



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:36 AM UTC

PDB ID : 8WAU / pdb_00008wau
EMDB ID : EMD-37405
Title : De novo transcribing complex 11 (TC11), the early elongation complex with Pol II positioned 11nt downstream of TSS
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-08
Resolution : 2.78 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:

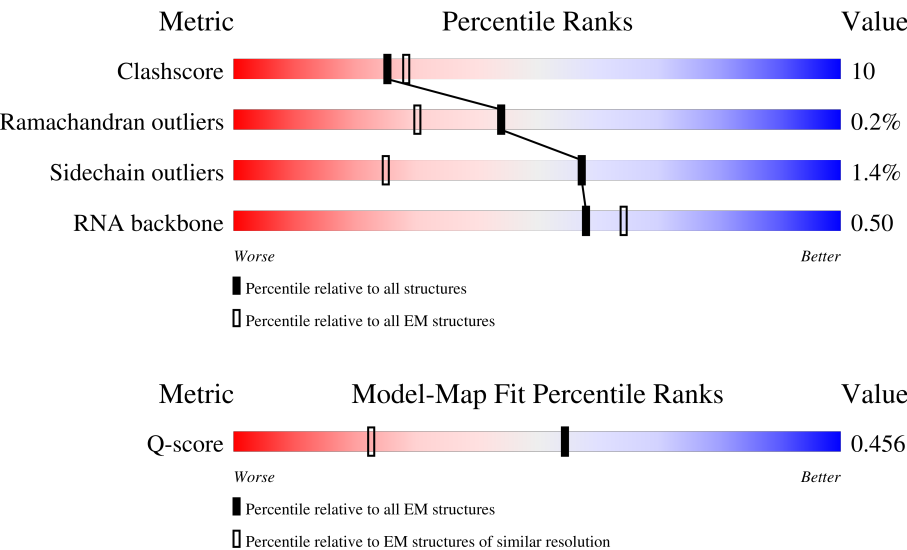
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.78 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10754 (2.28 - 3.28)

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	N	8	
2	S	517	
3	T	249	

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Mol	Chain	Length	Quality of chain
4	X	99	
5	Y	99	
6	Z	11	
7	o	1970	
8	p	1174	
9	q	275	
10	r	142	
11	s	210	
12	t	127	
13	u	172	
14	v	150	
15	w	125	
16	x	67	
17	y	117	
18	z	58	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 35728 atoms, of which 30 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	8	Total	C	H	N	O	S	
			94	39	30	10	14	1	
								0	0

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	138	Total	C	N	O	S		
			1138	719	208	208	3		
								0	0

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	103	Total	C	N	O	S		
			789	492	142	154	1		
								0	0

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	43	Total	C	N	O	P		
			878	418	155	262	43		
								0	0

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	54	Total	C	N	O	P		
			1112	527	211	320	54		
								0	0

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	11	Total	C	N	O	P		
			241	105	40	83	13		
								0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	1146	Total	C	N	O	S	0	0
			9149	5782	1610	1693	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

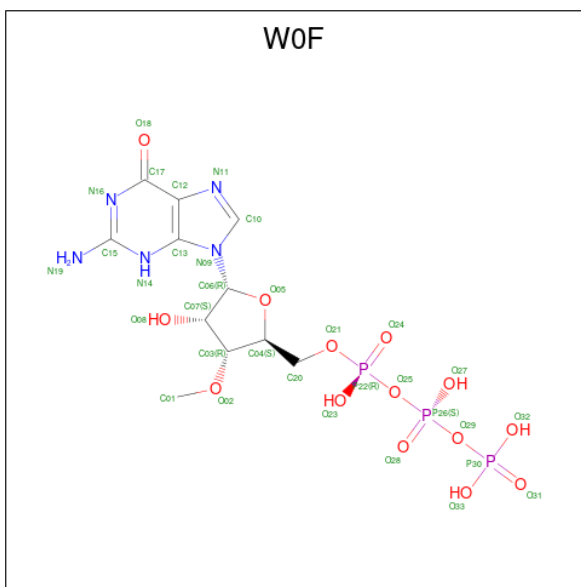
- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 18 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 19 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	Z	1	Total	C	N	O	P	0
			33	11	5	14	3	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	o	2	Total	Zn	0
			2	2	
20	p	1	Total	Zn	0
			1	1	
20	q	1	Total	Zn	0
			1	1	
20	w	2	Total	Zn	0
			2	2	
20	x	1	Total	Zn	0
			1	1	
20	z	1	Total	Zn	0
			1	1	

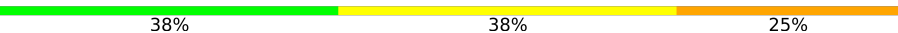
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

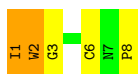
Mol	Chain	Residues	Atoms		AltConf
21	o	1	Total	Mg	0
			1	1	

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.

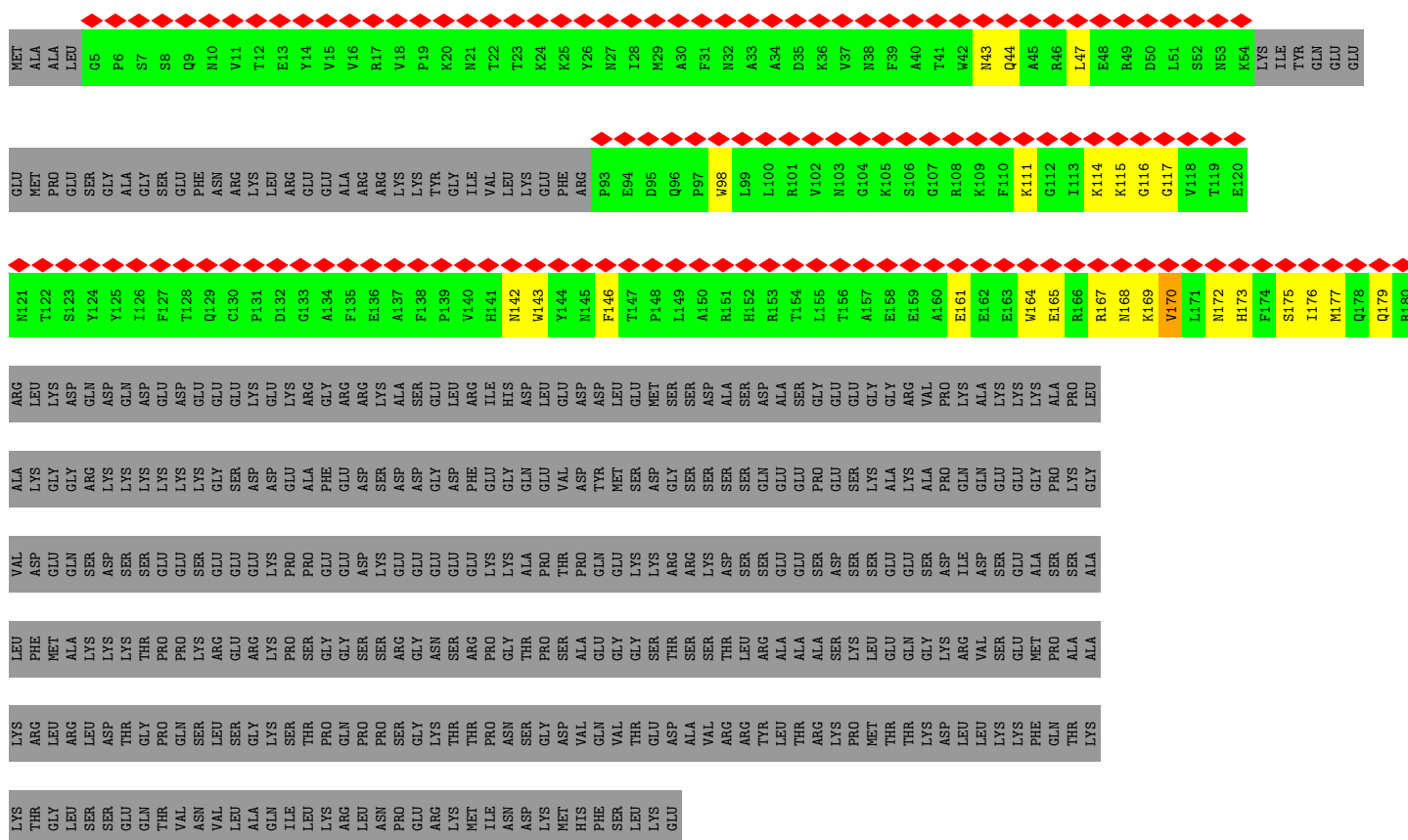
• Molecule 1: Alpha-amanitin

Chain N: 

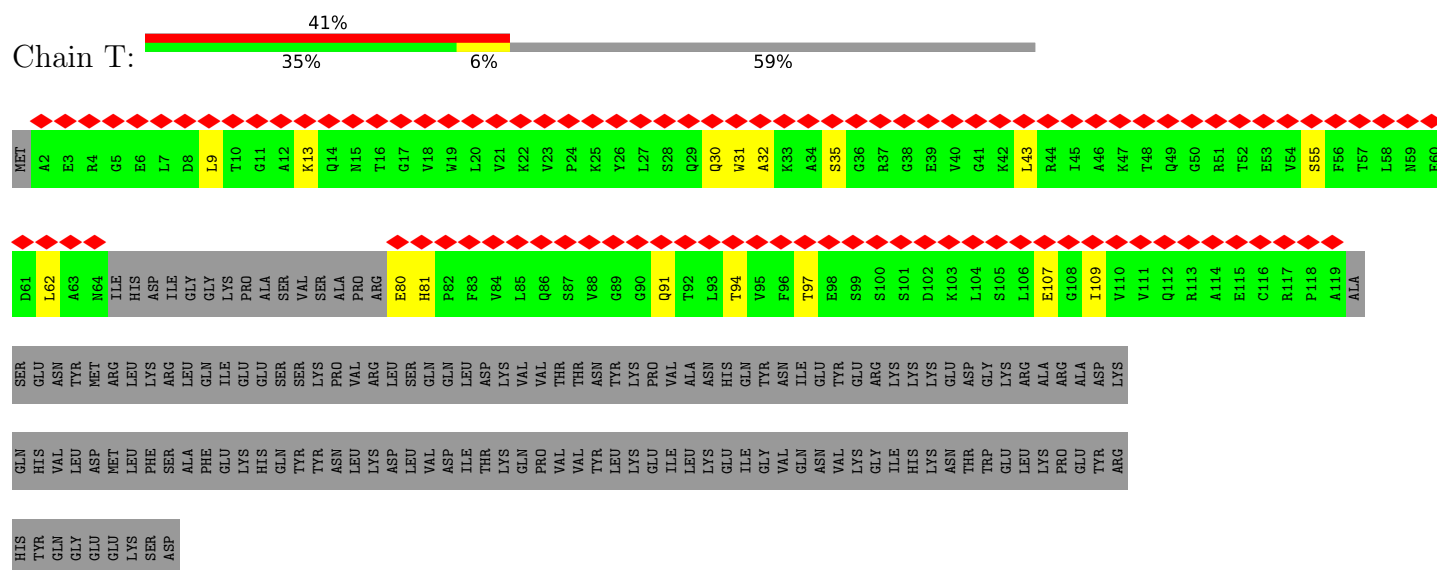


• Molecule 2: General transcription factor IIF subunit 1

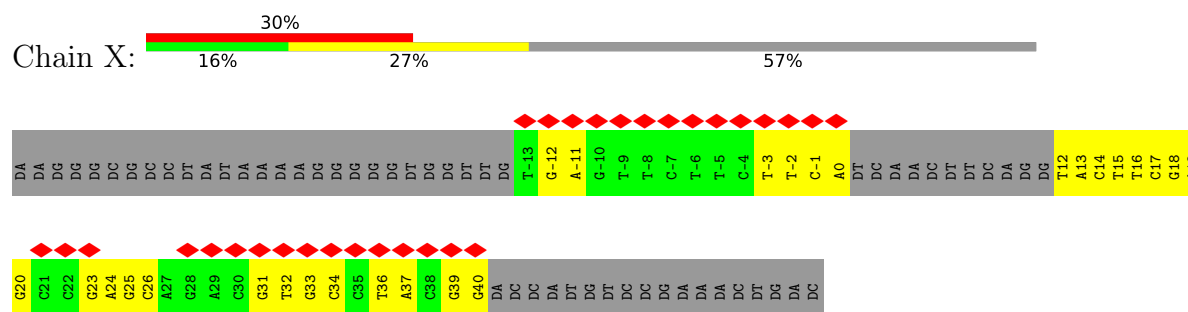
Chain S: 



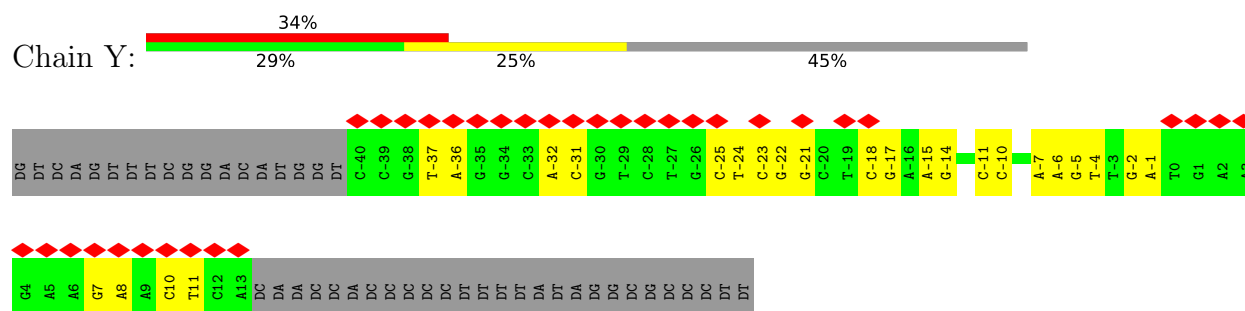
• Molecule 3: General transcription factor IIF subunit 2



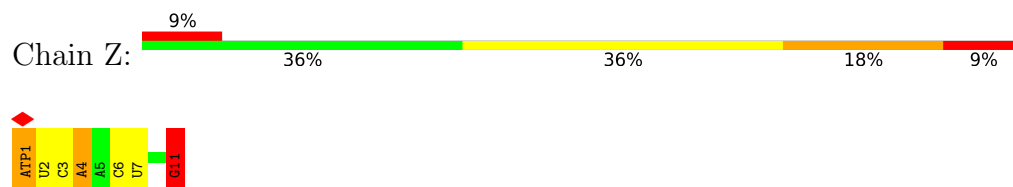
- Molecule 4: non-template DNA



- Molecule 5: template DNA



- Molecule 6: RNA



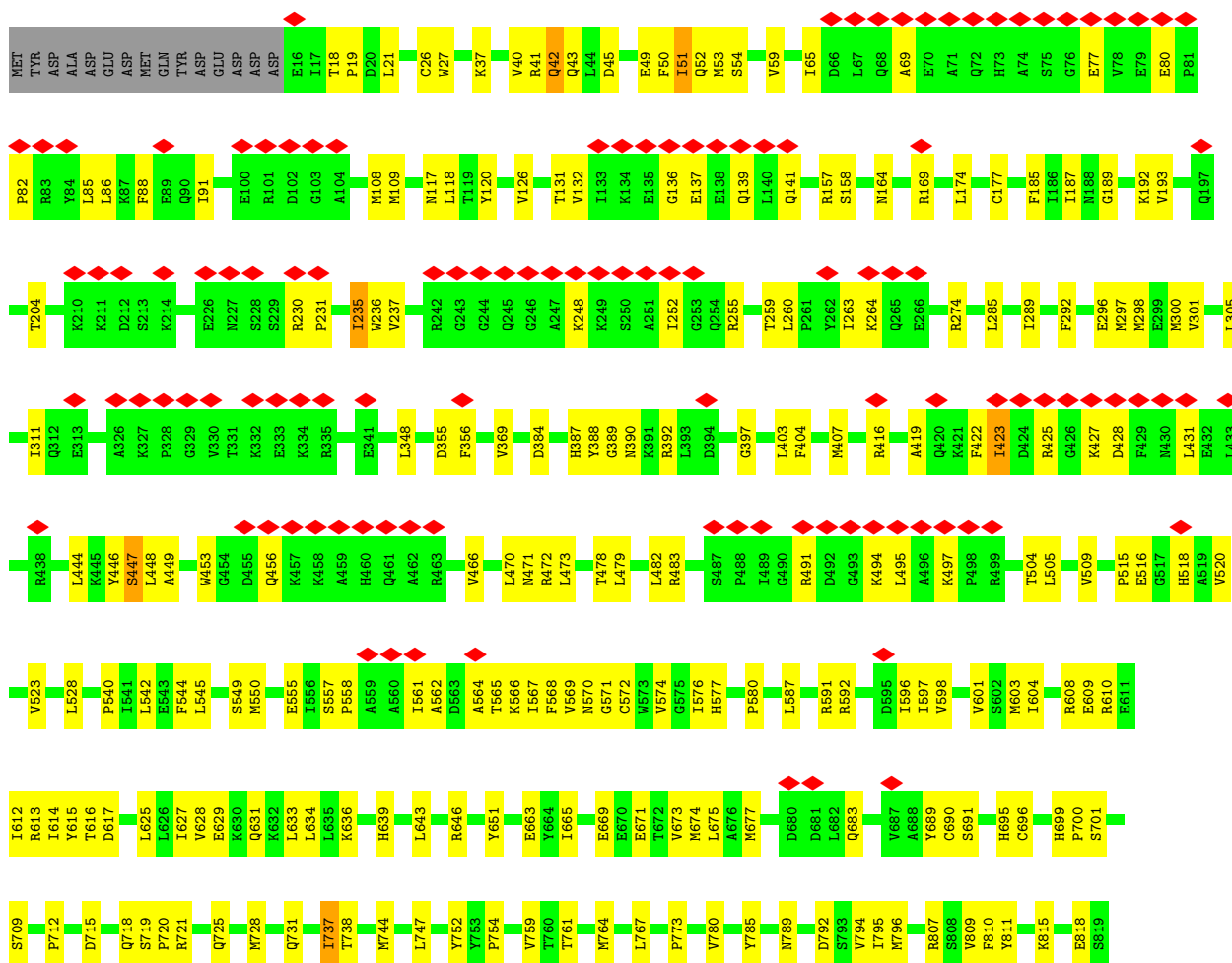
- Molecule 7: DNA-directed RNA polymerase subunit

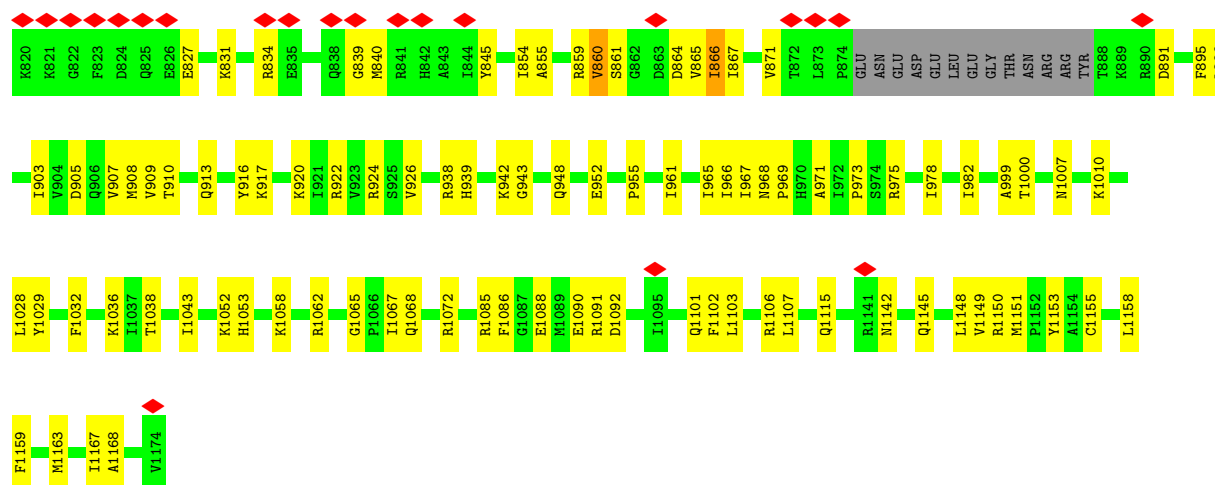


GLY	E1433	L1298	K1219	T1118	V939	G789	L640	M620	G379	S269	ASP	L100	MET
ILE	Q1299	Q1299	T1227	K1225	I948	Q790	L645	V521	V380	A270	GLU	V101	HIS
SER	E1434	G1300				Q791		P522	P381	R271	LEU	K102	GLY
ALA	T1435	V1307	Q1230	I1128	E953	F802	F668	M524	Y413	D282	THR	V106	GLY
MET	M1440		K1234	N1129	E953	T611	V669	V525	R421	I286	LYS	L107	PRO
THR	A1443	Q1313	K1234	I1130	M959	P817	S670	V526	R421		GLU	V110	PRO
TRP	A1444	T1314	I1235	K1135	R960	P817	N671	V527	I427		LYS	F112	SER
ASN	H1445	D1315	N1236	K1135	R963	P817	W671				LYS	F113	GLY
GLN	H1456	N1316		L1139	R963	G821	W672	S530	H181		GLY	S11	ASP
ALA	N1457	K1317	F1239	Q1146	P971	G821	V675	N531	G182			L15	
THR	I1458	K1318	G1240	S1147	T972	F822	W676	R532	G183			I18	
PRO	I1320	K1319	D1241	S1147	T972	V823	L680	F533	C184			L26	
ALA	Q1462	I1321	D1242	A1148	V978	E824	V534	M535	G185			L26	
TYR		I1321	L1243	R1149	V978	L828	H685	M535	R186			L26	
GLY	G1467	E1324		E1152	L963	L831	W689	A544	Y187			L31	
ALA	T1468	R1153	N1248	R1153	W988	L831		V545	R190			L31	
TRP	F1471	E1327	D1249	I1157	N989	F838	T693	F548	S194			M34	
SER	D1472	A1330	D1250	L1158	N989	L847	D695	T549	S194			M34	
SER	L1473	L1331	N1251	C1159	K992	L847	D695	T549	Y199			G40	
VAL	L1474	Q1332	A1252	R1160	I956	V852	I706	D552	A200			I41	
GLY	E1333	E1333	E1253	L1161	I956	K853	A709	F554	E201			T46	
SER	A1477	E1333	E1253	E1162	H1005	V852	A709	F554	W202			T47	
GLY	E1478	V1346	K1254	H1163	P1006	R863	V713	L555	K203			E48	
MET	K1479	L1347	L1255	H1163	I1007	R863	V713	L555	H204			G49	
THR	C1480	V1256	V1256	I1175	I1007	R863	V713	L555	V205			G50	
PRO	K1481	L1257	L1257	I1175	L1016	L864	I717	M665	N206			R51	
GLY	Y1482	R1258	R1258	M1180	L1016	L864	I717	M665	E207			R52	
ALA	G1483	I1259	I1259	P1181	L1020	R866	H721	T569	D208			K53	
ALA	L1473	R1260	R1260	P1181	L1020	R866	H721	T569	S209			L57	
GLY	M1484	I1261	I1261	S1182	V1021	S867	E726	Q876	Q210			Q62	
PHE	E1485	M1262	M1262	S1182	I1022	Q885	P727	P577	E211			I65	
SER	I1486	N1263	N1263	T1184	H1044	Q885	P727	P577	K212			E86	
PRO	P1487	S1264	S1264	D1189	H1044	D894	L733	L580	I214			R67	
SER		D1265	D1265	Q1190	R1052	D894	L733	L580	P218			K149	
ALA	Y1392	E1266	E1266	Q1190	R1052	V901	T736	P582	E219			G150	
ALA	Y1392	E1266	E1266	Q1190	R1052	V901	T736	P582	R220			K151	
ASP	L1398	E1267	E1267	E1191	L1060	L909	F737	L585	V221			N152	
PRO	A1399	K1268	K1268	W1192	H1082	L909	F737	L585	K226			I153	
SER	L1400	M1269	M1269	E1198	H1082	P911	L745	K589	R227			C154	
LEU	L1401	Q1270	Q1270	M1199	V1087	S912	A748	Q590	E219			E155	
GLY	G1402	Q1271	E1271	P1200	V1087	N913	R749	T591	R227			GLY	
ALA	D1403	E1271	E1271	P1200	V1087	N913	R749	T591	E219			GLY	
GLY	T1404	E1272	E1272	E1198	H1082	P911	L745	K589	E219			GLU	
PRO	C1407	E1273	E1273	M1199	V1087	S912	A748	Q590	E219			GLU	
THR	R1408	E1274	E1274	P1200	V1087	N913	R749	T591	E219			MET	
SER	L1411	V1275	V1275	E1198	H1082	P911	L745	K589	E219			ASP	
ALA	L1411	V1276	V1276	E1198	H1082	P911	L745	K589	E219			ASP	
THR	T1414	K1277	K1277	M1199	V1087	S912	A748	Q590	E219			GLY	
PRO	R1416	D1278	D1278	P1200	V1087	N913	R749	T591	E219			GLY	
GLY	H1417	M1279	M1279	E1198	H1082	P911	L745	K589	E219			GLU	
ALA	R1421	D1280	D1280	L1211	L1211	E936	V784	E631	E219			MET	
PRO	R1421	D1281	D1281	L1212	L1212	D937	V784	E631	E219			ASP	
GLY	R1421	D1282	D1282	L1213	L1213	D937	V784	E631	E219			ASN	
SER	L1427	I1288	I1288	E1215	V1117	L938	V788	M637	E219			LYS	
		E1289	E1289	E1215	V1117	L938	V788	M637	E219			PHE	
		L1293	L1293	R1218	V1117	L938	V788	M637	E219			VAL	
		T1294	T1294	R1218	V1117	L938	V788	M637	E219			VAL	
		D1295	D1295	R1218	V1117	L938	V788	M637	E219			GLN	
		M1296	M1296	R1218	V1117	L938	V788	M637	E219			GLN	
		T1297	T1297	R1218	V1117	L938	V788	M637	E219			PRO	
				R1218	V1117	L938	V788	M637	E219			GLY	

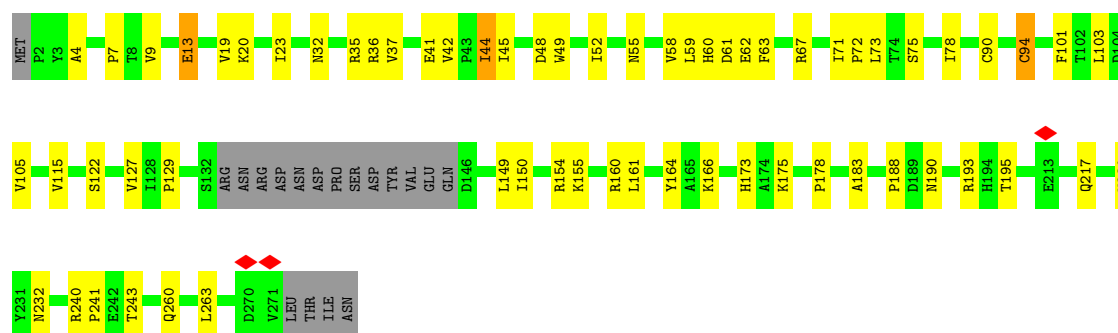
[illegible]

- Molecule 8: DNA-directed RNA polymerase subunit beta

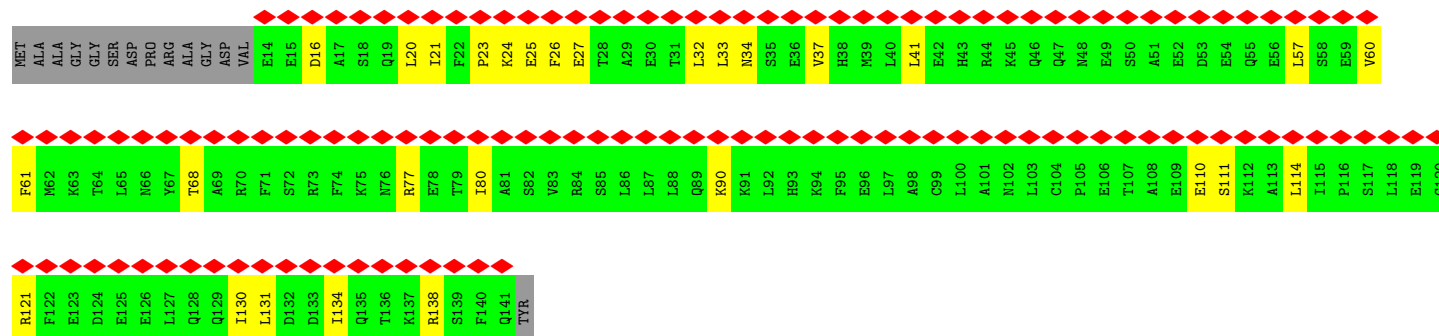
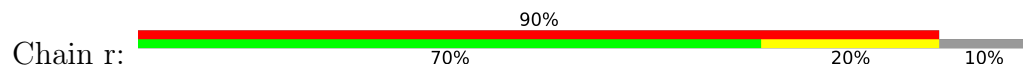




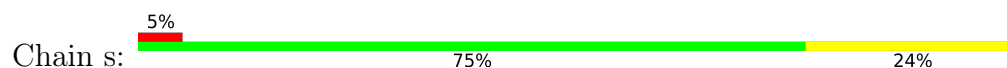
• Molecule 9: DNA-directed RNA polymerase II subunit RPB3

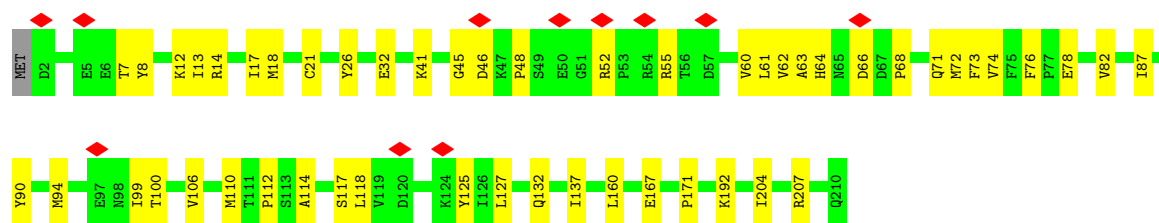


• Molecule 10: DNA-directed RNA polymerase II subunit RPB4

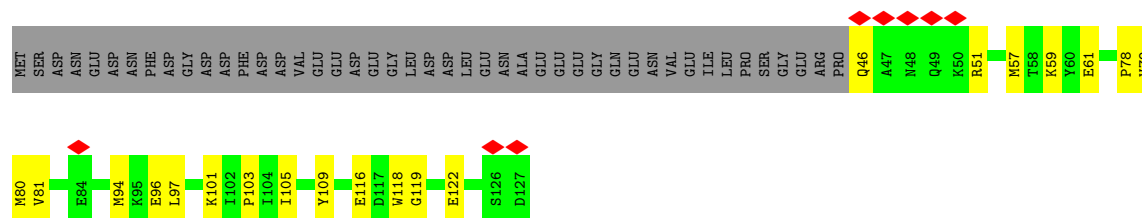


• Molecule 11: DNA-directed RNA polymerase II subunit E

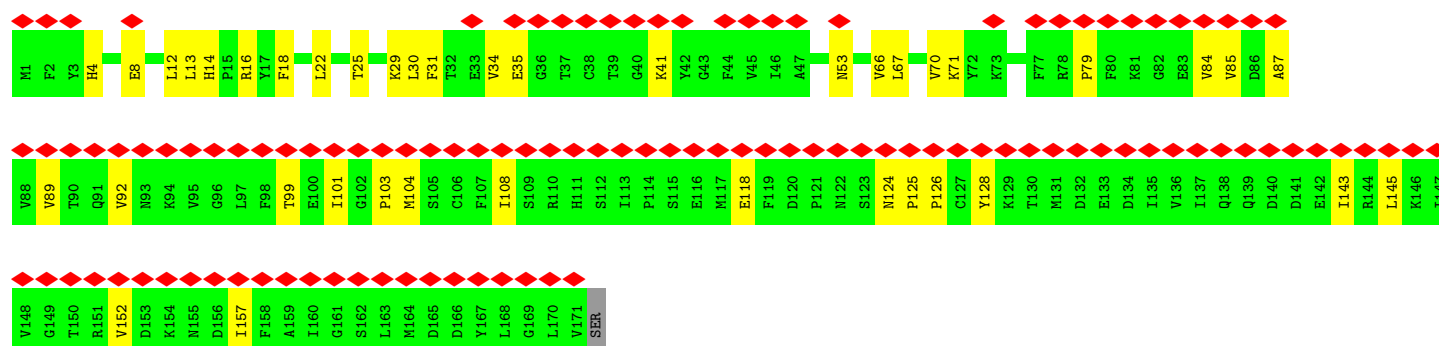
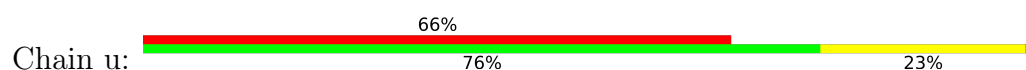




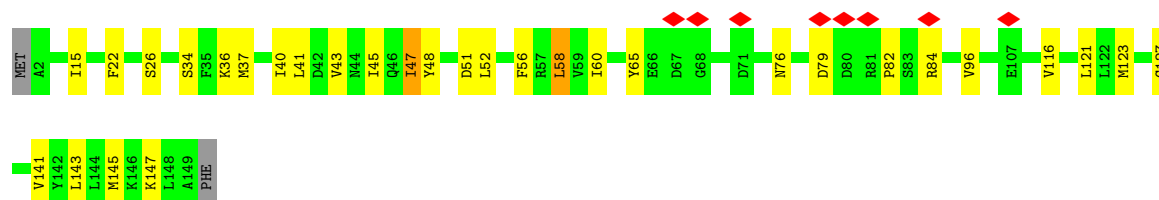
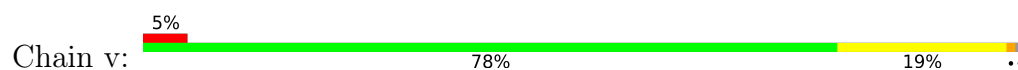
- Molecule 12: DNA-directed RNA polymerase II subunit F



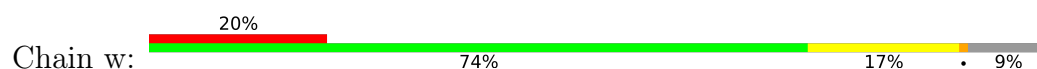
- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

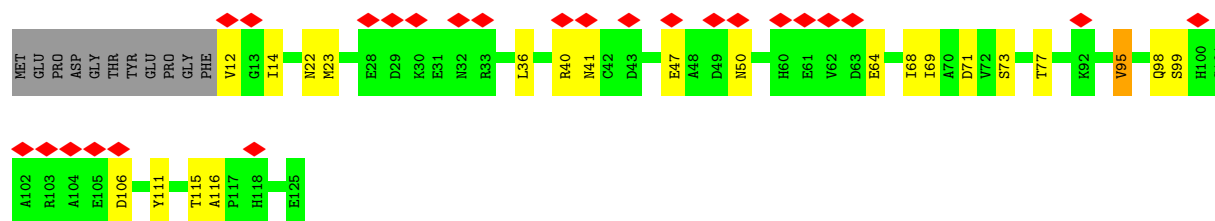


- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

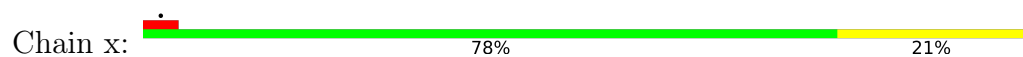


- Molecule 15: DNA-directed RNA polymerase II subunit RPB9

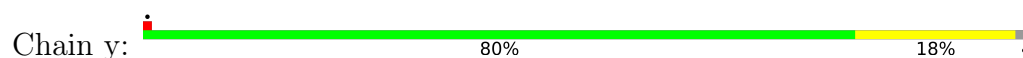




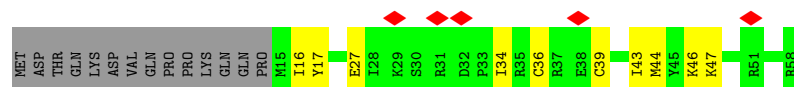
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 17: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 18: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	461083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.464	Depositor
Minimum map value	-5.345	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.93	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G2L, ATP, ILX, CSX, W0F, MG, TRX, ZN, HYP

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	N	0.41	0/22	0.98	0/26
2	S	0.09	0/1167	0.23	0/1576
3	T	0.09	0/799	0.25	0/1077
4	X	0.30	0/981	0.60	0/1509
5	Y	0.34	0/1249	0.56	0/1926
6	Z	0.32	0/206	0.44	0/317
7	o	0.30	0/11723	0.39	0/15830
8	p	0.33	0/9332	0.42	1/12598 (0.0%)
9	q	0.34	0/2102	0.40	0/2857
10	r	0.13	0/1064	0.22	0/1428
11	s	0.26	0/1751	0.36	1/2366 (0.0%)
12	t	0.31	0/667	0.31	0/901
13	u	0.17	0/1382	0.32	0/1874
14	v	0.32	0/1207	0.36	0/1628
15	w	0.24	0/948	0.35	0/1284
16	x	0.31	0/542	0.34	0/730
17	y	0.32	0/939	0.34	0/1271
18	z	0.26	0/377	0.38	0/500
All	All	0.30	0/36458	0.40	2/49698 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	46	ASP	CB-CA-C	-5.41	109.88	117.23
8	p	355	ASP	CB-CA-C	-5.27	110.06	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	N	64	30	51	6	0
2	S	1138	0	1103	18	0
3	T	789	0	795	9	0
4	X	878	0	487	27	0
5	Y	1112	0	606	23	0
6	Z	241	0	118	6	0
7	o	11510	0	11616	253	0
8	p	9149	0	9178	251	0
9	q	2059	0	2007	59	0
10	r	1050	0	1033	18	0
11	s	1720	0	1737	39	0
12	t	657	0	684	17	0
13	u	1351	0	1358	26	0
14	v	1186	0	1147	23	0
15	w	927	0	859	17	0
16	x	533	0	553	11	0
17	y	920	0	942	16	0
18	z	372	0	378	8	0
19	Z	33	0	0	6	0
20	o	2	0	0	0	0
20	p	1	0	0	0	0
20	q	1	0	0	0	0
20	w	2	0	0	0	0
20	x	1	0	0	0	0
20	z	1	0	0	0	0
21	o	1	0	0	0	0
All	All	35698	30	34652	731	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 10.

The worst 5 of 731 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)
3:T:91:GLN:HB2	8:p:555:GLU:HG3	1.56	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:2500:W0F:O32	8:p:975:ARG:NH2	2.11	0.83
8:p:866:ILE:HG22	8:p:867:ILE:HG13	1.62	0.81
8:p:926:VAL:HG21	9:q:62:GLU:HG3	1.63	0.81
4:X:31:DG:H2''	4:X:32:DT:H72	1.61	0.80

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	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
2	S	134/517 (26%)	134 (100%)	0	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1395 (96%)	51 (4%)	2 (0%)	48	75
8	p	1142/1174 (97%)	1076 (94%)	64 (6%)	2 (0%)	43	70
9	q	253/275 (92%)	244 (96%)	9 (4%)	0	100	100
10	r	126/142 (89%)	126 (100%)	0	0	100	100
11	s	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
12	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
13	u	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
14	v	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	18	44
15	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	3	10
17	y	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
18	z	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
All	All	4140/5361 (77%)	3970 (96%)	163 (4%)	7 (0%)	44	70

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	549	SER
14	v	34	SER
16	x	6	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	N	2/2 (100%)	2 (100%)	0	100	100
2	S	121/448 (27%)	120 (99%)	1 (1%)	73	89
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1257 (98%)	23 (2%)	51	79
8	p	1001/1027 (98%)	984 (98%)	17 (2%)	53	80
9	q	234/252 (93%)	230 (98%)	4 (2%)	53	80
10	r	118/126 (94%)	118 (100%)	0	100	100
11	s	191/192 (100%)	191 (100%)	0	100	100
12	t	71/111 (64%)	71 (100%)	0	100	100
13	u	152/153 (99%)	151 (99%)	1 (1%)	76	90
14	v	129/131 (98%)	127 (98%)	2 (2%)	55	81
15	w	103/112 (92%)	102 (99%)	1 (1%)	68	86
16	x	56/56 (100%)	55 (98%)	1 (2%)	51	79
17	y	104/106 (98%)	103 (99%)	1 (1%)	68	86
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3637 (99%)	51 (1%)	57	82

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	p	235	ILE
8	p	737	ILE
16	x	14	VAL
8	p	292	PHE
8	p	466	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
9	q	18	ASN
15	w	41	ASN
9	q	232	ASN
11	s	64	HIS
17	y	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	10/11 (90%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	4	A
6	Z	11	G2L

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	Z	1	ATP

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	G2L	Z	11	5,21,6	23,26,30	1.38	4 (17%)	31,38,44	3.15	15 (48%)
1	HYP	N	8	1	7,8,9	0.84	0	5,10,12	2.35	2 (40%)
1	TRX	N	2	1	15,16,17	1.12	1 (6%)	17,22,24	0.97	0
1	CSX	N	6	1	3,6,7	1.08	0	1,6,8	2.10	1 (100%)
1	ILX	N	1	1	8,9,10	0.61	0	8,11,13	1.41	1 (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
6	G2L	Z	11	5,21,6	-	2/9/27/31	0/3/3/3
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1
1	TRX	N	2	1	-	2/5/6/8	0/2/2/2
1	CSX	N	6	1	-	2/2/5/7	-
1	ILX	N	1	1	-	7/11/12/14	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	11	G2L	C5-C4	3.11	1.47	1.38
6	Z	11	G2L	C6-N1	-2.42	1.34	1.38
1	N	2	TRX	CD2-CE2	2.40	1.44	1.41
6	Z	11	G2L	O4'-C4'	-2.31	1.39	1.45
6	Z	11	G2L	C5-N7	-2.14	1.34	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	11	G2L	O4'-C4'-C5'	-6.90	87.22	109.33
6	Z	11	G2L	O4'-C1'-N9	6.66	123.44	108.36
6	Z	11	G2L	C5-C4-N3	-6.17	118.57	128.39
6	Z	11	G2L	C2-N3-C4	5.10	121.09	112.30
6	Z	11	G2L	O2'-C2'-C1'	-4.88	93.32	110.10

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	ILX	C-CA-CB-CG2
1	N	1	ILX	OD1-CD1-CG1-CB
1	N	1	ILX	OD1-CD1-CG1-OG1
1	N	6	CSX	N-CA-CB-SG
1	N	6	CSX	C-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	11	G2L	1	0
1	N	2	TRX	2	0
1	N	1	ILX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	$\# Z > 2$
19	W0F	Z	2500	-	34,35,35	4.06	14 (41%)	43,55,55	3.45	17 (39%)

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
19	W0F	Z	2500	-	-	3/24/40/40	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	2500	W0F	P26-O29	13.80	1.74	1.59
19	Z	2500	W0F	C03-C04	-9.77	1.27	1.52
19	Z	2500	W0F	P22-O25	8.44	1.68	1.59
19	Z	2500	W0F	O05-C04	6.86	1.60	1.45
19	Z	2500	W0F	O05-C06	-6.01	1.28	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	2500	W0F	O05-C06-N09	-14.54	75.41	108.36
19	Z	2500	W0F	C07-C06-N09	8.28	136.30	113.25
19	Z	2500	W0F	O05-C04-C03	-5.80	92.69	104.92
19	Z	2500	W0F	O27-P26-O25	-5.27	93.03	107.27
19	Z	2500	W0F	O05-C04-C20	4.93	125.14	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

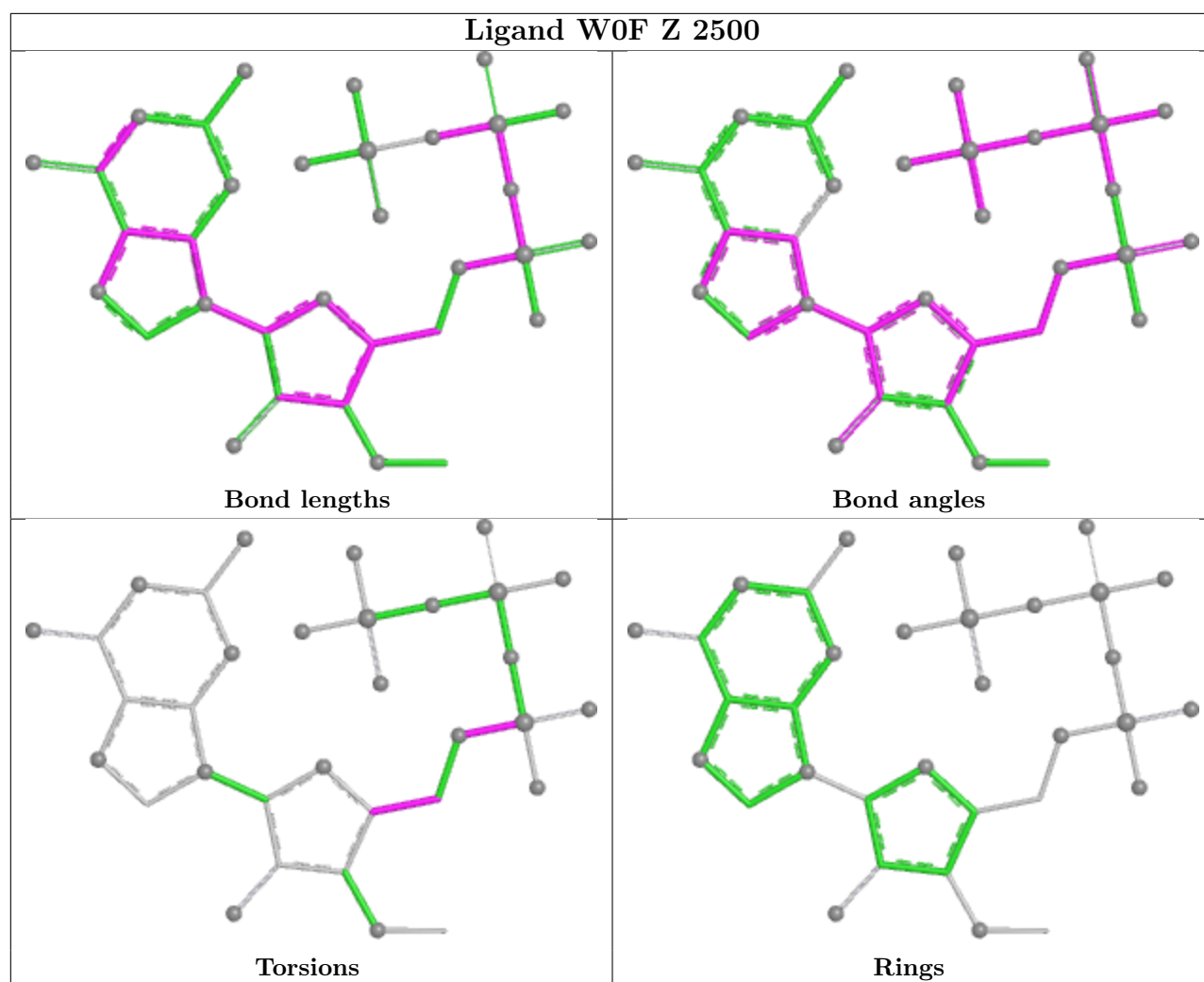
Mol	Chain	Res	Type	Atoms
19	Z	2500	W0F	C20-O21-P22-O24
19	Z	2500	W0F	C20-O21-P22-O25
19	Z	2500	W0F	C03-C04-C20-O21

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	2500	W0F	6	0

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.

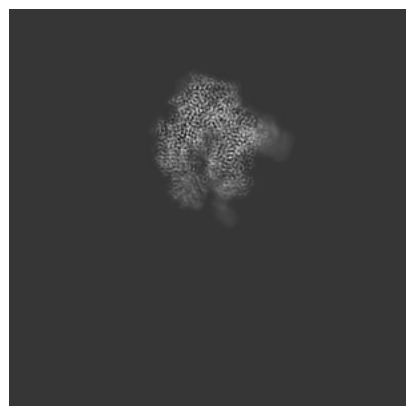
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37405. These allow visual inspection of the internal detail of the map and identification of artifacts.

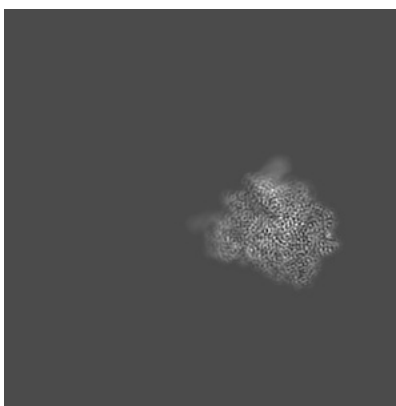
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

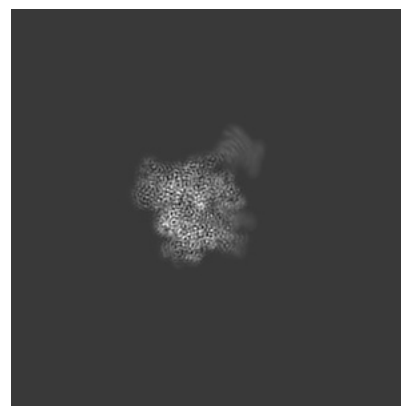
6.1.1 Primary map



X

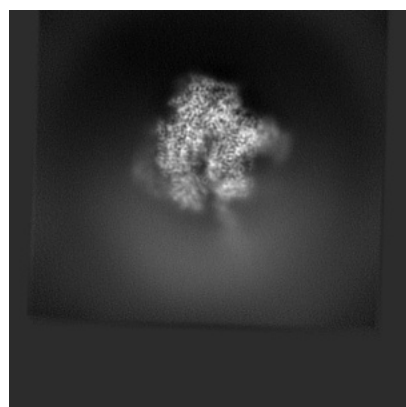


Y

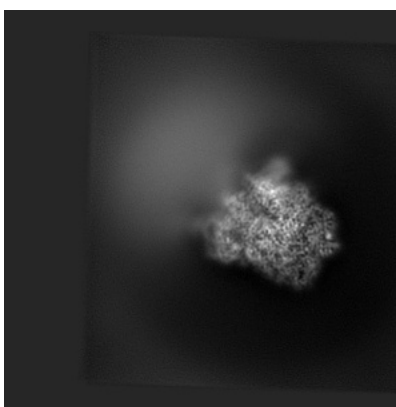


Z

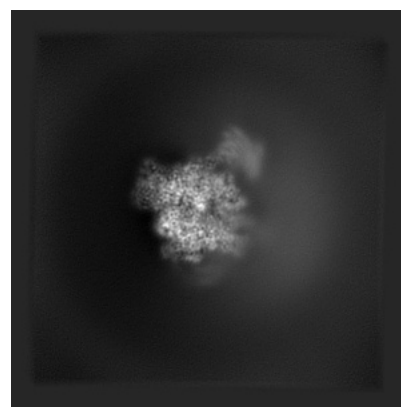
6.1.2 Raw map



X



Y

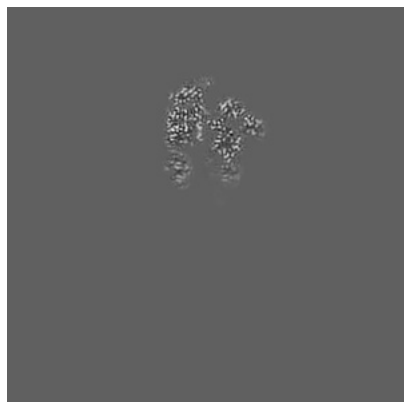


Z

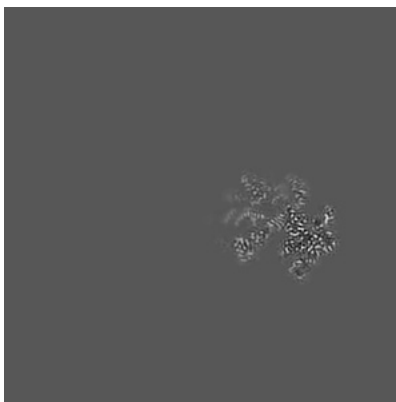
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

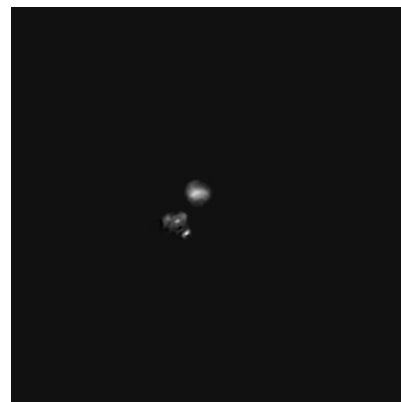
6.2.1 Primary map



X Index: 160

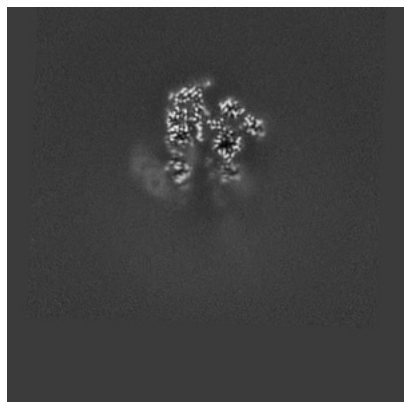


Y Index: 160

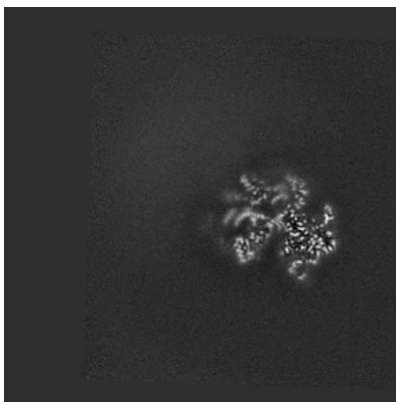


Z Index: 160

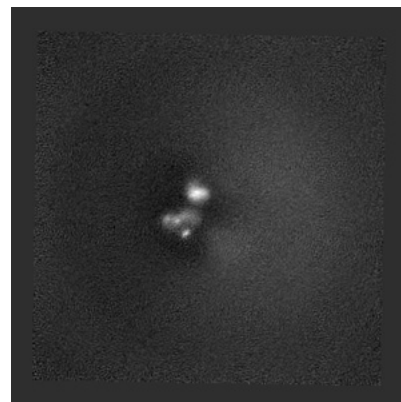
6.2.2 Raw map



X Index: 160



Y Index: 160

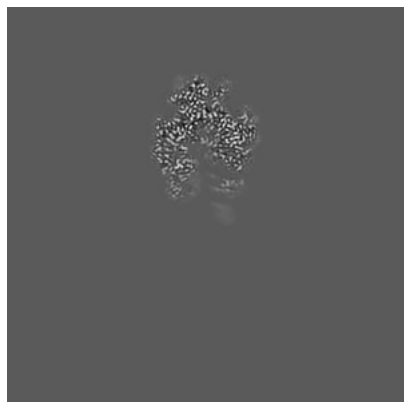


Z Index: 160

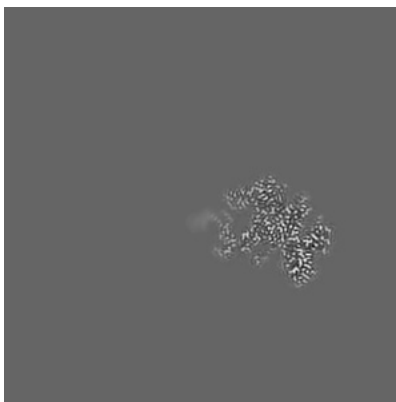
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

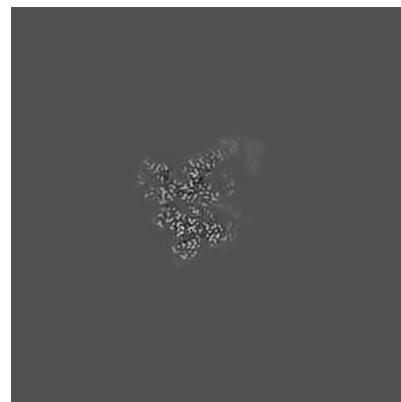
6.3.1 Primary map



X Index: 144

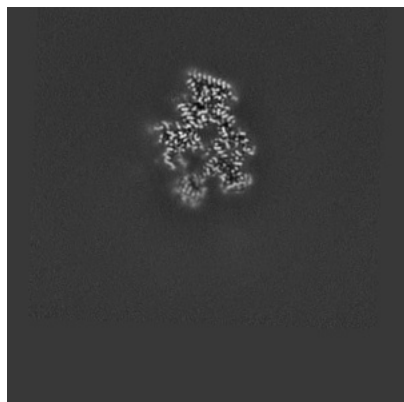


Y Index: 172

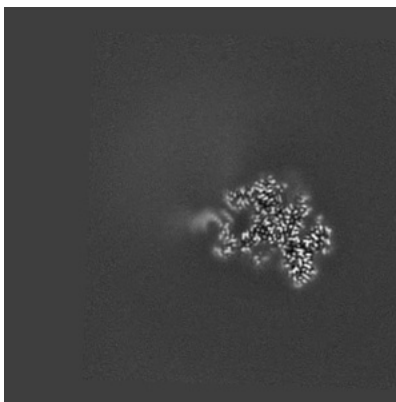


Z Index: 224

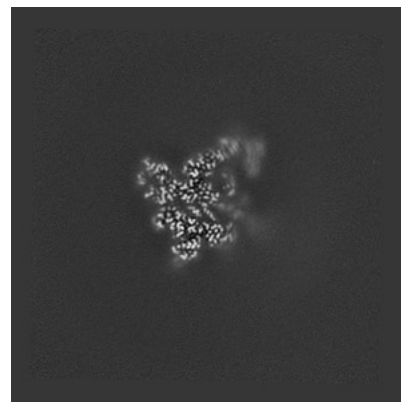
6.3.2 Raw map



X Index: 133



Y Index: 172

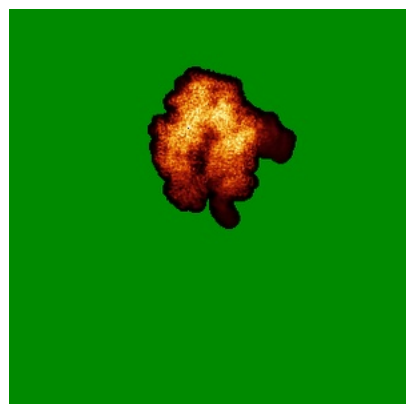


Z Index: 224

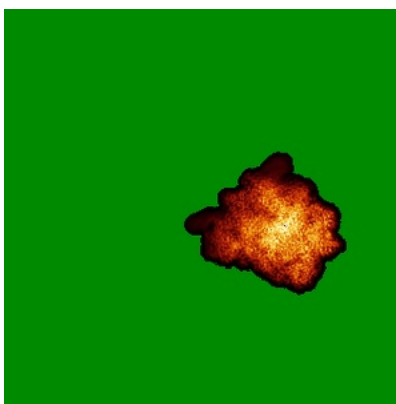
The images above show the largest variance slices of the map in three orthogonal directions.

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

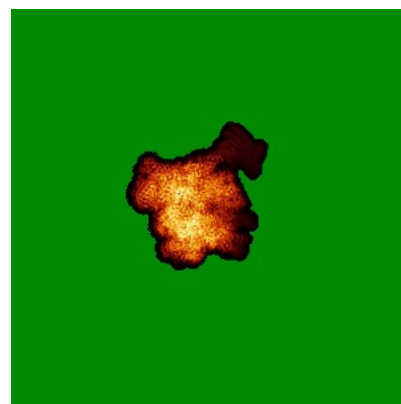
6.4.1 Primary map



X



Y

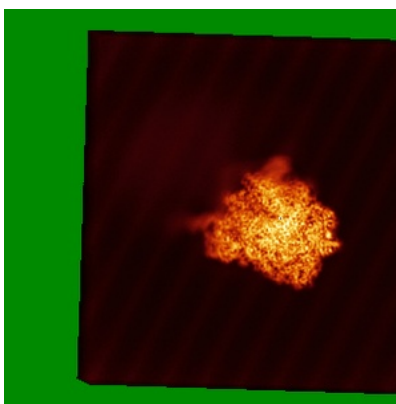


Z

6.4.2 Raw map



X



Y

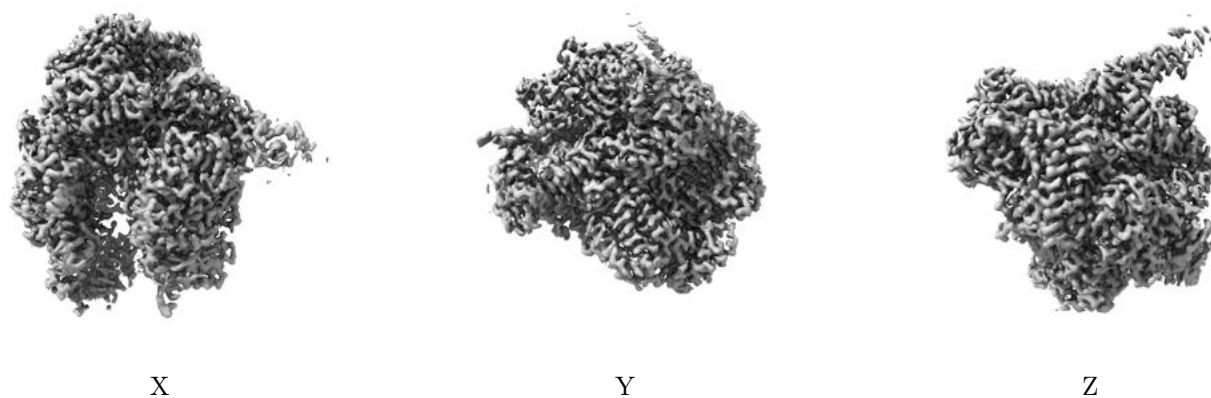


Z

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.

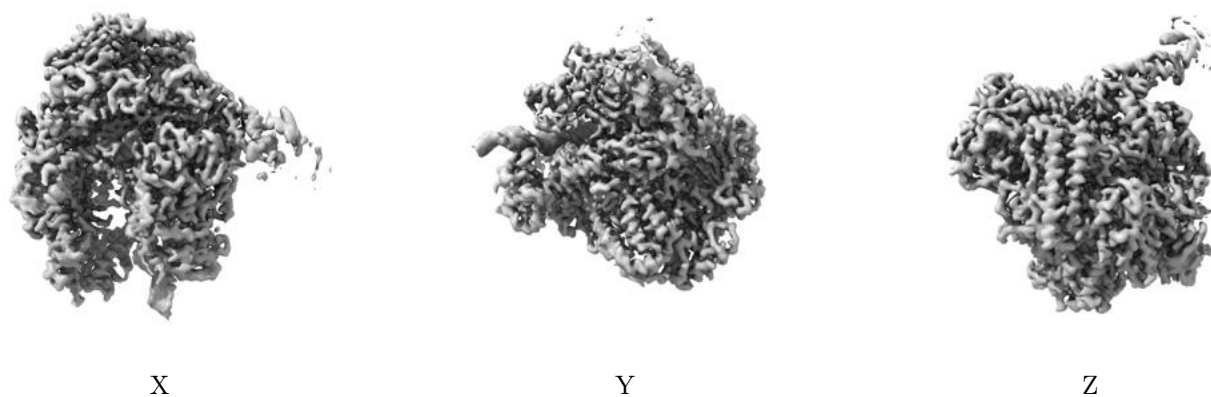
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.93. 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.

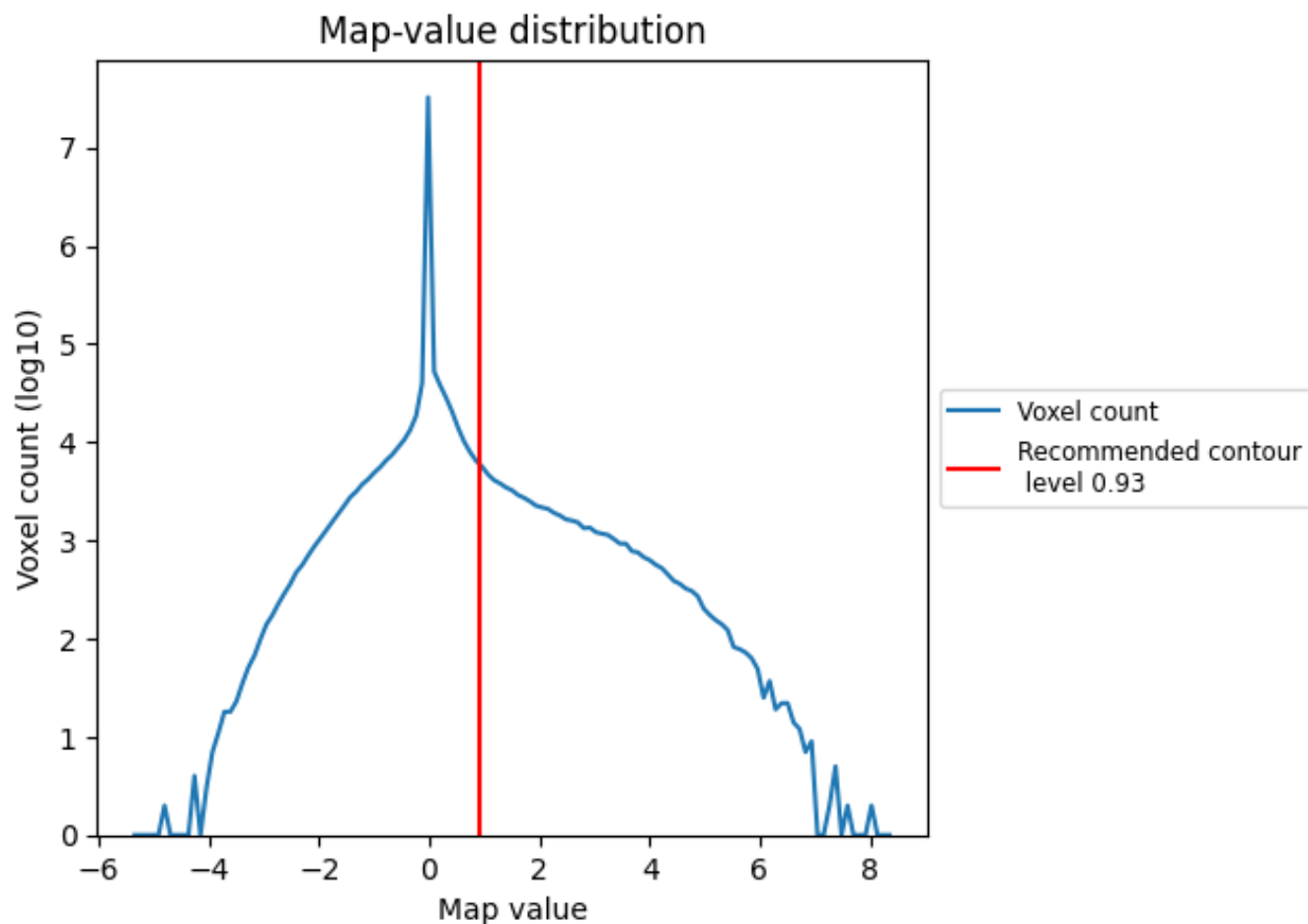
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

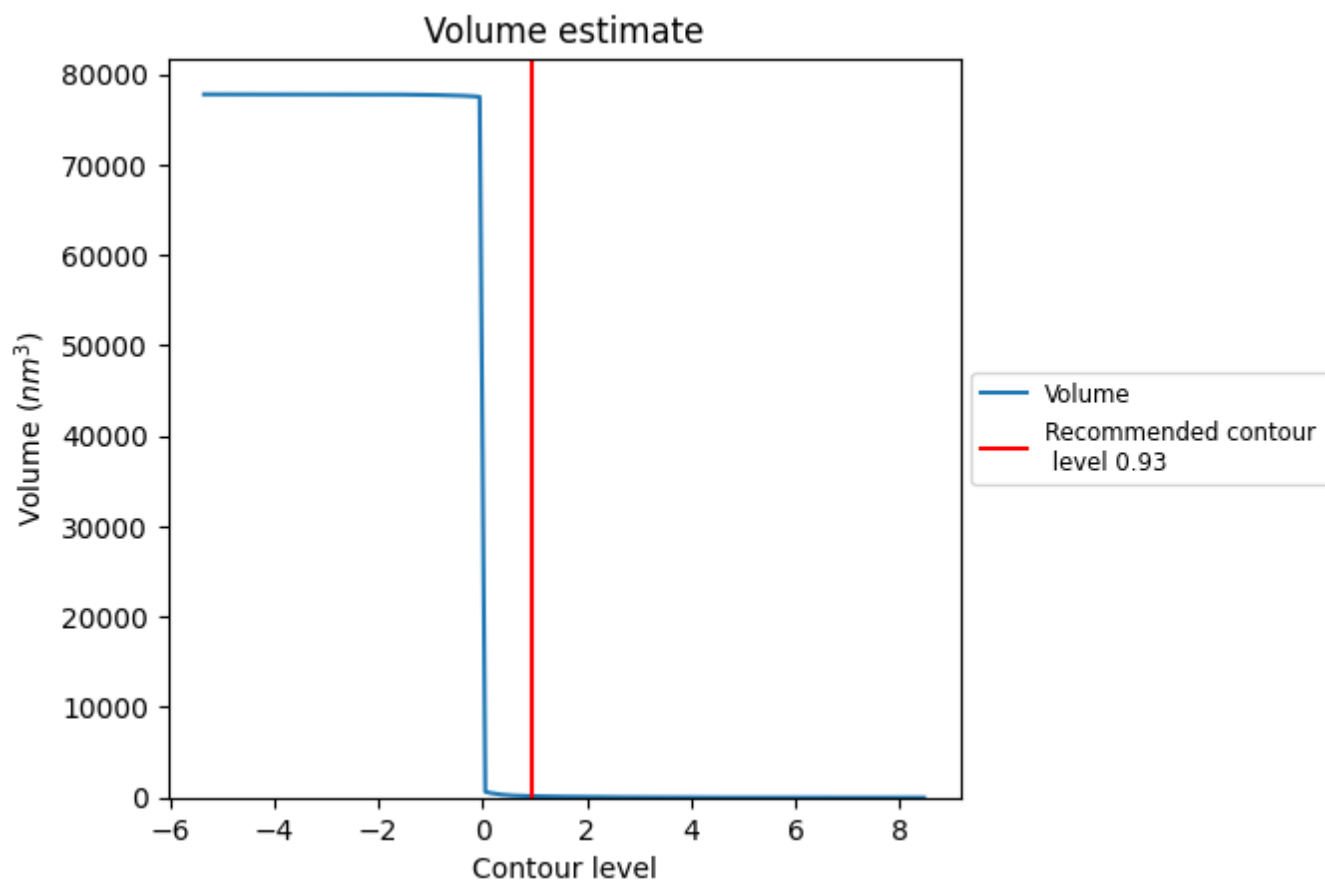
This section contains the results of statistical analysis of the map.

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.

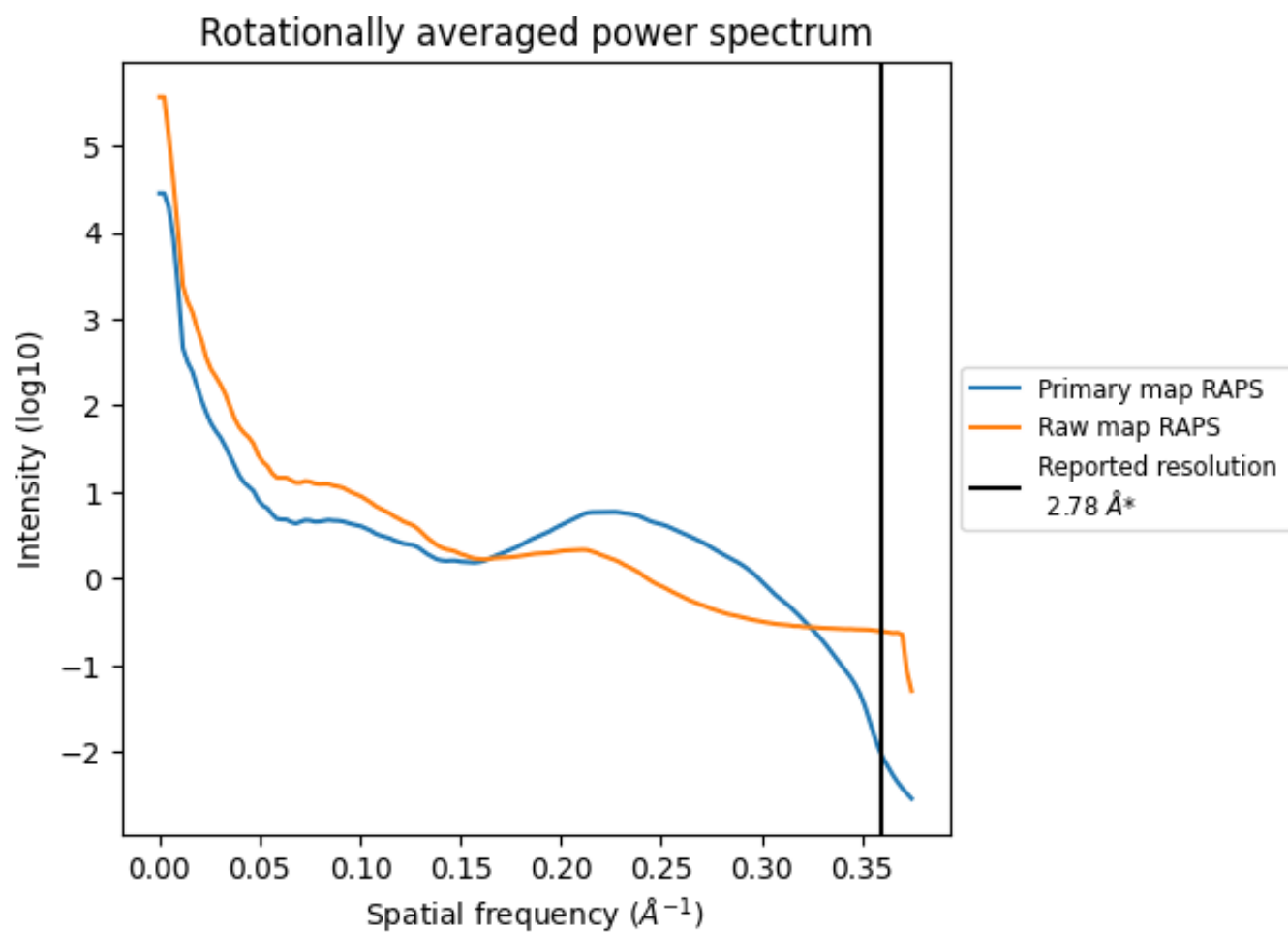
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 ⓘ

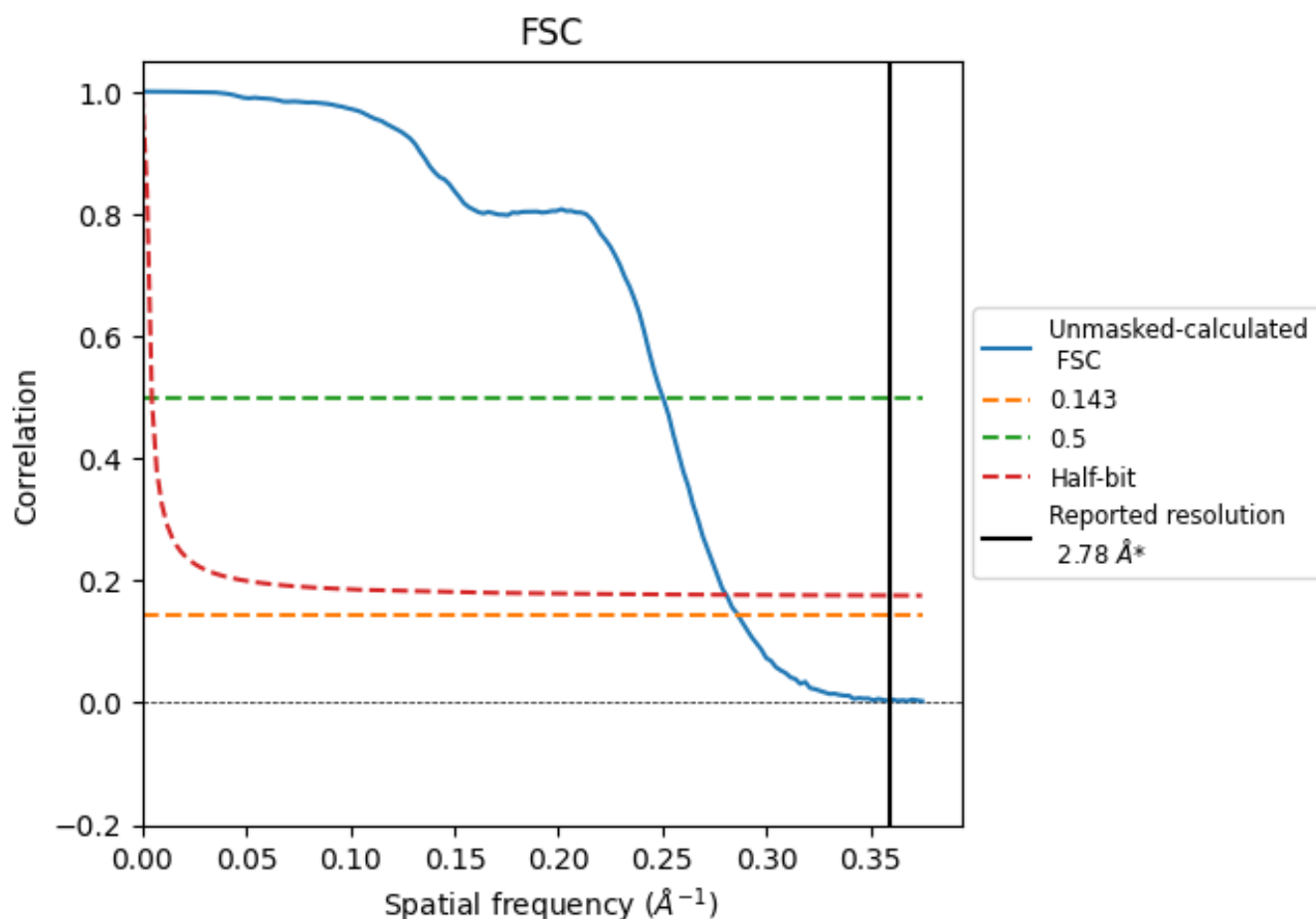


*Reported resolution corresponds to spatial frequency of $0.360 \text{ \AA}^{-1}$

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 0.360 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	4.00	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.78 by more than 10 %

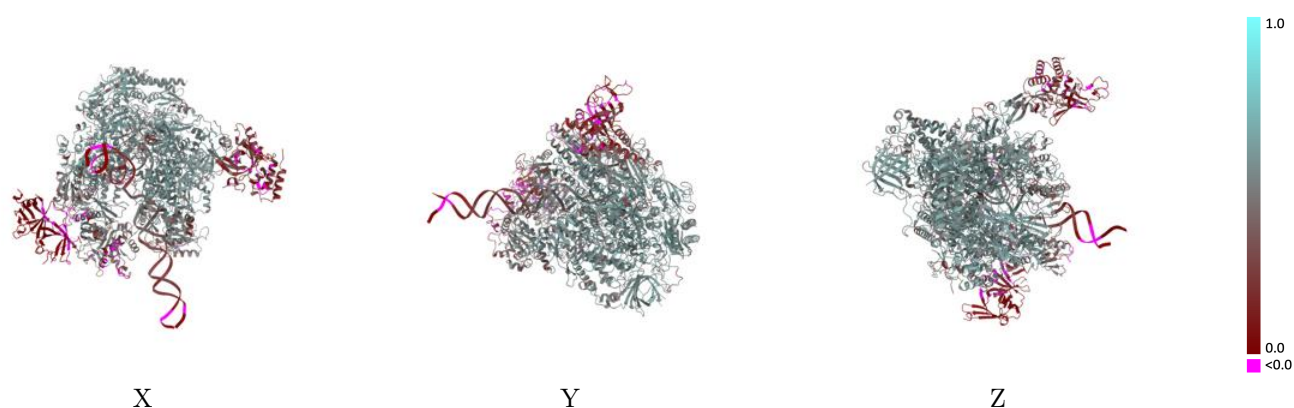
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37405 and PDB model 8WAU. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

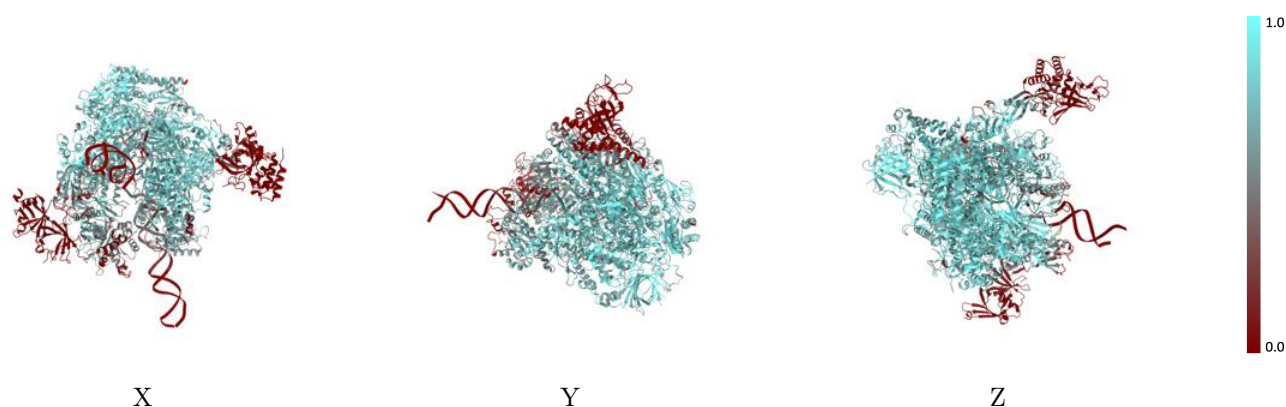
This section was not generated.

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



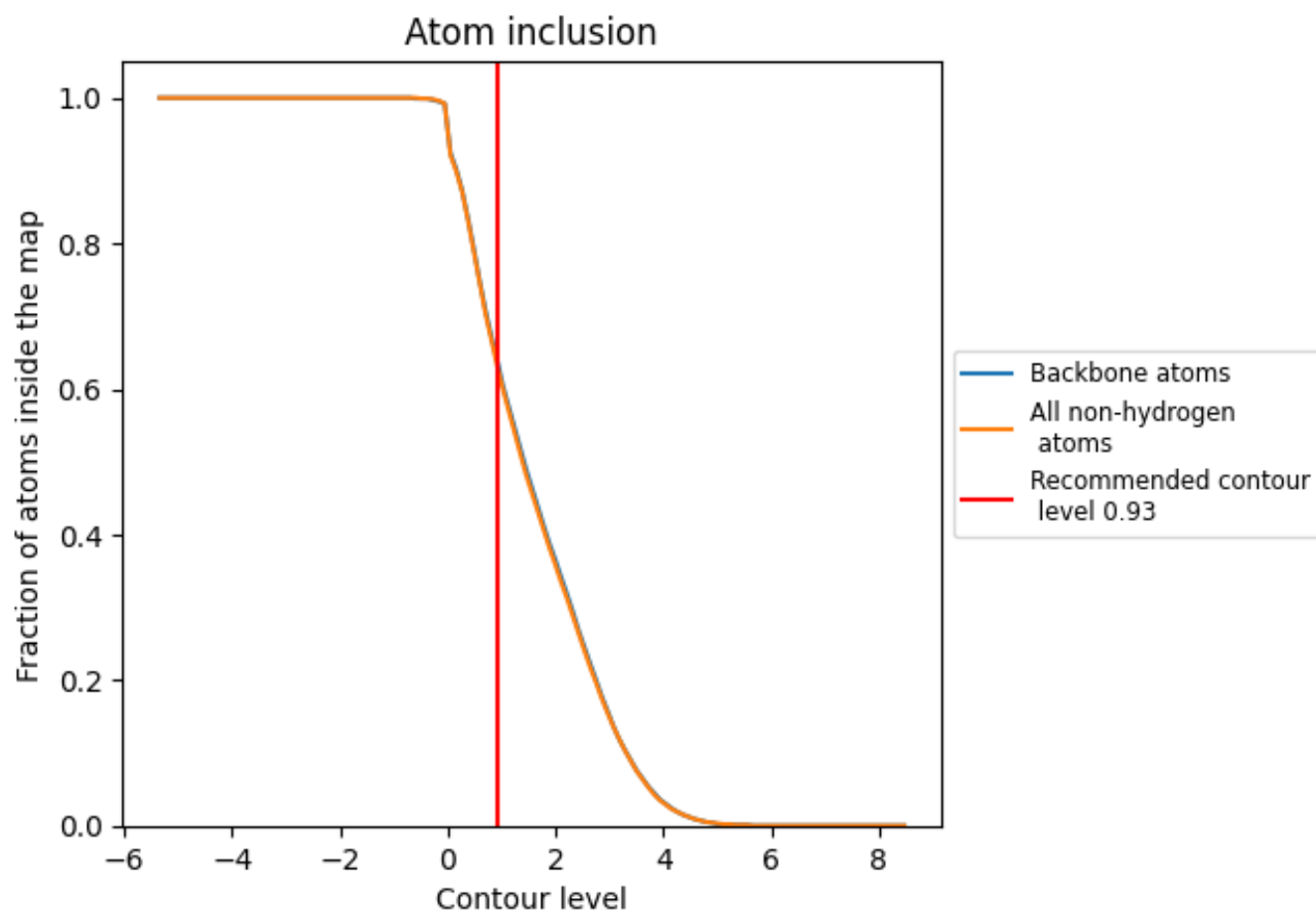
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.93).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.93) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6270	 0.4560
N	 0.9030	 0.5800
S	 0.0000	 0.0210
T	 0.0000	 -0.0050
X	 0.1900	 0.2020
Y	 0.3290	 0.2900
Z	 0.6570	 0.4760
o	 0.7270	 0.5170
p	 0.7300	 0.5100
q	 0.8260	 0.5460
r	 0.0240	 0.1930
s	 0.7310	 0.5000
t	 0.7820	 0.5400
u	 0.2670	 0.2870
v	 0.7810	 0.5200
w	 0.6230	 0.4430
x	 0.8310	 0.5700
y	 0.8190	 0.5580
z	 0.6990	 0.4840

