (100%)	0	100	100
32	K	99/102 (97%)	99 (100%)	0	100	100
33	L	38/57 (67%)	38 (100%)	0	100	100
All	All	7103/9873 (72%)	7076 (100%)	27 (0%)	88	93

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	u	1	MET
18	u	120	ARG
23	B	327	ARG
18	u	100	LYS
18	u	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
22	A	471	ASN
22	A	1211	GLN
28	G	131	GLN
28	G	122	ASN
9	h	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	q	1
18	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	318:ASN	C	319:LYS	N	5.82
1	u	80:LEU	C	81:PRO	N	3.18

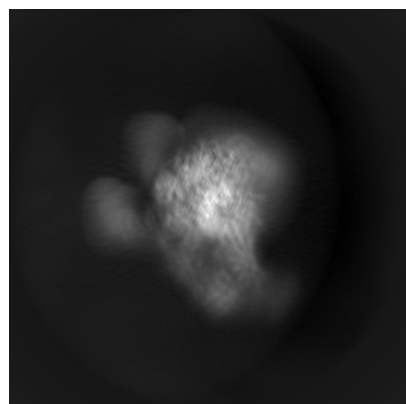
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26542. These allow visual inspection of the internal detail of the map and identification of artifacts.

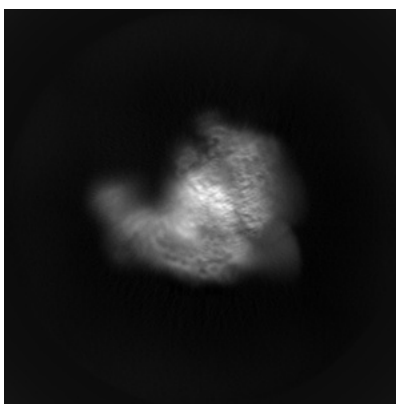
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

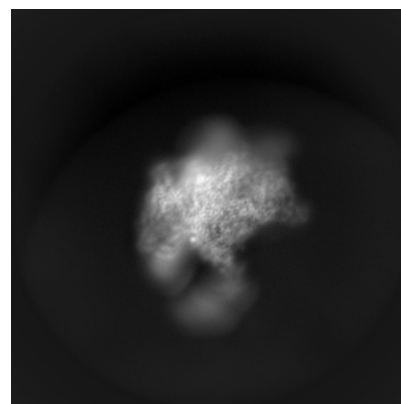
6.1.1 Primary map



X

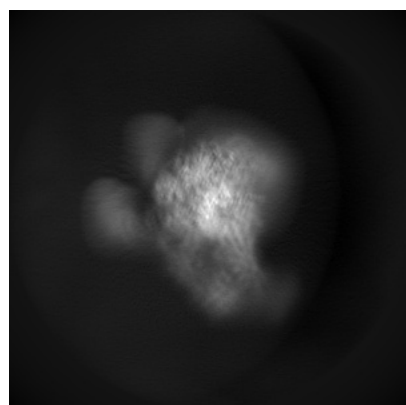


Y

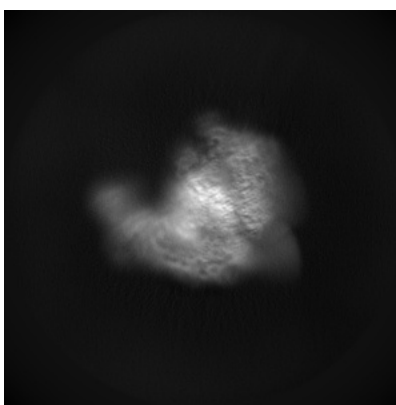


Z

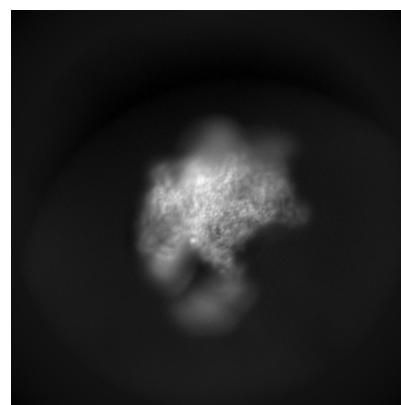
6.1.2 Raw map



X



Y

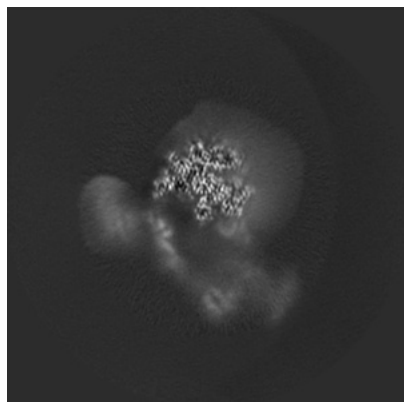


Z

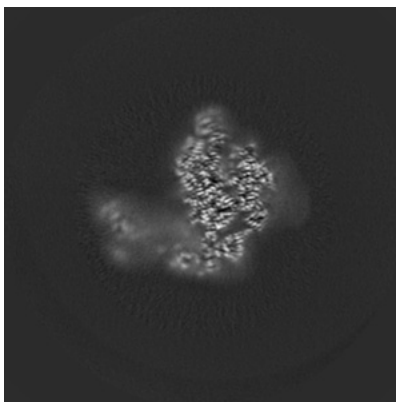
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

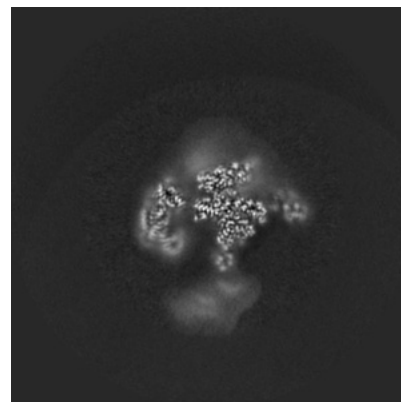
6.2.1 Primary map



X Index: 180

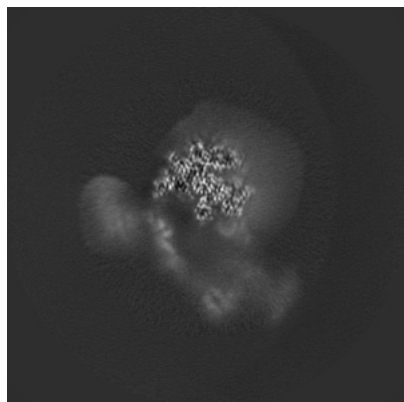


Y Index: 180

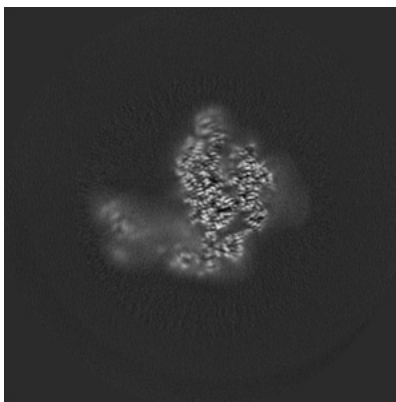


Z Index: 180

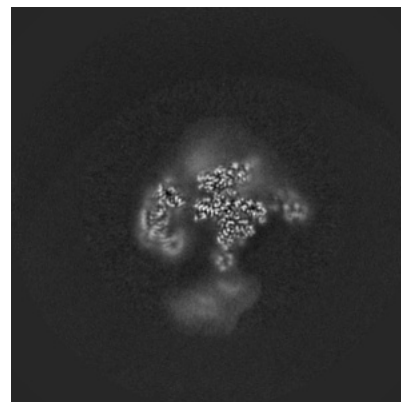
6.2.2 Raw map



X Index: 180



Y Index: 180

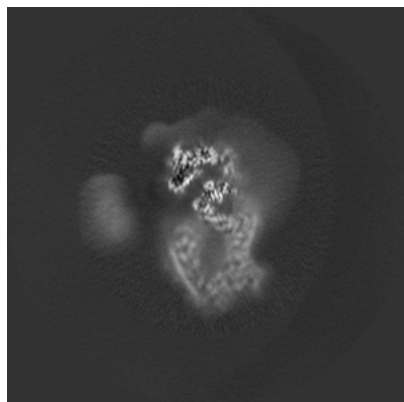


Z Index: 180

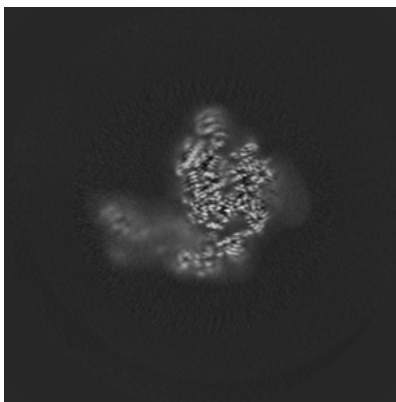
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

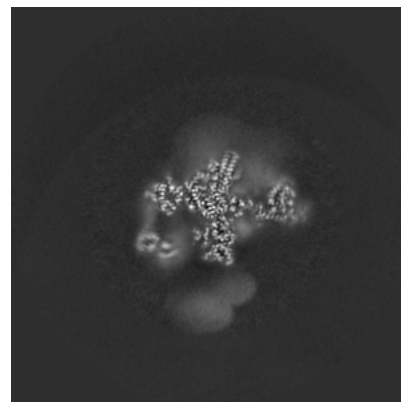
6.3.1 Primary map



X Index: 166

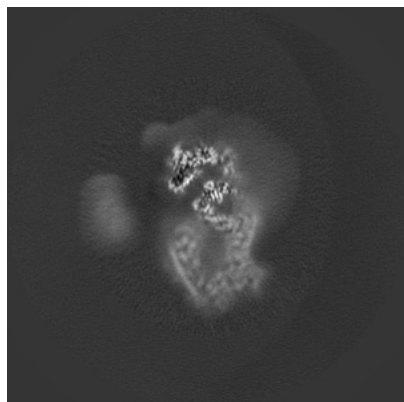


Y Index: 178

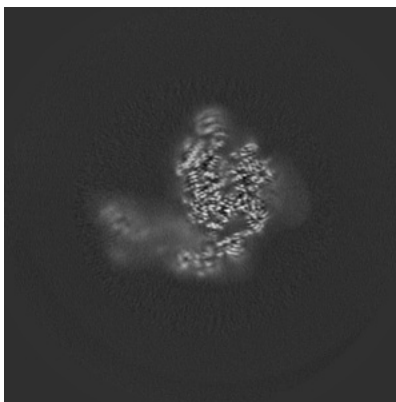


Z Index: 193

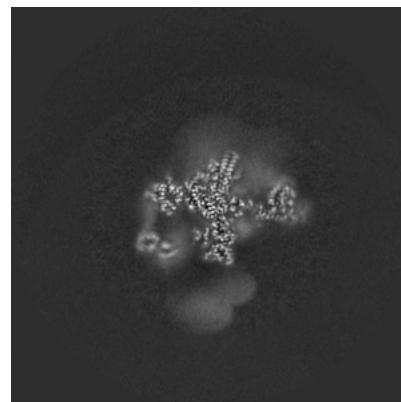
6.3.2 Raw map



X Index: 166



Y Index: 178

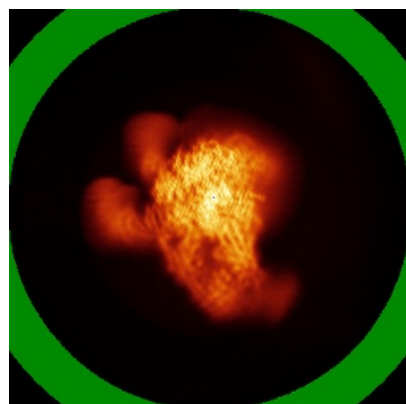


Z Index: 193

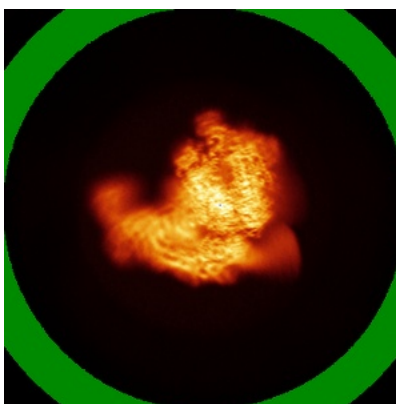
The images above show the largest variance slices of the map in three orthogonal directions.

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

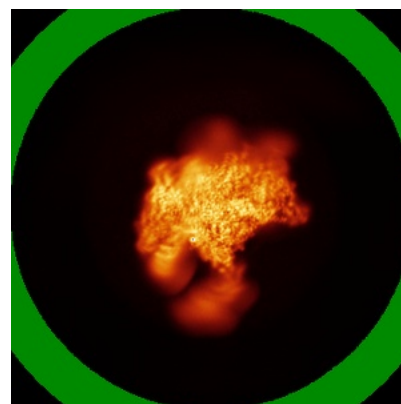
6.4.1 Primary map



X

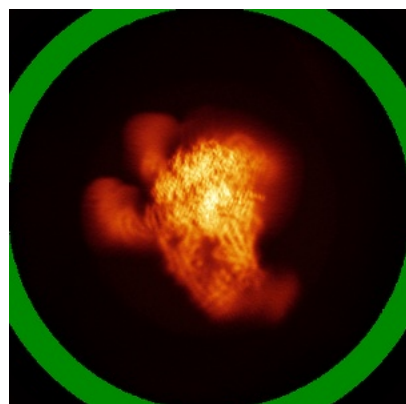


Y

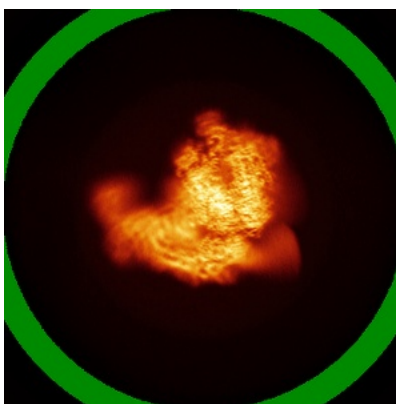


Z

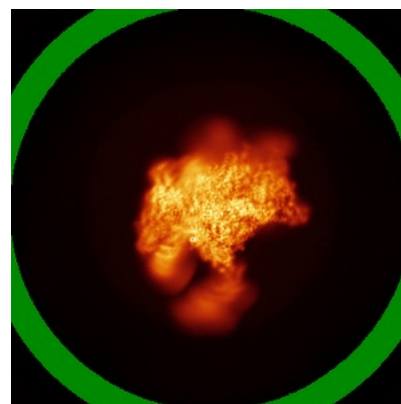
6.4.2 Raw map



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 0.0125. 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.

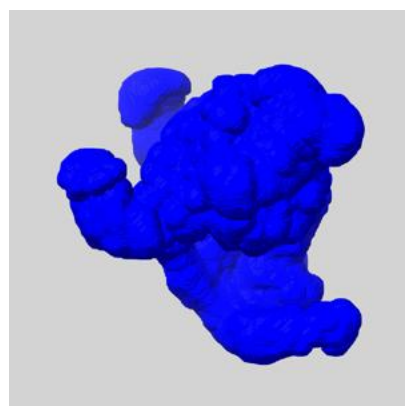
6.6 Mask visualisation [i](#)

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

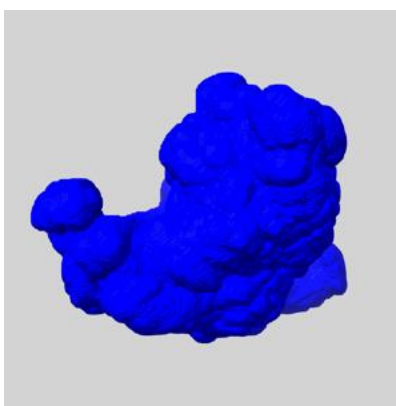
A mask typically either:

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

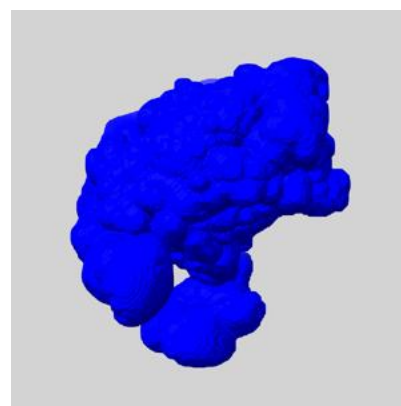
6.6.1 emd_26542_msk_1.map [i](#)



X



Y

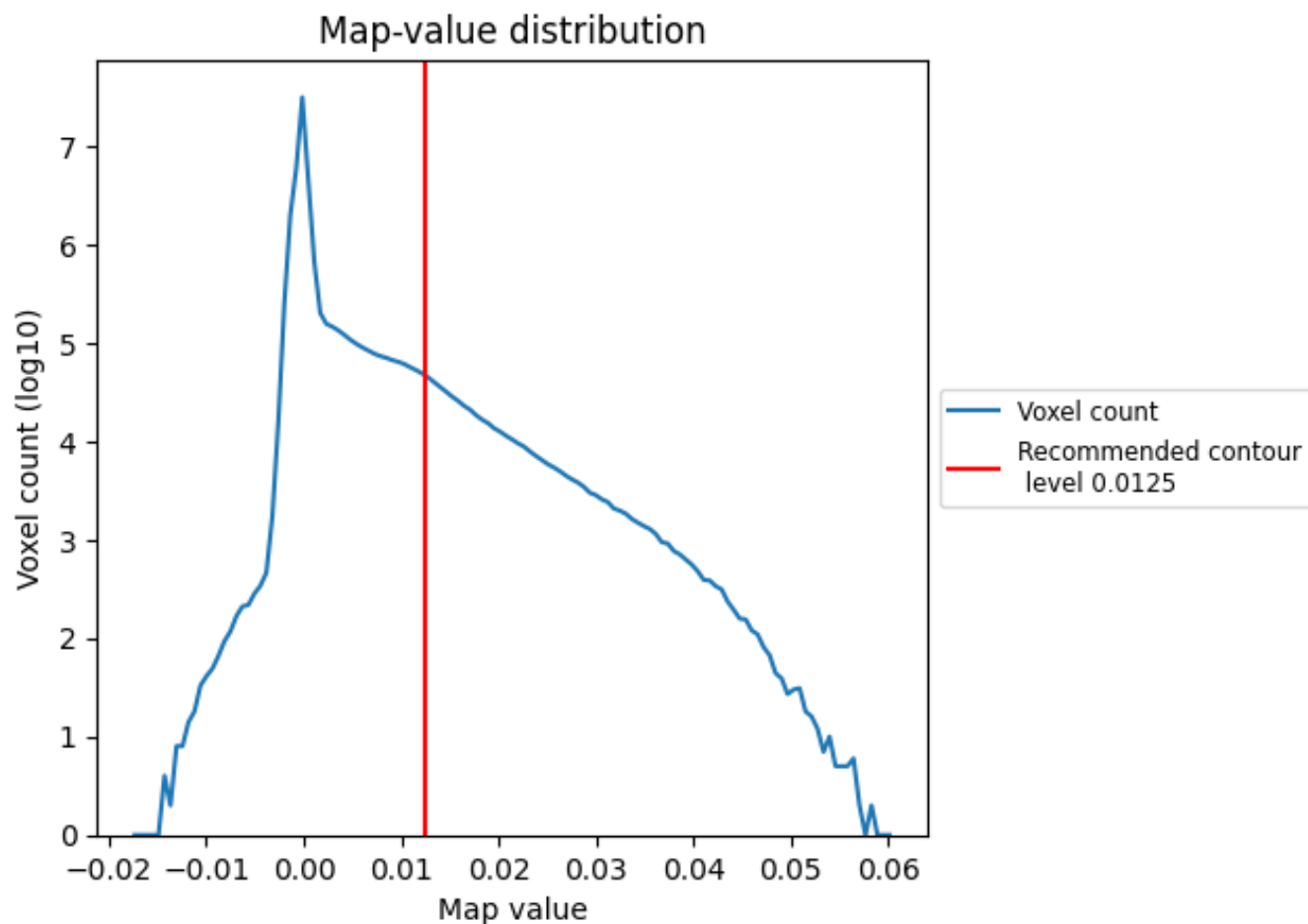


Z

7 Map analysis [i](#)

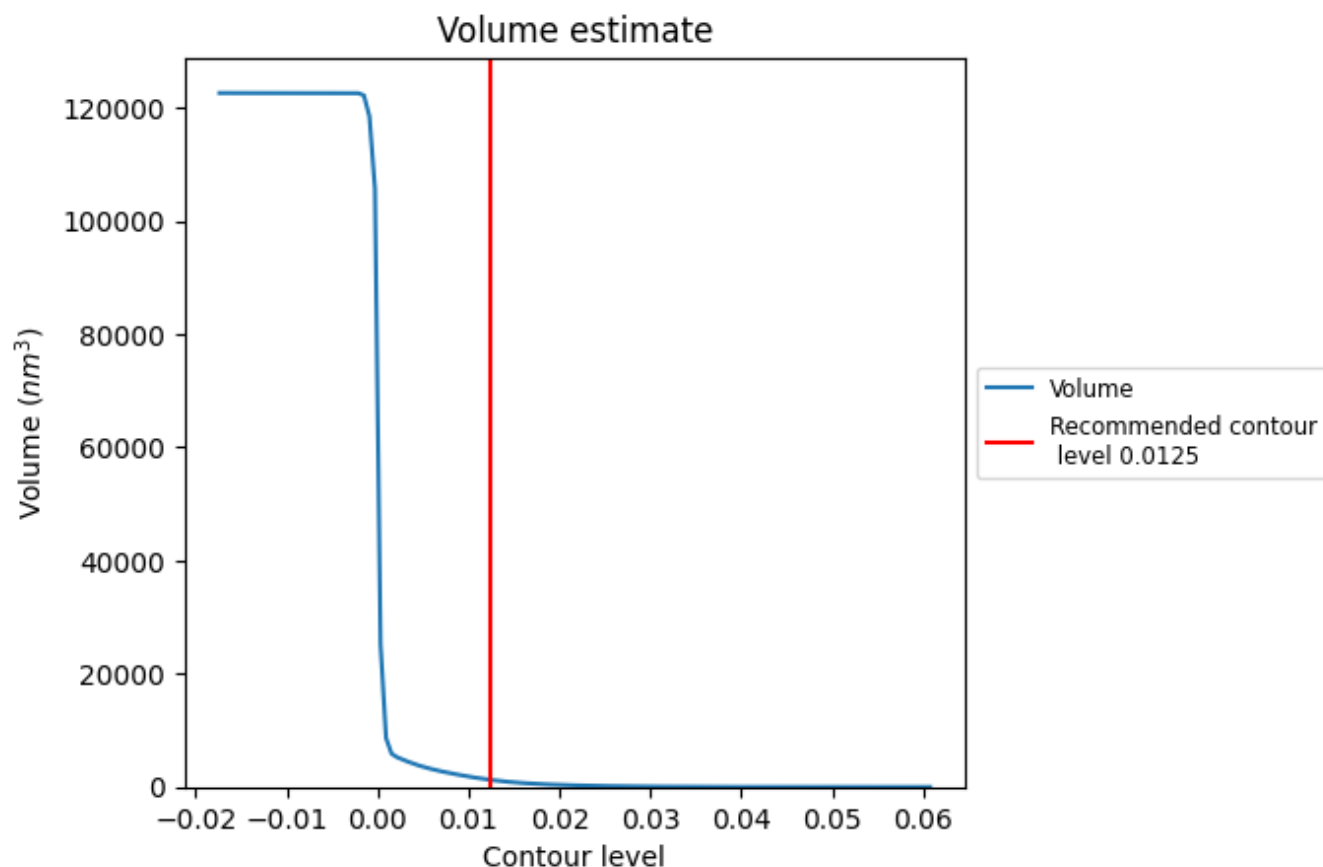
This section contains the results of statistical analysis of the map.

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.

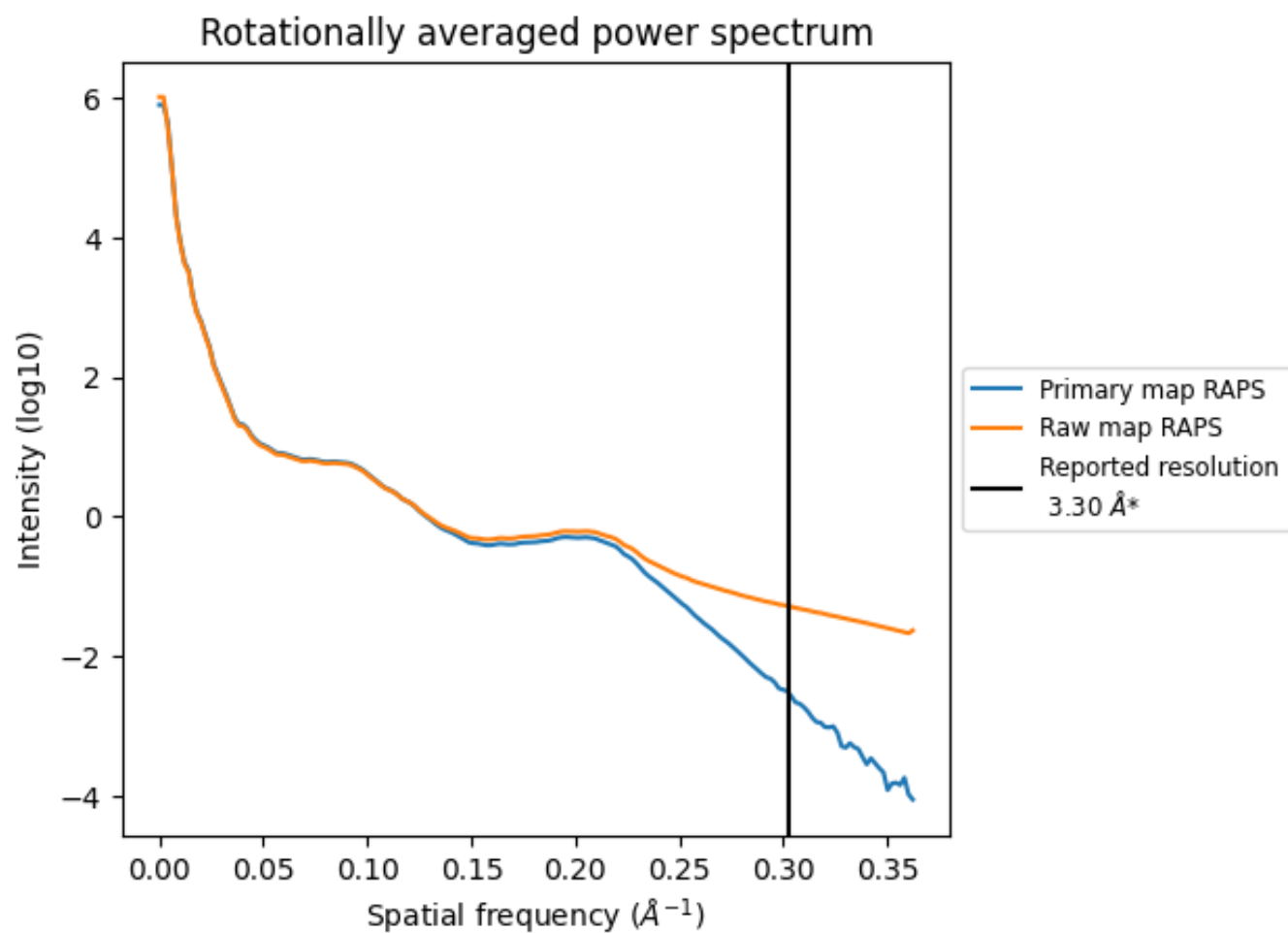
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1241 nm³; this corresponds to an approximate mass of 1121 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 ⓘ

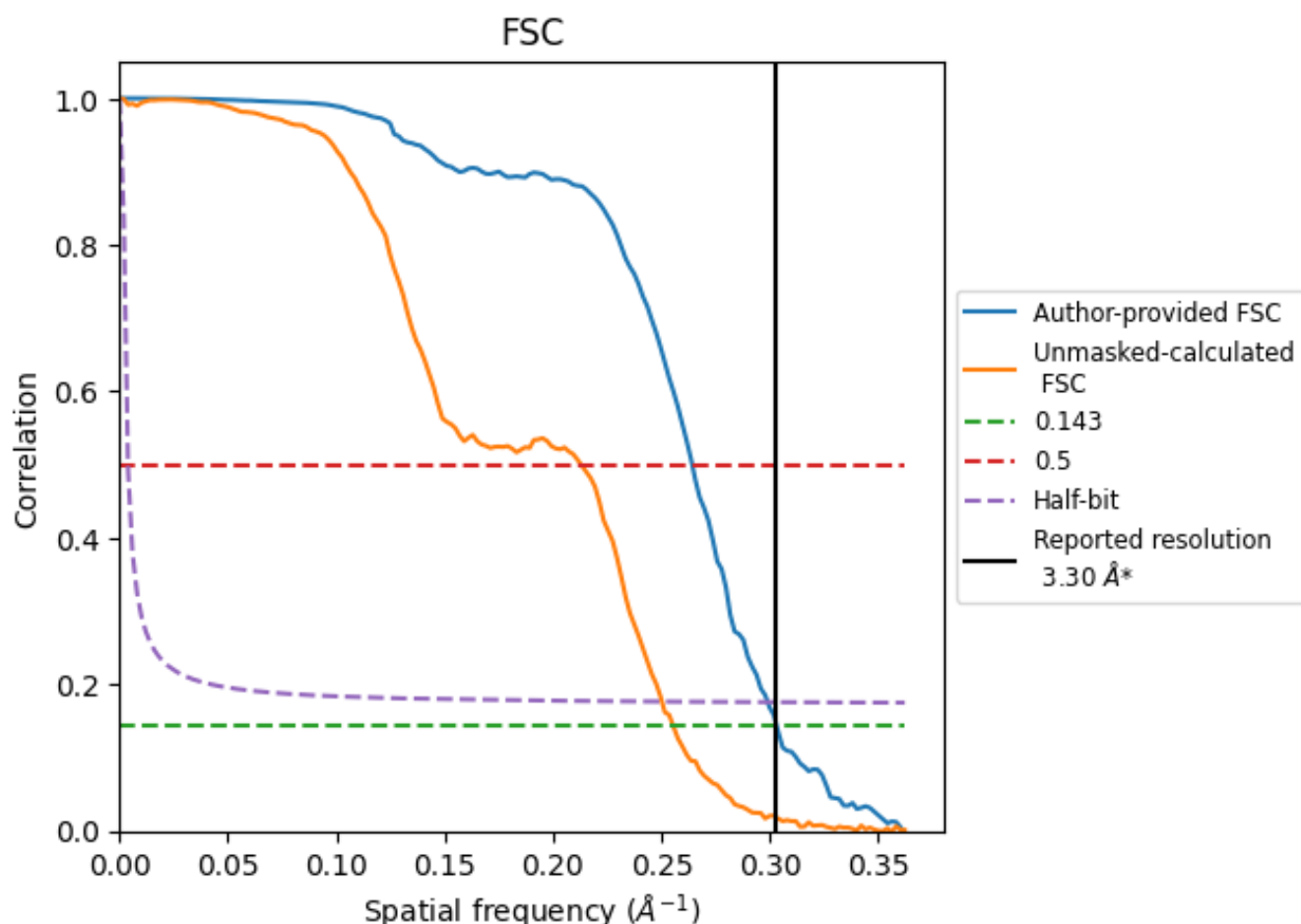


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

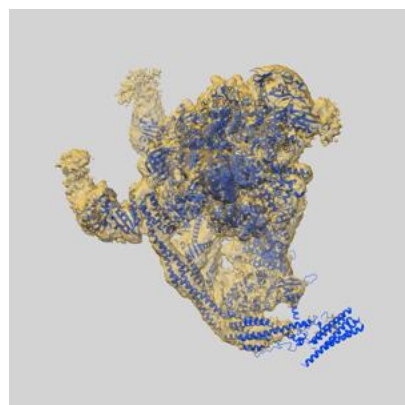
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.79	3.34
Unmasked-calculated*	3.91	4.70	4.00

*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 3.91 differs from the reported value 3.3 by more than 10 %

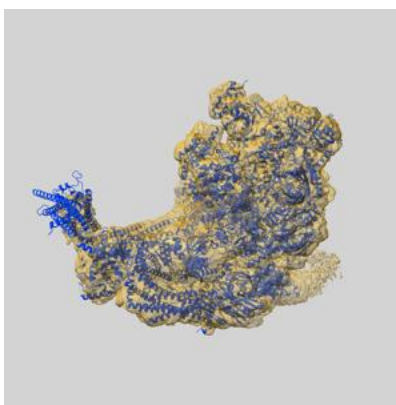
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26542 and PDB model 7UI9. Per-residue inclusion information can be found in section 3 on page 9.

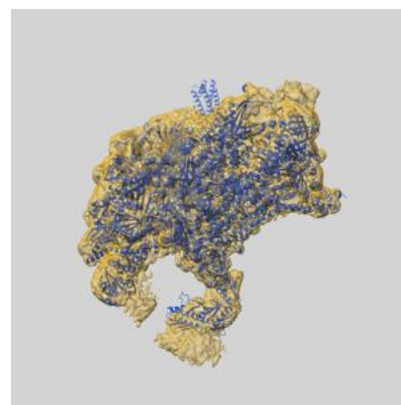
9.1 Map-model overlay [i](#)



X



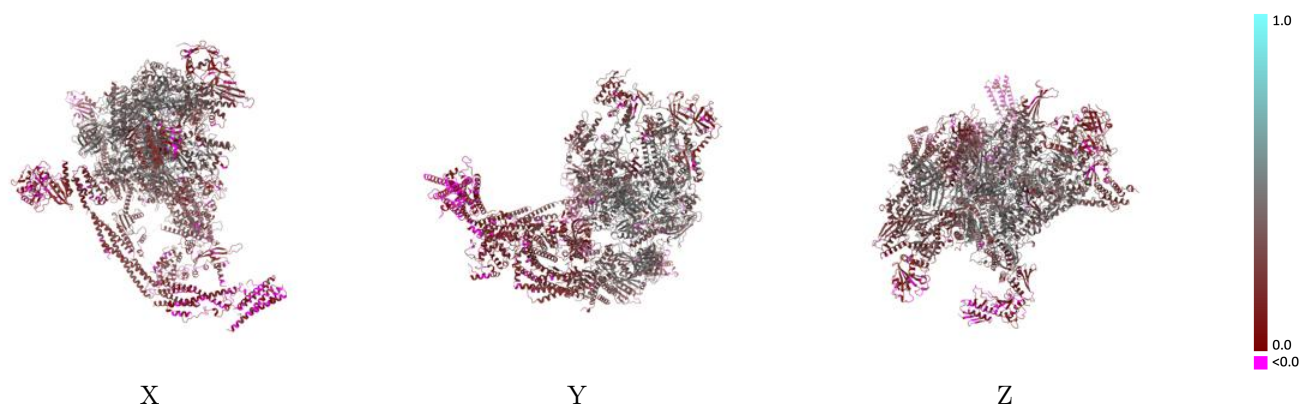
Y



Z

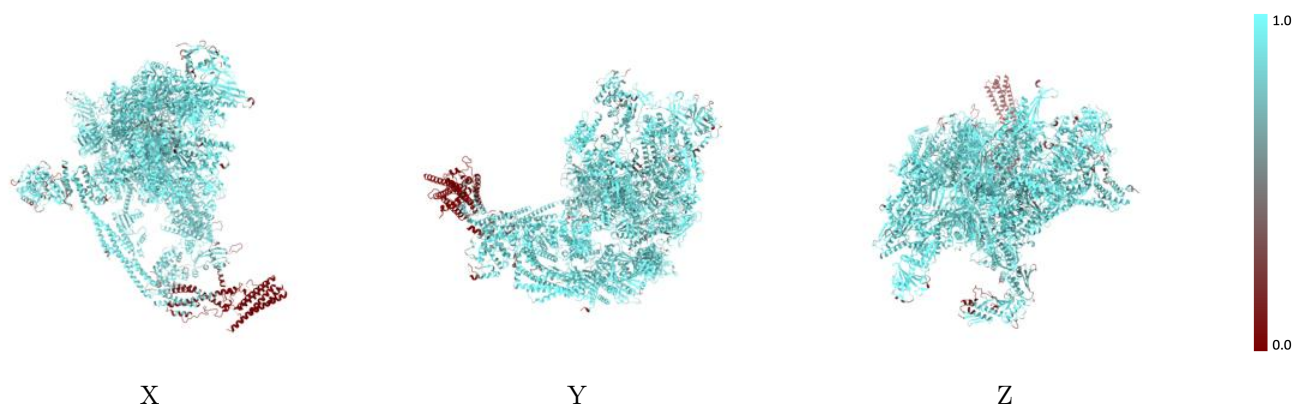
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



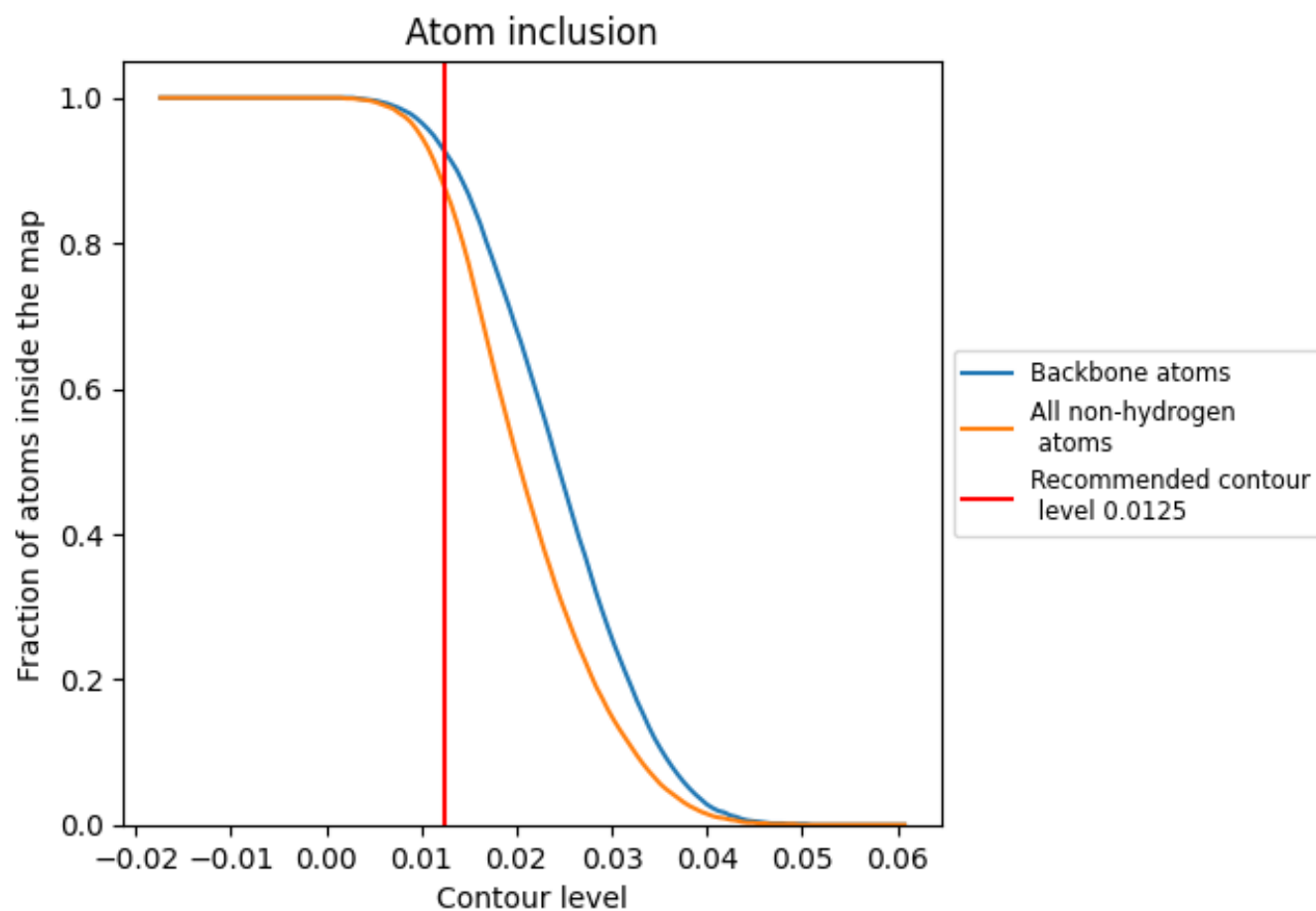
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.2940
A	 0.9300	 0.3960
B	 0.9450	 0.3960
C	 0.9390	 0.4190
D	 0.9840	 0.1810
E	 0.9660	 0.3800
F	 0.9350	 0.4230
G	 0.9730	 0.2730
H	 0.8940	 0.4240
I	 0.9190	 0.3600
J	 0.9090	 0.3550
K	 0.9260	 0.4140
L	 0.8400	 0.3210
M	 0.9730	 0.4370
P	 0.8710	 0.2170
Q	 0.7460	 0.1730
S	 0.8020	 0.2400
a	 0.7470	 0.1030
d	 0.8760	 0.1560
f	 0.7750	 0.1640
g	 0.7730	 0.1470
h	 0.9840	 0.2170
i	 0.8920	 0.1800
j	 0.1590	 0.0540
k	 0.9480	 0.2530
n	 0.8220	 0.1790
q	 0.9320	 0.2370
r	 0.9400	 0.4050
s	 0.0230	 0.0530
t	 0.9430	 0.4020
u	 0.6940	 0.1490
v	 0.9220	 0.2140
w	 0.9330	 0.1760
z	 0.9560	 0.1970

