



wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 06:58 PM JST

PDB ID : 8ITY
EMDB ID : EMD-35712
Title : human RNA polymerase III pre-initiation complex closed DNA 1
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on : 2023-03-23
Resolution : 3.90 Å(reported)

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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:

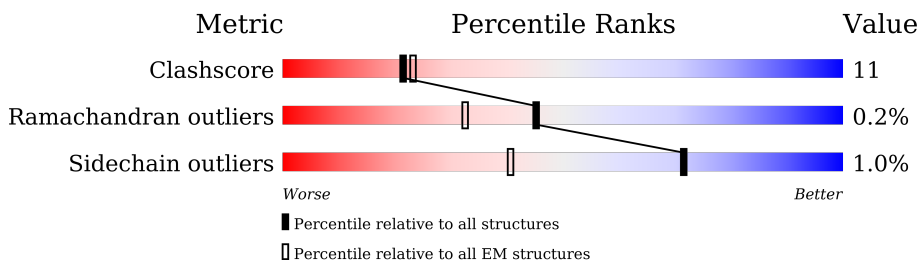
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)
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	1	368	
2	3	411	
3	4	1469	
4	A	1390	
5	B	1133	
6	C	346	
7	D	148	
8	E	210	

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Mol	Chain	Length	Quality of chain
9	F	127	46% 13% 40%
10	G	204	6% 48% 33% 19%
11	H	150	5% 77% 22%
12	I	108	42% 10% 48%
13	J	67	63% 34%
14	K	133	53% 24% 23%
15	L	58	7% 45% 34% 21%
16	M	708	42% 14% 44%
17	N	317	6% 32% 14% 54%
18	O	534	22% 63% 31%
19	P	316	48% 49% 24% 27%
20	Q	223	13% 26% 13% 61%
21	U	339	45% 6% 48%
22	V	419	15% 74% 12% 14%
23	W	2624	96%
24	X	464	7% 12% 82%
25	Y	464	5% 12% 82%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 57140 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	146	1233	804	212	209	8	0	0

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	374	3037	1925	521	570	21	0	0

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	365	3058	1921	573	555	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1105	8741	5538	1529	1605	69	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	343	2736	1723	488	514	11	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	122	985	614	172	196	3	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	209	1715	1083	300	324	8	0	0

- Molecule 9 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		
9	F	76	610	392	103	110	5	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	166	1337	876	211	245	5	0	0

- Molecule 11 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		
11	H	148	1186	750	194	237	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	56	435	272	81	76	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 13 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		
13	J	65	512	331	87	88	6	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	103	822	513	145	157	7	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	46	388	241	75	66	6	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	394	3167	2013	550	584	20	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	146	1128	710	191	221	6	0	0

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	512	4075	2565	712	774	24	0	0

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	232	1837	1166	305	353	13	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	176	Total	C	N	O	S	1	0
			1396	907	244	238	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (82-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	82	Total	C	N	O	P	0	0
			1677	804	291	500	82		

- Molecule 25 is a DNA chain called DNA (82-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	82	Total	C	N	O	P	0	0
			1685	804	315	484	82		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	

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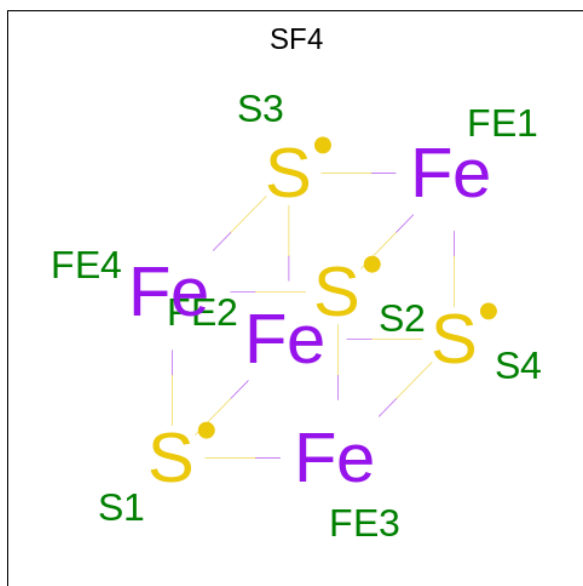
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Mol	Chain	Residues	Atoms		AltConf
26	I	1	Total	Zn	0
			1	1	
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

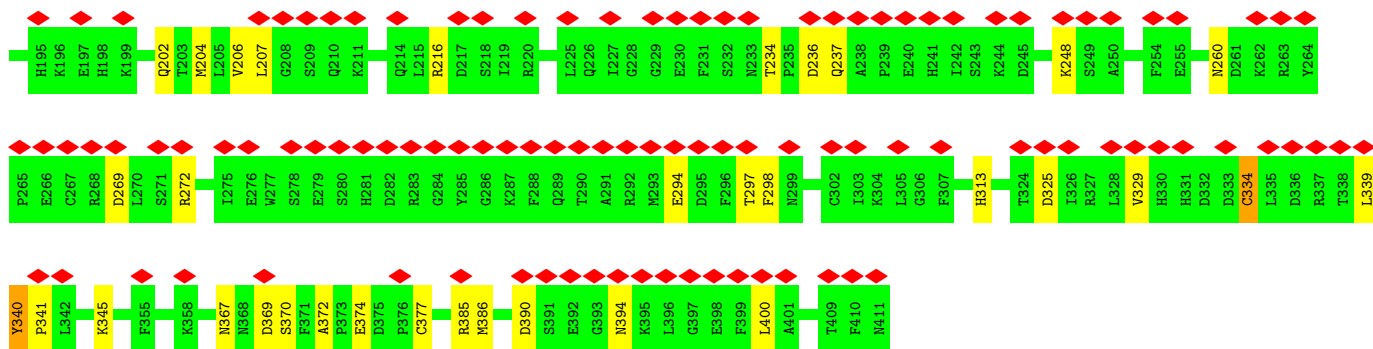
- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

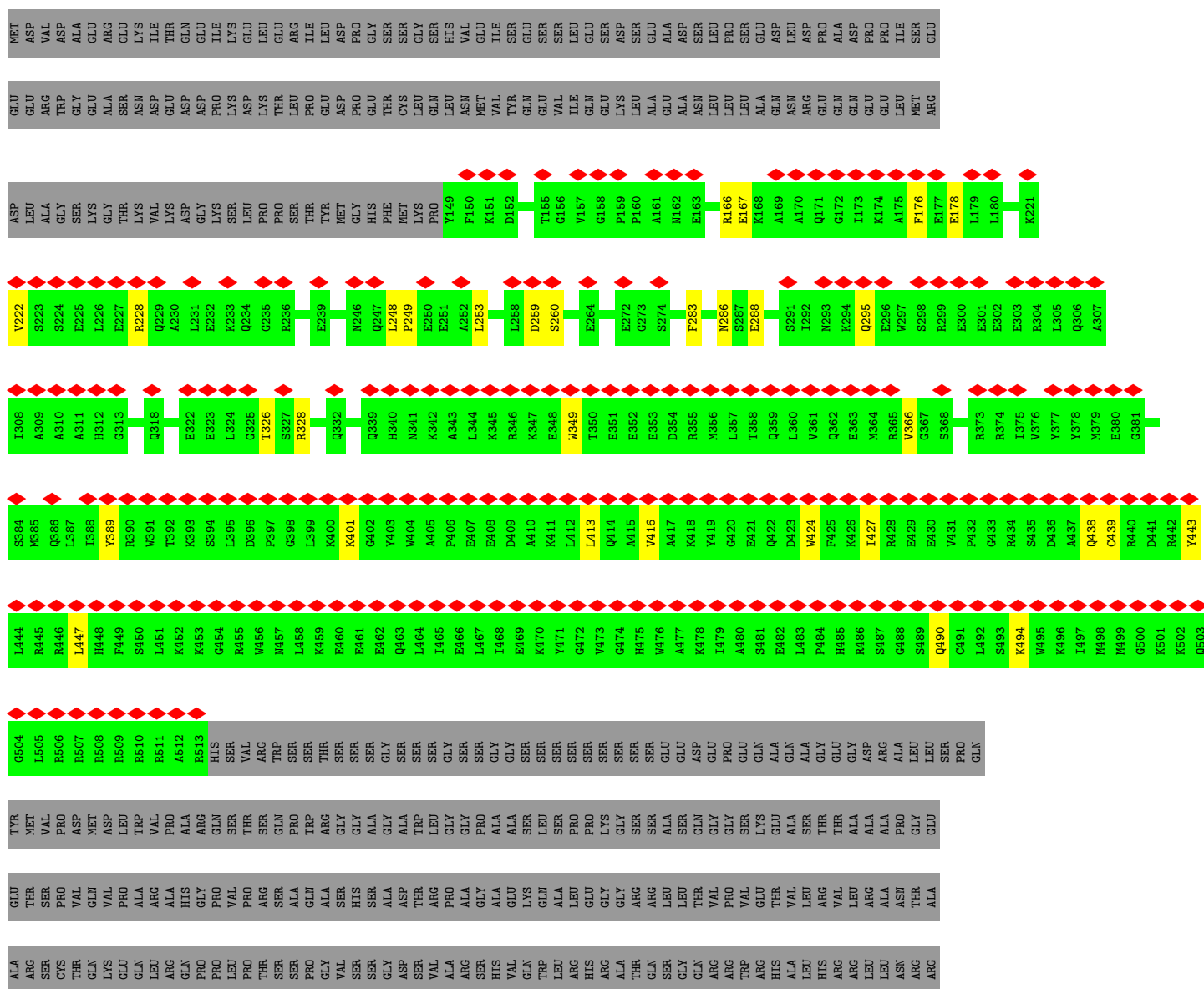
- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).

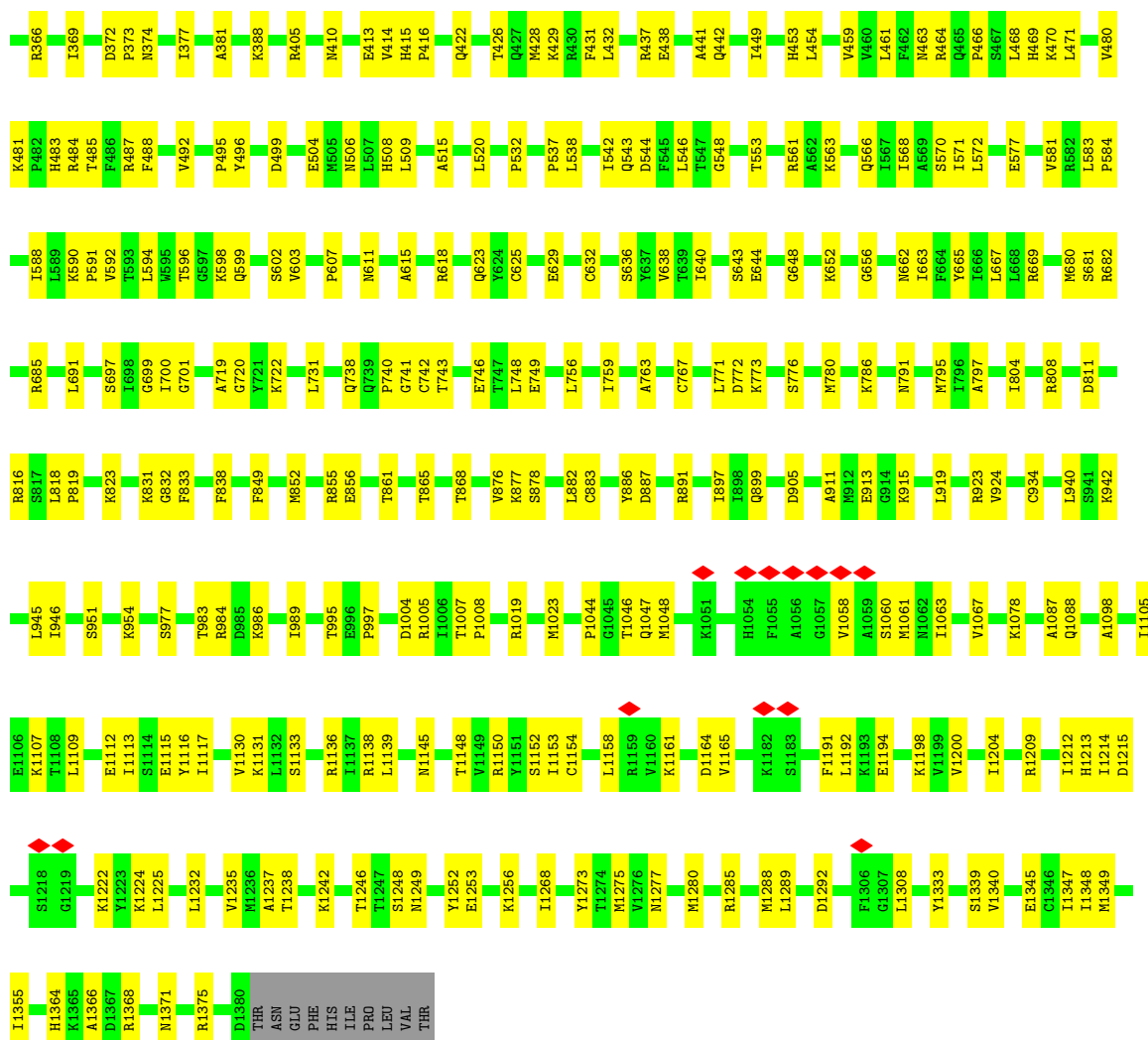


Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	Fe	S	0
			8	4	4	



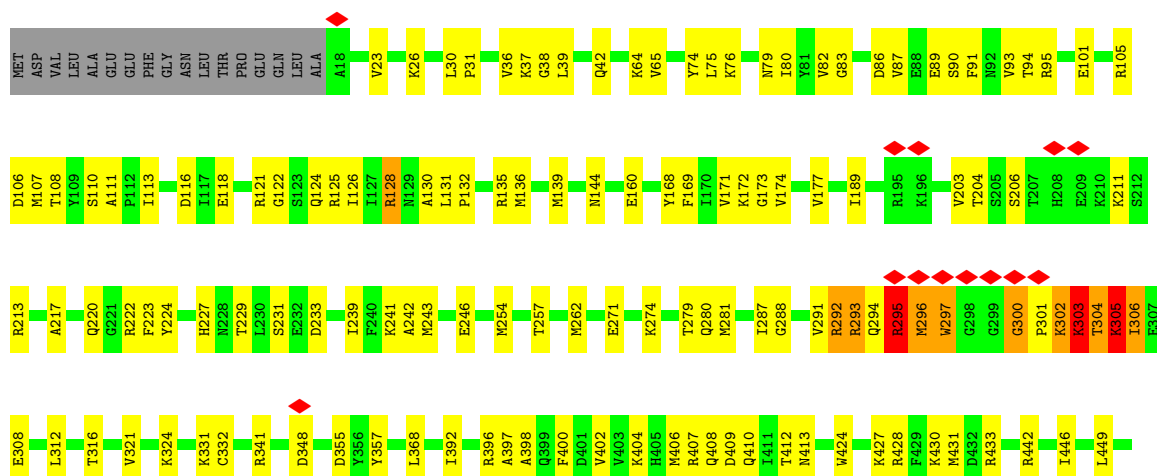
• Molecule 3: snRNA-activating protein complex subunit 4



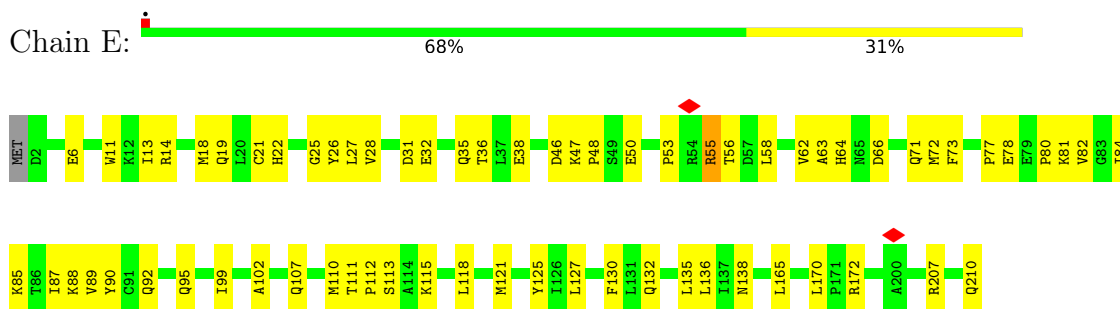


- Molecule 5: DNA-directed RNA polymerase III subunit RPC2

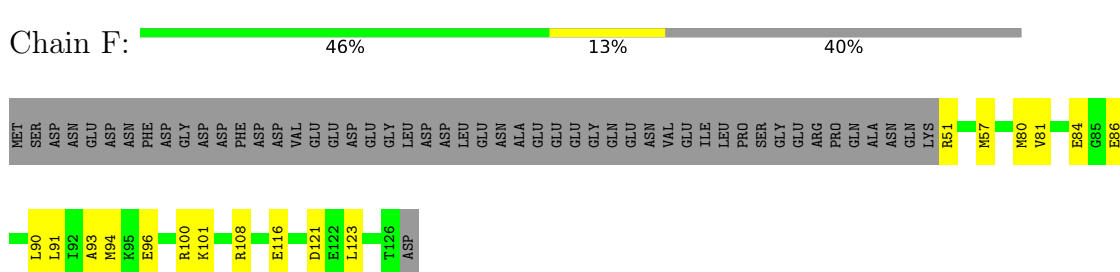
Chain B:  67% 29%



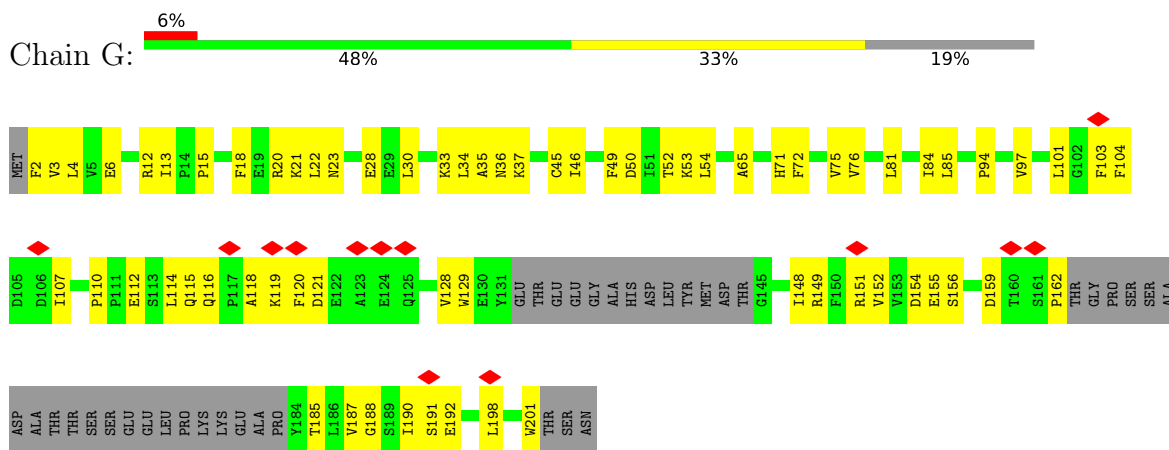
● Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



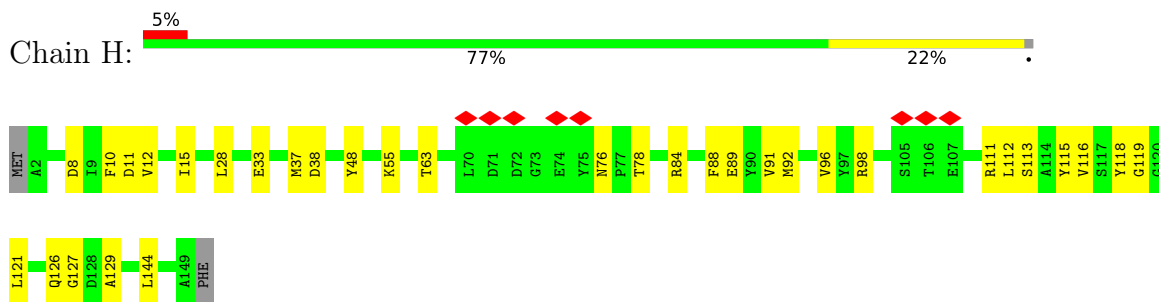
● Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



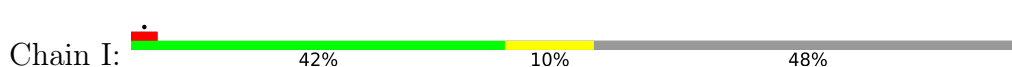
● Molecule 10: DNA-directed RNA polymerase III subunit RPC8

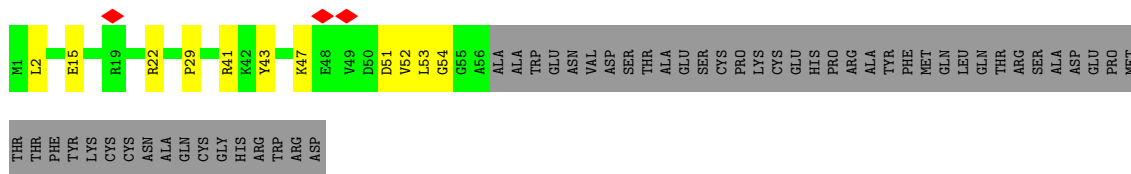


● Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

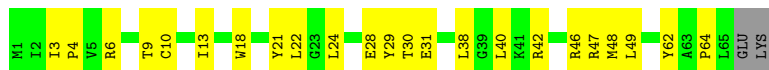


● Molecule 12: DNA-directed RNA polymerase III subunit RPC10

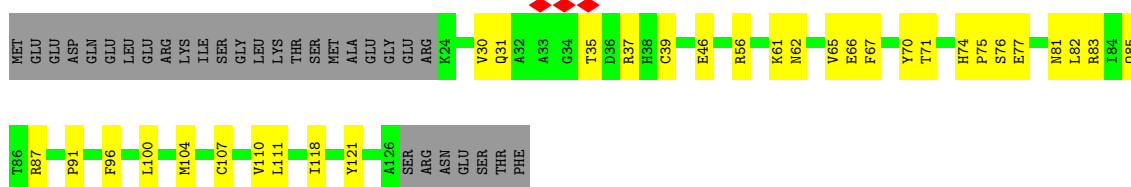




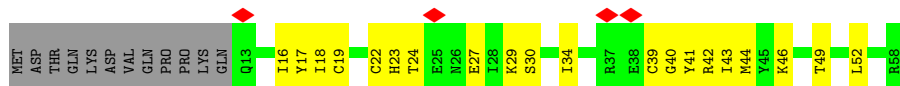
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5



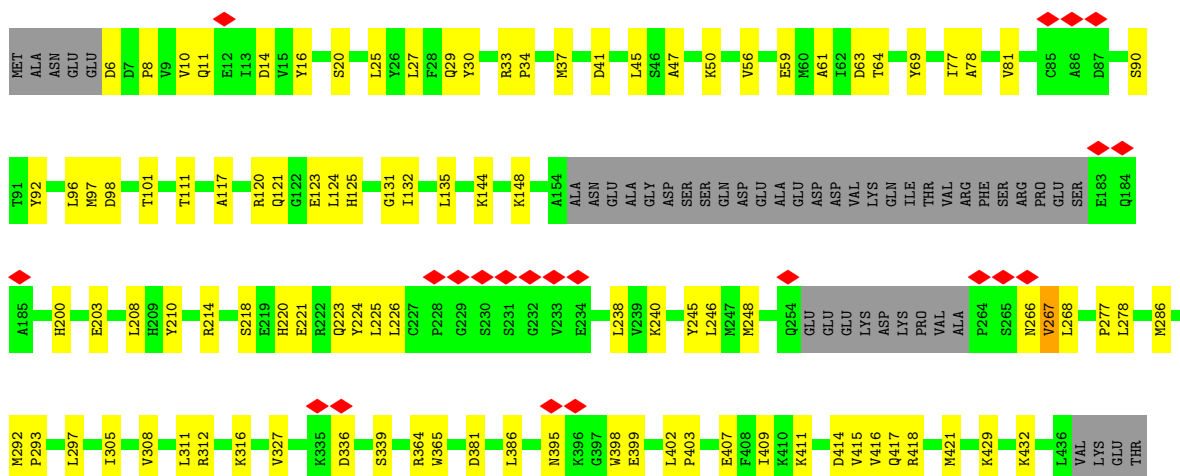
- Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

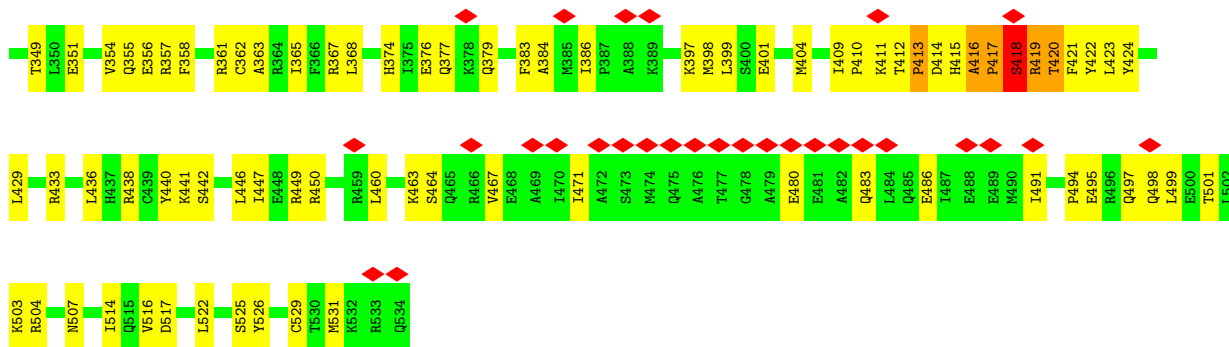


- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

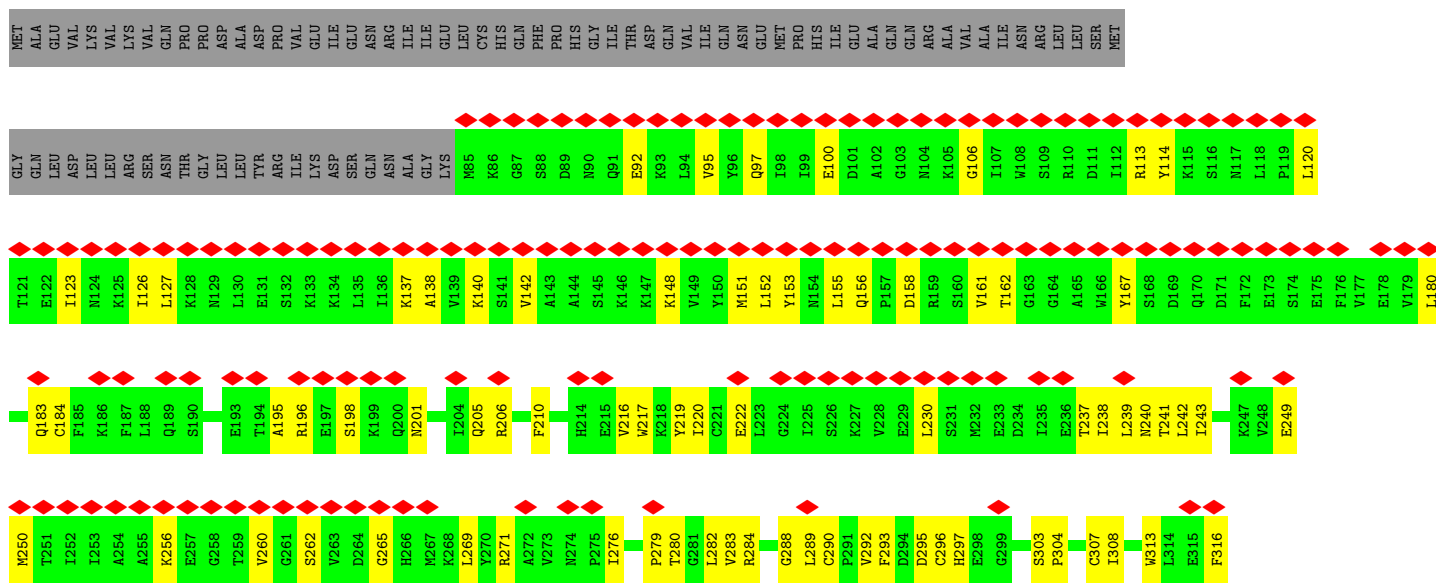


- Molecule 16: DNA-directed RNA polymerase III subunit RPC5

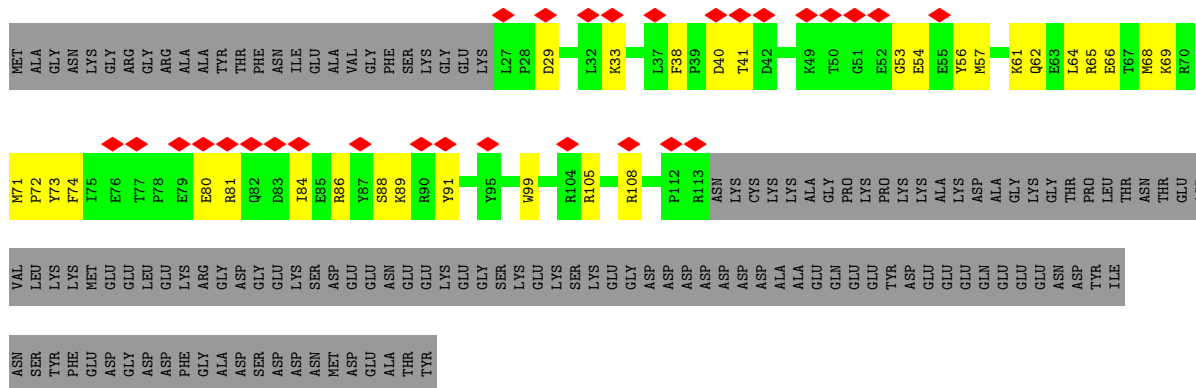




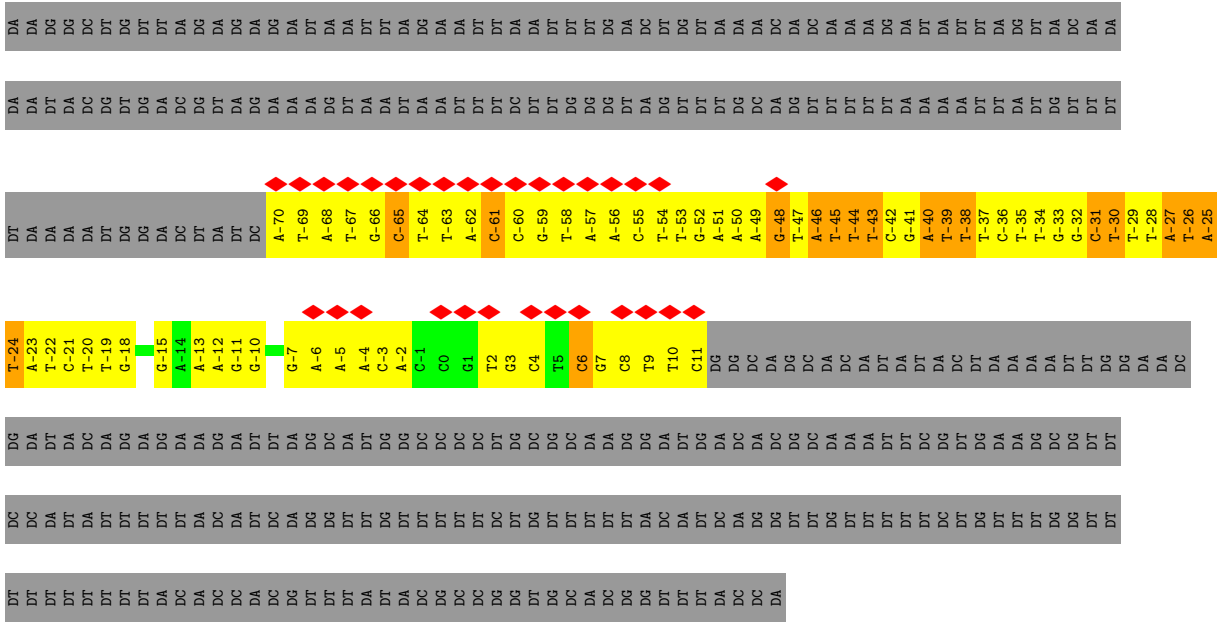
• Molecule 19: DNA-directed RNA polymerase III subunit RPC6



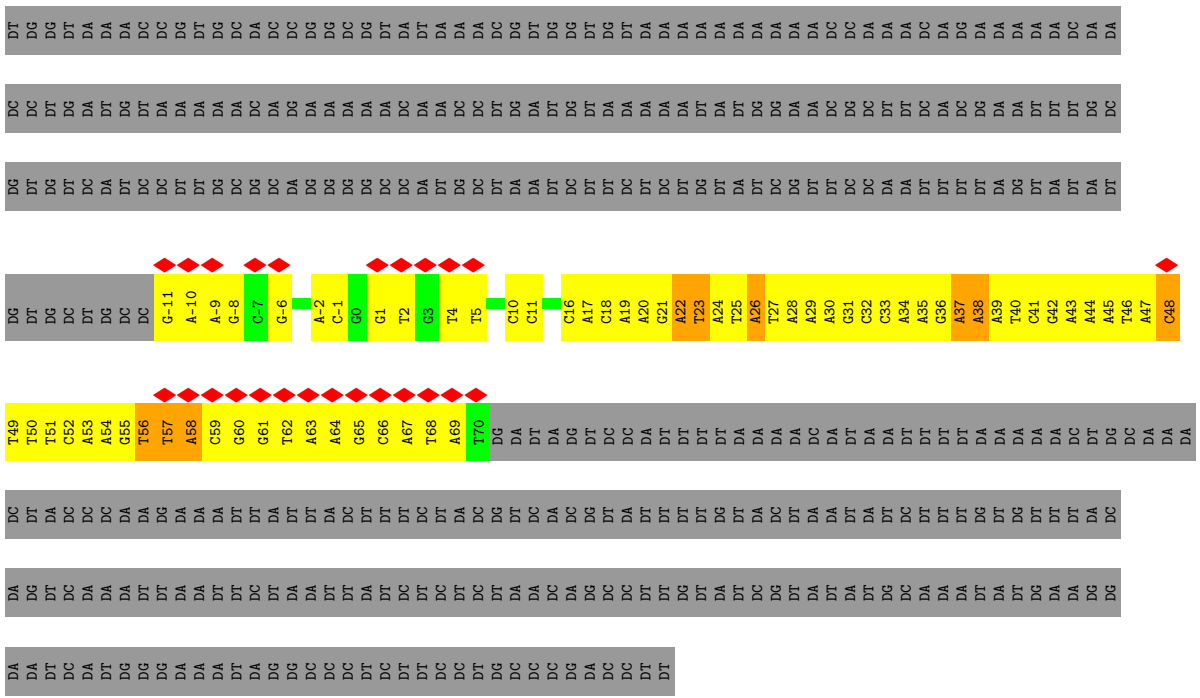
• Molecule 20: DNA-directed RNA polymerase III subunit RPC7



• Molecule 21: TATA-box-binding protein



• Molecule 25: DNA (82-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70361	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.334, 1.334, 1.334	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, SF4, 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	1	0.24	0/1266	0.37	0/1708
2	3	0.23	0/3112	0.40	0/4206
3	4	0.23	0/3121	0.40	1/4181 (0.0%)
4	A	0.27	0/11008	0.49	0/14842
5	B	0.28	0/8910	0.50	2/12018 (0.0%)
6	C	0.27	0/2790	0.51	0/3782
7	D	0.23	0/997	0.46	0/1343
8	E	0.26	0/1745	0.51	0/2358
9	F	0.27	0/620	0.55	0/839
10	G	0.26	0/1374	0.49	0/1868
11	H	0.27	0/1207	0.51	0/1628
12	I	0.28	0/443	0.54	0/596
13	J	0.27	0/521	0.46	0/703
14	K	0.29	0/837	0.52	0/1129
15	L	0.34	0/394	0.69	0/524
16	M	0.25	0/3237	0.46	0/4377
17	N	0.25	0/1137	0.51	0/1530
18	O	0.25	0/4141	0.52	0/5592
19	P	0.25	0/1872	0.45	0/2525
20	Q	0.25	0/777	0.55	0/1050
21	U	0.24	0/1424	0.44	1/1918 (0.1%)
22	V	0.25	0/2904	0.50	3/3941 (0.1%)
23	W	0.26	0/967	0.49	2/1293 (0.2%)
24	X	0.47	0/1877	1.95	91/2895 (3.1%)
25	Y	0.48	0/1893	2.17	88/2919 (3.0%)
All	All	0.28	0/58574	0.73	188/79765 (0.2%)

There are no bond length outliers.

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	49	DT	OP1-P-O3'	-37.68	22.30	105.20
25	Y	67	DA	OP1-P-O3'	-37.60	22.48	105.20
25	Y	69	DA	OP1-P-O3'	-37.59	22.50	105.20
24	X	-70	DA	OP1-P-O3'	-37.54	22.62	105.20
25	Y	50	DT	OP1-P-O3'	-37.37	22.98	105.20

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	1	1233	0	1231	7	0
2	3	3037	0	2911	38	0
3	4	3058	0	3064	19	0
4	A	10814	0	11059	322	0
5	B	8741	0	8867	286	0
6	C	2736	0	2712	68	0
7	D	985	0	1006	37	0
8	E	1715	0	1733	43	0
9	F	610	0	642	9	0
10	G	1337	0	1306	63	0
11	H	1186	0	1147	23	0
12	I	435	0	436	10	0
13	J	512	0	526	19	0
14	K	822	0	810	35	0
15	L	388	0	395	13	0
16	M	3167	0	3184	74	0
17	N	1128	0	1181	36	0
18	O	4075	0	4149	137	0
19	P	1837	0	1835	60	0
20	Q	754	0	759	22	0
21	U	1396	0	1490	15	0
22	V	2853	0	2890	39	0
23	W	943	0	924	54	0
24	X	1677	0	932	42	0
25	Y	1685	0	924	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	1	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	0	0
All	All	57140	0	56113	1293	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 11.

The worst 5 of 1293 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)
23:W:328:LEU:HD13	23:W:367:PHE:CE1	1.56	1.37
8:E:85:LYS:NZ	25:Y:-8:DG:OP2	1.71	1.23
23:W:363:ASP:OD2	23:W:366:PHE:HB3	1.28	1.22
23:W:328:LEU:CD1	23:W:367:PHE:CE1	2.24	1.18
5:B:287:ILE:O	5:B:291:VAL:HG23	1.48	1.13

There are no symmetry-related clashes.

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	1	144/368 (39%)	144 (100%)	0	0	100 100
2	3	368/411 (90%)	352 (96%)	16 (4%)	0	100 100
3	4	363/1469 (25%)	345 (95%)	18 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1376/1390 (99%)	1323 (96%)	50 (4%)	3 (0%)	44	75
5	B	1101/1133 (97%)	1047 (95%)	51 (5%)	3 (0%)	37	70
6	C	341/346 (99%)	337 (99%)	4 (1%)	0	100	100
7	D	120/148 (81%)	112 (93%)	8 (7%)	0	100	100
8	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
9	F	74/127 (58%)	71 (96%)	3 (4%)	0	100	100
10	G	160/204 (78%)	137 (86%)	23 (14%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	54/108 (50%)	51 (94%)	3 (6%)	0	100	100
13	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
14	K	101/133 (76%)	93 (92%)	8 (8%)	0	100	100
15	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	M	388/708 (55%)	374 (96%)	13 (3%)	1 (0%)	37	70
17	N	140/317 (44%)	134 (96%)	6 (4%)	0	100	100
18	O	508/534 (95%)	485 (96%)	19 (4%)	4 (1%)	16	51
19	P	230/316 (73%)	223 (97%)	7 (3%)	0	100	100
20	Q	85/223 (38%)	85 (100%)	0	0	100	100
21	U	175/339 (52%)	173 (99%)	2 (1%)	0	100	100
22	V	358/419 (85%)	347 (97%)	11 (3%)	0	100	100
23	W	109/2624 (4%)	106 (97%)	2 (2%)	1 (1%)	14	48
All	All	6655/11802 (56%)	6385 (96%)	258 (4%)	12 (0%)	45	75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	O	416	ALA
18	O	418	SER
5	B	305	LYS
16	M	267	VAL
4	A	334	PRO

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	1	130/334 (39%)	127 (98%)	3 (2%)	45	64
2	3	330/356 (93%)	323 (98%)	7 (2%)	48	67
3	4	321/1213 (26%)	317 (99%)	4 (1%)	67	78
4	A	1200/1212 (99%)	1190 (99%)	10 (1%)	79	84
5	B	964/988 (98%)	950 (98%)	14 (2%)	60	74
6	C	299/302 (99%)	299 (100%)	0	100	100
7	D	114/136 (84%)	113 (99%)	1 (1%)	75	83
8	E	191/192 (100%)	190 (100%)	1 (0%)	86	90
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	148 (99%)	1 (1%)	81	86
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	48/93 (52%)	48 (100%)	0	100	100
13	J	53/56 (95%)	53 (100%)	0	100	100
14	K	92/119 (77%)	92 (100%)	0	100	100
15	L	43/55 (78%)	42 (98%)	1 (2%)	45	64
16	M	353/622 (57%)	353 (100%)	0	100	100
17	N	131/276 (48%)	130 (99%)	1 (1%)	79	84
18	O	458/476 (96%)	452 (99%)	6 (1%)	65	76
19	P	206/280 (74%)	205 (100%)	1 (0%)	86	90
20	Q	84/195 (43%)	83 (99%)	1 (1%)	67	78
21	U	152/293 (52%)	151 (99%)	1 (1%)	81	86
22	V	325/365 (89%)	321 (99%)	4 (1%)	67	78
23	W	102/2381 (4%)	100 (98%)	2 (2%)	50	68
All	All	5940/10367 (57%)	5882 (99%)	58 (1%)	71	81

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	295	ARG
22	V	368	ARG
5	B	306	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	V	55	TYR
19	P	156	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
10	G	36	ASN
18	O	310	GLN
18	O	306	GLN
19	P	156	GLN
3	4	463	GLN

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 9 ligands modelled in this entry, 8 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	$\# Z > 2$
28	SF4	P	401	19	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
28	SF4	P	401	19	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

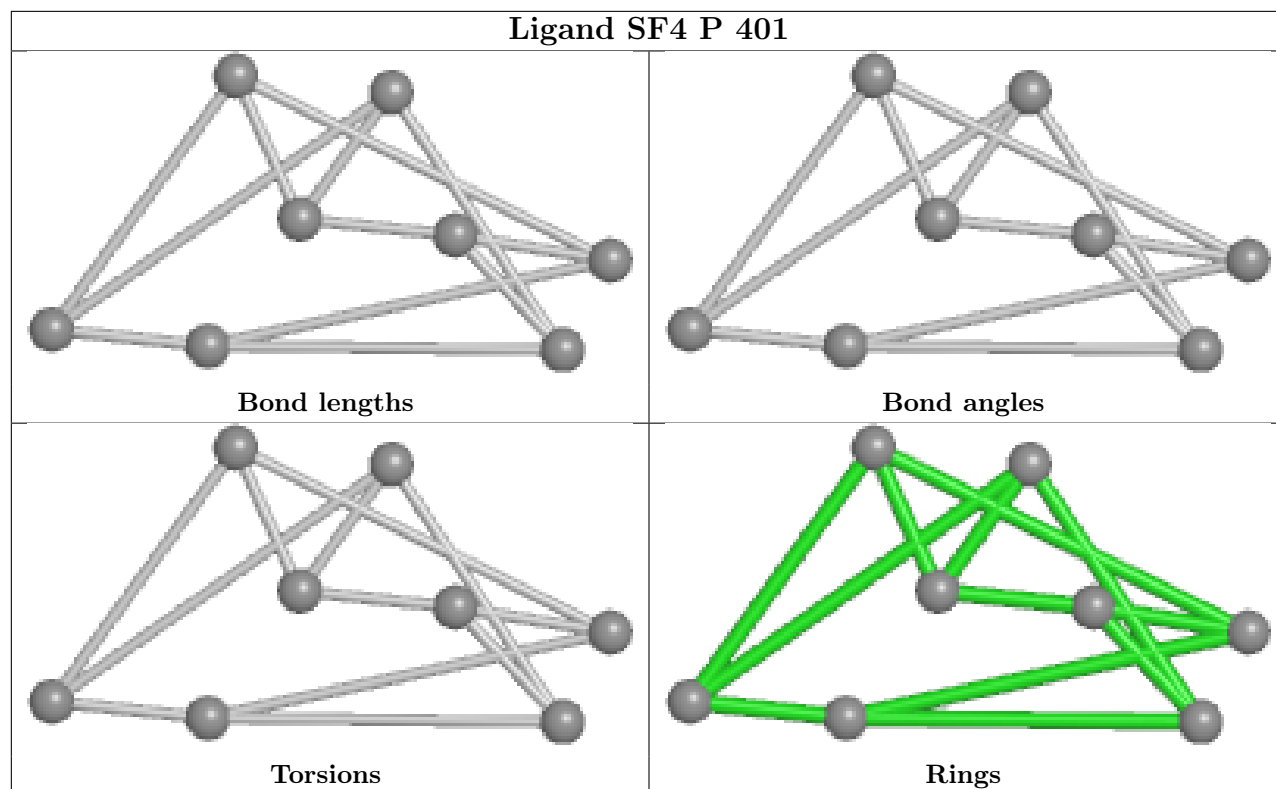
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

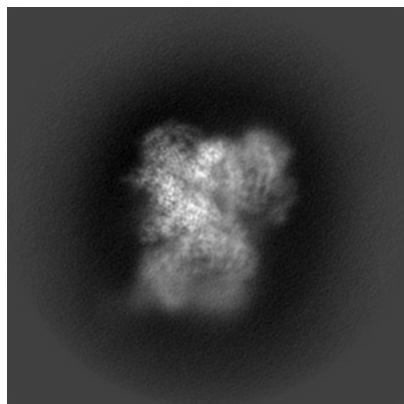
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35712. These allow visual inspection of the internal detail of the map and identification of artifacts.

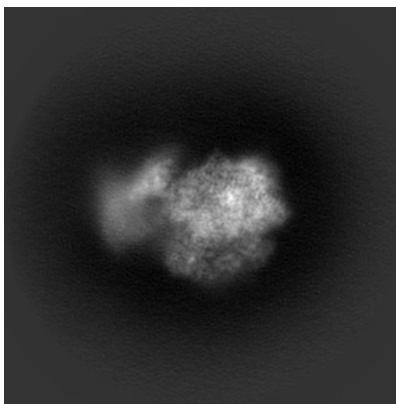
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

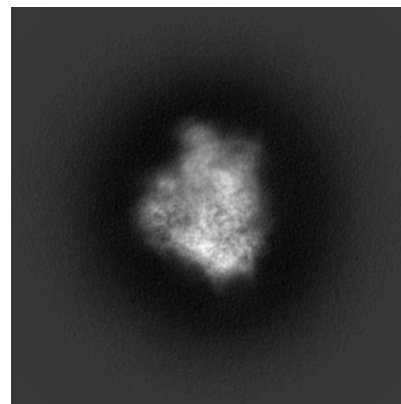
6.1.1 Primary map



X

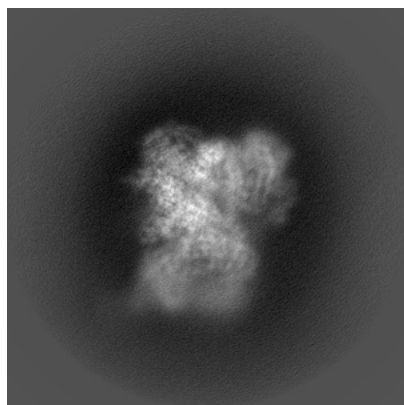


Y

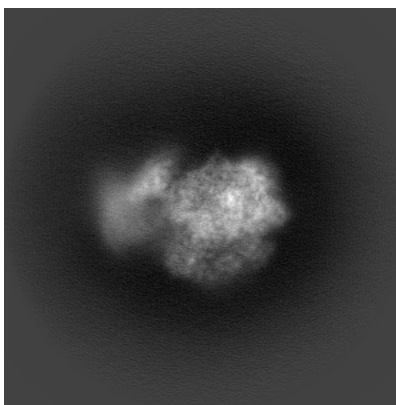


Z

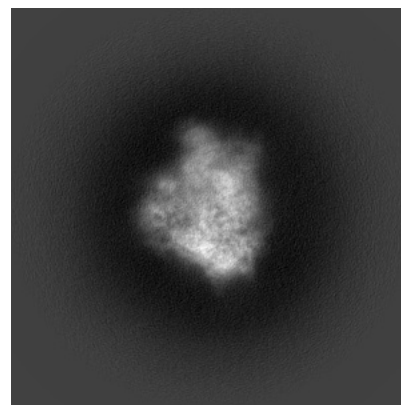
6.1.2 Raw map



X



Y

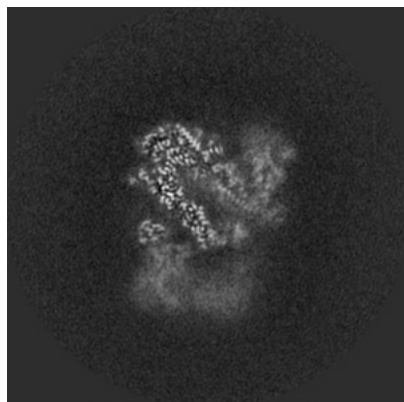


Z

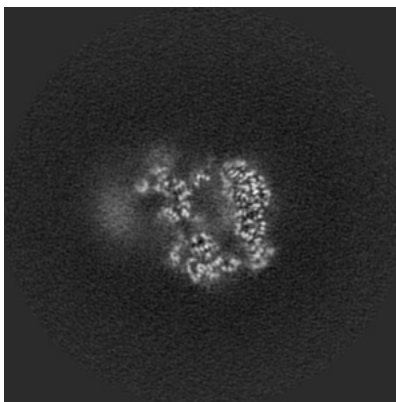
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

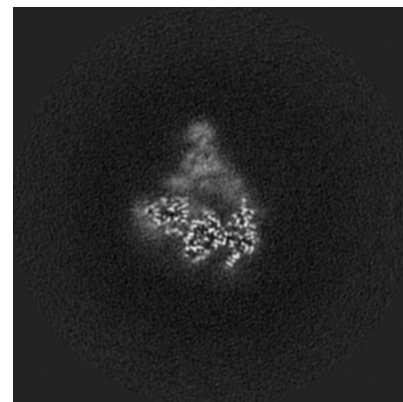
6.2.1 Primary map



X Index: 160

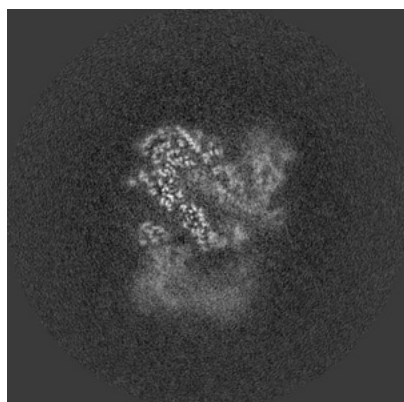


Y Index: 160

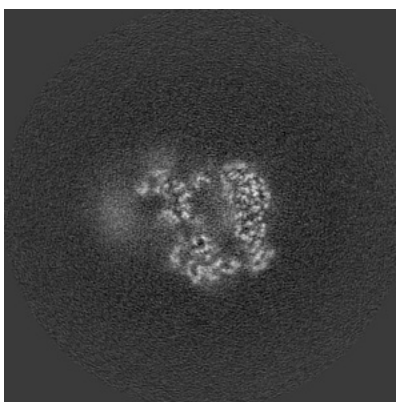


Z Index: 160

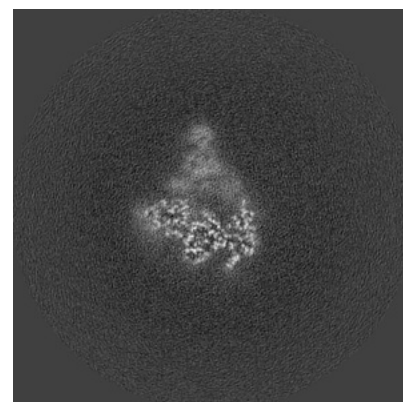
6.2.2 Raw map



X Index: 160



Y Index: 160

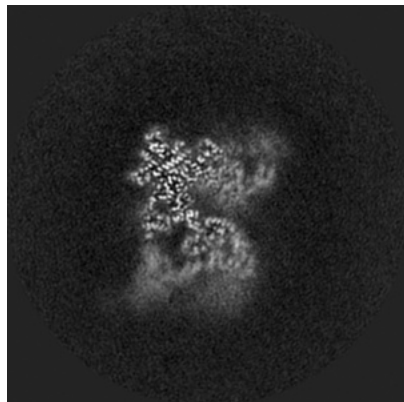


Z Index: 160

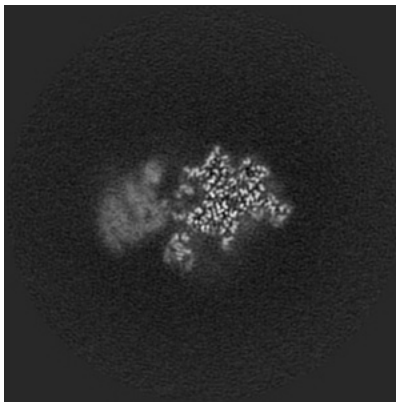
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

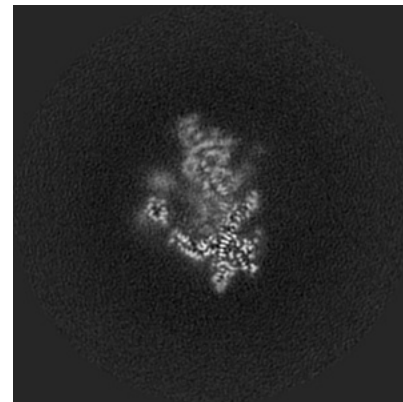
6.3.1 Primary map



X Index: 171

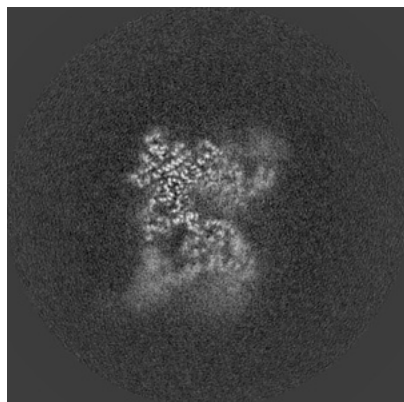


Y Index: 128

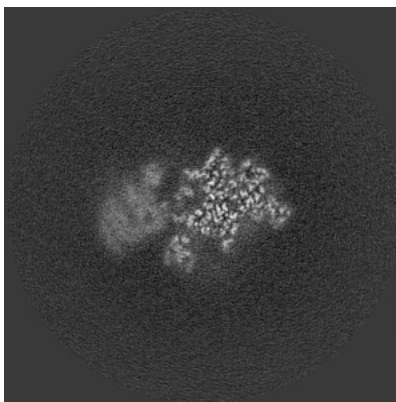


Z Index: 181

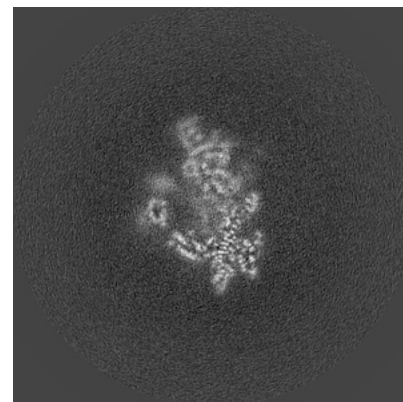
6.3.2 Raw map



X Index: 171



Y Index: 128

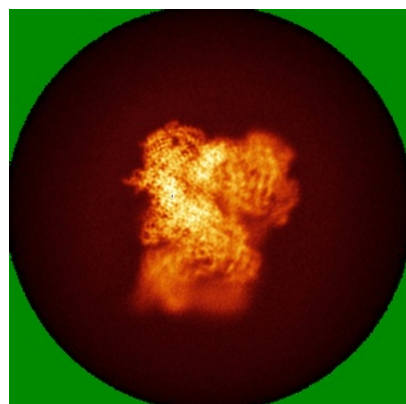


Z Index: 180

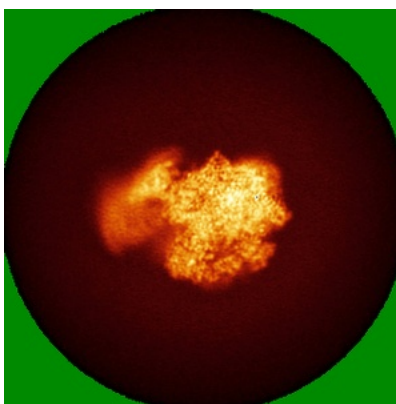
The images above show the largest variance slices of the map in three orthogonal directions.

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

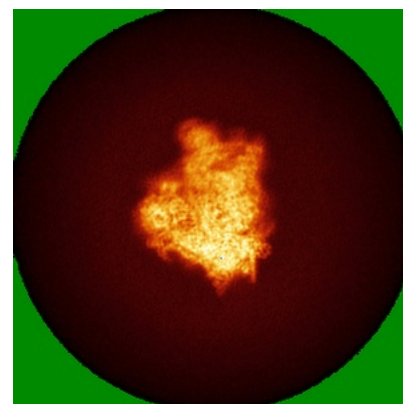
6.4.1 Primary map



X

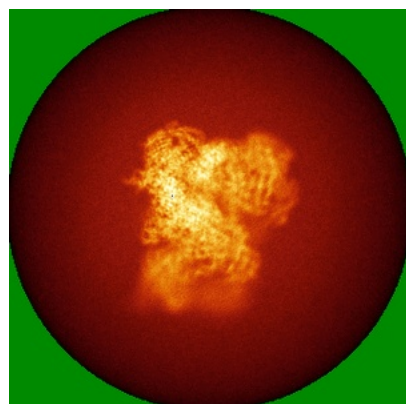


Y

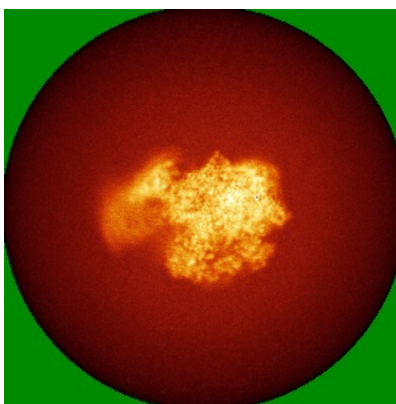


Z

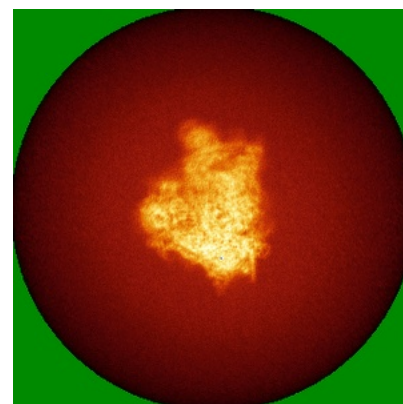
6.4.2 Raw map



X



Y



Z

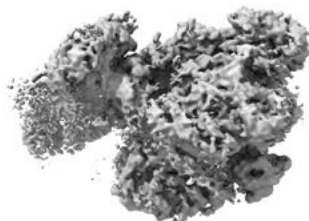
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

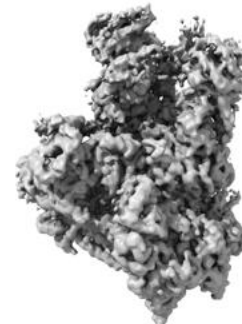
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

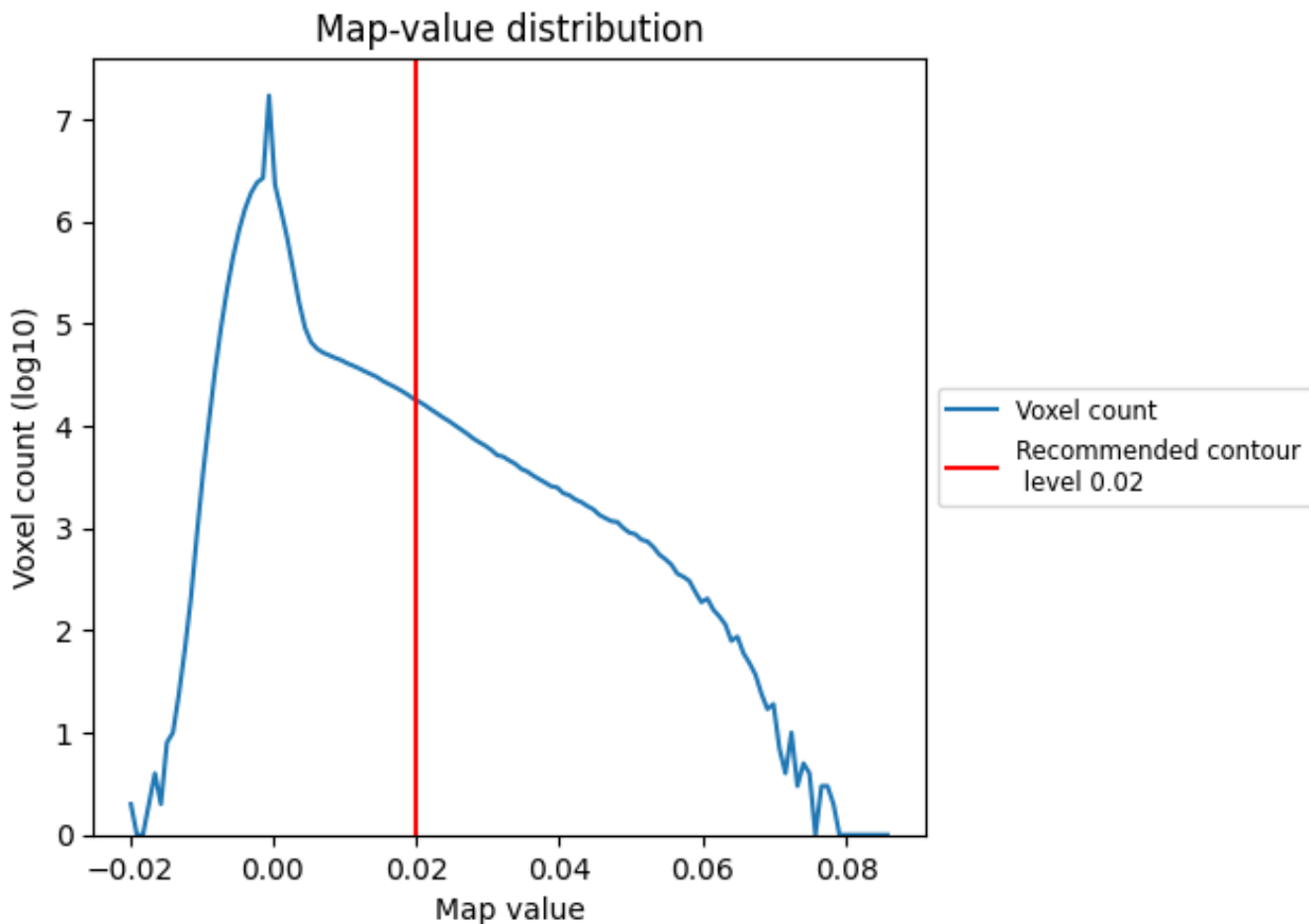
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

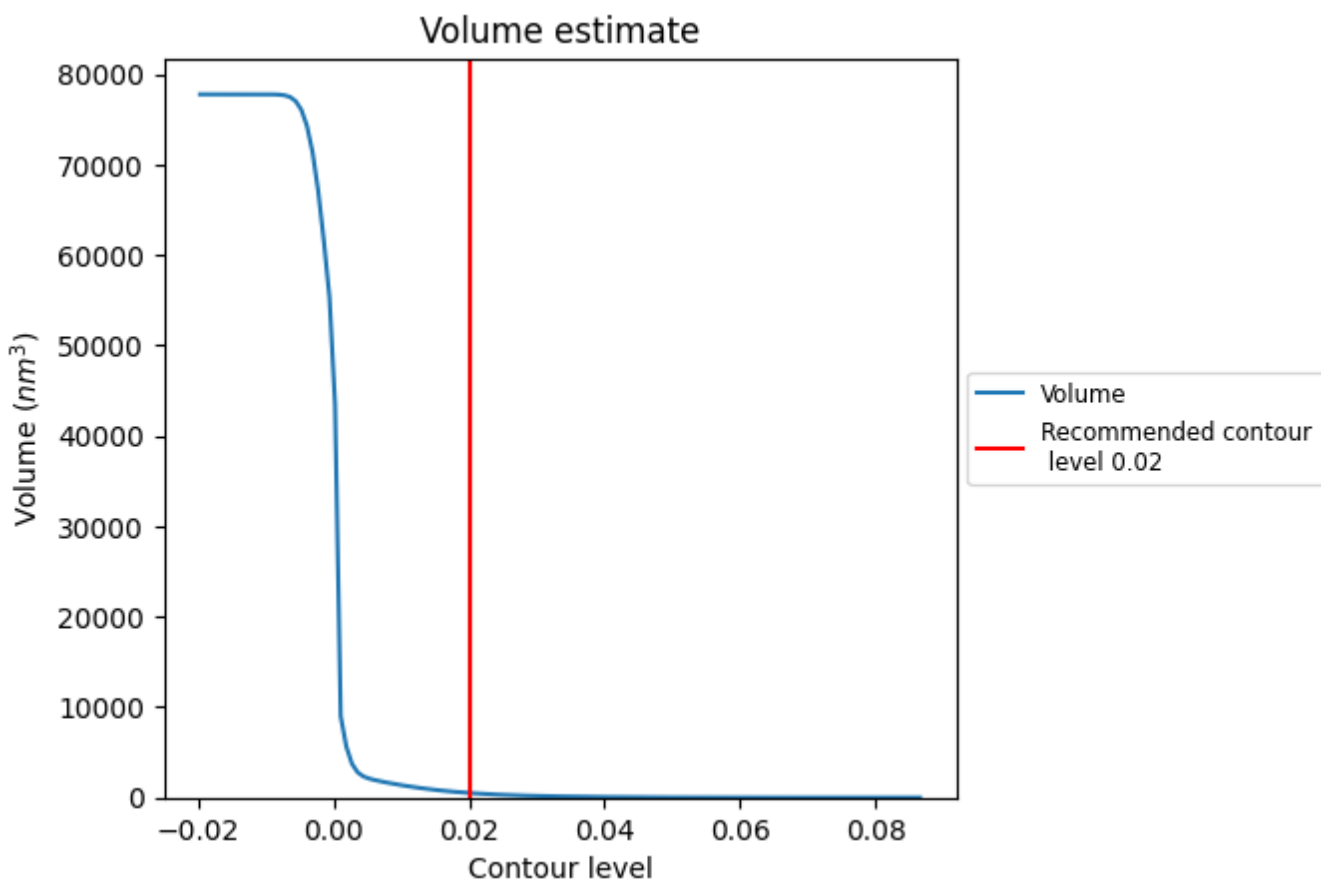
This section contains the results of statistical analysis of the map.

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.

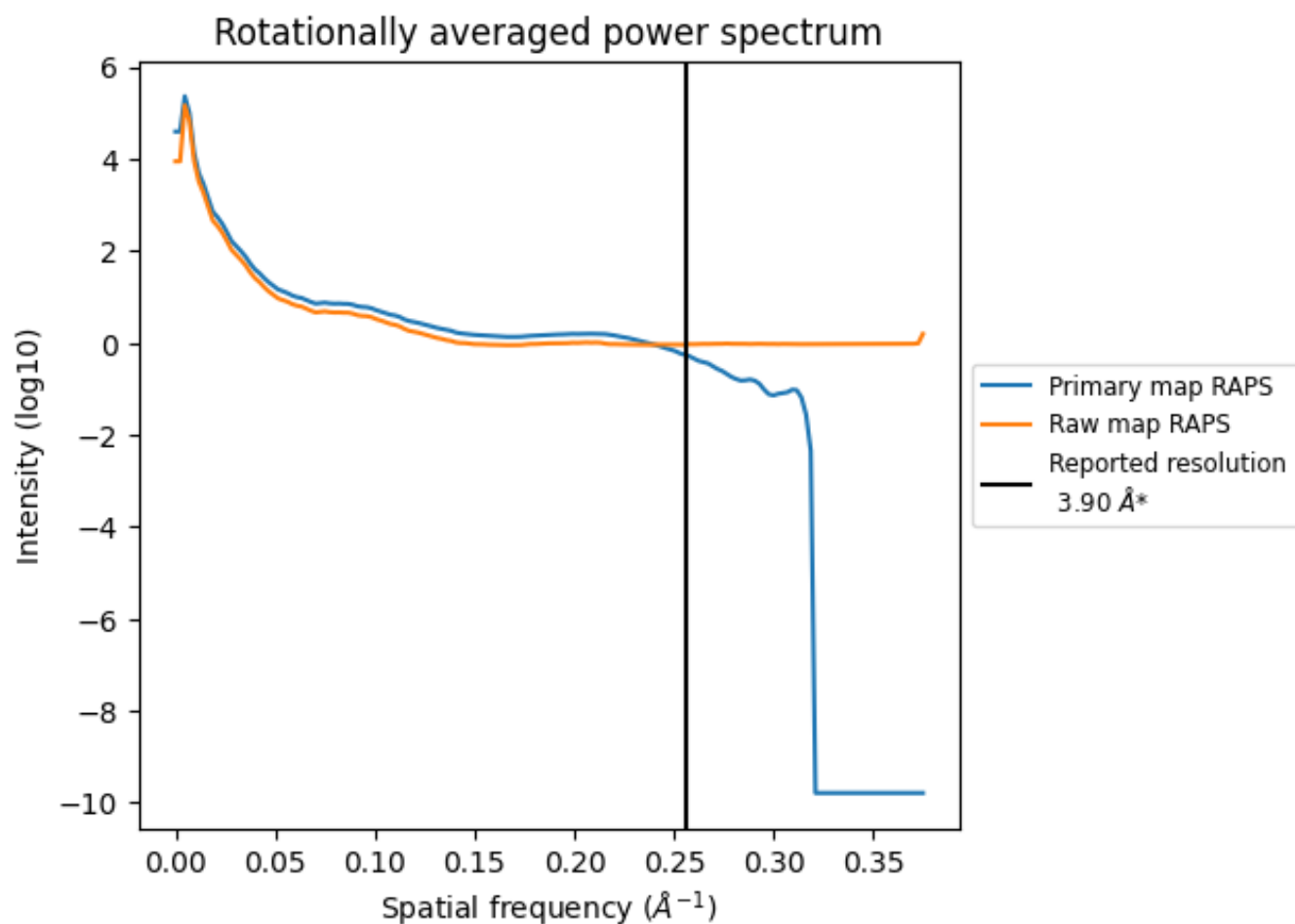
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 507 nm^3 ; this corresponds to an approximate mass of 458 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](#)

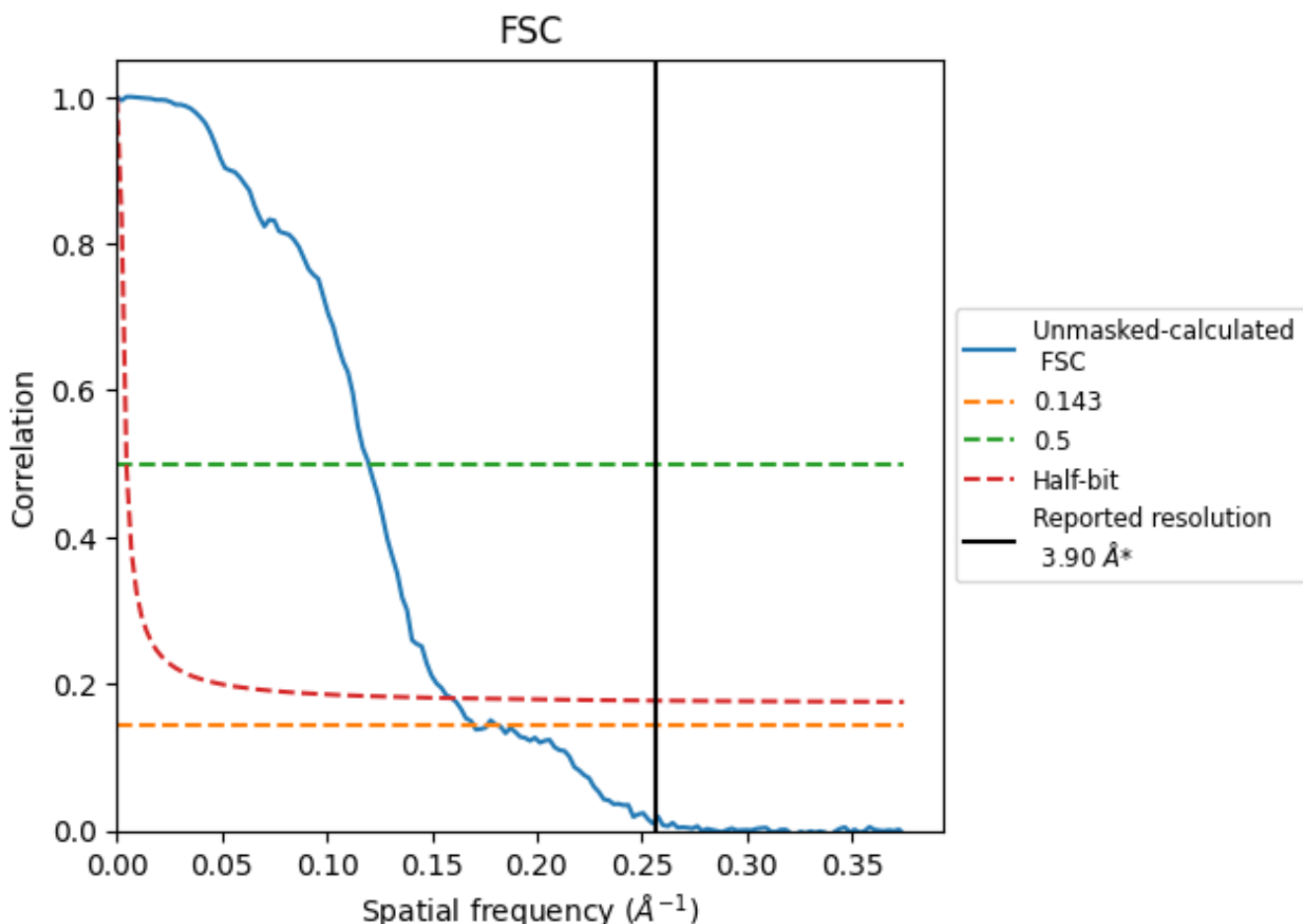


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

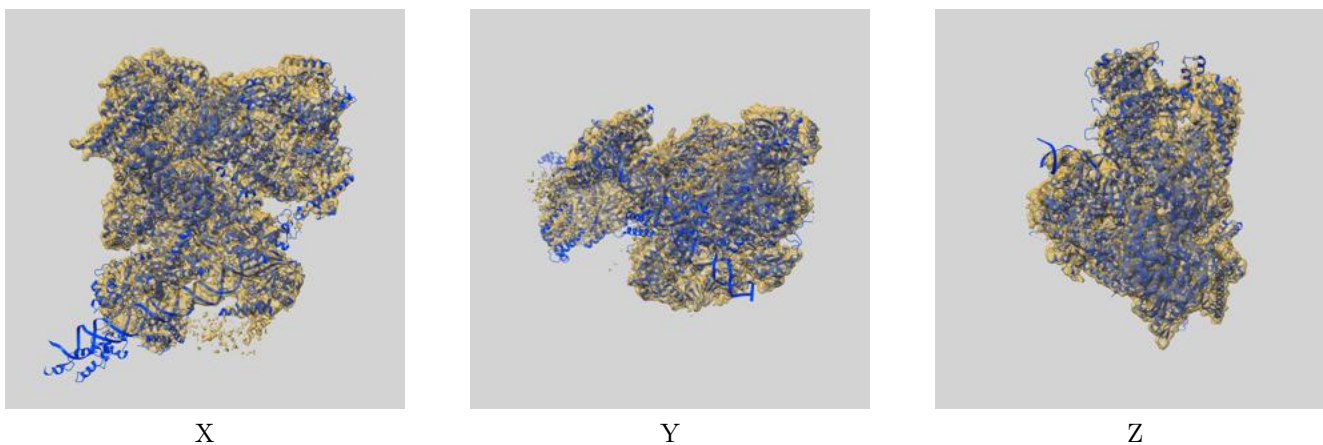
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.89	8.34	6.27

*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 5.89 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

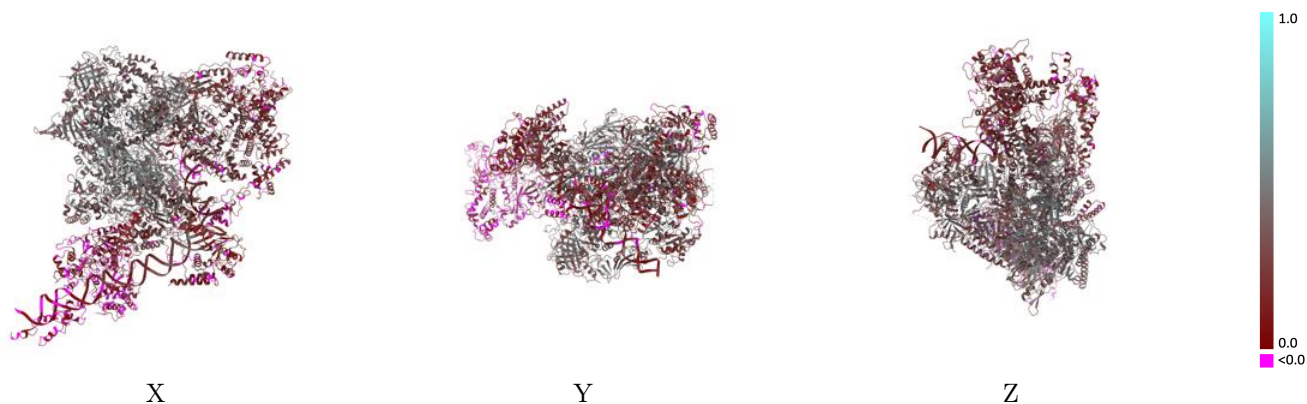
This section contains information regarding the fit between EMDB map EMD-35712 and PDB model 8ITY. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



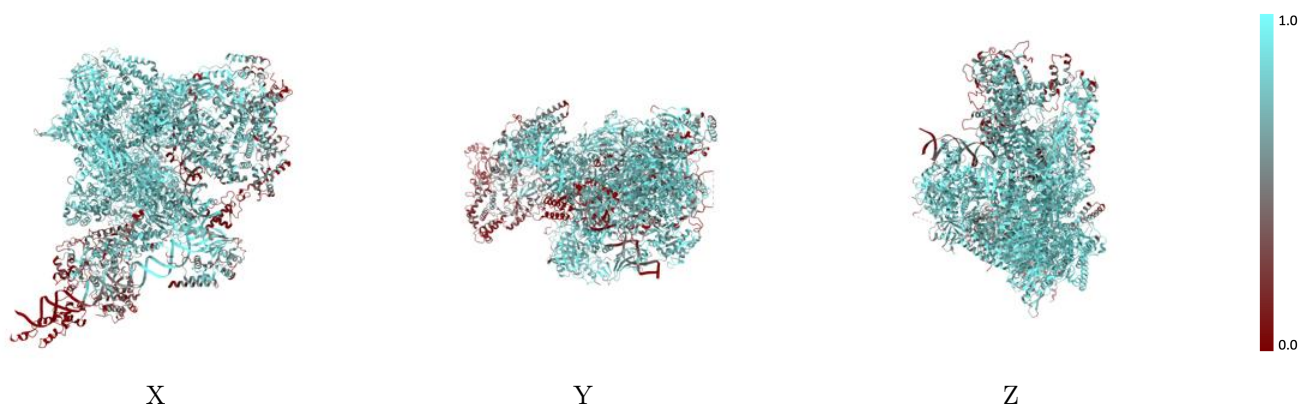
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



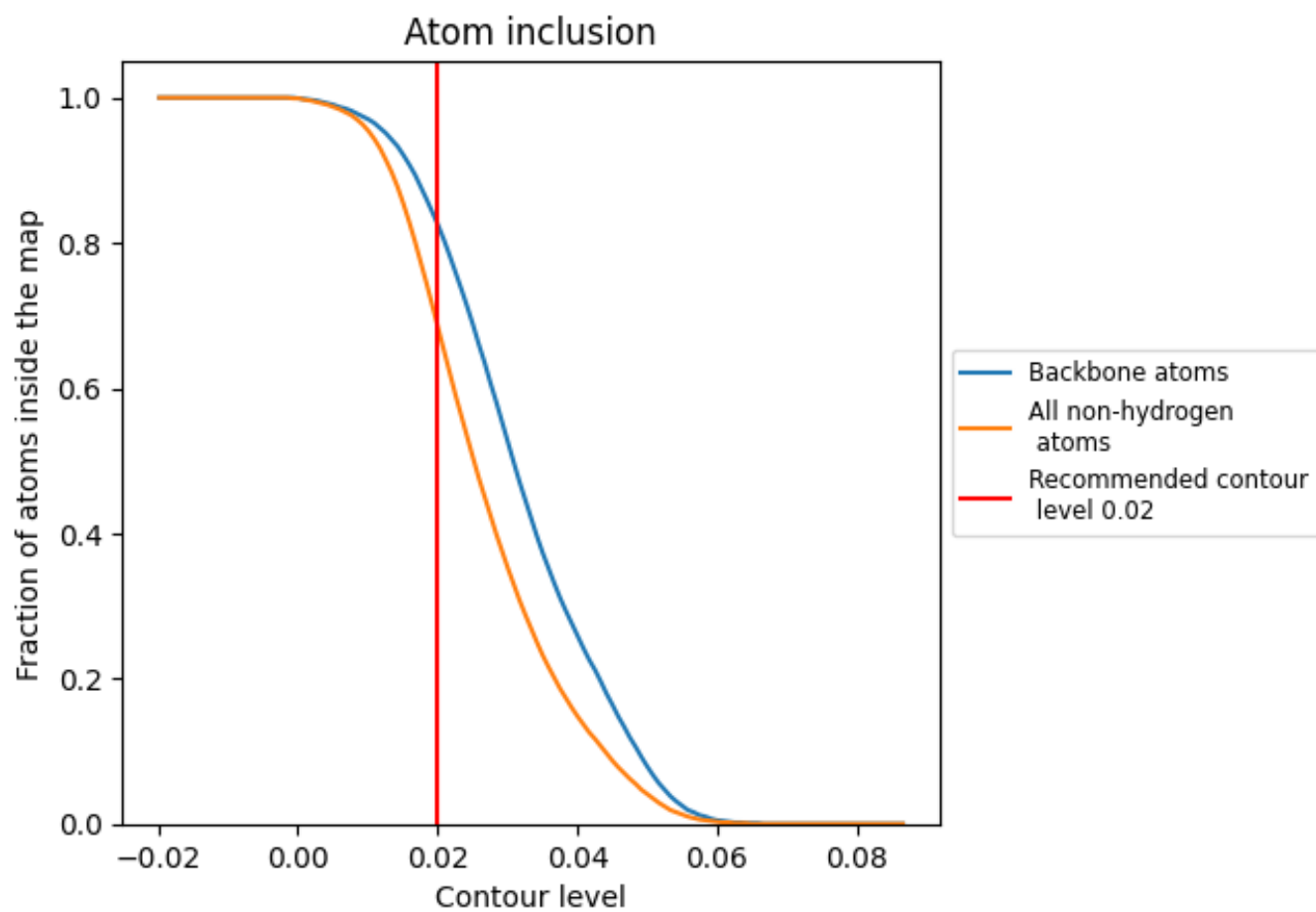
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 69% 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	 0.6860	 0.2910
1	 0.3140	 0.0520
3	 0.3420	 0.0470
4	 0.2820	 0.0910
A	 0.8060	 0.3660
B	 0.8560	 0.4260
C	 0.8460	 0.4350
D	 0.6650	 0.2070
E	 0.8000	 0.3420
F	 0.8700	 0.4210
G	 0.7840	 0.2740
H	 0.7880	 0.4100
I	 0.8170	 0.3700
J	 0.8980	 0.4530
K	 0.8540	 0.4170
L	 0.8170	 0.3780
M	 0.7610	 0.3630
N	 0.7110	 0.3530
O	 0.6030	 0.2180
P	 0.3090	 0.1460
Q	 0.5560	 0.2040
U	 0.7340	 0.2040
V	 0.6650	 0.2470
W	 0.6020	 0.1580
X	 0.5470	 0.1380
Y	 0.5640	 0.1550

