



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 09:04 pm GMT

PDB ID : 6GYM
EMDB ID : EMD-0092
Title : Structure of a yeast closed complex with distorted DNA (CCdist)
Authors : Dienemann, C.; Schwalb, B.; Schilbach, S.; Cramer, P.
Deposited on : 2018-06-30
Resolution : 6.70 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 : 1.8.4, CSD as541be (2020)
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

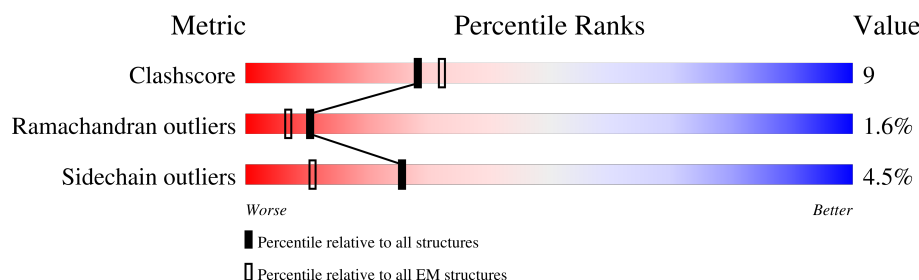
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








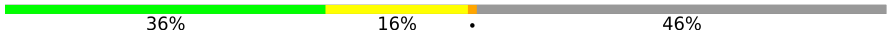





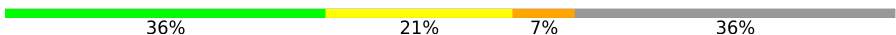




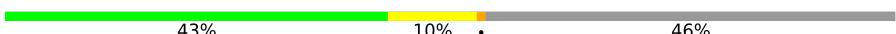




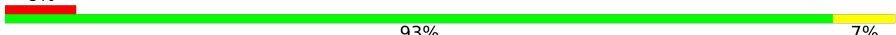
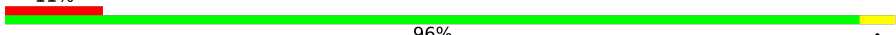
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	778	<div> <div>11%</div> <div>76%</div> <div>13%</div> <div>10%</div> </div>
2	1	641	<div> <div>15%</div> <div>70%</div> <div>6%</div> <div>23%</div> </div>
3	2	462	<div> <div>23%</div> <div>83%</div> <div>15%</div> </div>
4	3	321	<div> <div>5%</div> <div>37%</div> <div>6%</div> <div>57%</div> </div>
5	4	338	<div> <div>6%</div> <div>84%</div> <div>12%</div> </div>
6	5	72	<div> <div>54%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>
7	6	461	<div> <div>61%</div> <div>11%</div> <div>27%</div> </div>
8	7	843	<div> <div>36%</div> <div>12%</div> <div>52%</div> </div>

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Mol	Chain	Length	Quality of chain
9	A	1733	
10	B	1224	
11	C	318	
12	D	221	
13	E	215	
14	F	155	
15	G	171	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	345	
22	O	240	
23	Q	735	
24	R	400	
25	U	171	
26	V	122	
27	W	332	
28	X	328	
29	Z	43	
30	N	75	
31	T	75	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 63012 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 General transcription and DNA repair factor IIIH helicase subunit XPD,General transcription and DNA repair factor IIIH helicase subunit XPD,DNA repair helicase RAD3,DNA repair helicase RAD3,General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	698	Total	C	N	O	S	0	0
			4844	3051	856	907	30		

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	491	Total	C	N	O	S	0	0
			3060	1893	570	590	7		

- Molecule 3 is a protein called General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	395	Total	C	N	O	0	0
			2160	1317	413	430		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4,General transcription and DNA repair factor IIH subunit TFB4,RNA polymerase II transcription factor B subunit 4,General transcription and DNA repair factor IIH subunit TFB4,General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	297	Total	C	N	O	S	0	0
			1474	876	297	297	4		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1,General transcription and DNA repair factor IIH subunit SSL1,General transcription and DNA repair factor IIH subunit SSL1,General transcription and DNA repair factor IIH subunit SSL1,General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	335	Total	C	N	O	S	0	0
			2197	1355	399	422	21		

- [illegible]

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	408	Total	C	N	O	S	0	0
			3148	2000	557	572	19		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1152	Total	C	N	O	S	0	0
			9178	5807	1608	1708	55		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 22 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 23 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 24 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 25 is a protein called Transcription initiation factor IIA large subunit,Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 26 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 27 is a protein called Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	258	Total	C	N	O	S	0	0
			1825	1147	321	351	6		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	160	Total	C	N	O	S	0	0
			1004	620	184	196	4		

- Molecule 29 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Z	43	Total	C	N	O	0	0
			215	129	43	43		

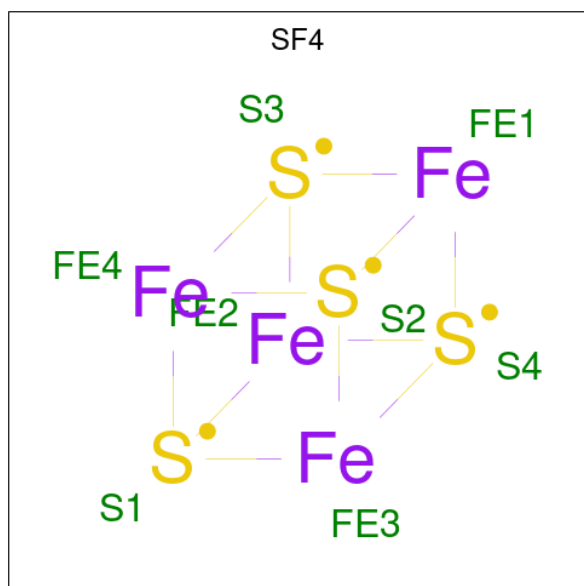
- Molecule 30 is a DNA chain called non-template DNA (HIS4).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	75	Total	C	N	O	P	0	0
			1531	736	281	439	75		

- Molecule 31 is a DNA chain called Template DNA (HIS4).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	75	Total	C	N	O	P	0	0
			1524	735	273	441	75		

- Molecule 32 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
32	0	1	Total	Fe	S	0
			8	4	4	

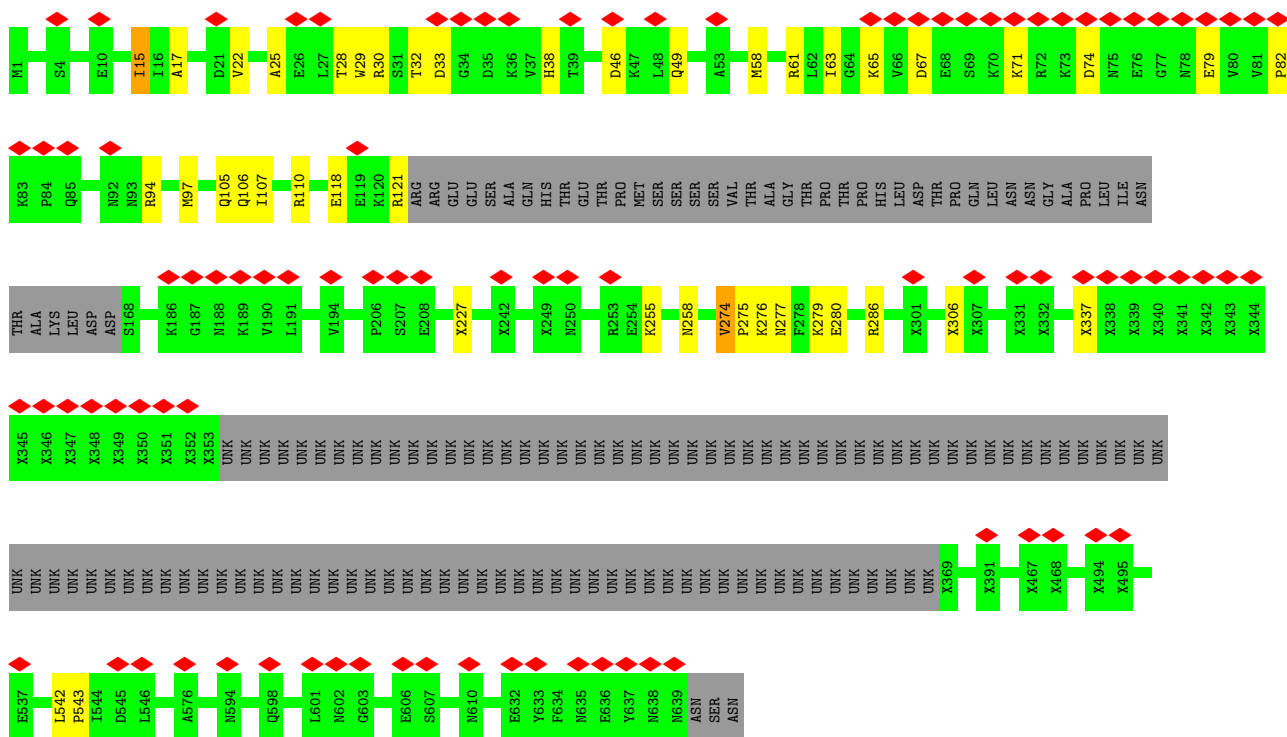
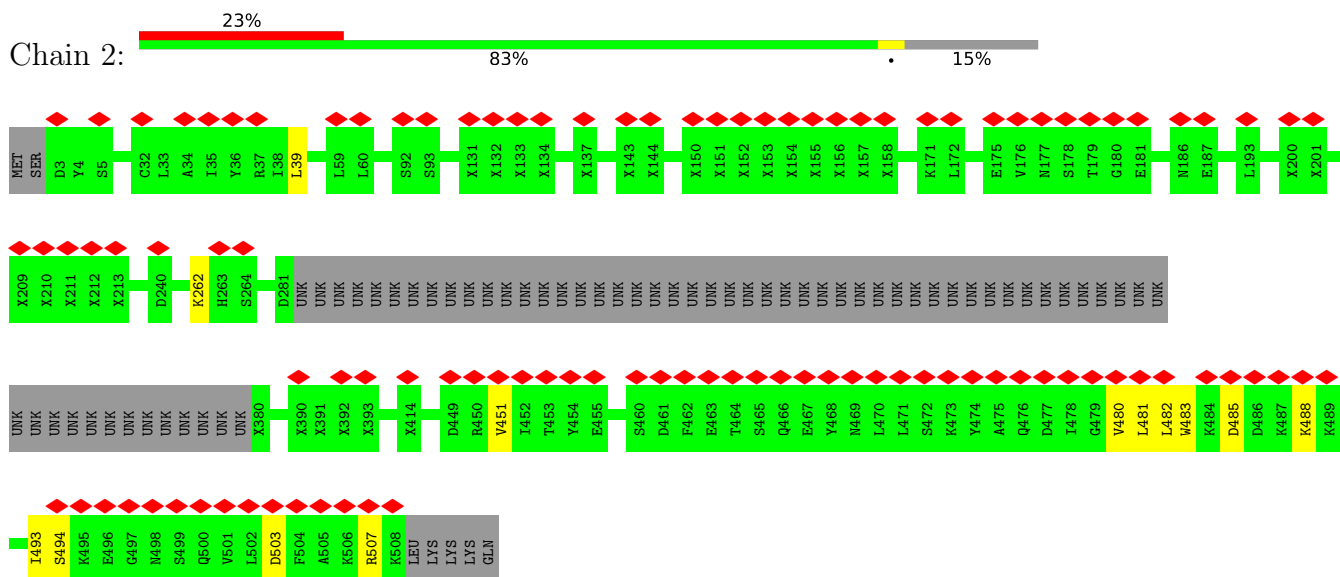
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	3	2	Total 2	Zn 2	0
33	4	1	Total 1	Zn 1	0
33	6	3	Total 3	Zn 3	0
33	A	2	Total 2	Zn 2	0
33	B	1	Total 1	Zn 1	0
33	C	1	Total 1	Zn 1	0
33	I	2	Total 2	Zn 2	0
33	J	1	Total 1	Zn 1	0
33	L	1	Total 1	Zn 1	0
33	M	1	Total 1	Zn 1	0
33	W	1	Total 1	Zn 1	0

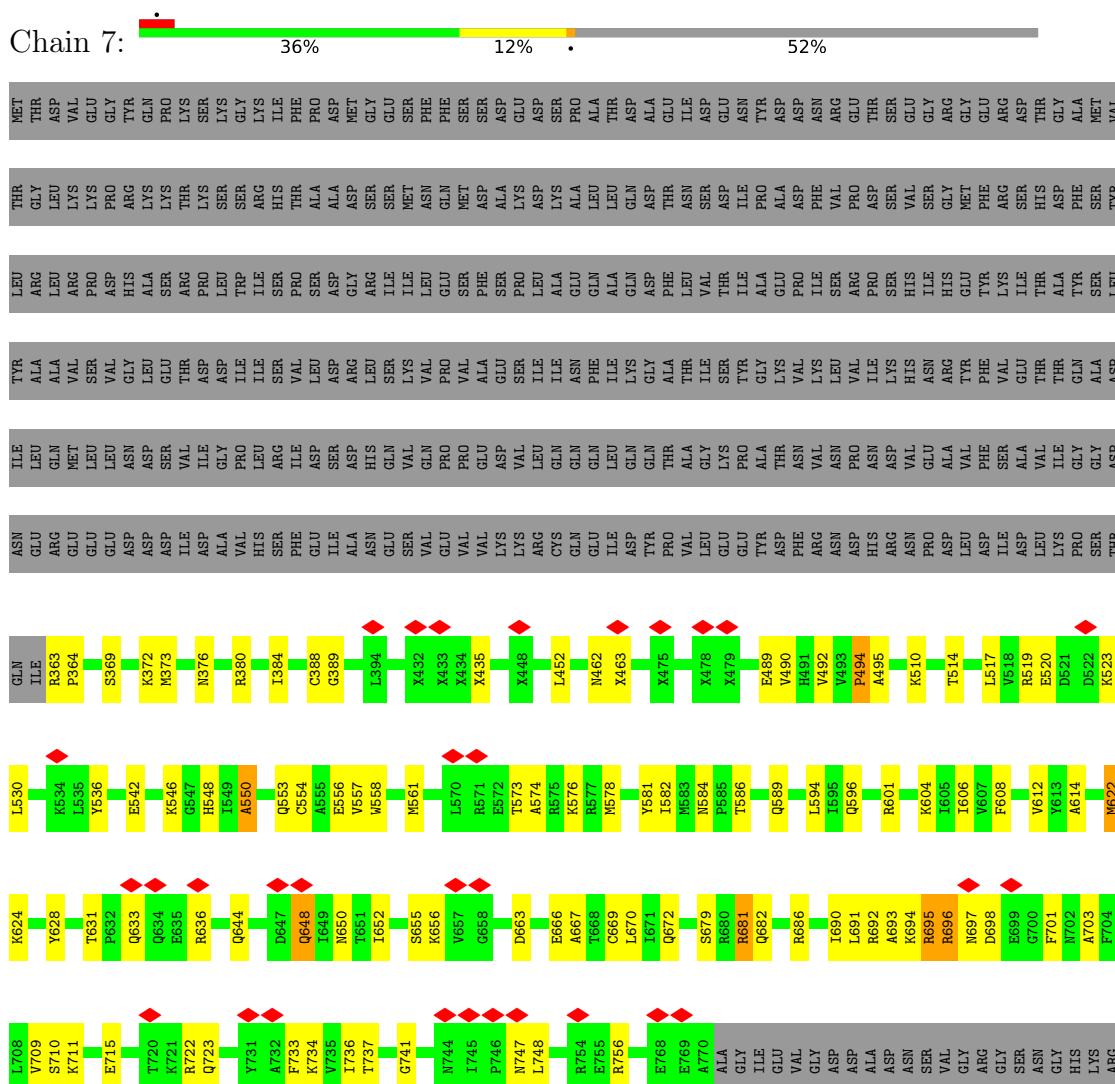
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Chain 1:  15% 70% 6% 9%

[illegible]

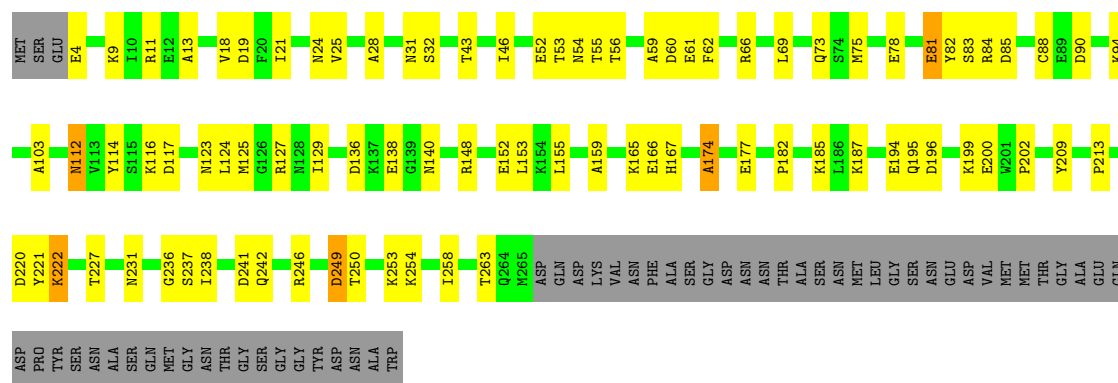
- Molecule 4: RNA polymerase II transcription factor B subunit 3



Chain A: 59% 20% • 19%

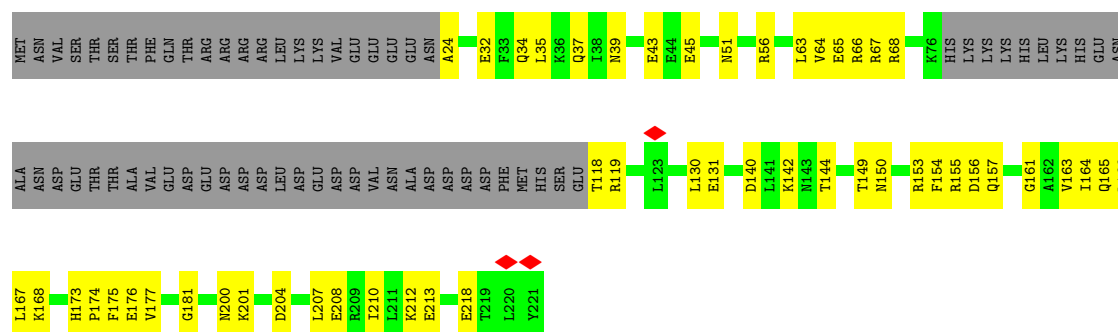


Chain C:  55% 26% 18%



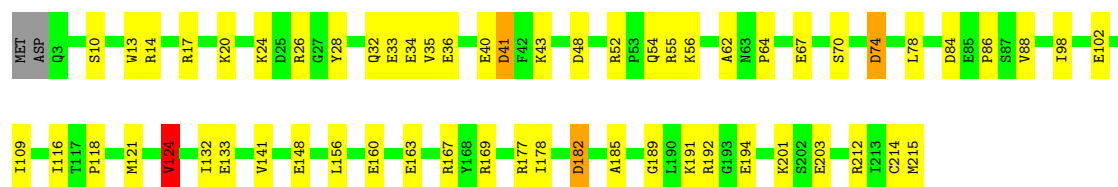
- Molecule 12: DNA-directed RNA polymerase II subunit RPB4

Chain D:  48% 24% 29%

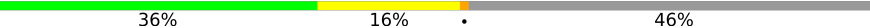


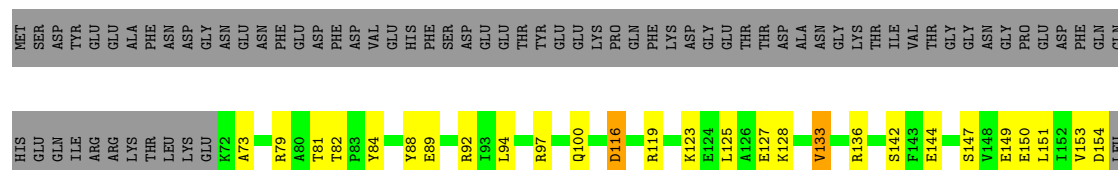
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  72% 26% ..

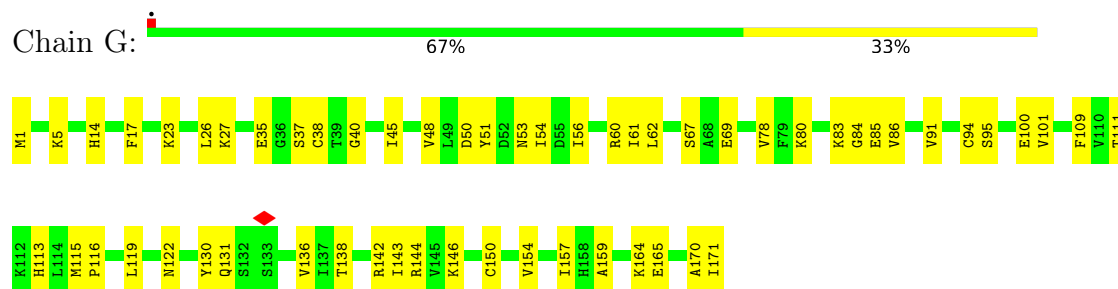


- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

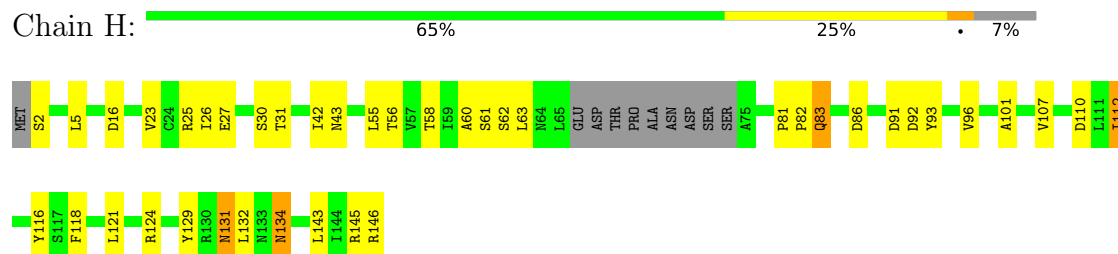
Chain F:  36% 16% 46%



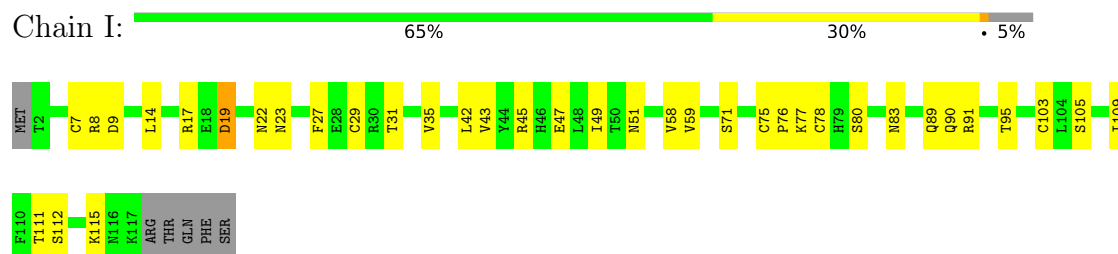
- Molecule 15: DNA-directed RNA polymerase II subunit RPB7



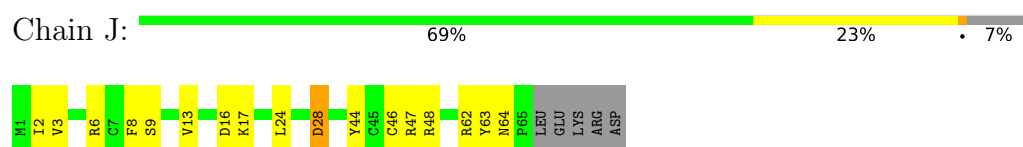
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

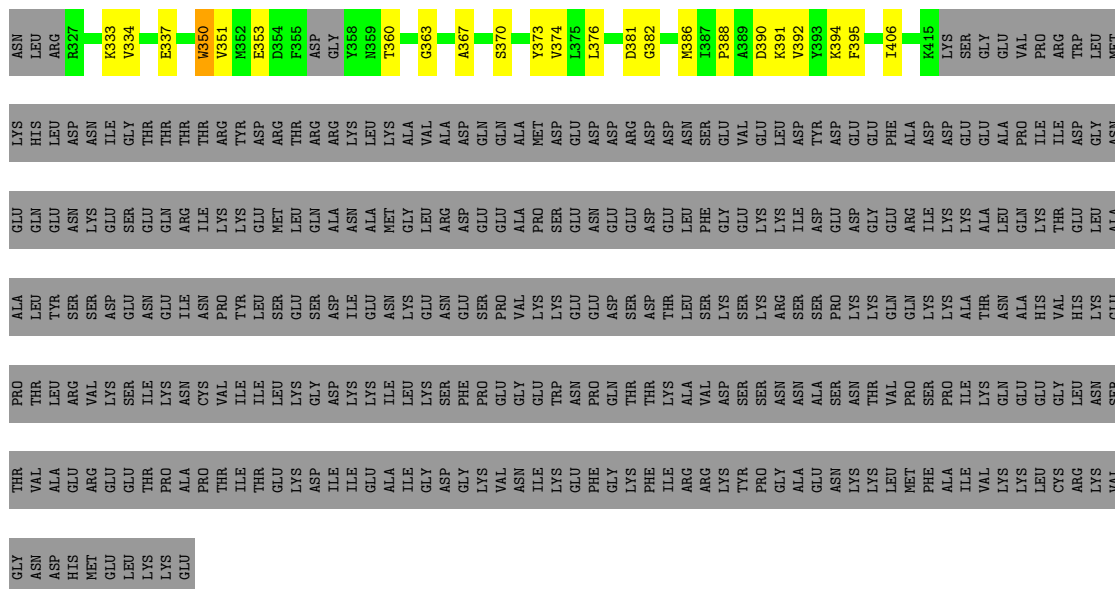


- Molecule 17: DNA-directed RNA polymerase II subunit RPB9

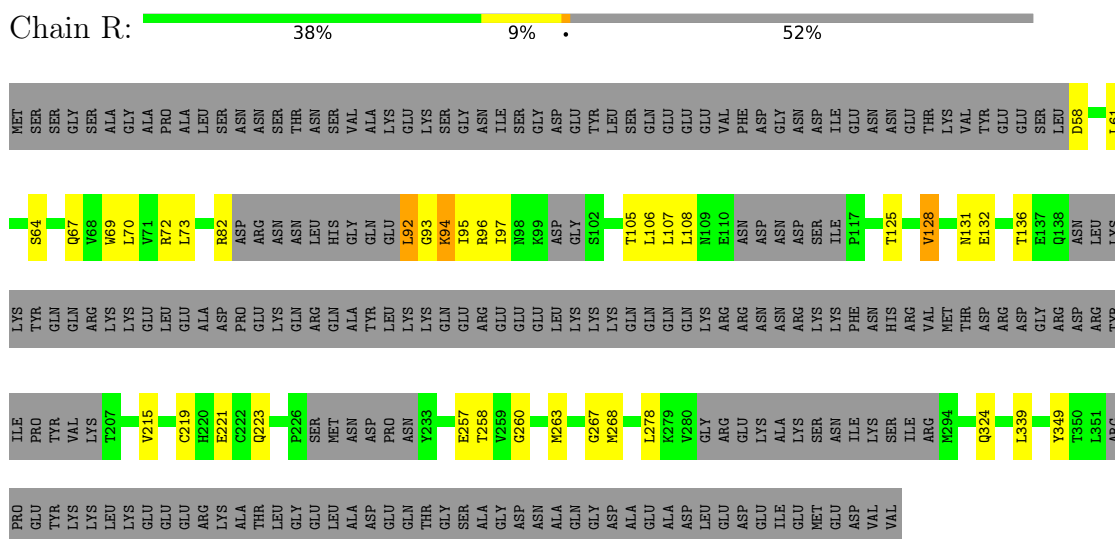


- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

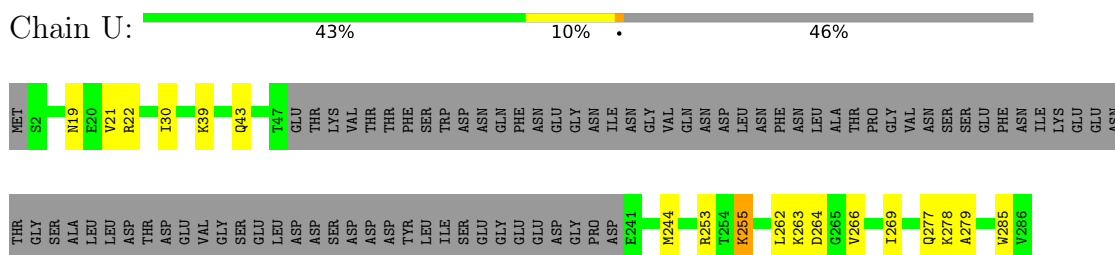




- Molecule 24: Transcription initiation factor IIF subunit beta

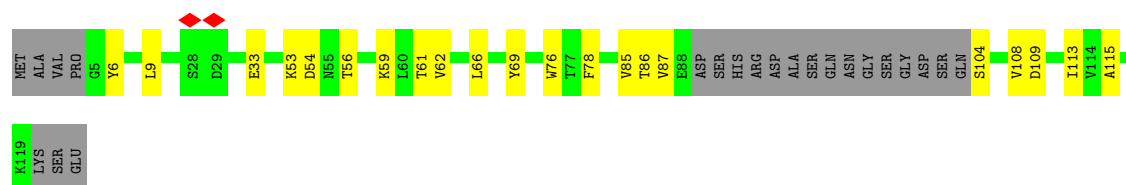


● Molecule 25: Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit

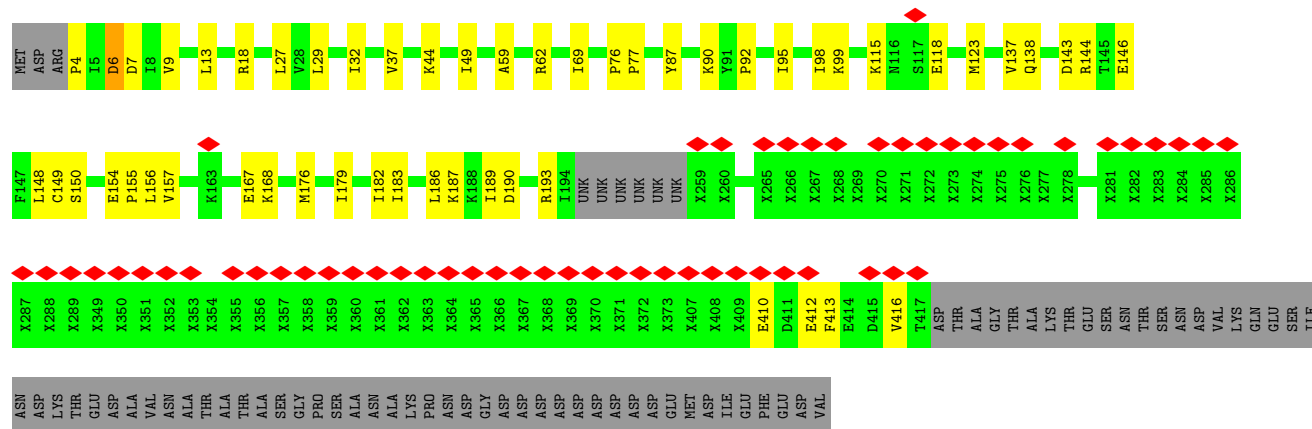


- Molecule 26: Transcription initiation factor IIA subunit 2

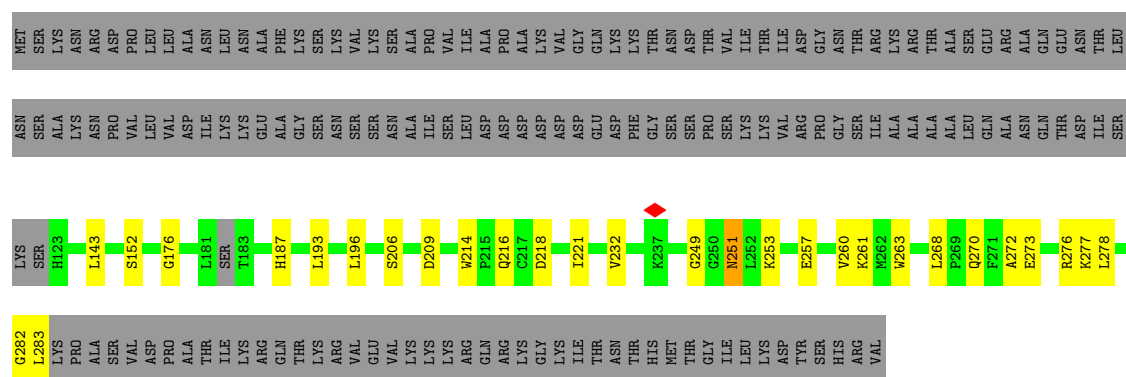




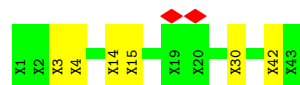
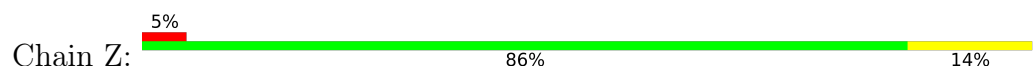
- Molecule 27: Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha,Transcription initiation factor IIE subunit alpha



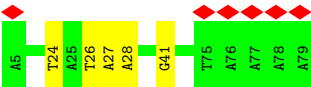
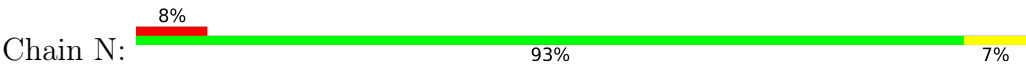
- Molecule 28: Transcription initiation factor IIE subunit beta



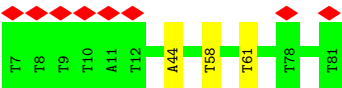
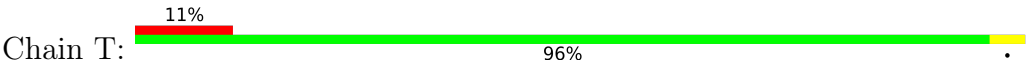
- Molecule 29: Unknown protein



- Molecule 30: non-template DNA (HIS4)



• Molecule 31: Template DNA (HIS4)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0057	Depositor
Map size (Å)	479.5, 479.5, 479.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: SF4, 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	0	0.25	0/4739	0.42	0/6431
2	1	0.25	0/2238	0.40	0/3039
3	2	0.24	0/1631	0.39	0/2243
4	3	0.25	0/870	0.43	0/1190
5	4	0.25	0/1367	0.51	2/1900 (0.1%)
6	5	0.23	0/502	0.46	0/677
7	6	0.24	0/1996	0.42	0/2713
8	7	0.24	0/2980	0.40	0/4019
9	A	0.27	0/11192	0.44	0/15128
10	B	0.28	0/9357	0.44	0/12618
11	C	0.28	0/2099	0.43	0/2845
12	D	0.24	0/1262	0.39	0/1693
13	E	0.29	1/1780 (0.1%)	0.41	0/2395
14	F	0.29	0/682	0.43	0/922
15	G	0.27	0/1368	0.46	0/1844
16	H	0.28	0/1107	0.47	0/1499
17	I	0.27	0/962	0.46	0/1295
18	J	0.30	0/541	0.47	0/727
19	K	0.27	0/922	0.42	0/1244
20	L	0.27	0/360	0.51	0/478
21	M	0.26	0/2204	0.46	0/2963
22	O	0.28	0/1443	0.46	0/1942
23	Q	0.26	0/1168	0.44	0/1579
24	R	0.25	0/1312	0.44	0/1777
25	U	0.26	0/766	0.46	0/1032
26	V	0.26	0/789	0.44	0/1066
27	W	0.26	0/1551	0.42	0/2096
28	X	0.25	0/1014	0.44	0/1388
30	N	0.54	0/1719	0.92	0/2638
31	T	0.57	0/1709	0.92	0/2621
All	All	0.29	1/61630 (0.0%)	0.48	2/84002 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	124	VAL	C-N	5.04	1.43	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	260	PRO	N-CA-CB	6.07	110.59	103.30
5	4	265	PRO	N-CA-CB	5.94	110.43	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4844	0	4244	59	0
2	1	3060	0	2056	24	0
3	2	2160	0	1075	6	0
4	3	860	0	623	13	0
5	4	1474	0	641	2	0
6	5	498	0	506	6	0
7	6	2197	0	1740	29	0
8	7	3148	0	2999	61	0
9	A	10997	0	11083	246	0
10	B	9178	0	9196	213	0
11	C	2061	0	2030	64	0
12	D	1253	0	1275	31	0
13	E	1744	0	1772	38	0
14	F	670	0	690	17	0
15	G	1340	0	1357	38	0
16	H	1089	0	1062	27	0
17	I	944	0	900	18	0
18	J	532	0	543	14	0
19	K	904	0	911	24	0
20	L	358	0	381	19	0
21	M	2175	0	2286	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	1416	0	1493	33	0
23	Q	1144	0	1034	27	0
24	R	1303	0	1110	31	0
25	U	757	0	747	15	0
26	V	782	0	790	11	0
27	W	1825	0	1545	38	0
28	X	1004	0	731	18	0
29	Z	215	0	47	3	0
30	N	1531	0	848	4	0
31	T	1524	0	850	5	0
32	0	8	0	0	1	0
33	3	2	0	0	0	0
33	4	1	0	0	0	0
33	6	3	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	I	2	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	W	1	0	0	0	0
34	A	1	0	0	0	0
All	All	63012	0	56565	1045	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1045 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:875:GLU:OE2	10:B:934:LYS:NZ	1.91	1.02
14:F:123:LYS:NZ	14:F:127:GLU:OE2	1.95	0.98
13:E:56:LYS:NZ	13:E:84:ASP:OD2	1.97	0.95
18:J:13:VAL:O	18:J:17:LYS:NZ	2.05	0.90
9:A:362:ASP:OD2	9:A:459:ARG:NH1	2.05	0.88

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	659/778 (85%)	578 (88%)	71 (11%)	10 (2%)	8	40
2	1	316/641 (49%)	293 (93%)	16 (5%)	7 (2%)	5	29
3	2	284/462 (62%)	263 (93%)	18 (6%)	3 (1%)	12	47
4	3	136/321 (42%)	114 (84%)	20 (15%)	2 (2%)	8	40
5	4	274/338 (81%)	244 (89%)	23 (8%)	7 (3%)	4	25
6	5	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	8	38
7	6	289/461 (63%)	257 (89%)	27 (9%)	5 (2%)	7	37
8	7	361/843 (43%)	330 (91%)	23 (6%)	8 (2%)	5	29
9	A	1386/1733 (80%)	1253 (90%)	112 (8%)	21 (2%)	8	40
10	B	1136/1224 (93%)	1034 (91%)	87 (8%)	15 (1%)	10	43
11	C	260/318 (82%)	235 (90%)	21 (8%)	4 (2%)	8	40
12	D	153/221 (69%)	143 (94%)	9 (6%)	1 (1%)	19	57
13	E	211/215 (98%)	194 (92%)	15 (7%)	2 (1%)	14	51
14	F	81/155 (52%)	71 (88%)	9 (11%)	1 (1%)	11	44
15	G	169/171 (99%)	148 (88%)	20 (12%)	1 (1%)	22	60
16	H	132/146 (90%)	110 (83%)	21 (16%)	1 (1%)	16	55
17	I	114/122 (93%)	91 (80%)	20 (18%)	3 (3%)	4	25
18	J	63/70 (90%)	55 (87%)	7 (11%)	1 (2%)	8	38
19	K	110/120 (92%)	105 (96%)	5 (4%)	0	100	100
20	L	43/70 (61%)	36 (84%)	4 (9%)	3 (7%)	1	11
21	M	273/345 (79%)	238 (87%)	25 (9%)	10 (4%)	2	20
22	O	178/240 (74%)	165 (93%)	12 (7%)	1 (1%)	22	60
23	Q	140/735 (19%)	124 (89%)	12 (9%)	4 (3%)	3	23
24	R	176/400 (44%)	150 (85%)	24 (14%)	2 (1%)	12	47
25	U	88/171 (52%)	81 (92%)	5 (6%)	2 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	V	96/122 (79%)	94 (98%)	1 (1%)	1 (1%)	13	49
27	W	196/332 (59%)	181 (92%)	12 (6%)	3 (2%)	8	40
28	X	158/328 (48%)	127 (80%)	26 (16%)	5 (3%)	3	21
All	All	7546/11154 (68%)	6771 (90%)	651 (9%)	124 (2%)	10	38

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	275	PRO
5	4	87	TYR
5	4	88	PRO
5	4	263	VAL
9	A	47	ARG

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	0	413/676 (61%)	396 (96%)	17 (4%)	26	47
2	1	179/341 (52%)	174 (97%)	5 (3%)	38	57
3	2	53/273 (19%)	52 (98%)	1 (2%)	52	69
4	3	53/303 (18%)	50 (94%)	3 (6%)	17	38
5	4	4/276 (1%)	4 (100%)	0	100	100
6	5	53/66 (80%)	53 (100%)	0	100	100
7	6	173/378 (46%)	172 (99%)	1 (1%)	84	88
8	7	315/695 (45%)	304 (96%)	11 (4%)	31	51
9	A	1221/1520 (80%)	1160 (95%)	61 (5%)	20	41
10	B	1000/1061 (94%)	948 (95%)	52 (5%)	19	40
11	C	230/274 (84%)	217 (94%)	13 (6%)	17	38
12	D	139/200 (70%)	132 (95%)	7 (5%)	20	41
13	E	195/197 (99%)	190 (97%)	5 (3%)	41	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	F	73/137 (53%)	69 (94%)	4 (6%)	18	39
15	G	152/152 (100%)	145 (95%)	7 (5%)	23	44
16	H	119/128 (93%)	114 (96%)	5 (4%)	25	46
17	I	110/116 (95%)	105 (96%)	5 (4%)	23	45
18	J	60/65 (92%)	56 (93%)	4 (7%)	13	34
19	K	97/102 (95%)	95 (98%)	2 (2%)	48	66
20	L	40/57 (70%)	33 (82%)	7 (18%)	1	8
21	M	245/299 (82%)	225 (92%)	20 (8%)	9	28
22	O	152/205 (74%)	150 (99%)	2 (1%)	65	77
23	Q	109/641 (17%)	99 (91%)	10 (9%)	7	23
24	R	107/363 (30%)	102 (95%)	5 (5%)	22	44
25	U	84/154 (54%)	81 (96%)	3 (4%)	30	50
26	V	90/108 (83%)	86 (96%)	4 (4%)	24	45
27	W	161/244 (66%)	157 (98%)	4 (2%)	42	61
28	X	62/295 (21%)	62 (100%)	0	100	100
All	All	5689/9326 (61%)	5431 (96%)	258 (4%)	26	45

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	O	124	THR
23	Q	350	TRP
9	A	1384	VAL
9	A	1334	ASP
24	R	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
11	C	73	GLN
17	I	12	ASN
11	C	195	GLN
12	D	216	ASN
18	J	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	SF4	0	801	-	0,12,12	-	-	-		

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
32	SF4	0	801	-	-	-	0/6/5/5

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	801	SF4	1	0

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
27	W	2
2	1	2
3	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	373:UNK	C	407:UNK	N	84.71
1	1	394:UNK	C	465:UNK	N	82.85
1	W	289:UNK	C	349:UNK	N	45.78
1	2	419:UNK	C	433:LEU	N	13.35
1	1	519:UNK	C	537:GLU	N	11.39

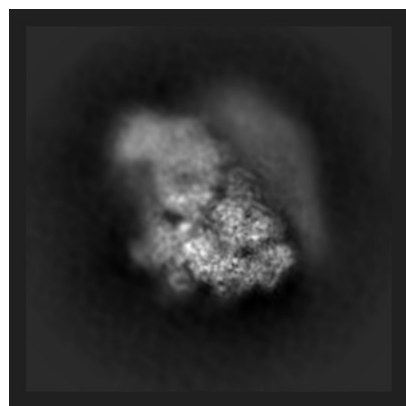
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0092. These allow visual inspection of the internal detail of the map and identification of artifacts.

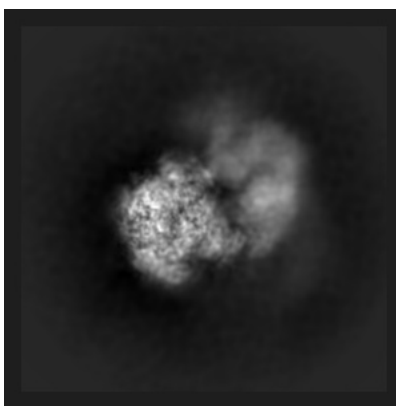
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

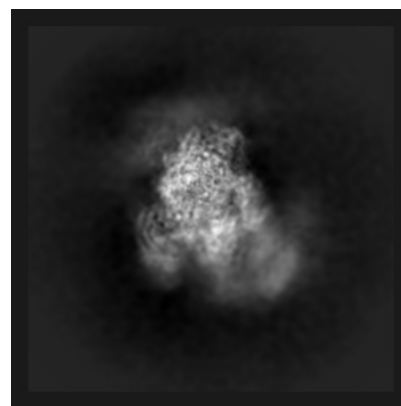
6.1.1 Primary map



X

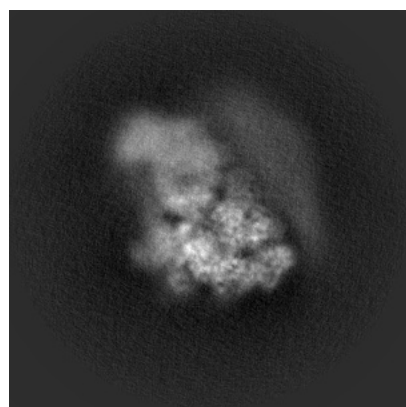


Y

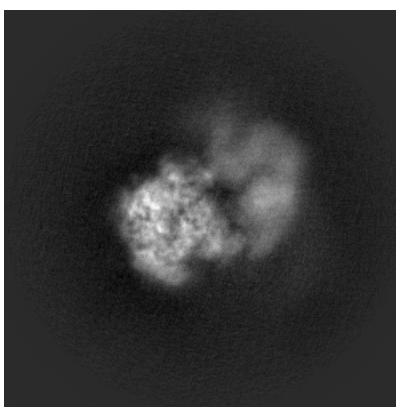


Z

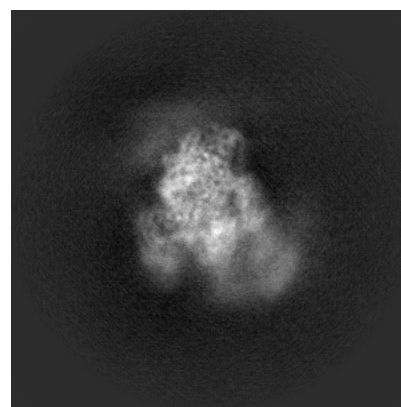
6.1.2 Raw map



X



Y

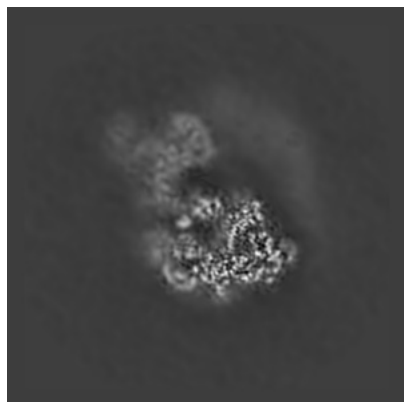


Z

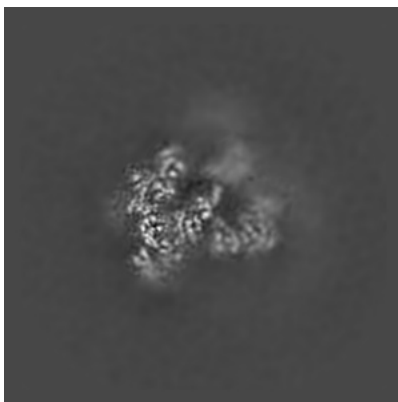
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

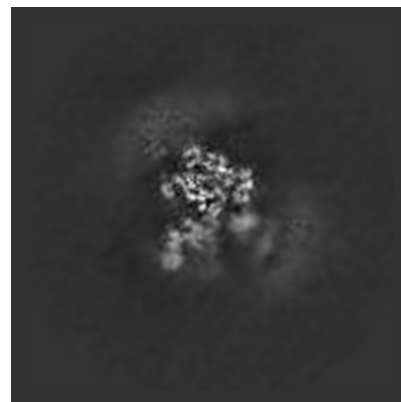
6.2.1 Primary map



X Index: 175

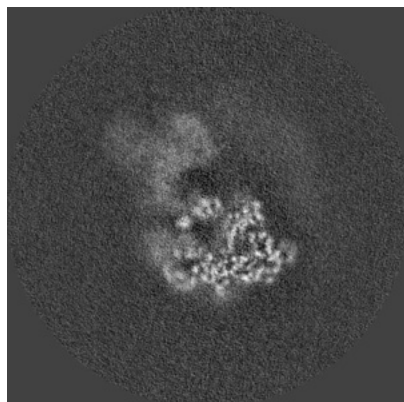


Y Index: 175

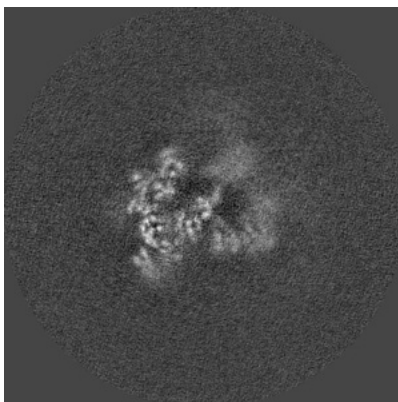


Z Index: 175

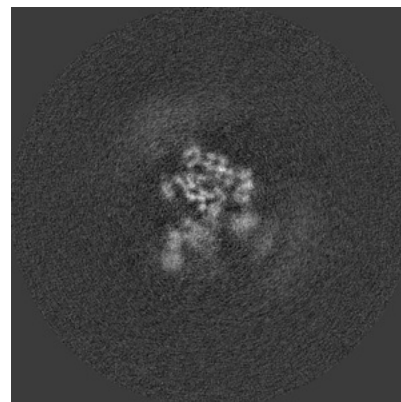
6.2.2 Raw map



X Index: 175



Y Index: 175

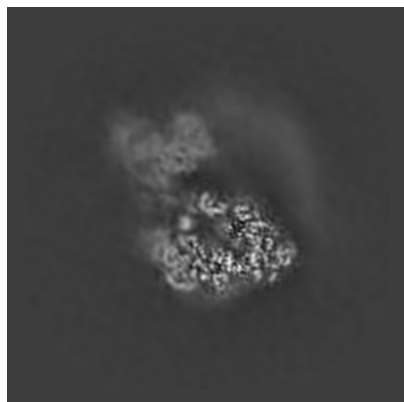


Z Index: 175

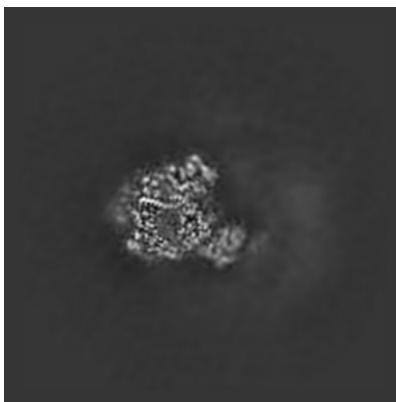
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

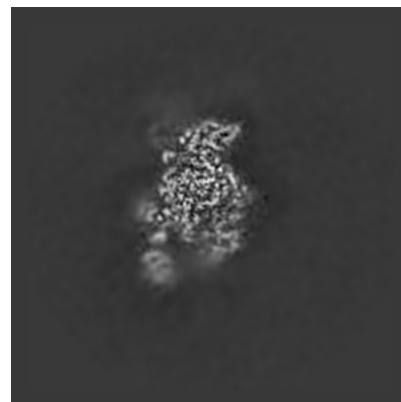
6.3.1 Primary map



X Index: 180

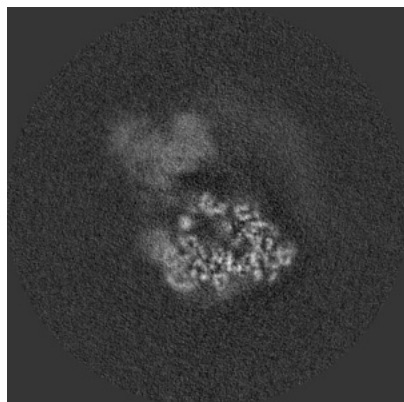


Y Index: 194

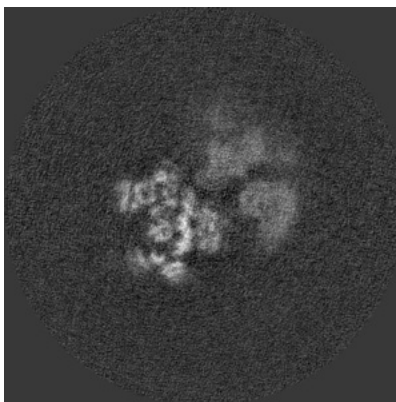


Z Index: 129

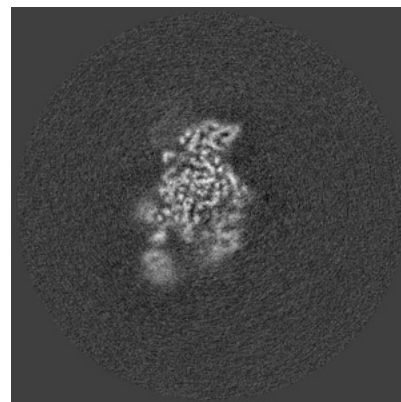
6.3.2 Raw map



X Index: 180



Y Index: 152

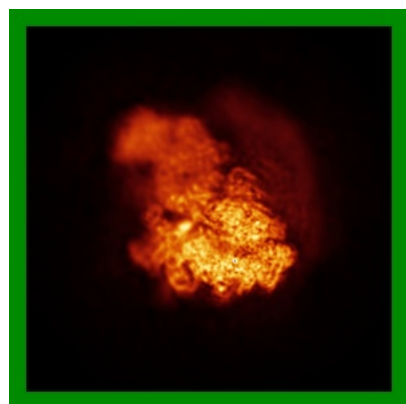


Z Index: 129

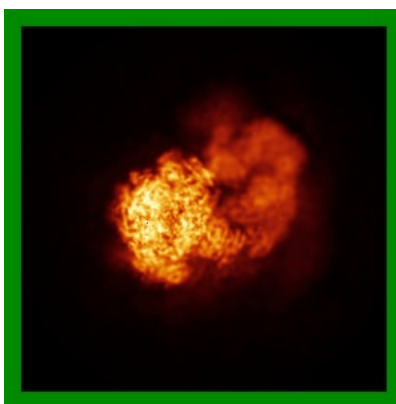
The images above show the largest variance slices of the map in three orthogonal directions.

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

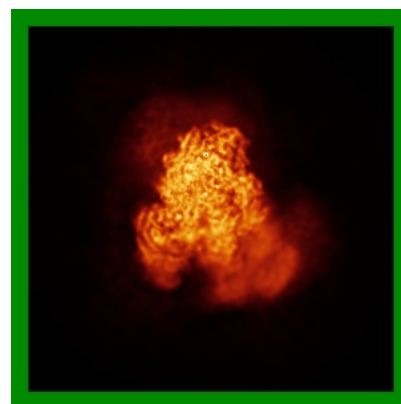
6.4.1 Primary map



X

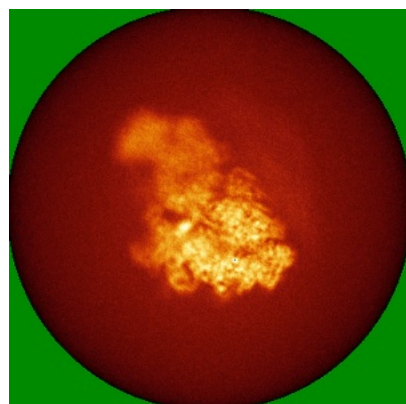


Y

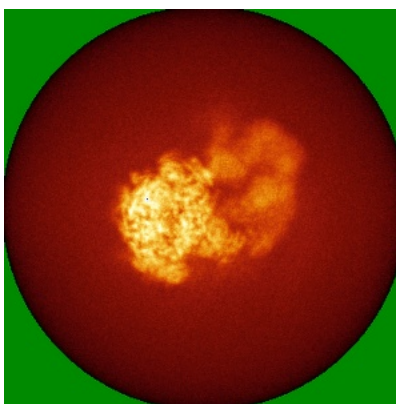


Z

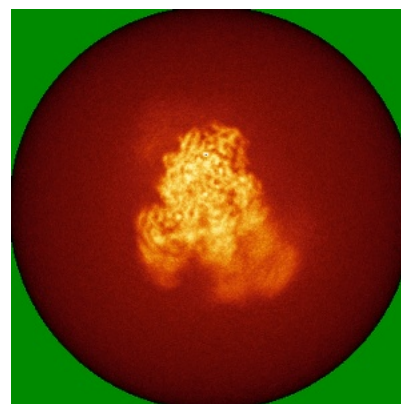
6.4.2 Raw map



X



Y

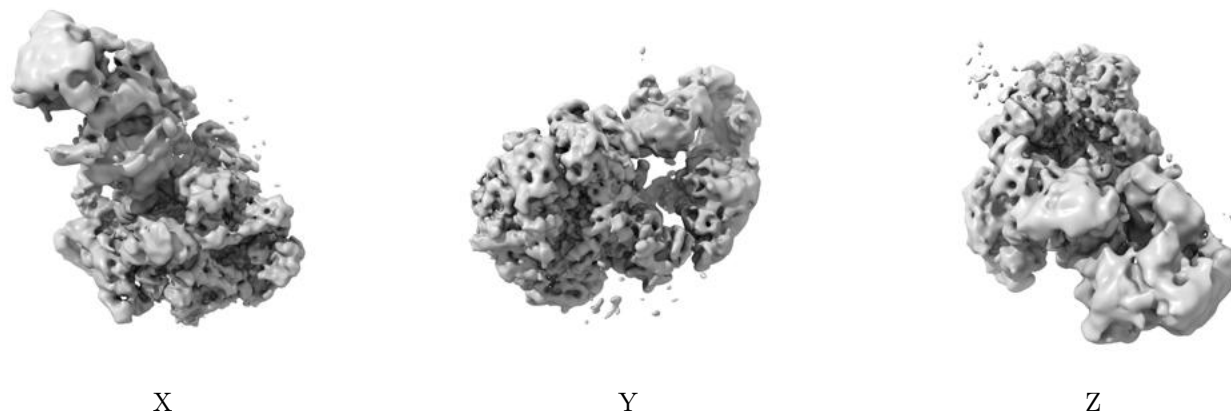


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0057. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

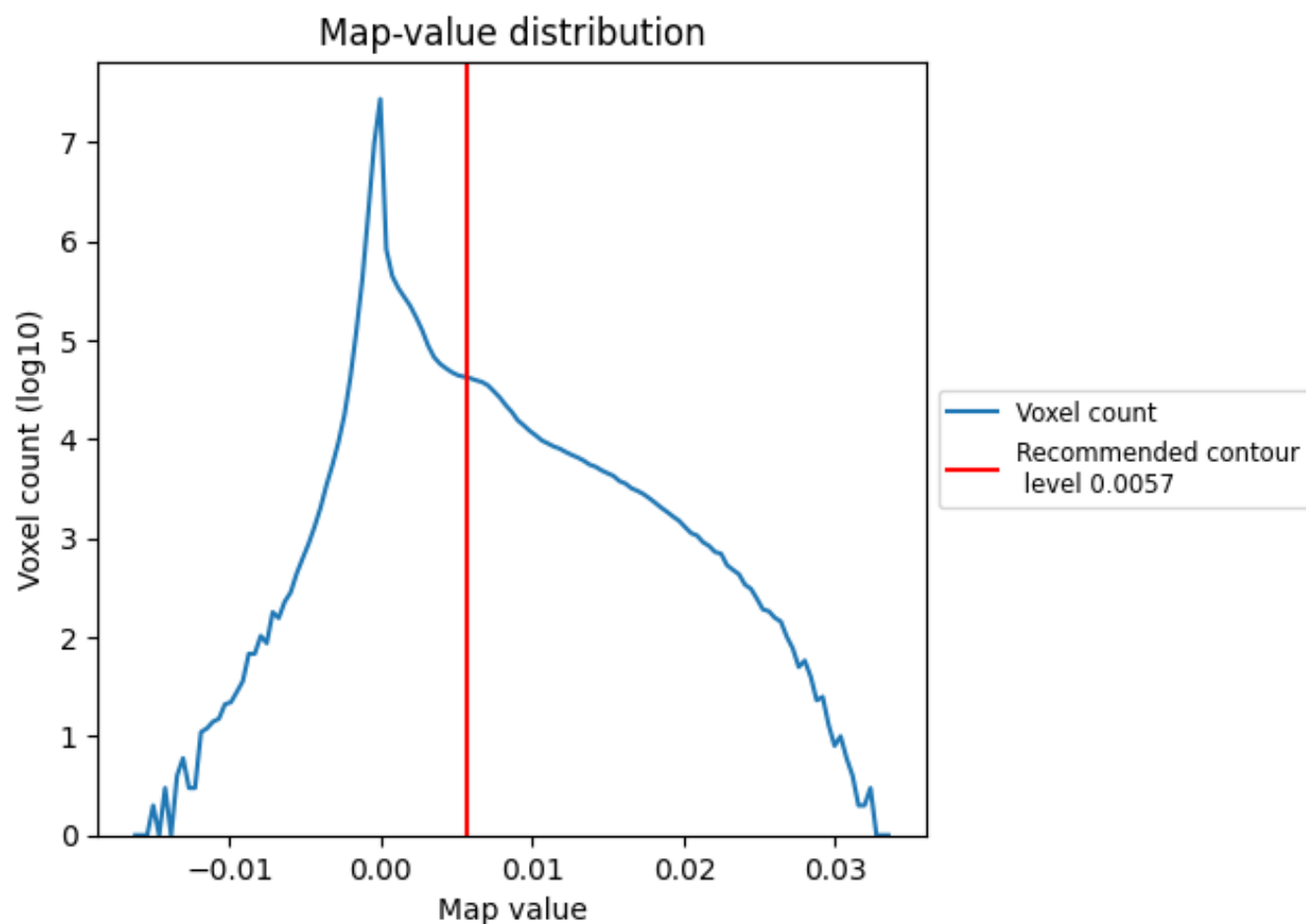
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

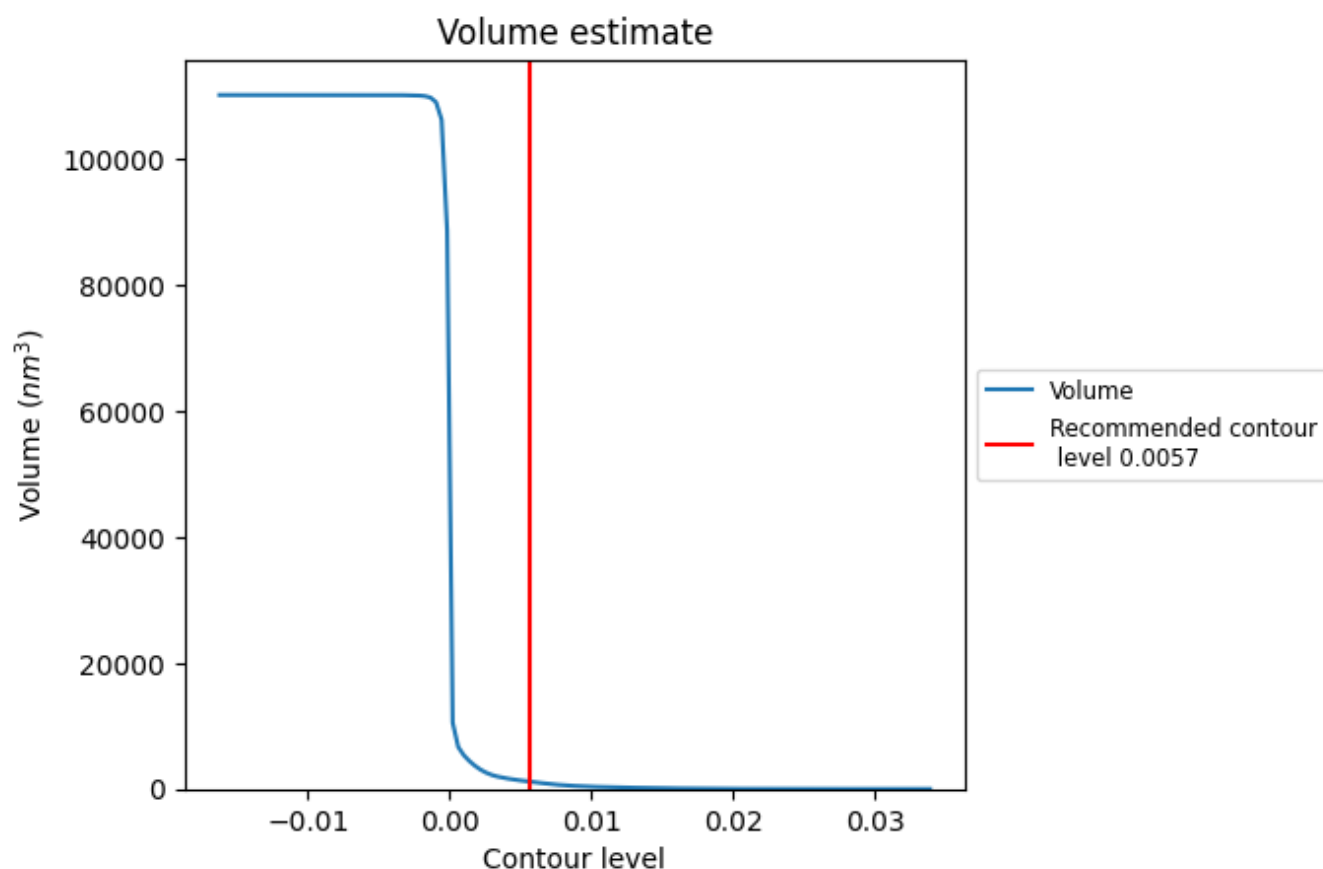
This section contains the results of statistical analysis of the map.

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.

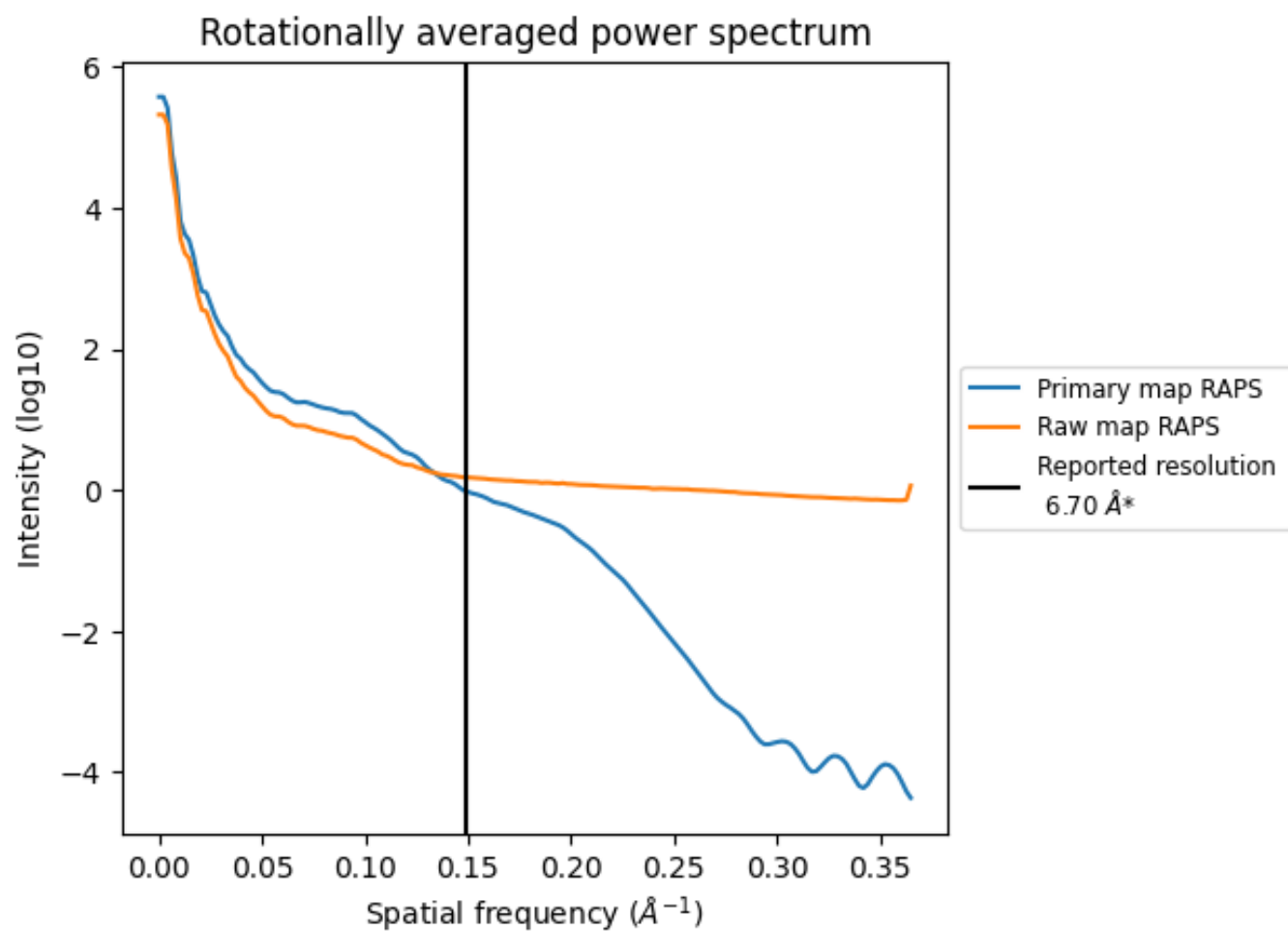
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1149 nm^3 ; this corresponds to an approximate mass of 1038 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 ⓘ

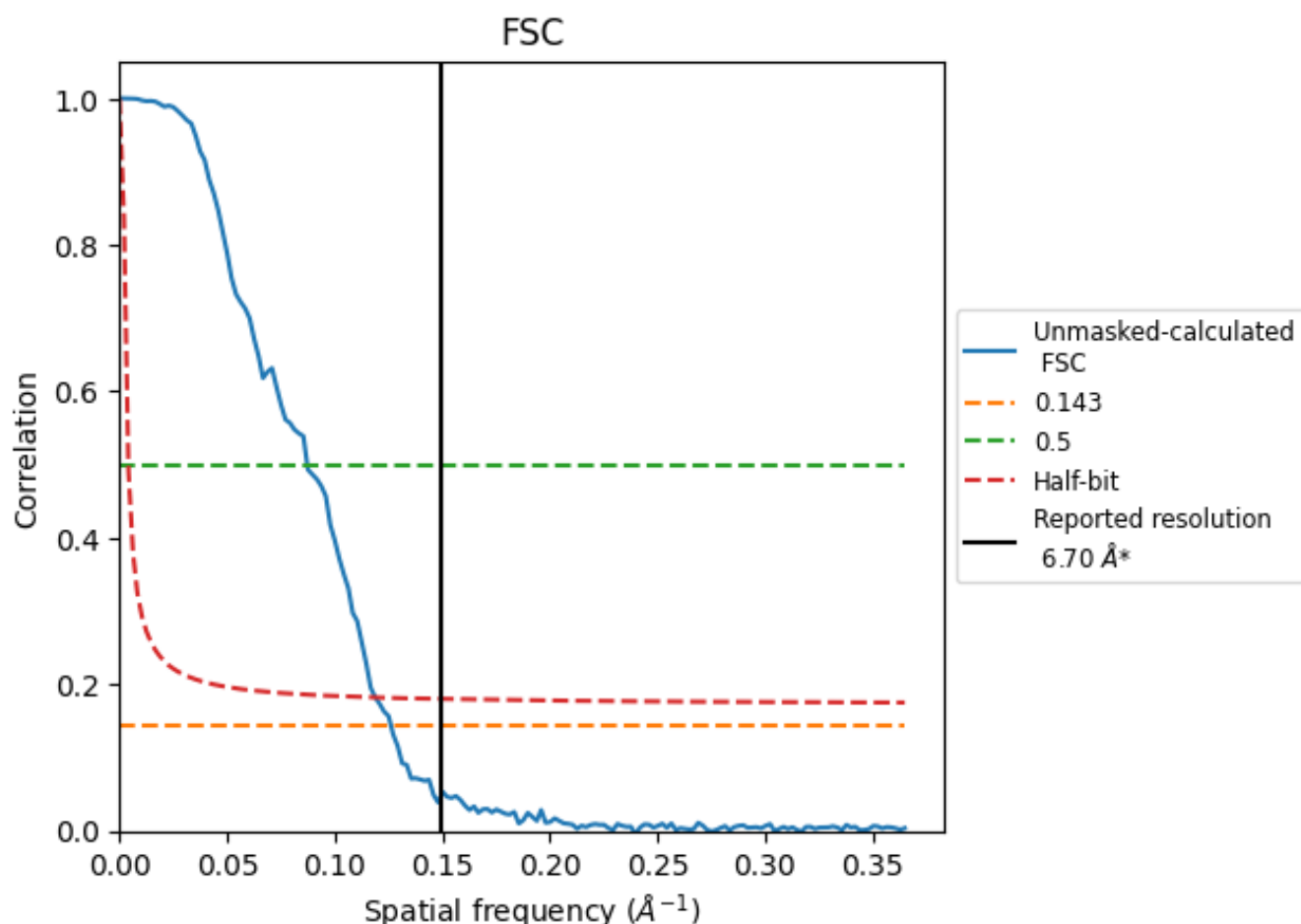


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

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 0.149 Å⁻¹

8.2 Resolution estimates [i](#)

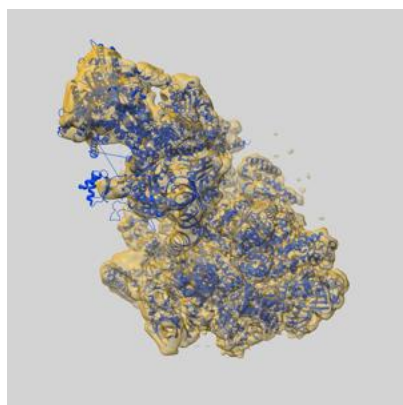
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.92	11.45	8.41

*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 7.92 differs from the reported value 6.7 by more than 10 %

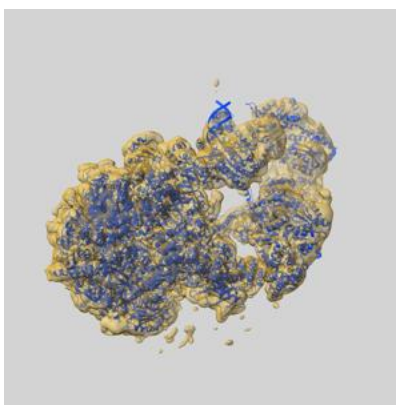
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0092 and PDB model 6GYM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

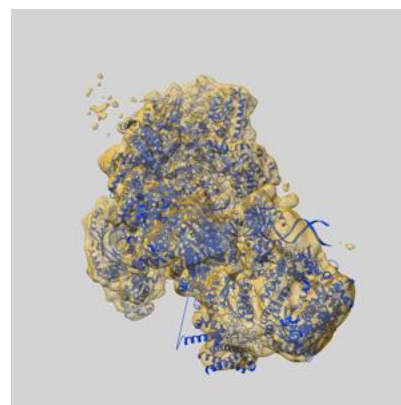
9.1 Map-model overlay [i](#)



X



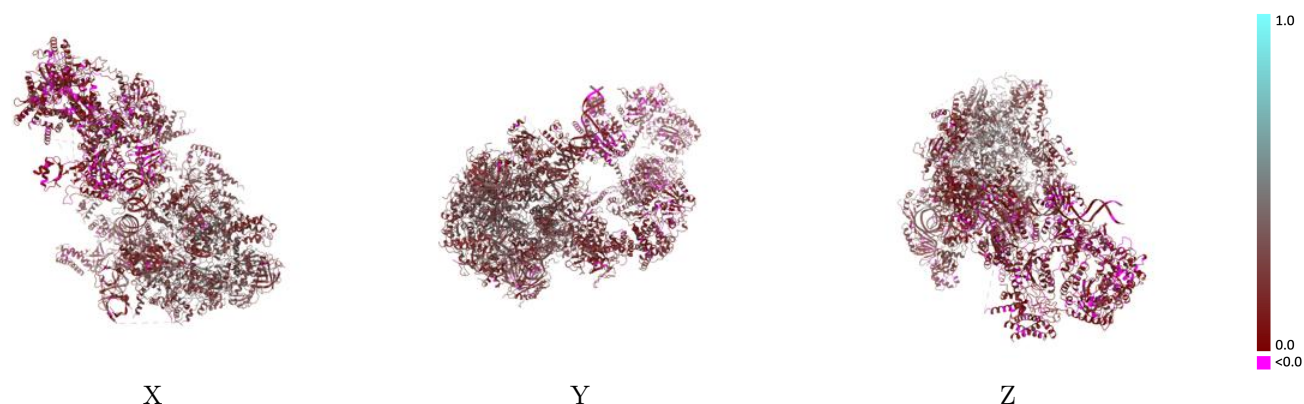
Y



Z

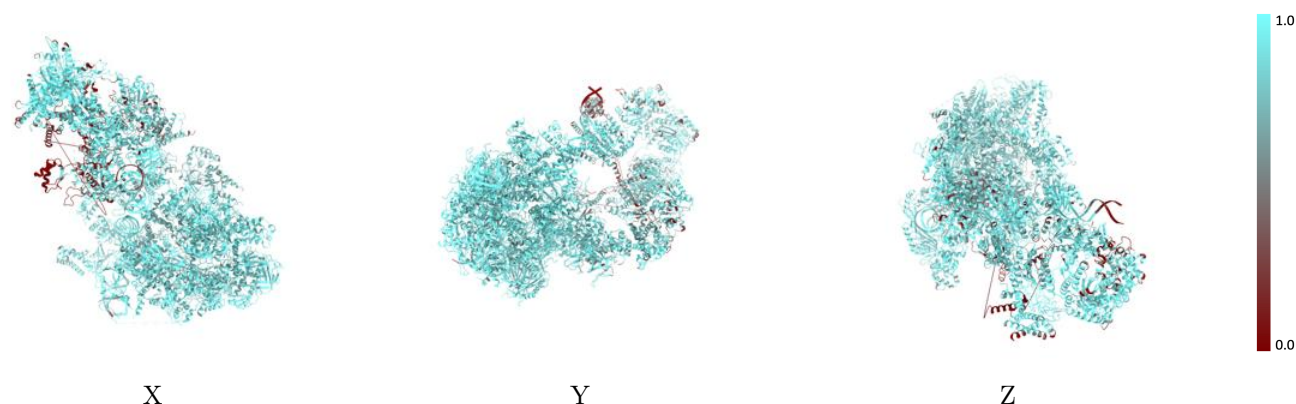
The images above show the 3D surface view of the map at the recommended contour level 0.0057 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



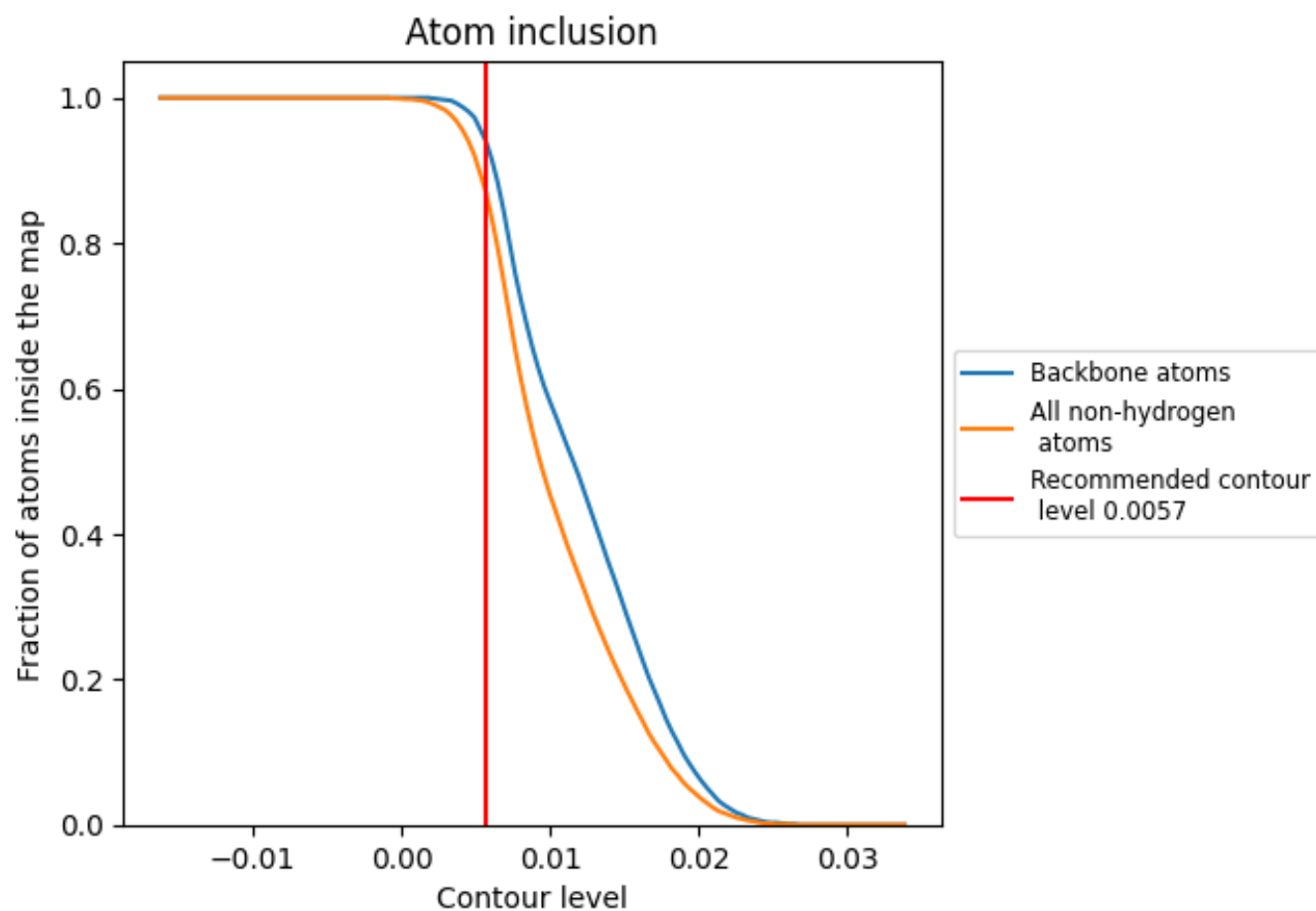
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0057).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0057) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.2190
0	 0.7850	 0.1370
1	 0.7310	 0.1470
2	 0.6780	 0.0910
3	 0.8210	 0.1930
4	 0.9190	 0.1090
5	 0.3860	 0.0900
6	 0.8950	 0.1170
7	 0.8840	 0.0870
A	 0.9050	 0.2860
B	 0.9110	 0.3130
C	 0.9380	 0.3170
D	 0.7890	 0.1930
E	 0.9320	 0.2430
F	 0.9220	 0.3170
G	 0.8560	 0.2310
H	 0.9290	 0.2770
I	 0.9340	 0.2420
J	 0.9380	 0.2870
K	 0.9190	 0.2910
L	 0.9310	 0.3010
M	 0.8540	 0.2270
N	 0.9010	 0.2050
O	 0.9290	 0.1820
Q	 0.9420	 0.2200
R	 0.9580	 0.2400
T	 0.8690	 0.2040
U	 0.9110	 0.1450
V	 0.8890	 0.1250
W	 0.7540	 0.1640
X	 0.9430	 0.2180
Z	 0.9630	 0.1140

