



## Full wwPDB EM Validation Report ⓘ

Sep 17, 2023 – 01:07 PM JST

PDB ID : 7YCX  
EMDB ID : EMD-33741  
Title : The structure of INTAC-PEC complex  
Authors : Zheng, H.; Jin, Q.; Wang, X.; Qi, Y.; Liu, W.; Ren, Y.; Zhao, D.; Chen, F.X.;  
Cheng, J.; Chen, X.; Xu, Y.  
Deposited on : 2022-07-02  
Resolution : 4.18 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

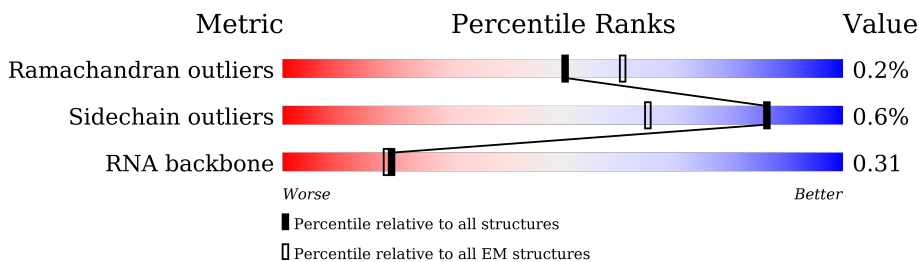
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.18 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2190	
2	B	1204	
3	D	963	
4	E	1019	
5	F	887	
6	G	962	
7	H	995	
8	I	658	


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Mol	Chain	Length	Quality of chain
9	K	600	13% 97% ..
10	M	17	100%
11	P	589	98% .
12	Q	309	95% 5%
13	U	27	100%
14	1	1970	73% 26%
15	2	1174	94% 5%
16	3	271	96% .
17	4	210	99% .
18	5	127	7% 63% 36%
19	6	150	7% 97% ..
20	7	125	5% 94% 6%
21	8	67	99% .
22	9	117	100%
23	a	58	78% 21%
24	b	48	10% 75% 25%
25	c	23	35% 65%
26	d	48	15% 94% 6%
27	e	528	12% 34% 65%
28	f	580	26% 83% 17%
29	g	590	27% 90% 9%
30	h	380	5% 94%
31	i	121	95% 95% ..
32	j	1087	23% 44% 56%
33	k	172	11% 98% ..

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Mol	Chain	Length	Quality of chain
34	1	142	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '9%', a large green segment in the middle labeled '89%', and a grey segment on the right labeled '10%'. The segments are separated by thin white lines.</p>

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 113089 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 Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1779	13054	8226	2322	2432	74	0	0

- Molecule 2 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1061	8328	5322	1412	1530	64	0	0

- Molecule 3 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	828	6205	3931	1085	1158	31	0	0

- Molecule 4 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	798	5244	3284	988	958	14	0	0

- Molecule 5 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	560	4395	2809	750	813	23	0	0

- Molecule 6 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	910	6928	4382	1212	1293	41	0	0

- Molecule 7 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	937	7440	4761	1274	1361	44	0	0

- Molecule 8 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	633	4985	3210	815	926	34	0	0

- Molecule 9 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	590	4646	2964	806	841	35	0	0

- Molecule 10 is a protein called Unknown2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	M	17	85	51	17	17	0	0

- Molecule 11 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	581	4527	2877	763	860	27	0	0

- Molecule 12 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Q	293	2366	1497	405	449	15	0	0

- Molecule 13 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	U	27	135	81	27	27	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB1, DNA-directed RNA polymerase II subunit RPB1, CTD1, CTD2, CTD3, CTD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	1	1451	11345	7135	2033	2109	68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	2	1113	8649	5489	1515	1581	64	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	3	259	2048	1289	354	399	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	4	209	1721	1089	300	324	8	0	0

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	5	81	649	413	111	120	5	0	0

- Molecule 19 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		
19	6	148	1186	750	194	237	5	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	7	117	950	587	169	183	11	0	0

- Molecule 21 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 22 is a protein called RNA\_pol\_L\_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 23 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 24 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	36	Total	C	N	O	P	0	0
			752	351	153	212	36		

- Molecule 25 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	23	Total	C	N	O	P	0	0
			406	179	56	148	23		

- Molecule 26 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	45	Total	C	N	O	P	0	0
			909	431	157	276	45		

- Molecule 27 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	183	Total	C	N	O	S	0	0
			1410	895	239	269	7		

- Molecule 28 is a protein called Negative elongation factor B.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	f	480	1920	960	480	480	0	0

- Molecule 29 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	g	534	3764	2382	653	710	19	0	0

- Molecule 30 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	h	22	109	65	22	22	0	0

- Molecule 31 is a protein called Transcription elongation factor SPT4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 32 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	j	482	3854	2448	681	708	17	0	0

- Molecule 33 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	k	171	1299	849	205	238	7	0	0

- Molecule 34 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	128	Total	C	N	O	S	0	0
			997	629	169	195	4		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	K	2	Total	Zn	0
			2	2	
35	1	2	Total	Zn	0
			2	2	
35	2	1	Total	Zn	0
			1	1	
35	3	1	Total	Zn	0
			1	1	
35	7	2	Total	Zn	0
			2	2	
35	8	1	Total	Zn	0
			1	1	
35	a	1	Total	Zn	0
			1	1	

- Molecule 36 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
36	Q	2	Total	Mn	0
			2	2	

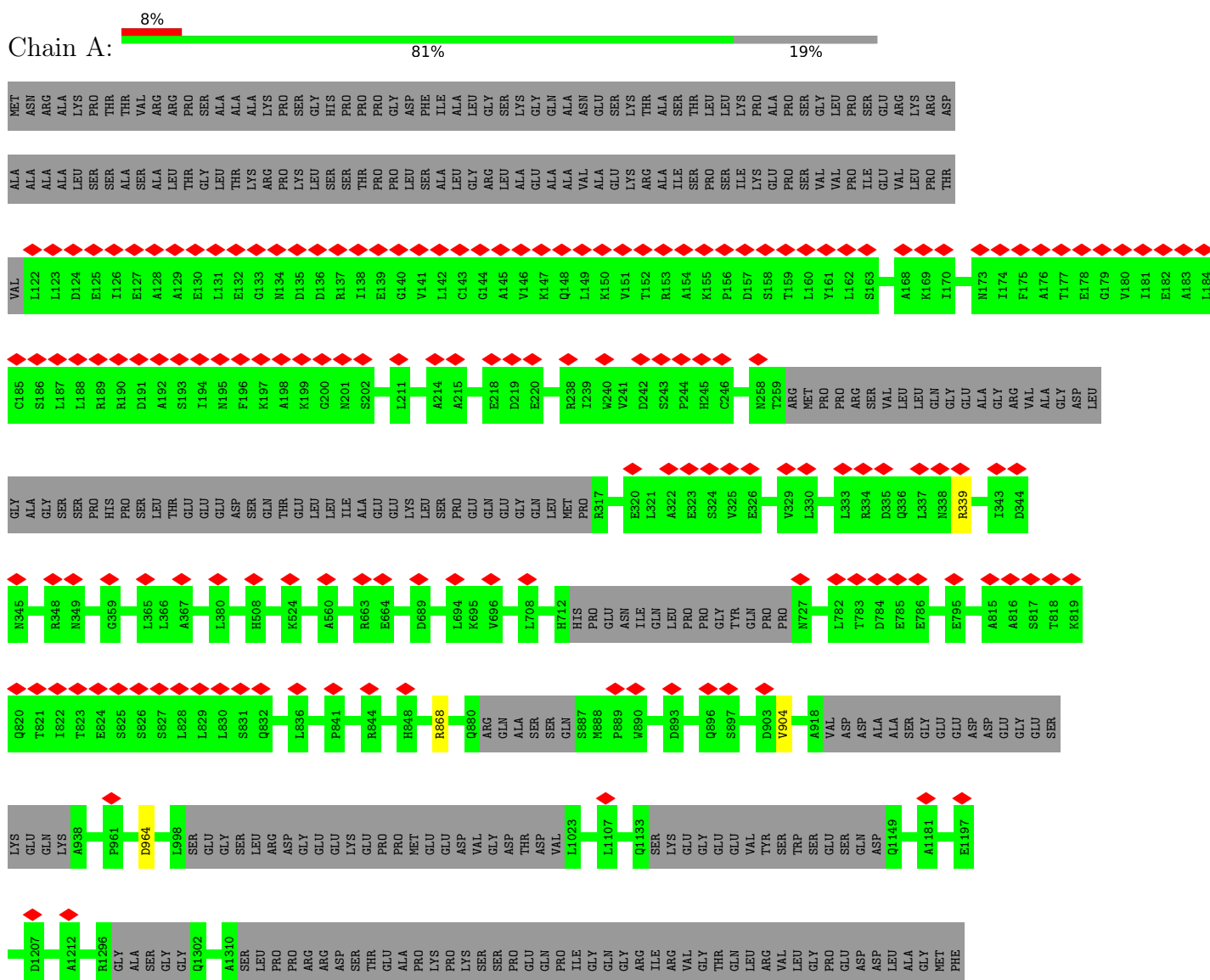
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	1	1	Total	Mg	0
			1	1	

### 3 Residue-property plots

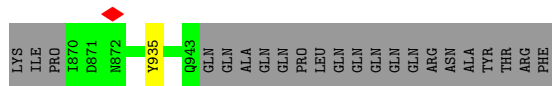
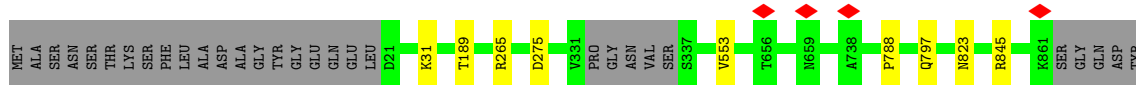
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Integrator complex subunit 1

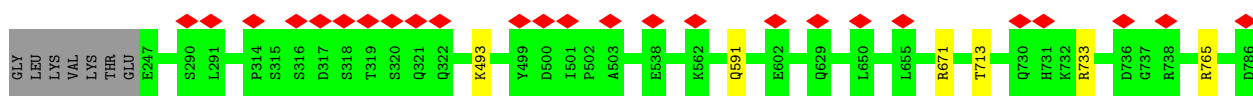
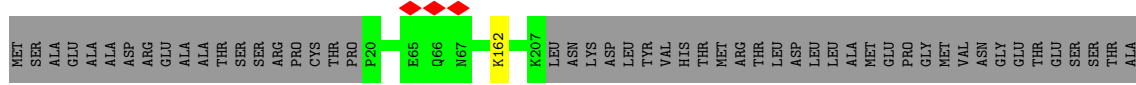




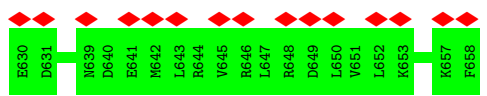
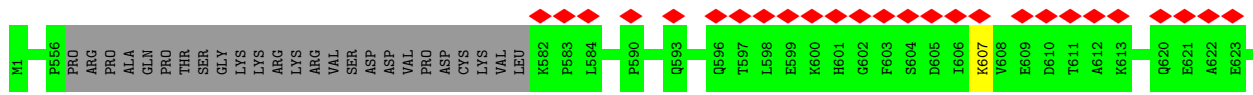




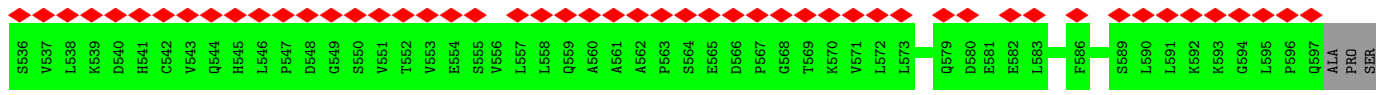
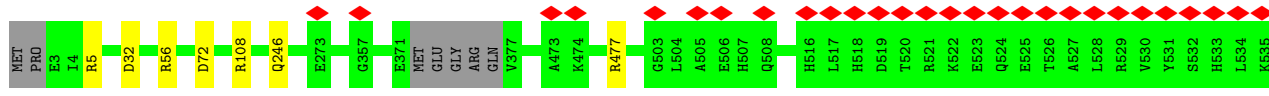
• Molecule 7: Integrator complex subunit 8



• Molecule 8: Integrator complex subunit 9



• Molecule 9: Integrator complex subunit 11

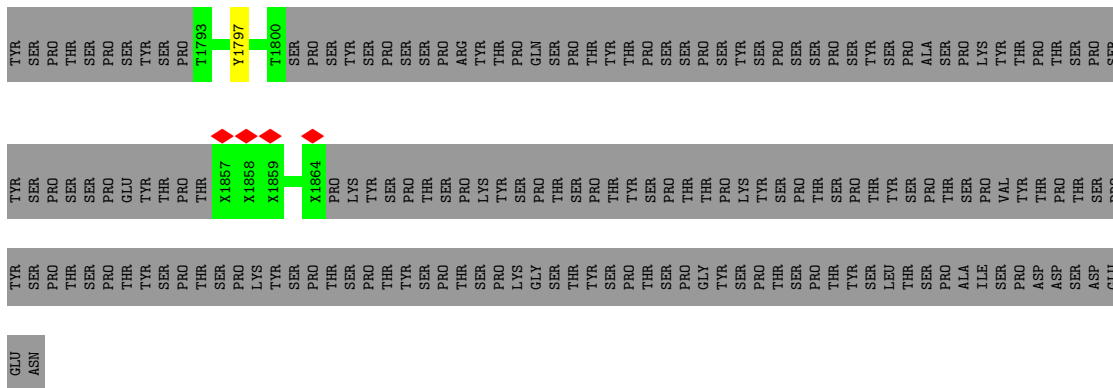


• Molecule 10: Unknown2



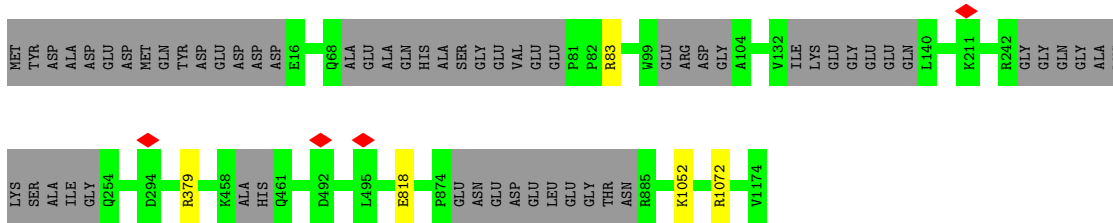
There are no outlier residues recorded for this chain.





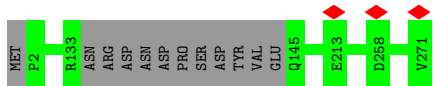
• Molecule 15: DNA-directed RNA polymerase subunit beta

Chain 2: 94% 5%



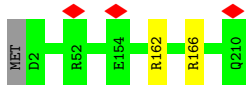
• Molecule 16: DNA-directed RNA polymerase II subunit RPB3

Chain 3: 96%



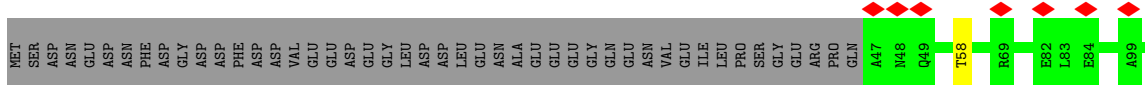
• Molecule 17: DNA-directed RNA polymerase II subunit E

Chain 4: 99%



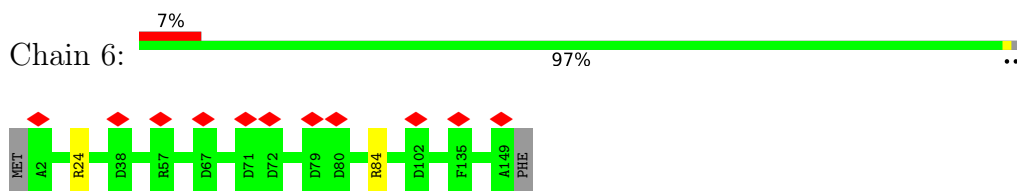
• Molecule 18: DNA-directed RNA polymerase II subunit F

Chain 5: 7% 63% 36%

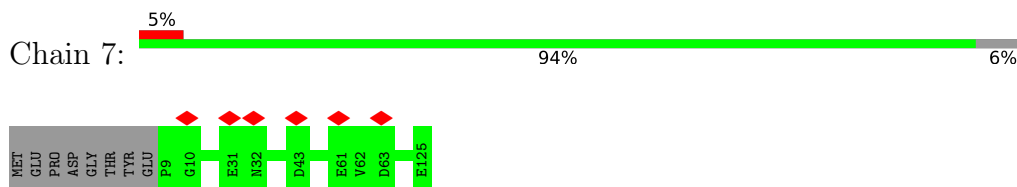




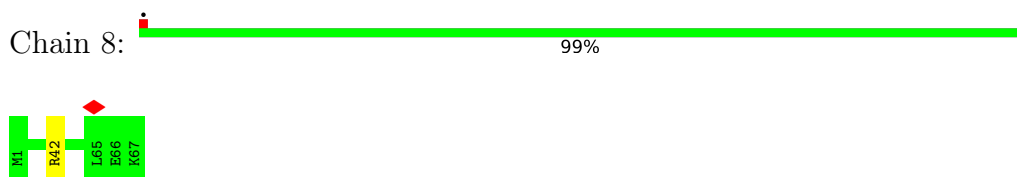
- Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC3



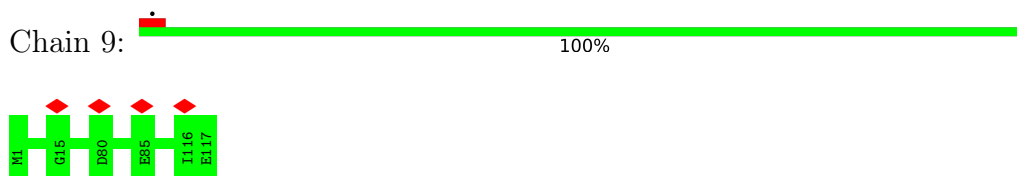
- Molecule 20: DNA-directed RNA polymerase II subunit RPB9



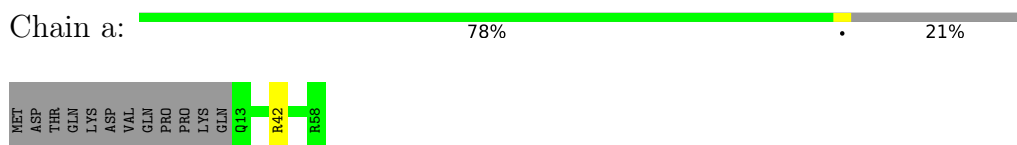
- Molecule 21: DNA-directed RNA polymerases I, II, and III subunit RPABC5



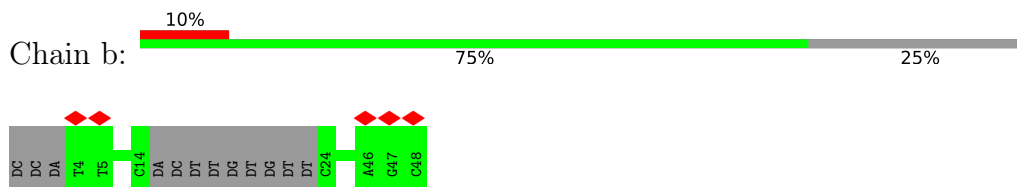
- Molecule 22: RNA\_pol\_L\_2 domain-containing protein



- Molecule 23: RPB12

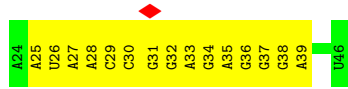


- Molecule 24: non-template DNA

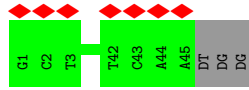
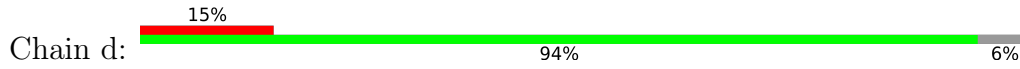


- Molecule 25: RNA

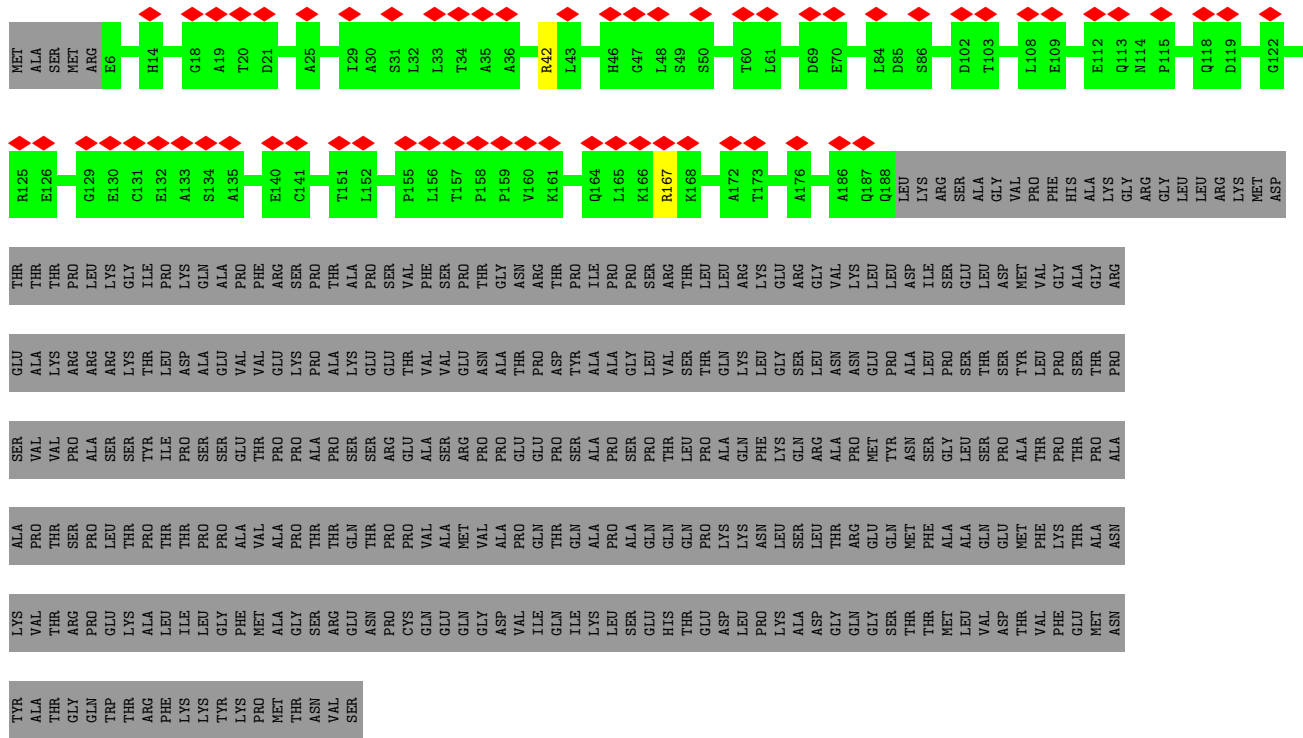




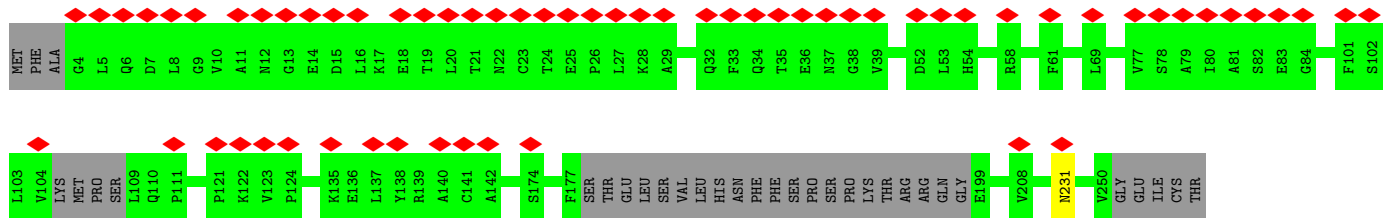
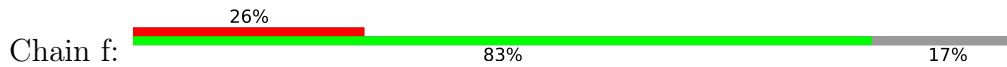
• Molecule 26: template DNA

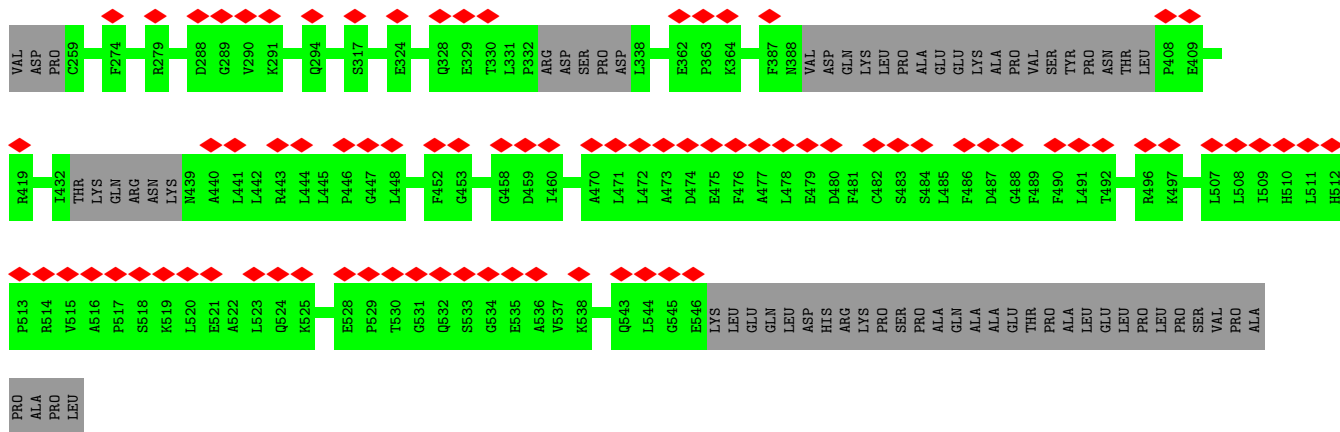


• Molecule 27: Negative elongation factor A

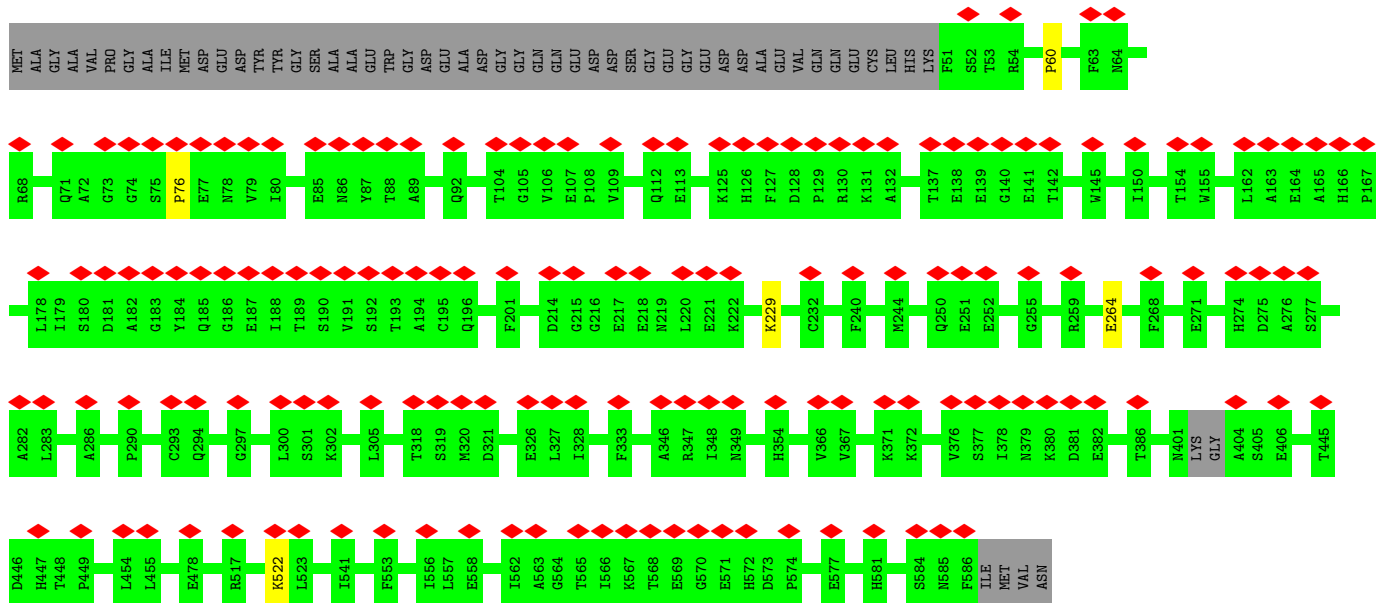
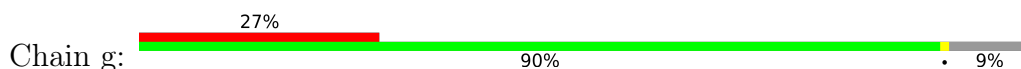


• Molecule 28: Negative elongation factor B

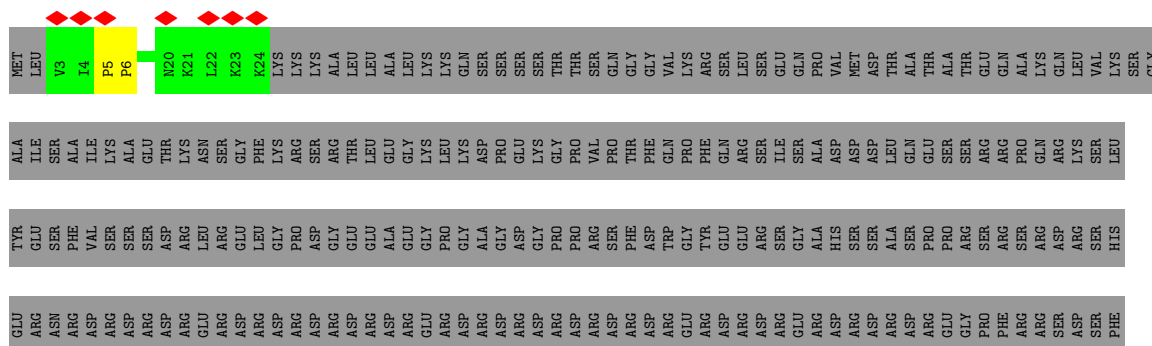




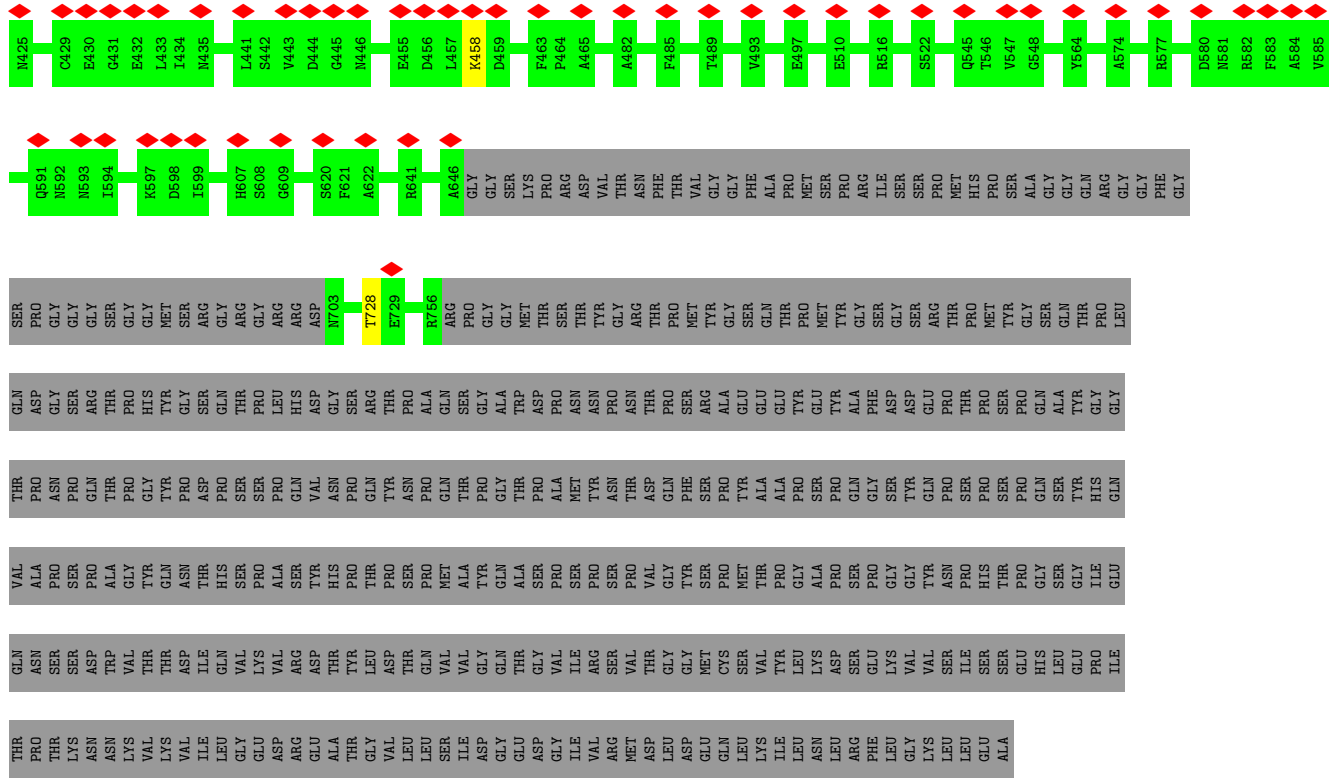
• Molecule 29: Negative elongation factor C/D



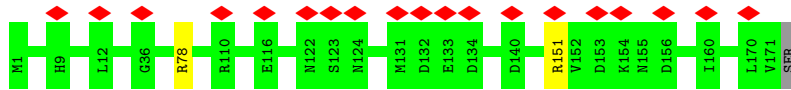
• Molecule 30: Negative elongation factor E



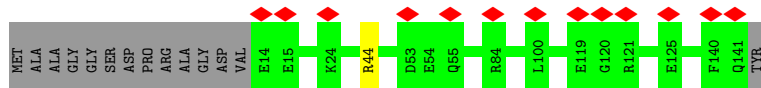
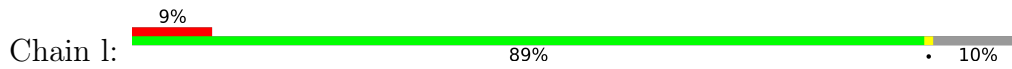




• Molecule 33: DNA-directed RNA polymerase II subunit RPB7



• Molecule 34: DNA-directed RNA polymerase II subunit RPB4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41201	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	442.68002, 442.68002, 442.68002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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: MN, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/13264	0.46	0/18049
2	B	0.31	0/8474	0.48	0/11498
3	D	0.31	0/6315	0.49	0/8583
4	E	0.26	0/5344	0.47	0/7312
5	F	0.27	0/4508	0.49	0/6131
6	G	0.32	0/7038	0.49	0/9532
7	H	0.27	0/7583	0.46	0/10280
8	I	0.32	0/5110	0.49	0/6959
9	K	0.30	0/4747	0.50	0/6412
11	P	0.27	0/4601	0.47	0/6246
12	Q	0.29	0/2423	0.51	0/3285
14	1	0.31	0/11492	0.52	0/15525
15	2	0.32	0/8823	0.52	0/11947
16	3	0.31	0/2091	0.50	0/2843
17	4	0.26	0/1752	0.52	0/2366
18	5	0.33	0/659	0.54	0/889
19	6	0.30	0/1207	0.56	0/1628
20	7	0.27	0/973	0.50	0/1316
21	8	0.38	0/542	0.54	0/730
22	9	0.28	0/956	0.48	0/1294
23	a	0.31	0/395	0.63	0/524
24	b	0.31	0/846	0.68	0/1304
25	c	0.51	0/450	0.88	1/696 (0.1%)
26	d	0.37	0/1014	0.73	0/1560
27	e	0.24	0/1434	0.47	0/1948
28	f	0.22	0/1913	0.40	0/2379
29	g	0.25	0/3830	0.44	2/5236 (0.0%)
30	h	0.27	0/108	0.74	2/149 (1.3%)
31	i	0.28	0/927	0.55	0/1250
32	j	0.26	0/3920	0.51	0/5276
33	k	0.26	0/1330	0.46	0/1813
34	l	0.25	0/1011	0.46	0/1364

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.29	0/115080	0.50	5/156324 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	38	G	C2'-C3'-O3'	5.75	122.90	113.70
29	g	60	PRO	N-CA-CB	5.70	110.14	103.30
30	h	5	PRO	N-CA-CB	5.62	110.05	103.30
30	h	6	PRO	N-CA-CB	5.59	110.01	103.30
29	g	76	PRO	N-CA-CB	5.02	109.33	103.30

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	A	1755/2190 (80%)	1671 (95%)	82 (5%)	2 (0%)	51	85
2	B	1045/1204 (87%)	998 (96%)	47 (4%)	0	100	100
3	D	814/963 (84%)	754 (93%)	54 (7%)	6 (1%)	22	62
4	E	794/1019 (78%)	734 (92%)	57 (7%)	3 (0%)	34	71
5	F	554/887 (62%)	541 (98%)	13 (2%)	0	100	100
6	G	904/962 (94%)	830 (92%)	70 (8%)	4 (0%)	34	71
7	H	933/995 (94%)	892 (96%)	41 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	629/658 (96%)	592 (94%)	37 (6%)	0	100	100
9	K	586/600 (98%)	551 (94%)	33 (6%)	2 (0%)	41	75
11	P	579/589 (98%)	559 (96%)	20 (4%)	0	100	100
12	Q	291/309 (94%)	267 (92%)	24 (8%)	0	100	100
14	1	1425/1970 (72%)	1335 (94%)	86 (6%)	4 (0%)	41	75
15	2	1099/1174 (94%)	995 (90%)	104 (10%)	0	100	100
16	3	255/271 (94%)	239 (94%)	16 (6%)	0	100	100
17	4	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
18	5	79/127 (62%)	77 (98%)	2 (2%)	0	100	100
19	6	146/150 (97%)	135 (92%)	11 (8%)	0	100	100
20	7	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
21	8	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
22	9	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
23	a	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
27	e	181/528 (34%)	177 (98%)	4 (2%)	0	100	100
28	f	466/580 (80%)	451 (97%)	14 (3%)	1 (0%)	47	80
29	g	530/590 (90%)	501 (94%)	29 (6%)	0	100	100
30	h	20/380 (5%)	20 (100%)	0	0	100	100
31	i	114/121 (94%)	111 (97%)	3 (3%)	0	100	100
32	j	470/1087 (43%)	451 (96%)	19 (4%)	0	100	100
33	k	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
34	l	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
All	All	14510/18245 (80%)	13686 (94%)	802 (6%)	22 (0%)	50	80

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1816	PRO
3	D	63	PRO
3	D	106	SER
3	D	561	MET
4	E	282	ILE
4	E	740	PRO
4	E	742	PRO

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Mol	Chain	Res	Type
6	G	553	VAL
14	1	910	LYS
1	A	904	VAL
3	D	141	LEU
28	f	231	ASN
3	D	688	LYS
9	K	72	ASP
6	G	189	THR
6	G	788	PRO
6	G	797	GLN
9	K	32	ASP
14	1	78	MET
3	D	147	ILE
14	1	1763	SER
14	1	188	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1253/1907 (66%)	1248 (100%)	5 (0%)	91	94
2	B	946/1072 (88%)	943 (100%)	3 (0%)	92	95
3	D	617/845 (73%)	613 (99%)	4 (1%)	86	92
4	E	395/812 (49%)	392 (99%)	3 (1%)	81	89
5	F	490/796 (62%)	488 (100%)	2 (0%)	91	94
6	G	744/840 (89%)	738 (99%)	6 (1%)	81	89
7	H	822/896 (92%)	815 (99%)	7 (1%)	78	87
8	I	575/600 (96%)	574 (100%)	1 (0%)	93	96
9	K	505/520 (97%)	500 (99%)	5 (1%)	76	86
11	P	508/512 (99%)	506 (100%)	2 (0%)	91	94
12	Q	259/274 (94%)	259 (100%)	0	100	100
14	1	1239/1736 (71%)	1232 (99%)	7 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	2	908/1027 (88%)	903 (99%)	5 (1%)	86	92
16	3	227/248 (92%)	227 (100%)	0	100	100
17	4	191/192 (100%)	189 (99%)	2 (1%)	76	86
18	5	70/111 (63%)	69 (99%)	1 (1%)	67	80
19	6	129/131 (98%)	127 (98%)	2 (2%)	62	78
20	7	105/112 (94%)	105 (100%)	0	100	100
21	8	56/56 (100%)	55 (98%)	1 (2%)	59	76
22	9	106/106 (100%)	106 (100%)	0	100	100
23	a	43/55 (78%)	42 (98%)	1 (2%)	50	69
27	e	158/451 (35%)	156 (99%)	2 (1%)	69	82
29	g	339/513 (66%)	336 (99%)	3 (1%)	78	87
31	i	102/105 (97%)	101 (99%)	1 (1%)	76	86
32	j	425/940 (45%)	423 (100%)	2 (0%)	88	93
33	k	136/153 (89%)	134 (98%)	2 (2%)	65	79
34	l	104/126 (82%)	103 (99%)	1 (1%)	76	86
All	All	11452/15136 (76%)	11384 (99%)	68 (1%)	86	92

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	ARG
1	A	868	ARG
1	A	964	ASP
1	A	2051	MET
1	A	2090	ARG
2	B	329	ARG
2	B	445	THR
2	B	748	ASN
3	D	182	LYS
3	D	387	MET
3	D	492	ASN
3	D	763	ARG
4	E	734	ARG
4	E	897	THR
4	E	940	ARG
5	F	103	ARG
5	F	407	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	G	31	LYS
6	G	265	ARG
6	G	275	ASP
6	G	823	ASN
6	G	845	ARG
6	G	935	TYR
7	H	162	LYS
7	H	493	LYS
7	H	591	GLN
7	H	671	ARG
7	H	713	THR
7	H	733	ARG
7	H	765	ARG
8	I	607	LYS
9	K	5	ARG
9	K	56	ARG
9	K	108	ARG
9	K	246	GLN
9	K	477	ARG
11	P	221	ARG
11	P	304	HIS
14	1	192	ARG
14	1	407	ARG
14	1	695	ASP
14	1	1046	ARG
14	1	1138	SER
14	1	1770	SER
14	1	1797	TYR
15	2	83	ARG
15	2	379	ARG
15	2	818	GLU
15	2	1052	LYS
15	2	1072	ARG
17	4	162	ARG
17	4	166	ARG
18	5	58	THR
19	6	24	ARG
19	6	84	ARG
21	8	42	ARG
23	a	42	ARG
27	e	42	ARG
27	e	167	ARG

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Mol	Chain	Res	Type
29	g	229	LYS
29	g	264	GLU
29	g	522	LYS
31	i	73	LYS
32	j	458	LYS
32	j	728	THR
33	k	78	ARG
33	k	151	ARG
34	l	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1666	HIS
2	B	66	GLN
2	B	773	GLN
2	B	777	HIS
2	B	934	GLN
2	B	1130	GLN
3	D	164	HIS
3	D	289	HIS
3	D	553	ASN
3	D	611	GLN
3	D	625	GLN
5	F	225	GLN
5	F	462	GLN
6	G	406	GLN
6	G	425	HIS
6	G	451	HIS
6	G	823	ASN
7	H	858	GLN
7	H	894	HIS
11	P	288	GLN
12	Q	12	GLN
14	1	278	HIS
14	1	432	HIS
14	1	531	ASN
14	1	780	ASN
15	2	111	ASN
15	2	197	GLN
15	2	980	HIS
15	2	1117	HIS

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Mol	Chain	Res	Type
15	2	1129	ASN
27	e	187	GLN
34	l	43	HIS
34	l	47	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	c	22/23 (95%)	14 (63%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	c	25	A
25	c	26	U
25	c	27	A
25	c	28	A
25	c	29	C
25	c	30	C
25	c	31	G
25	c	32	G
25	c	33	A
25	c	34	G
25	c	35	A
25	c	36	G
25	c	37	G
25	c	39	A

There are no RNA pucker outliers to report.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

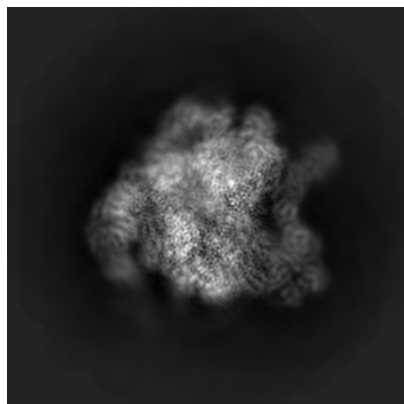
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33741. These allow visual inspection of the internal detail of the map and identification of artifacts.

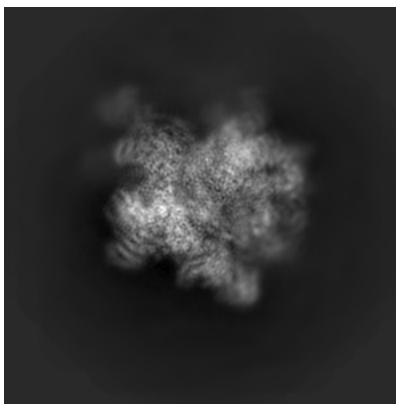
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

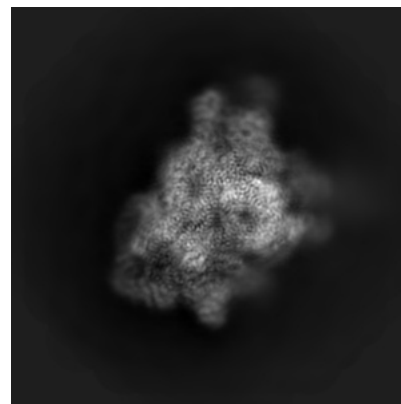
#### 6.1.1 Primary map



X

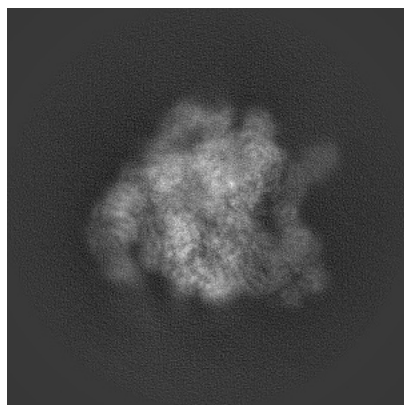


Y

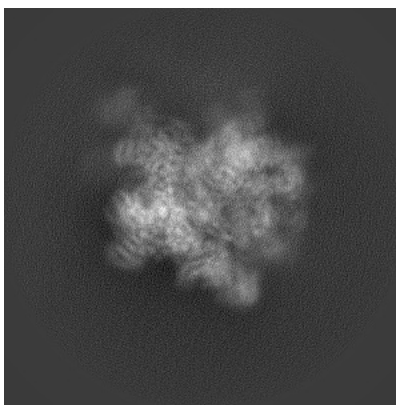


Z

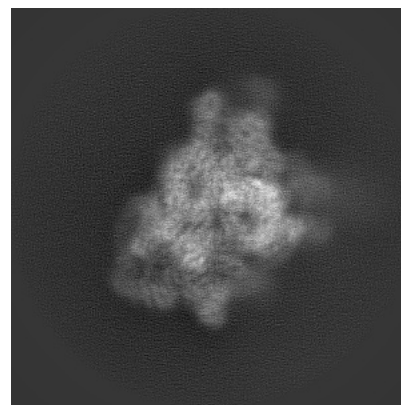
#### 6.1.2 Raw map



X



Y



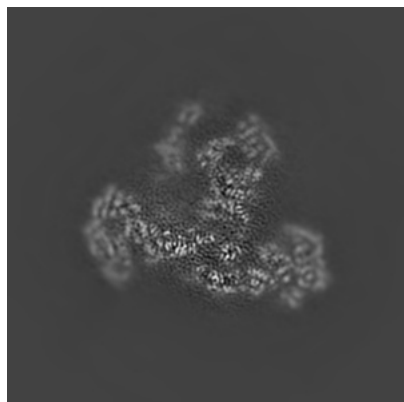
Z

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

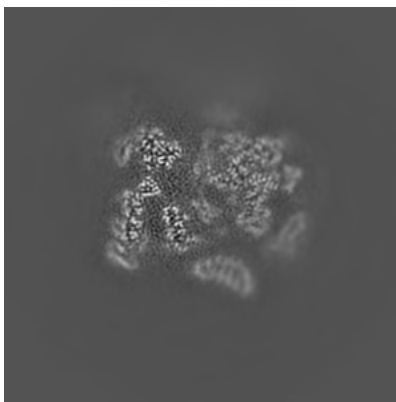


## 6.2 Central slices [i](#)

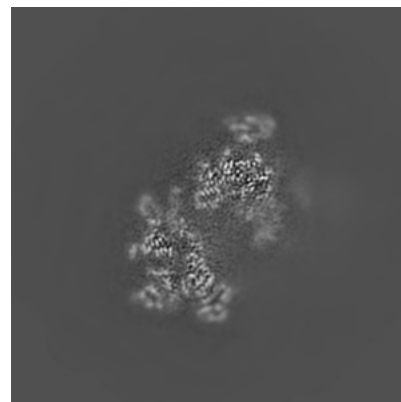
### 6.2.1 Primary map



X Index: 210

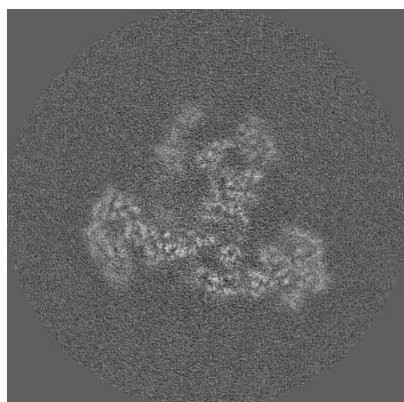


Y Index: 210

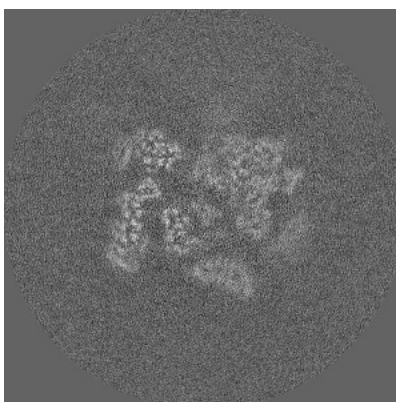


Z Index: 210

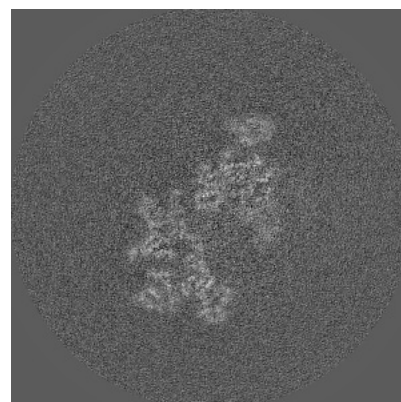
### 6.2.2 Raw map



X Index: 210



Y Index: 210

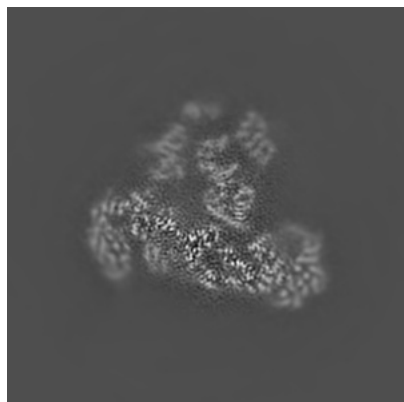


Z Index: 210

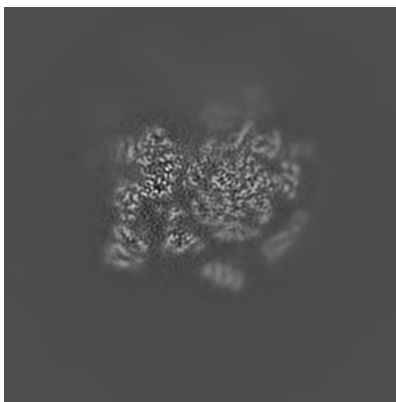
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

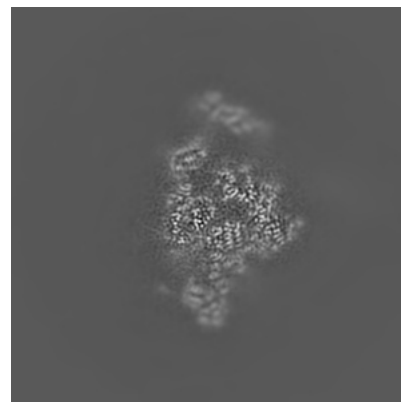
### 6.3.1 Primary map



X Index: 203

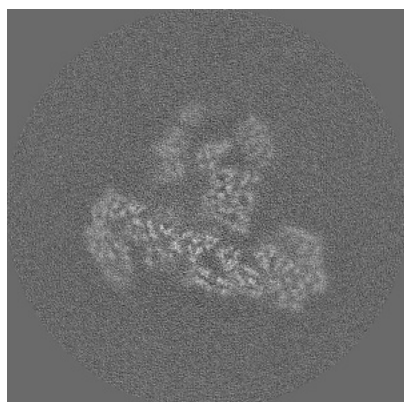


Y Index: 220

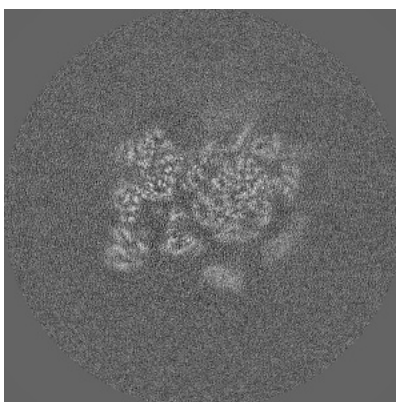


Z Index: 174

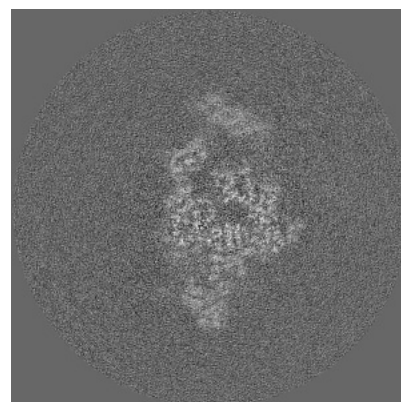
### 6.3.2 Raw map



X Index: 207



Y Index: 220

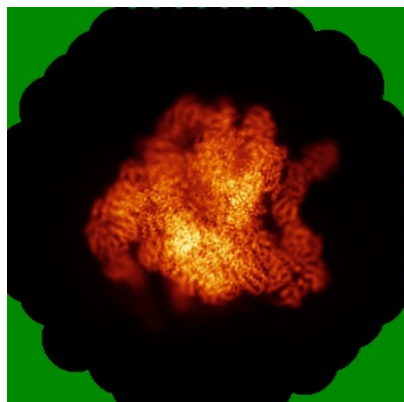


Z Index: 174

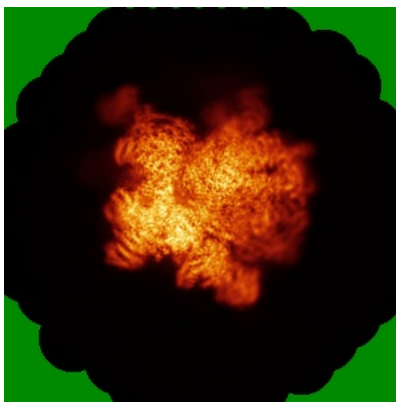
The images above show the largest variance slices of the map in three orthogonal directions.

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

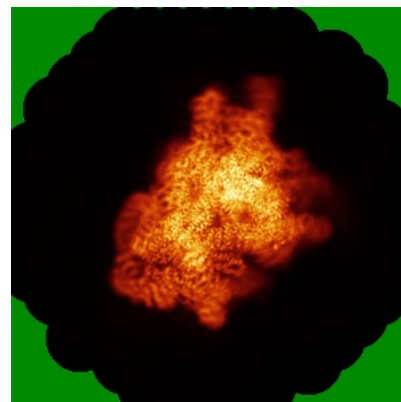
### 6.4.1 Primary map



X

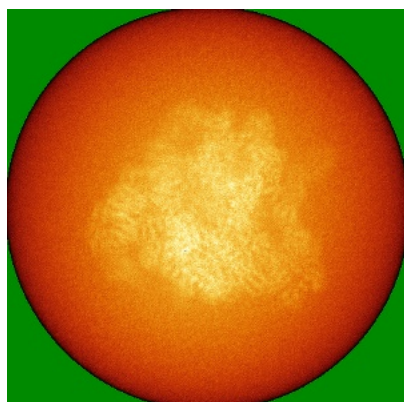


Y

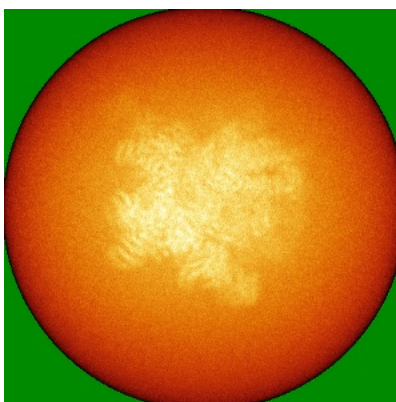


Z

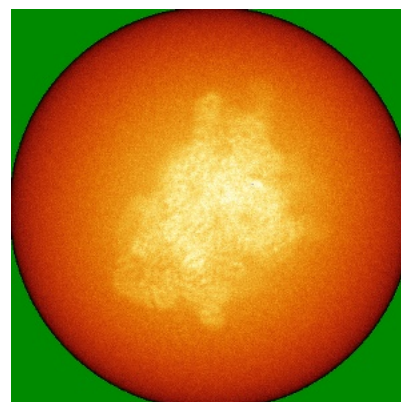
### 6.4.2 Raw map



X



Y

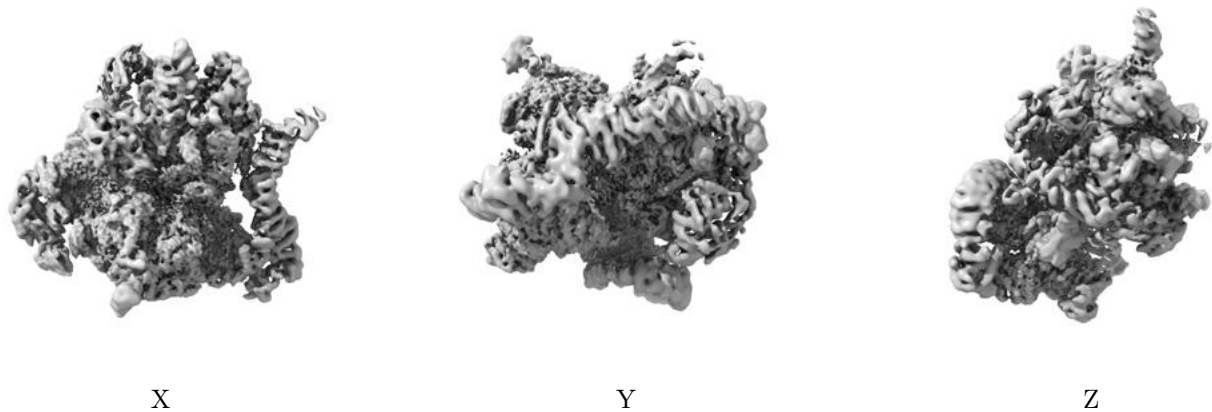


Z

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.

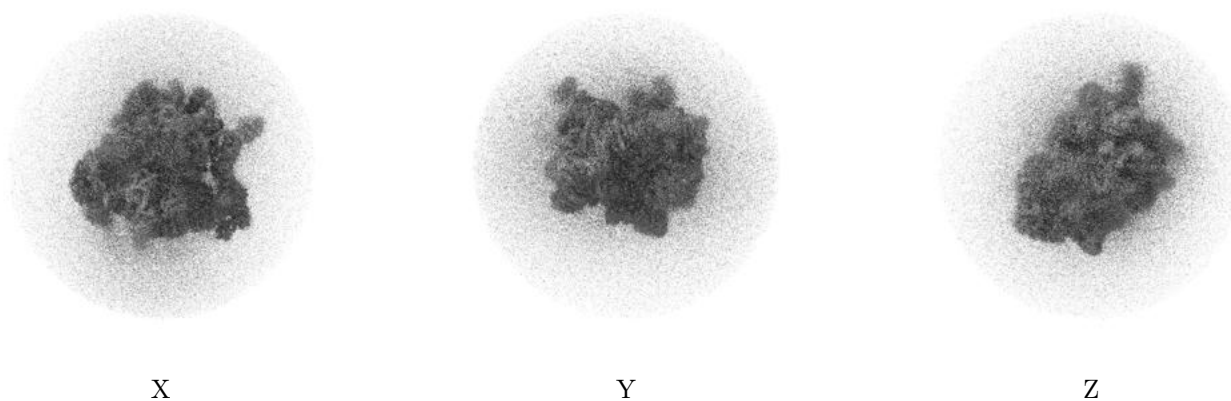
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

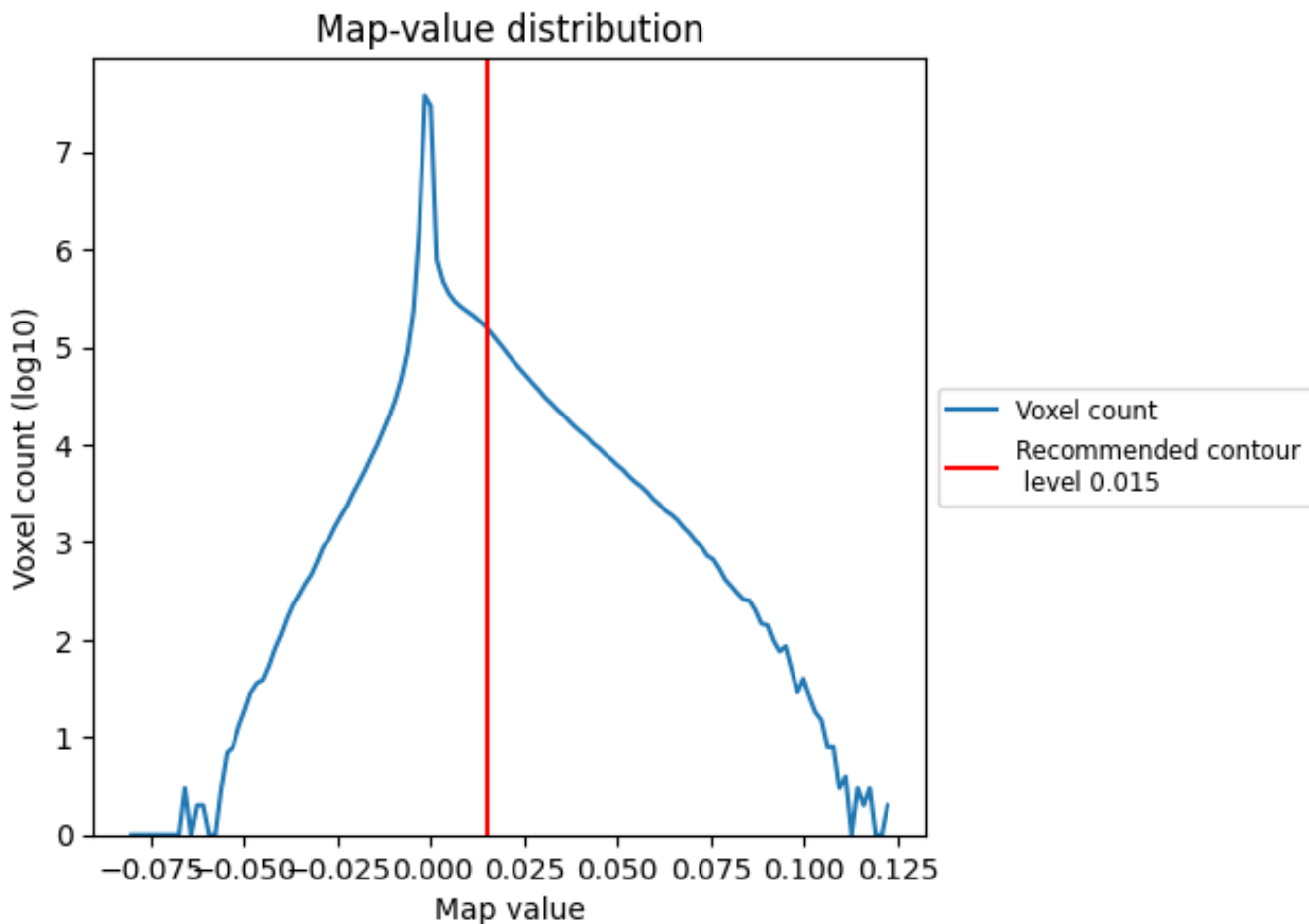
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

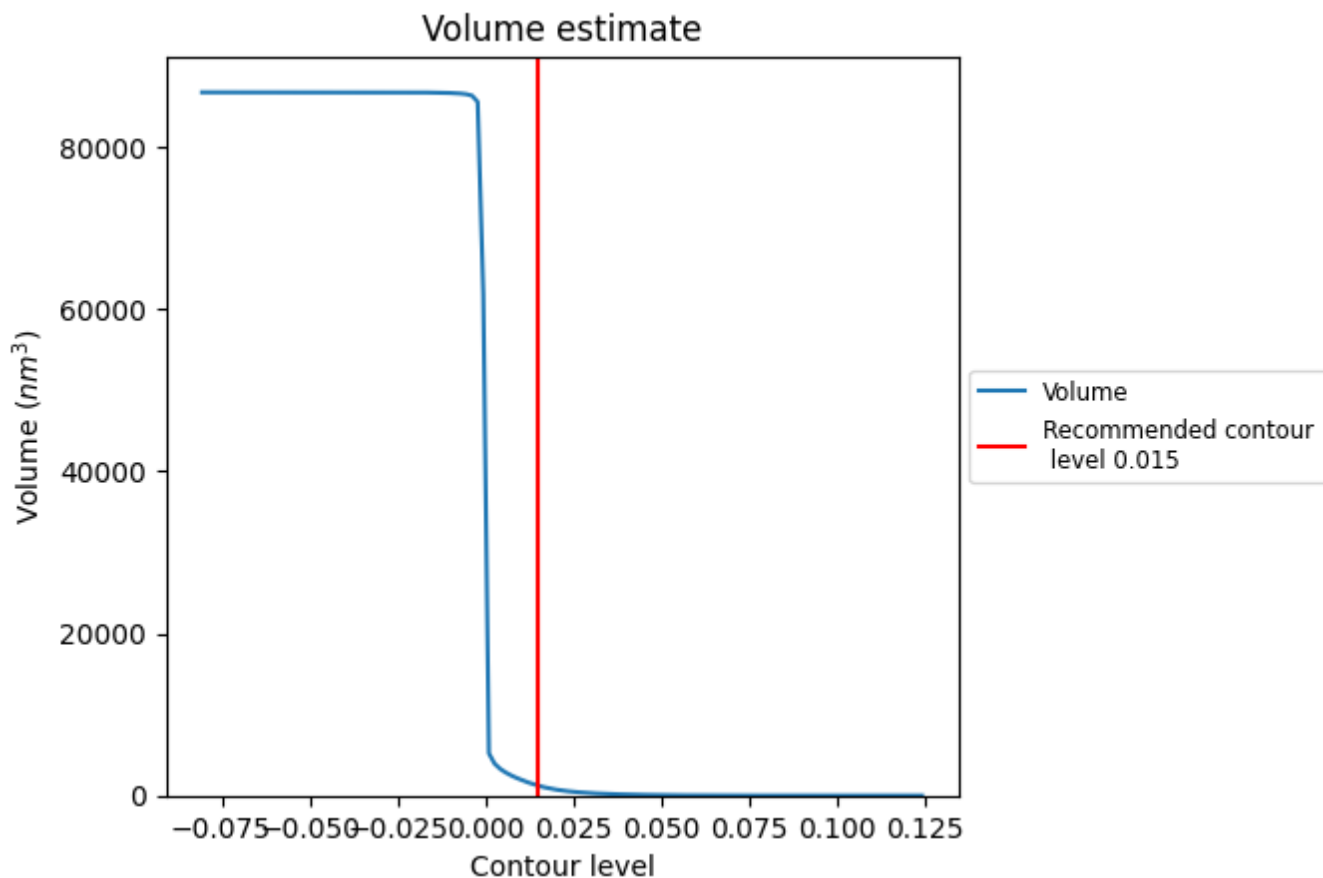
This section contains the results of statistical analysis of the map.

### 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](#)

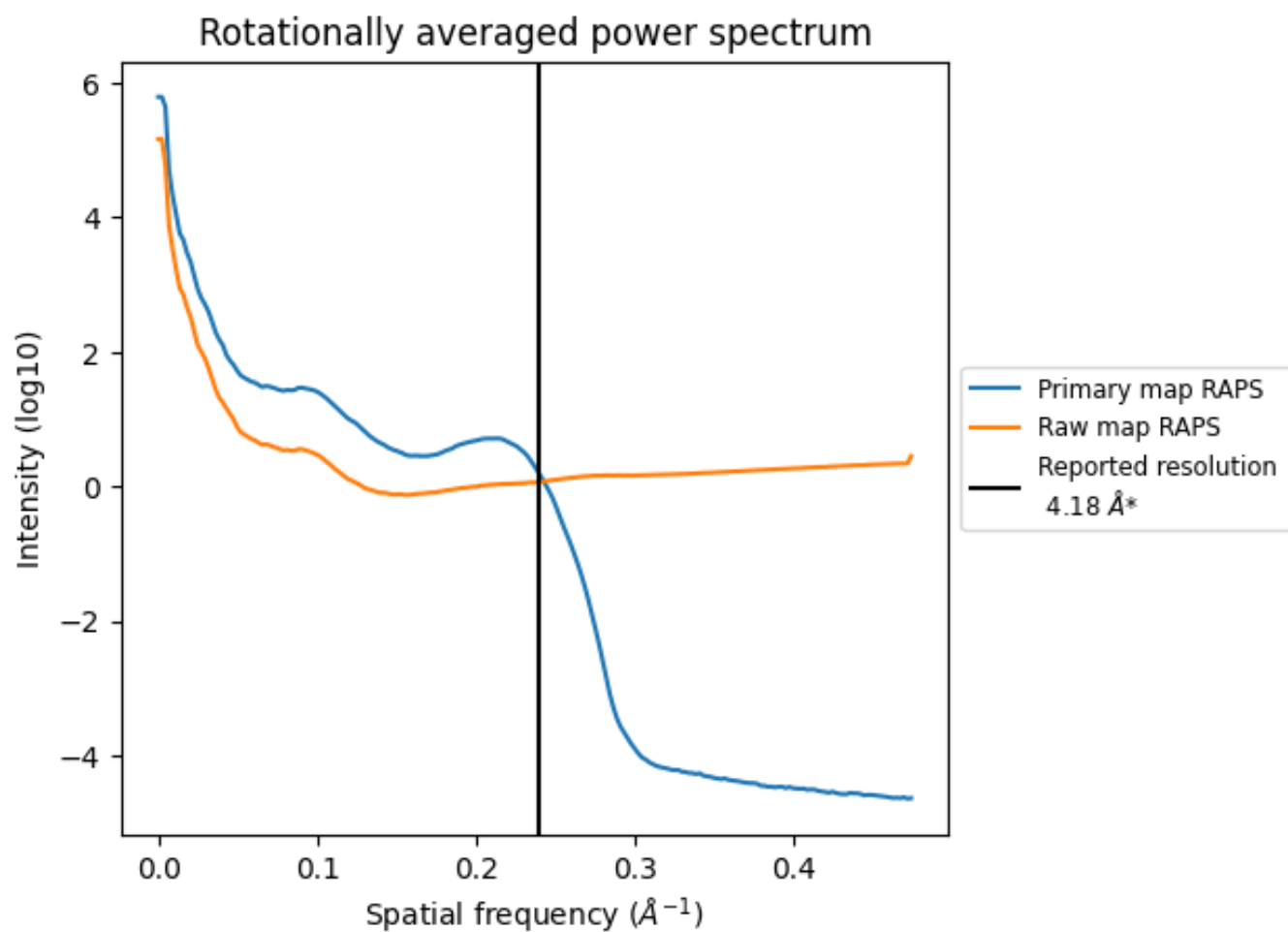


The volume at the recommended contour level is 1216 nm<sup>3</sup>; this corresponds to an approximate mass of 1099 kDa.

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

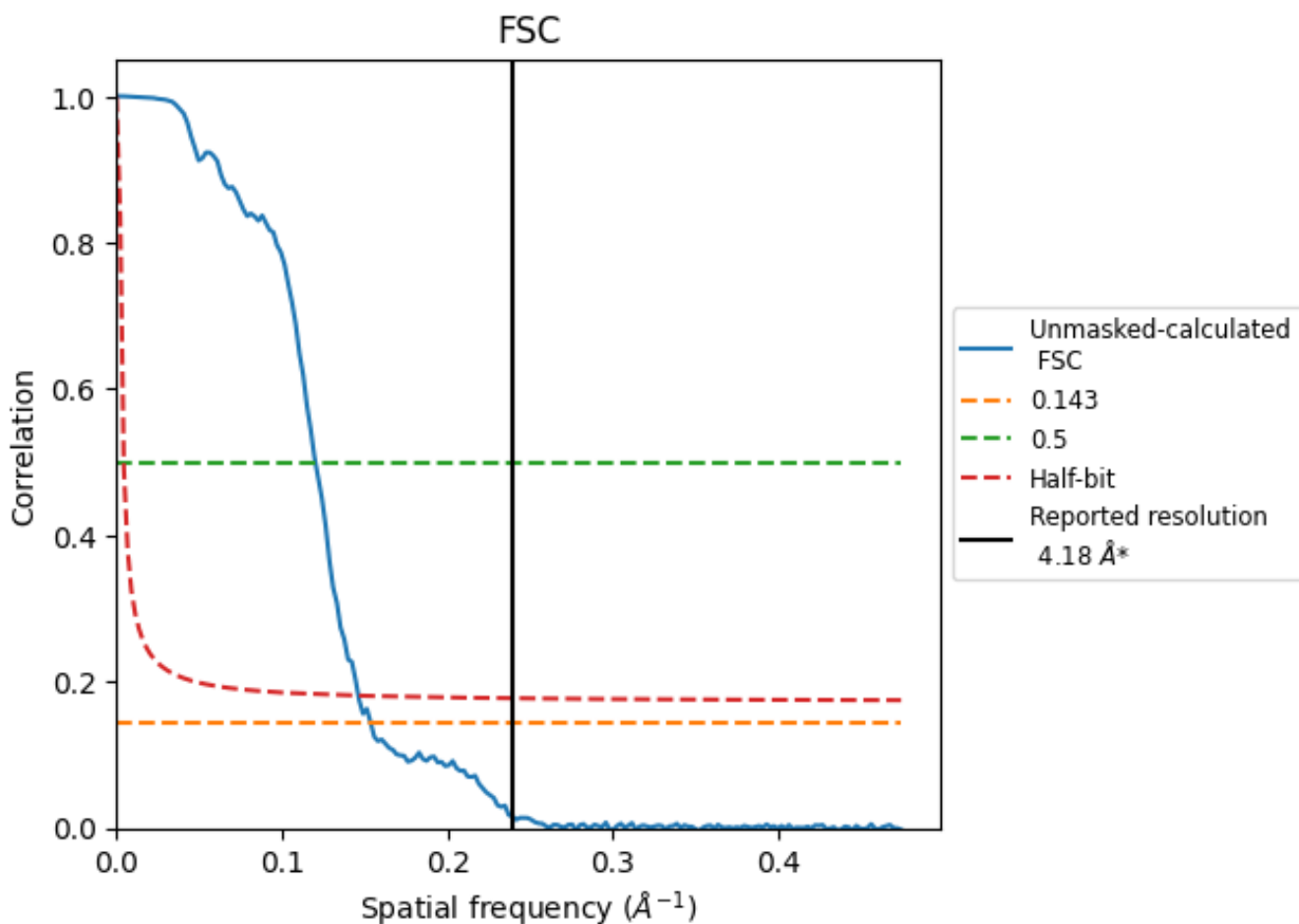


\*Reported resolution corresponds to spatial frequency of 0.239 Å<sup>-1</sup>

## 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 0.239 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

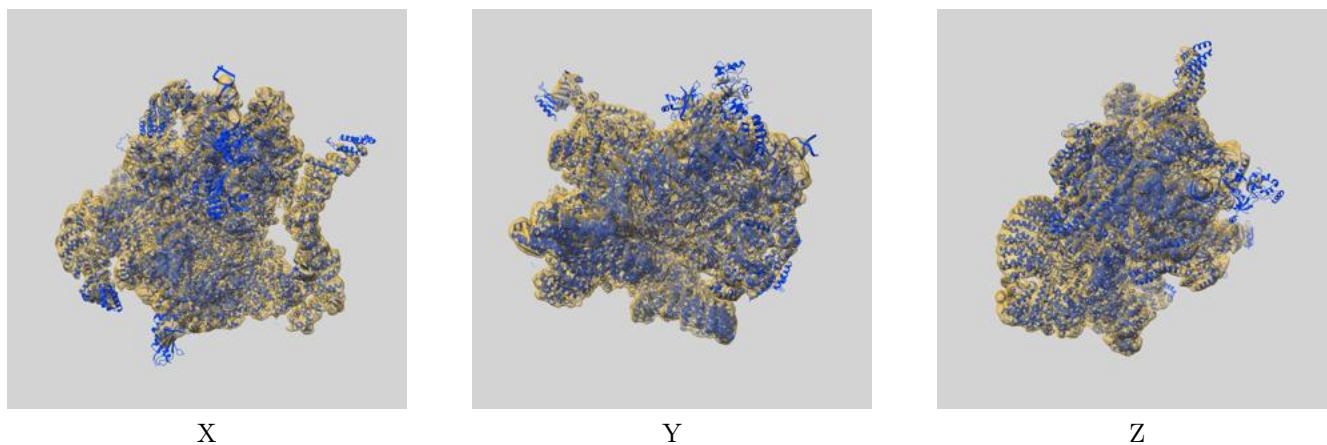
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.50	8.31	6.84

\*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 6.50 differs from the reported value 4.18 by more than 10 %

## 9 Map-model fit [i](#)

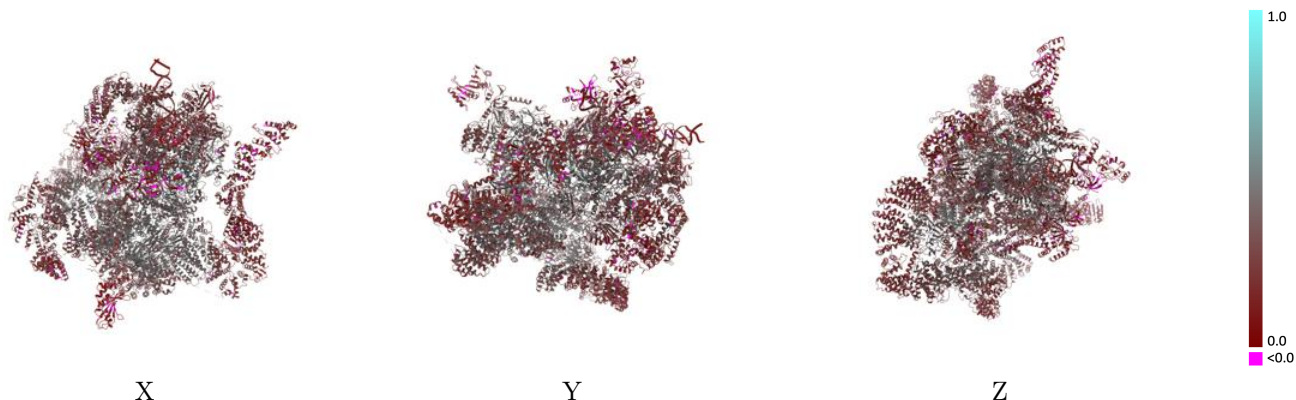
This section contains information regarding the fit between EMDB map EMD-33741 and PDB model 7YCX. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



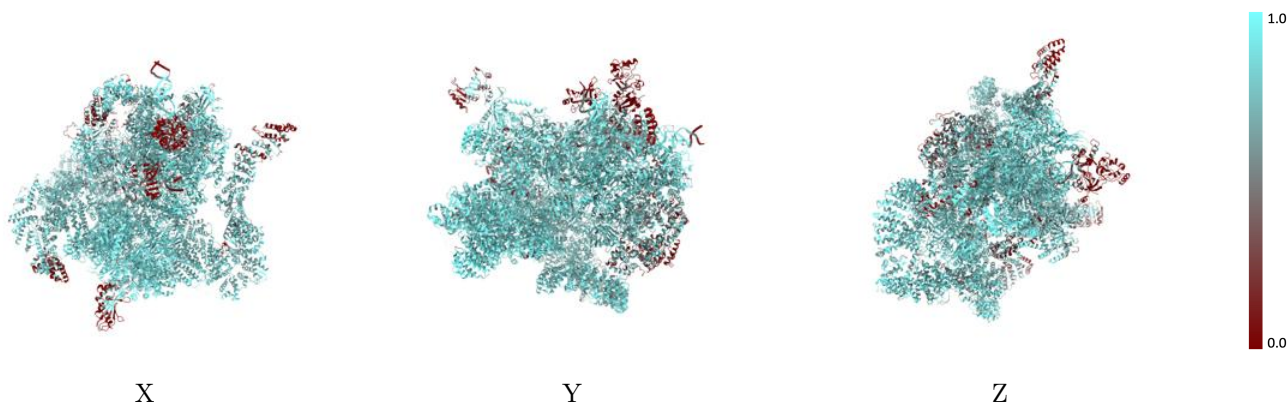
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



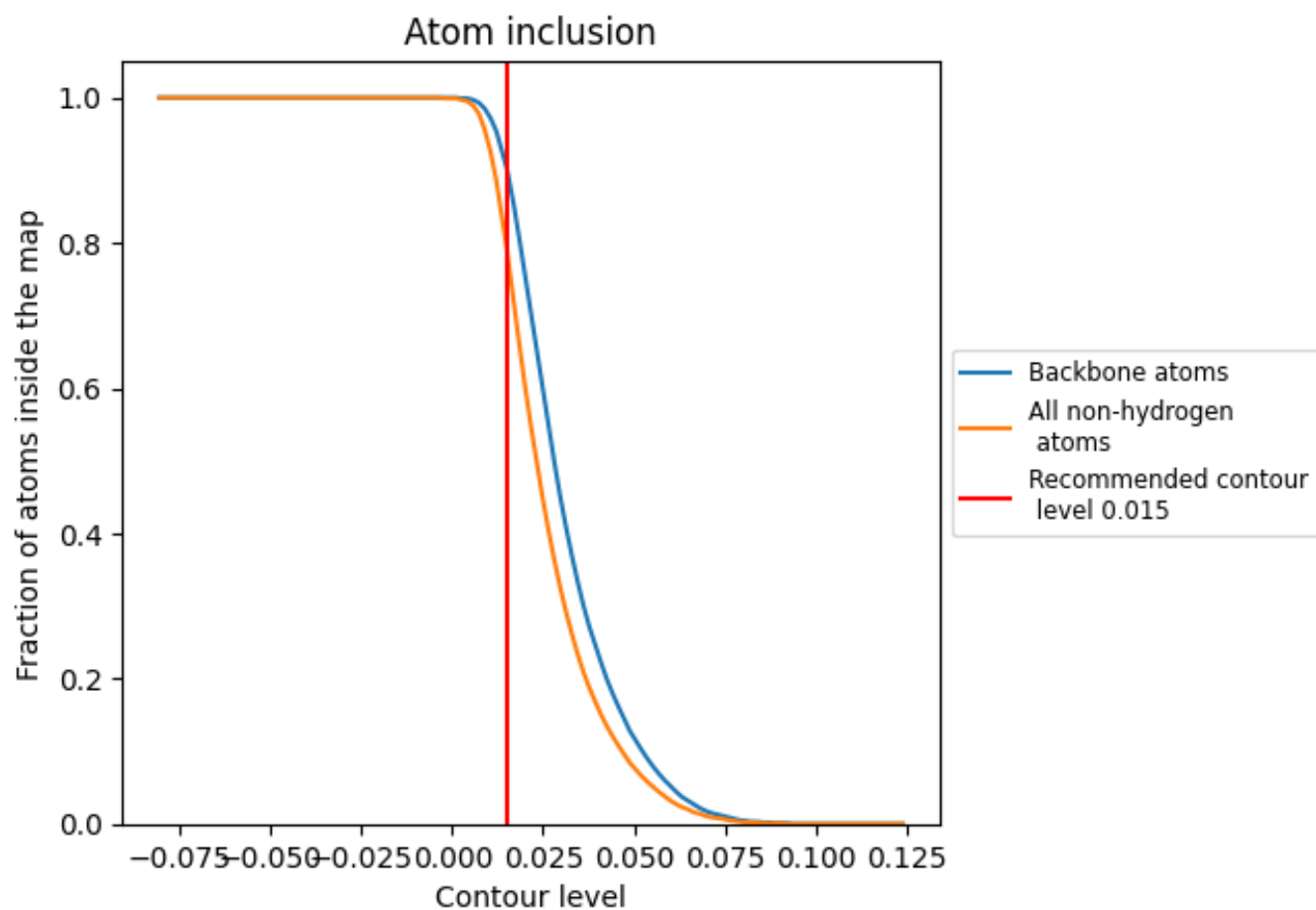
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.3110
1	 0.8490	 0.3500
2	 0.8960	 0.4060
3	 0.8970	 0.4240
4	 0.8170	 0.2900
5	 0.7870	 0.3040
6	 0.7760	 0.2510
7	 0.8220	 0.2580
8	 0.9190	 0.4570
9	 0.8390	 0.3640
A	 0.7480	 0.2340
B	 0.8730	 0.3770
D	 0.9070	 0.4000
E	 0.7750	 0.2950
F	 0.7790	 0.2680
G	 0.9070	 0.4090
H	 0.8120	 0.2520
I	 0.8410	 0.3820
K	 0.7610	 0.3240
M	 0.9650	 0.2830
P	 0.8260	 0.2400
Q	 0.8950	 0.3830
U	 0.9410	 0.4100
a	 0.9140	 0.4090
b	 0.7000	 0.1950
c	 0.8100	 0.2900
d	 0.7810	 0.2390
e	 0.5240	 0.1810
f	 0.6490	 0.2700
g	 0.5480	 0.2040
h	 0.5780	 0.2680
i	 0.0210	 0.1200
j	 0.3860	 0.1780
k	 0.7400	 0.2080
l	 0.7450	 0.1850

