



wwPDB EM Validation Summary Report ⓘ

Mar 18, 2026 – 10:41 AM UTC

PDB ID : 8WAT / pdb_00008wat
EMDB ID : EMD-37404
Title : De novo transcribing complex 10 (TC10), the early elongation complex with Pol II positioned 10nt 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 : 2.82 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:

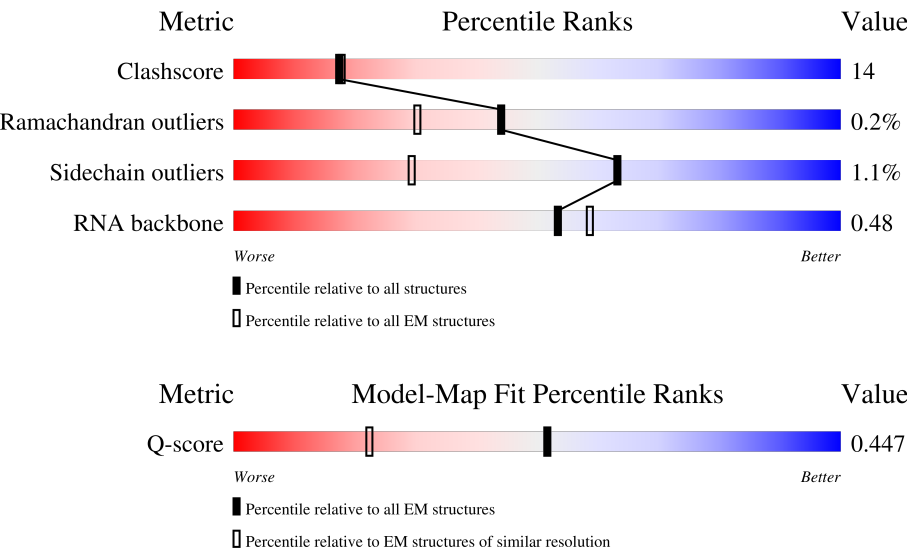
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.82 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	11795 (2.32 - 3.32)

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	10	
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 35676 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	8	Total	C	N	O	S	0	0
			64	39	10	14	1		

- 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	0	0
			1138	719	208	208	3		

- 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	0	0
			789	492	142	154	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	43	Total	C	N	O	P	0	0
			876	417	153	263	43		

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	54	Total	C	N	O	P	0	0
			1114	527	214	319	54		

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	10	Total	C	N	O	P	0	0
			219	95	35	77	12		

- 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		

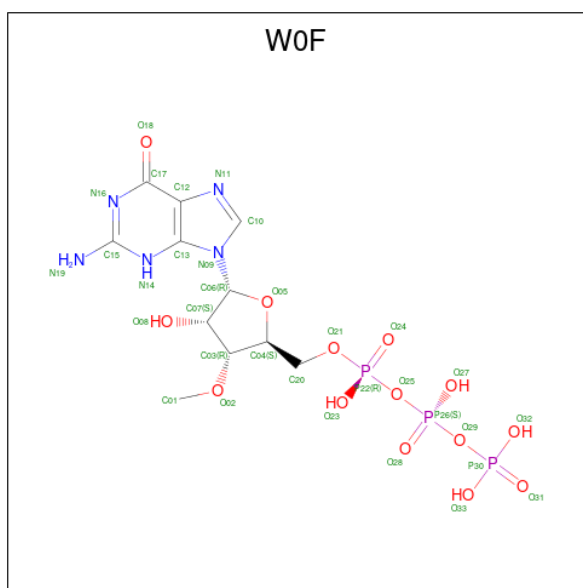
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

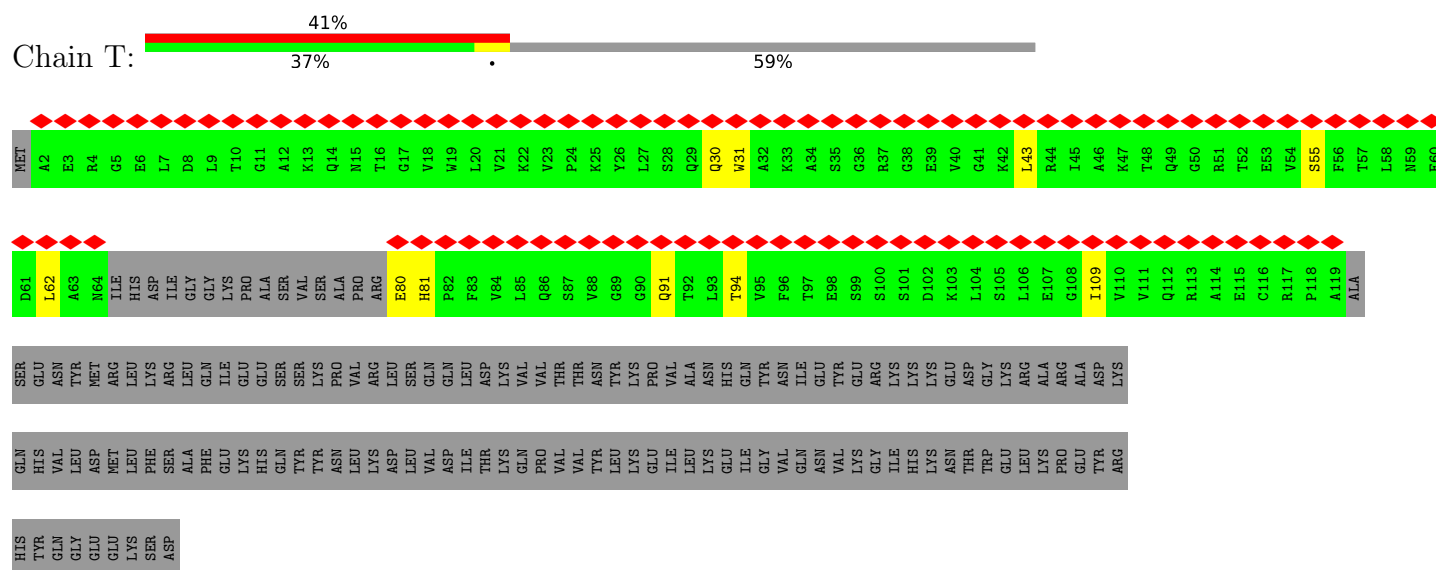
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

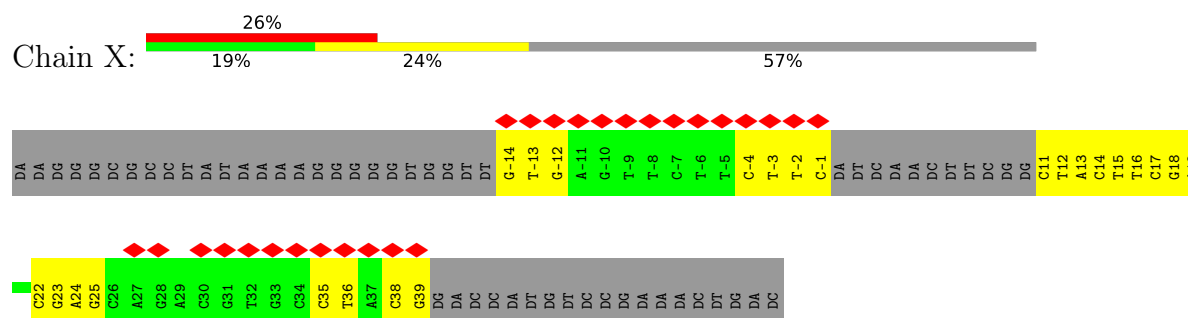
- Molecule 21 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



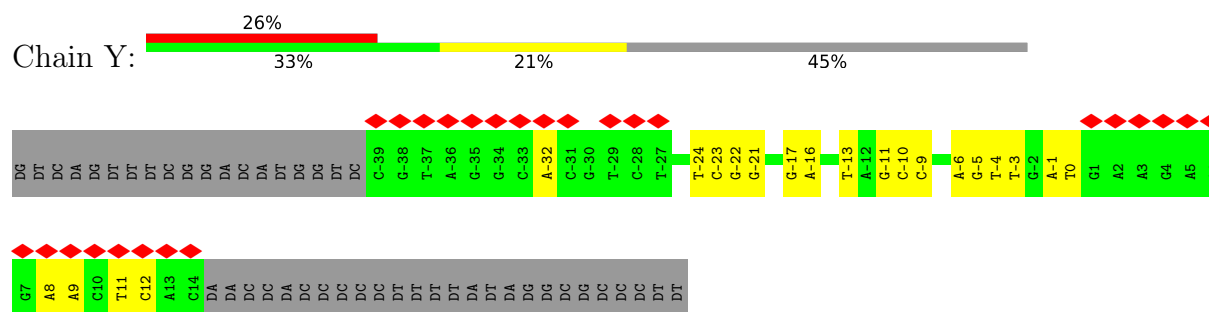
Mol	Chain	Residues	Atoms					AltConf
21	p	1	Total	C	N	O	P	0
			33	11	5	14	3	



- Molecule 4: non-template DNA



- Molecule 5: template DNA



- Molecule 6: RNA

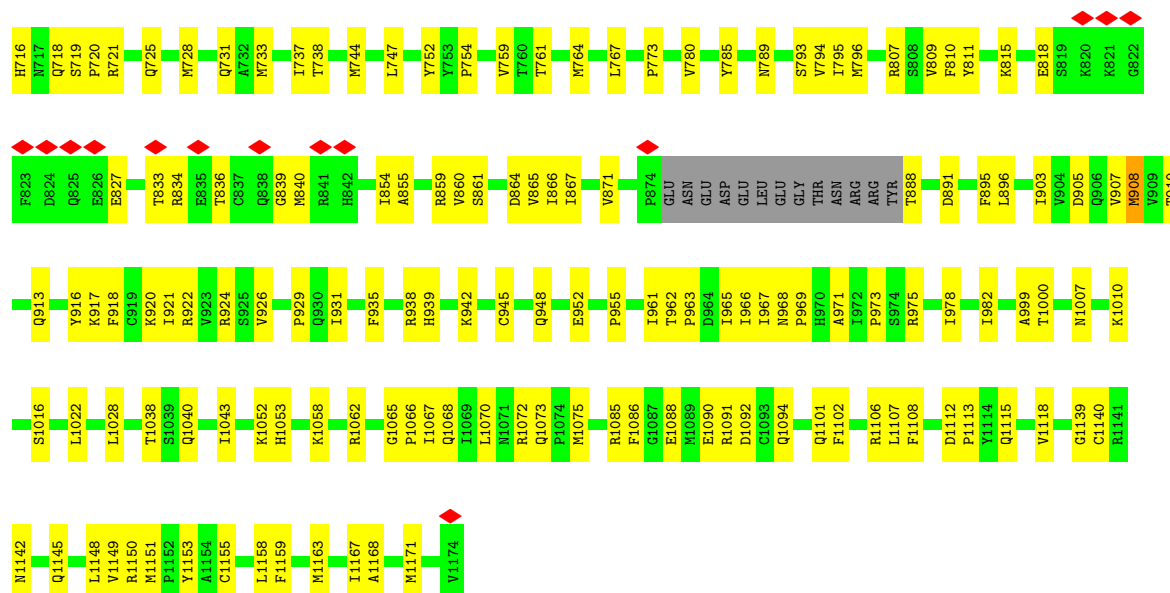


- Molecule 7: DNA-directed RNA polymerase subunit

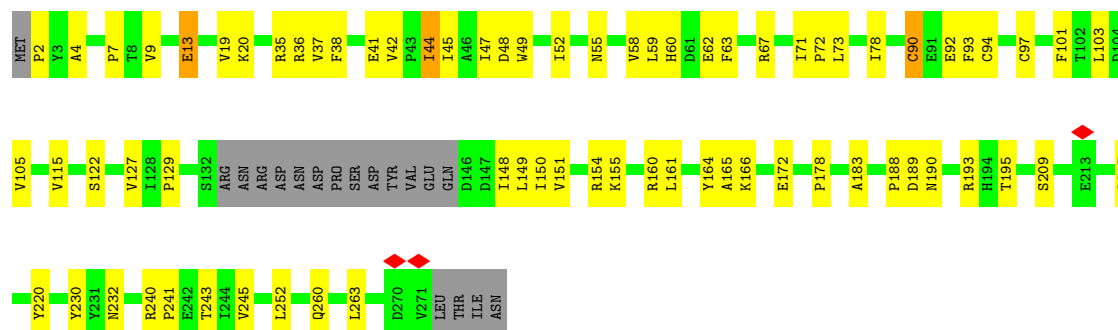


T1435	E1327	I1246	K1135	D894	R749	K627	S508	P381	Q295	C184	F112	MET
V1438	A1330	D1249	T1136	V901	A756	V628	L509	M388	A299	G185	F113	HIS
M1440	L1331	D1250	L1139	E902	V630	V630	E510	Y187	A299	R186	C114	GLY
A1443	Q1332	N1251	L1143	F903	L760	N632	E514	R408	V302	Y187	D120	GLY
A1444	E1333	E1252	L1147	N905	N765	N632	T515	Y413	I303	R190	S121	PRO
H1445	E1337	E1253	A1148	L906	N769	T636	Q516	P414	V307	I191	N122	PRO
E1456	R1345	K1254	R1153	T908	N769	N637	E517	R421	K308	R192	N123	GLY
N1457	V1346	L1255	R1157	L909	T781	N637	E520	R421	L309	R193	P124	ASP
I1458	L1347	L1256	L1157	K910	L781	N637	E521	I427	L316	S194	K125	S11
Q1462	S1346	L1257	L1158	P911	V784	L645	E522	H432	M317	L198	I126	L15
G1467	E1349	R1258	L1159	S912	I785	G646	E523	P433	D128	Y199	K127	L15
T1468	E1358	I1259	R1160	F916	A786	T647	V526	K434	E201	A200	E128	I18
F1471	T1358	I1261	E1161	F922	V788	R666	T527	H449	E202	W202	A131	L26
D1472	F1366	M1262	E1162	D933	Q791	F668	S530	H449	W202	K203	K132	L31
L1473	G1370	N1263	H1163	Y924	N792	V669	N531	M469	K203	H204	R32	R32
L1474	D1265	D1265	T1173	E927	F802	N671	P533	M459	V205	G135	K134	R33
A1477	V1374	E1266	I1175	E936	F802	Q673	V534	M460	E207	E135	G135	M34
E1478	E1381	N1267	P1181	L938	N808	Q673	N535	Q461	D208	K139	I141	G40
C1480	I1386	K1268	T1184	V939	F810	V675	V545	T463	S209	R140	L141	I41
Y1482	Y1392	M1269	D1189	L943	P817	H685	F548	M469	Q210	E211	D146	T46
G1483	L1398	Q1270	Q1190	L948	N823	T686	T549	M470	E211	K212	E146	E48
M1484	A1399	E1272	E1191	L952	E924	L687	D552	G471	K213	K214	K149	R51
I1485	L1400	E1274	W1192	E953	N828	G688	F564	R473	G333	L215	G150	P52
T1486	L1401	V1275	E1198	R960	L831	L695	L555	L477	K340	P218	I153	K53
P1487	C1402	D1277	M1199	L966	L847	D695	V560	P478	L343	E219	C154	L57
THR	T1406	K1278	D1201	T972	N848	T706	N565	Q481	K344	K226	GLY	Q62
ASN	C1407	D1280	V1202	V978	V852	A709	Q576	F482	R349	E246	GLU	E56
ILE	R1408	D1282	V1204	L983	K853	V713	P577	R483	V350	W247	GLU	GLU
GLY	L1411	E1289	A1205	N986	T860	I717	L580	L484	N353	M248	MET	MET
LEU	M1412	L1293	I1207	N987	R863	H721	K581	M485	L354	L253	ASN	ASN
ALA	I1413	T1294	S1208	W988	L864	N736	P582	S487	G355	P254	LYS	LYS
GLY	T1415	D1295	W1210	N989	L865	T736	N601	V488	K357	P255	PHE	PHE
GLY	R1417	M1296	L1211	A990	N866	P727	L585	T490	R358	V256	GLY	GLY
ALA	R1421	T1297	R1212	Q991	S867	L733	Q590	P491	S362	V260	VAL	VAL
PHE	L1427	L1298	R1213	Q991	S867	R734	L591	Y492	T365	R261	GLN	GLN
GLY	M1428	Q1299	V1214	Q992	N871	Q735	T591	D495	V366	V265	PRO	PRO
SER	C1430	I1301	E1215	T996	M872	E738	N601	F496	V367	M266	GLY	GLY
ALA	E1433	Q1313	Q1230	D1003	N873	L745	D612	D497	T368	Q267	ASP	ASP
PRO	E1434	T1314	K1234	L1004	K874	A748	Y618	G498	D370	G268	GLU	GLU
PRO		D1242	K1234	H1005	Q885			D499	I375	S269	LEU	LEU
GLY		L1243		P1006	E893			M501	D376	A270	THR	THR
				I1007				N502	Q377	R271	LYS	LYS
								L503	V378	L280	GLY	GLY
									V390	A281	H181	H181
										D282	G182	G182
										I286	G183	G183

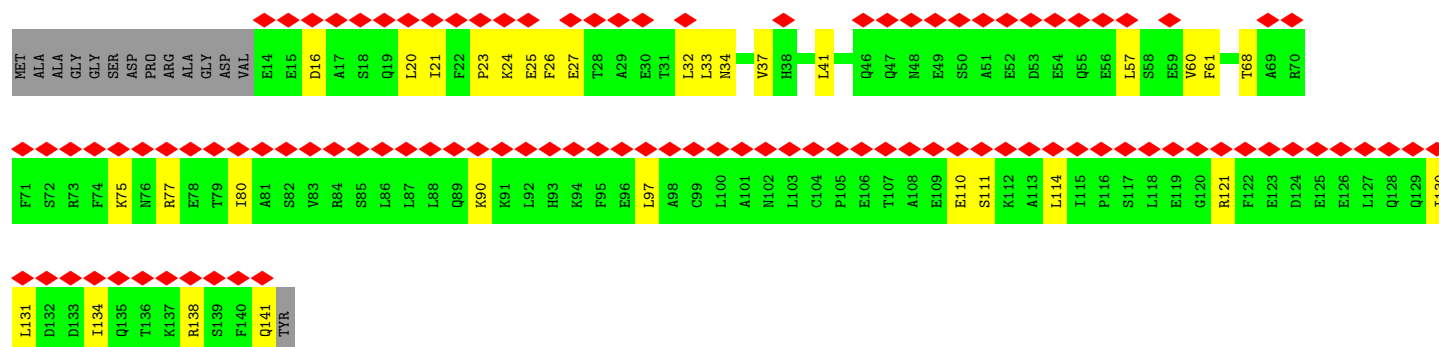




• Molecule 9: DNA-directed RNA polymerase II subunit RPB3

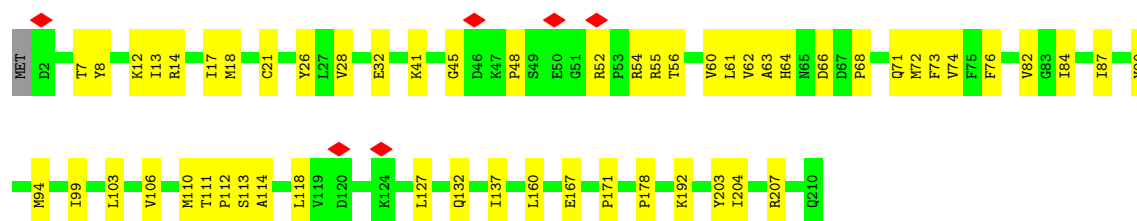


• Molecule 10: DNA-directed RNA polymerase II subunit RPB4

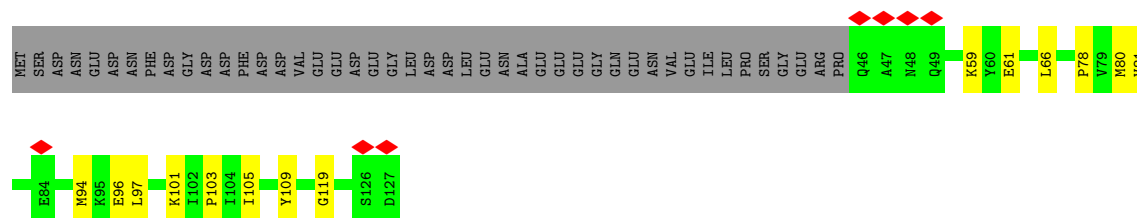


• Molecule 11: DNA-directed RNA polymerase II subunit E

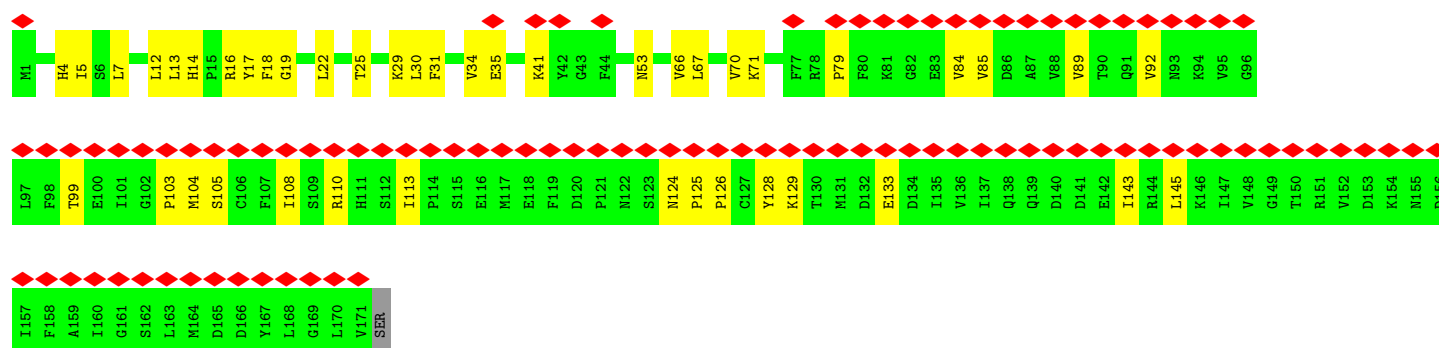
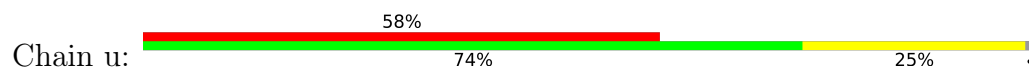




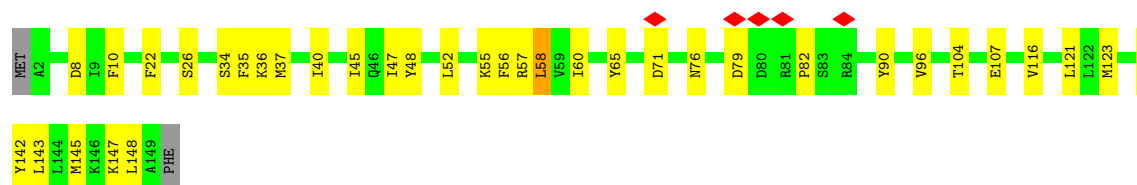
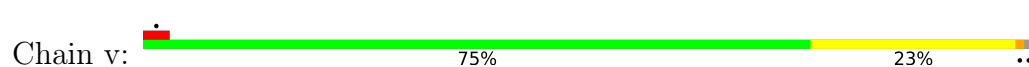
- Molecule 12: DNA-directed RNA polymerase II subunit F



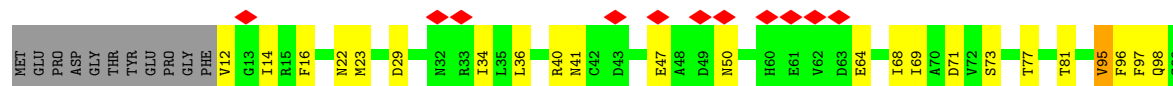
- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

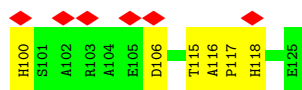


- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

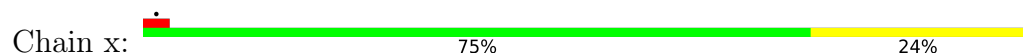


- Molecule 15: DNA-directed RNA polymerase II subunit RPB9

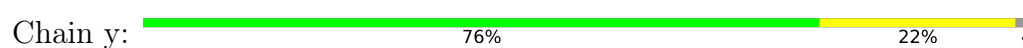




- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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	660714	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	5.668	Depositor
Minimum map value	-3.117	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.618	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: ATP, ILX, ZN, MG, CSX, TRX, G2L, WOF, 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	0.12	0/1167	0.26	0/1576
3	T	0.12	0/799	0.28	0/1077
4	X	0.28	0/978	0.59	0/1504
5	Y	0.28	0/1252	0.56	0/1931
6	Z	0.22	0/181	0.35	0/278
7	o	0.23	1/11723 (0.0%)	0.41	1/15830 (0.0%)
8	p	0.26	1/9332 (0.0%)	0.45	3/12598 (0.0%)
9	q	0.21	0/2102	0.39	0/2857
10	r	0.11	0/1064	0.26	0/1428
11	s	0.22	0/1751	0.40	0/2366
12	t	0.15	0/667	0.27	0/901
13	u	0.15	0/1382	0.36	0/1874
14	v	0.18	0/1207	0.39	0/1628
15	w	0.15	0/948	0.34	0/1284
16	x	0.19	0/542	0.35	0/730
17	y	0.19	0/939	0.32	0/1271
18	z	0.20	0/377	0.44	0/500
All	All	0.22	2/36433 (0.0%)	0.41	4/49659 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	558	PRO	N-CD	9.02	1.60	1.47
7	o	1098	PRO	N-CD	8.84	1.60	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	p	610	ARG	CG-CD-NE	5.95	125.08	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	p	535	GLY	CA-C-O	-5.59	118.38	122.23
7	o	1107	PHE	CA-C-O	-5.34	115.89	121.55
8	p	573	TRP	N-CA-C	-5.08	102.39	109.96

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	0	51	6	0
2	S	1138	0	1103	20	0
3	T	789	0	795	7	0
4	X	876	0	487	26	0
5	Y	1114	0	605	21	0
6	Z	219	0	107	9	0
7	o	11510	0	11616	367	0
8	p	9149	0	9178	325	0
9	q	2059	0	2007	71	0
10	r	1050	0	1032	27	0
11	s	1720	0	1737	50	0
12	t	657	0	684	12	0
13	u	1351	0	1358	33	0
14	v	1186	0	1147	34	0
15	w	927	0	859	22	0
16	x	533	0	553	14	0
17	y	920	0	942	26	0
18	z	372	0	378	10	0
19	o	2	0	0	0	0
19	p	1	0	0	0	0
19	q	1	0	0	0	0
19	w	2	0	0	0	0
19	x	1	0	0	0	0
19	z	1	0	0	0	0
20	o	1	0	0	0	0
21	p	33	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35676	0	34639	951	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 14.

The worst 5 of 951 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)
8:p:860:VAL:CG1	8:p:896:LEU:HD11	1.24	1.60
8:p:860:VAL:HG12	8:p:896:LEU:CD1	1.35	1.54
10:r:75:LYS:CE	10:r:141:GLN:OE1	1.69	1.39
10:r:75:LYS:NZ	10:r:141:GLN:OE1	1.58	1.36
10:r:75:LYS:CD	10:r:141:GLN:OE1	1.73	1.36

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%)	133 (99%)	1 (1%)	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1394 (96%)	52 (4%)	2 (0%)	48	75
8	p	1142/1174 (97%)	1083 (95%)	54 (5%)	5 (0%)	30	58
9	q	253/275 (92%)	245 (97%)	8 (3%)	0	100	100
10	r	126/142 (89%)	125 (99%)	1 (1%)	0	100	100
11	s	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
12	t	80/127 (63%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	u	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
14	v	146/150 (97%)	139 (95%)	6 (4%)	1 (1%)	18	45
15	w	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	3	11
17	y	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
18	z	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
All	All	4140/5361 (77%)	3976 (96%)	154 (4%)	10 (0%)	44	71

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	497	LYS
8	p	549	SER
8	p	570	ASN

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	90
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1259 (98%)	21 (2%)	55	82
8	p	1001/1027 (98%)	991 (99%)	10 (1%)	68	88
9	q	234/252 (93%)	231 (99%)	3 (1%)	61	85
10	r	118/126 (94%)	117 (99%)	1 (1%)	73	90
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	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	v	129/131 (98%)	128 (99%)	1 (1%)	73	90
15	w	103/112 (92%)	102 (99%)	1 (1%)	68	88
16	x	56/56 (100%)	56 (100%)	0	100	100
17	y	104/106 (98%)	103 (99%)	1 (1%)	68	88
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3648 (99%)	40 (1%)	63	86

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	p	598	VAL
10	r	97	LEU
8	p	908	MET
9	q	13	GLU
14	v	58	LEU

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

Mol	Chain	Res	Type
8	p	1142	ASN
15	w	118	HIS
9	q	190	ASN
11	s	35	GLN
18	z	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	3	C
6	Z	10	G2L

There are no RNA pucker outliers to report.

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

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	$\# Z > 2$
1	ILX	N	1	1	8,9,10	0.60	0	8,11,13	1.40	1 (12%)
1	TRX	N	2	1	15,16,17	1.10	1 (6%)	17,22,24	0.99	1 (5%)
1	CSX	N	6	1	3,6,7	1.07	0	1,6,8	2.11	1 (100%)
6	G2L	Z	10	5,6,20	23,26,30	1.26	2 (8%)	31,38,44	2.72	10 (32%)
1	HYP	N	8	1	7,8,9	0.83	0	5,10,12	2.35	2 (40%)

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
1	ILX	N	1	1	-	7/11/12/14	-
1	TRX	N	2	1	-	2/5/6/8	0/2/2/2
1	CSX	N	6	1	-	2/2/5/7	-
6	G2L	Z	10	5,6,20	-	1/9/27/31	0/3/3/3
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	10	G2L	C5-C4	3.10	1.47	1.38
6	Z	10	G2L	C6-N1	-2.39	1.34	1.38
1	N	2	TRX	CD2-CE2	2.29	1.44	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	10	G2L	O4'-C1'-N9	6.29	122.61	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	10	G2L	C5-C4-N3	-6.12	118.64	128.39
6	Z	10	G2L	O4'-C4'-C5'	-5.51	91.69	109.33
6	Z	10	G2L	C2-N3-C4	5.12	121.11	112.30
6	Z	10	G2L	C2'-C1'-N9	-4.58	100.49	113.25

There are no chirality outliers.

5 of 12 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.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	ILX	3	0
1	N	2	TRX	2	0
1	N	6	CSX	1	0
6	Z	10	G2L	5	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
21	W0F	p	1201	-	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
21	W0F	p	1201	-	-	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)
21	p	1201	W0F	P26-O29	13.80	1.74	1.59
21	p	1201	W0F	C03-C04	-9.77	1.27	1.52
21	p	1201	W0F	P22-O25	8.41	1.68	1.59
21	p	1201	W0F	O05-C04	6.90	1.60	1.45
21	p	1201	W0F	O05-C06	-5.98	1.28	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	p	1201	W0F	O05-C06-N09	-14.56	75.37	108.36
21	p	1201	W0F	C07-C06-N09	8.27	136.28	113.25
21	p	1201	W0F	O05-C04-C03	-5.79	92.70	104.92
21	p	1201	W0F	O27-P26-O25	-5.28	92.99	107.27
21	p	1201	W0F	O05-C04-C20	4.94	125.15	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

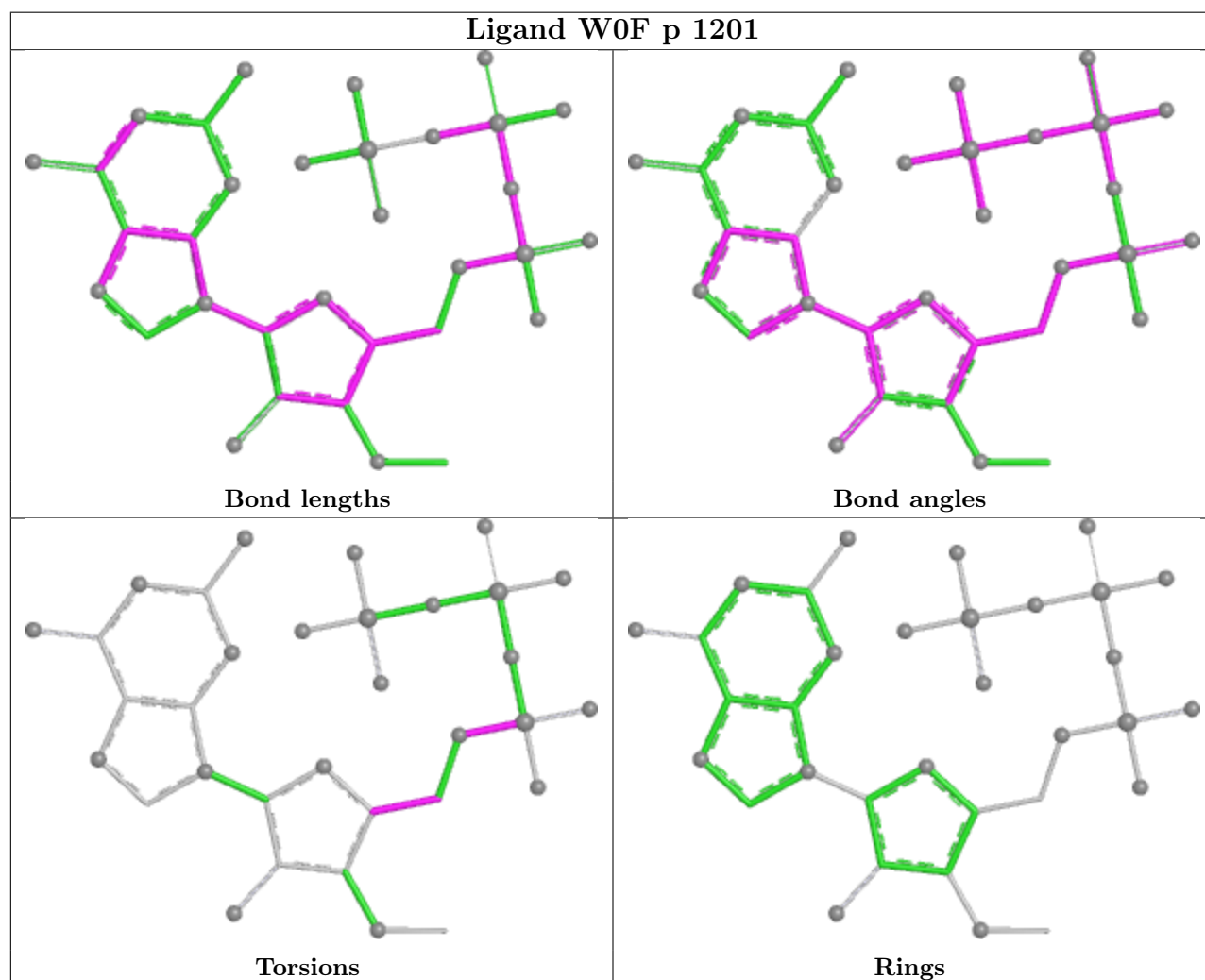
Mol	Chain	Res	Type	Atoms
21	p	1201	W0F	C20-O21-P22-O24
21	p	1201	W0F	C20-O21-P22-O25
21	p	1201	W0F	C03-C04-C20-O21

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	p	1201	W0F	5	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.

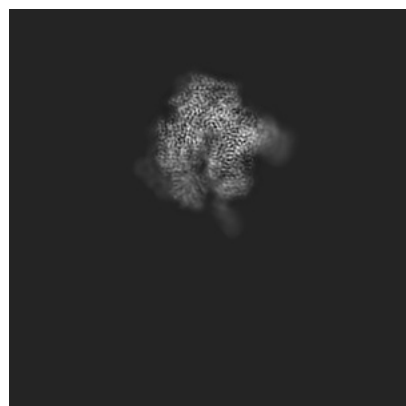
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37404. These allow visual inspection of the internal detail of the map and identification of artifacts.

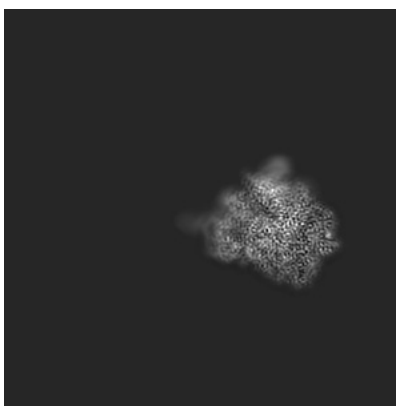
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

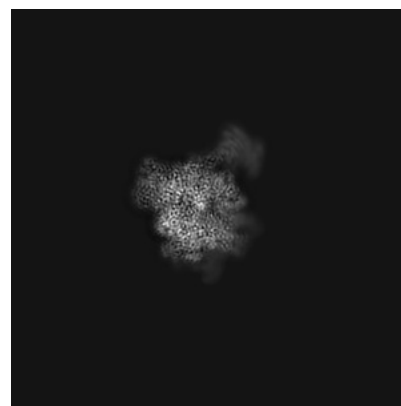
6.1.1 Primary map



X

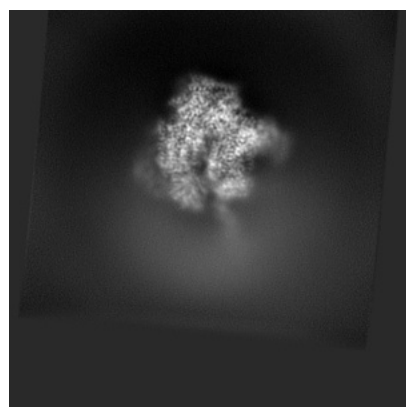


Y

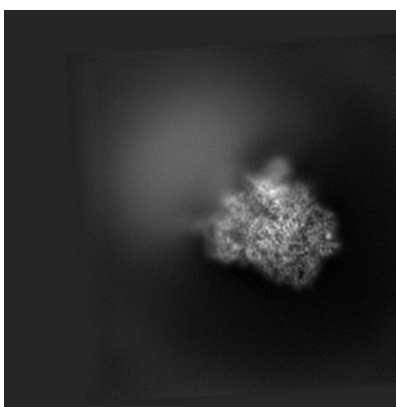


Z

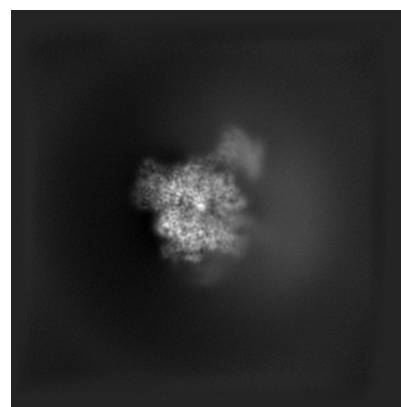
6.1.2 Raw map



X



Y

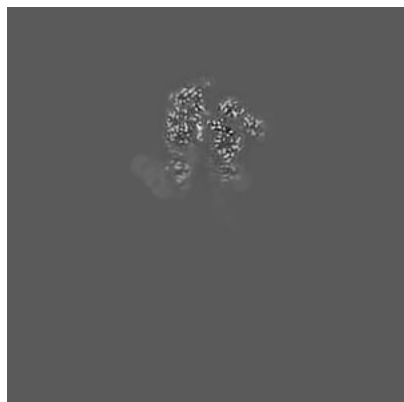


Z

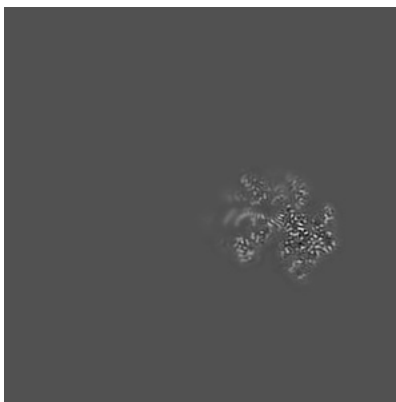
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

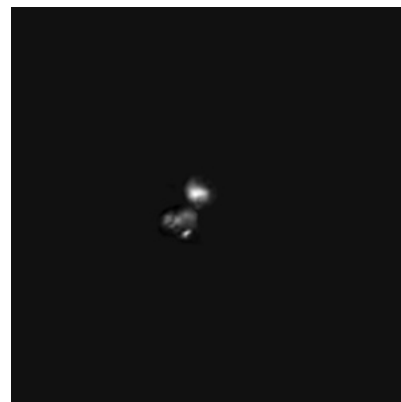
6.2.1 Primary map



X Index: 160

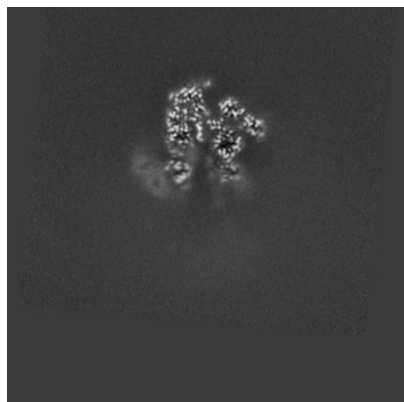


Y Index: 160

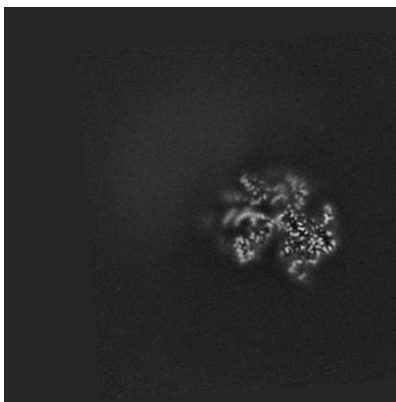


Z Index: 160

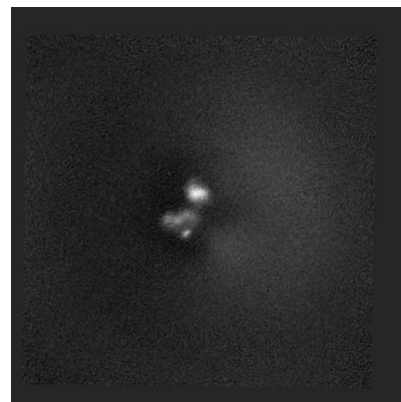
6.2.2 Raw map



X Index: 160



Y Index: 160

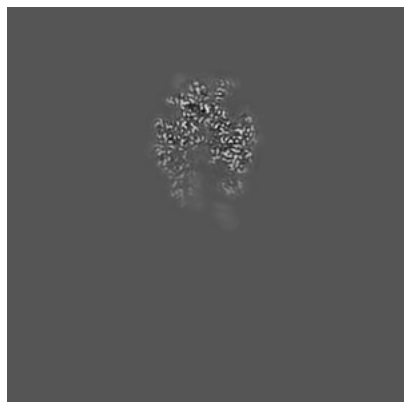


Z Index: 160

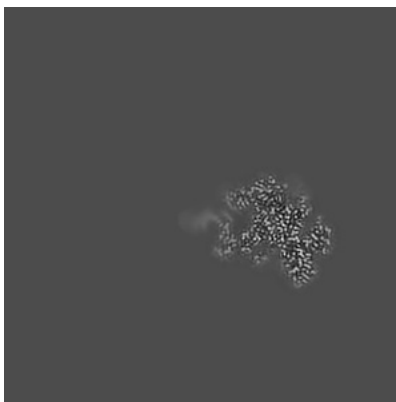
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

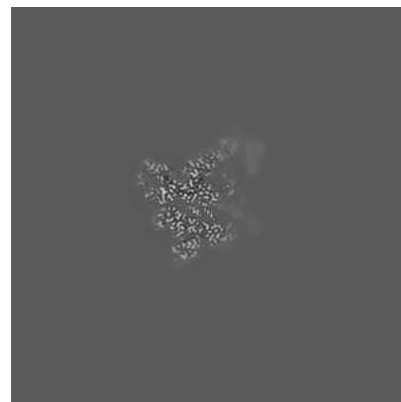
6.3.1 Primary map



X Index: 142

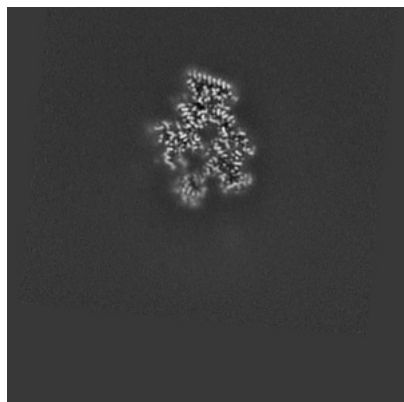


Y Index: 172

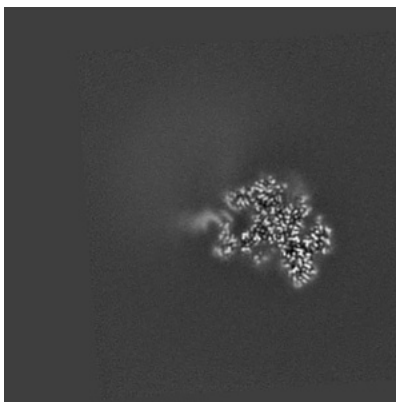


Z Index: 224

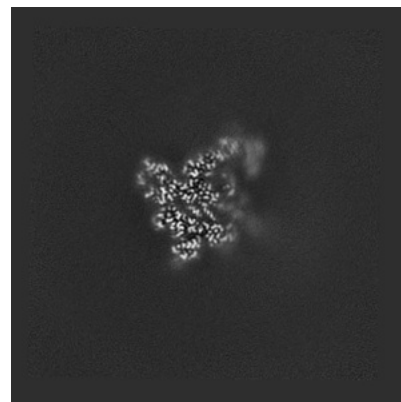
6.3.2 Raw map



X Index: 133



Y Index: 172

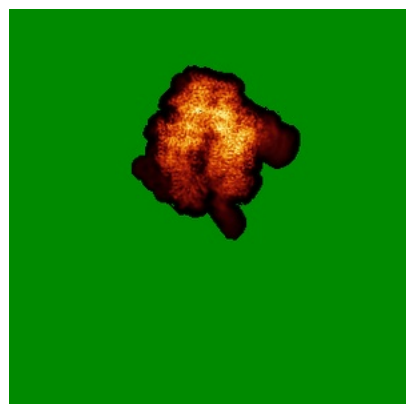


Z Index: 224

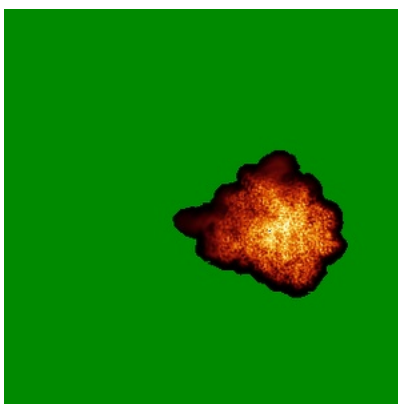
The images above show the largest variance slices of the map in three orthogonal directions.

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

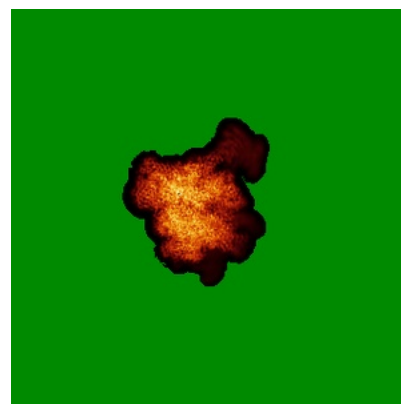
6.4.1 Primary map



X

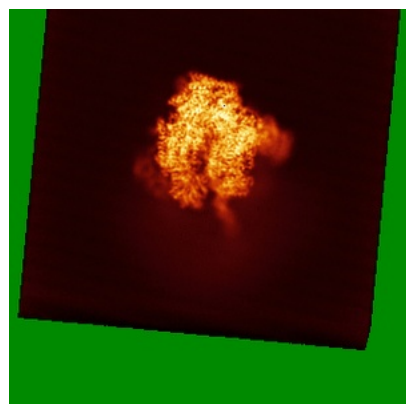


Y

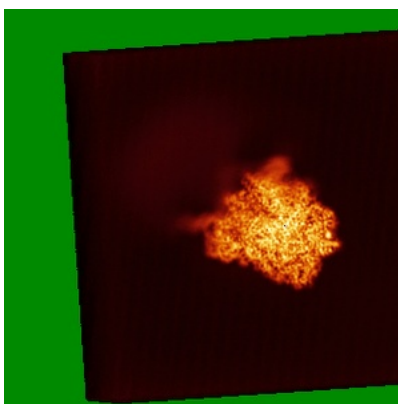


Z

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 0.618. 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.

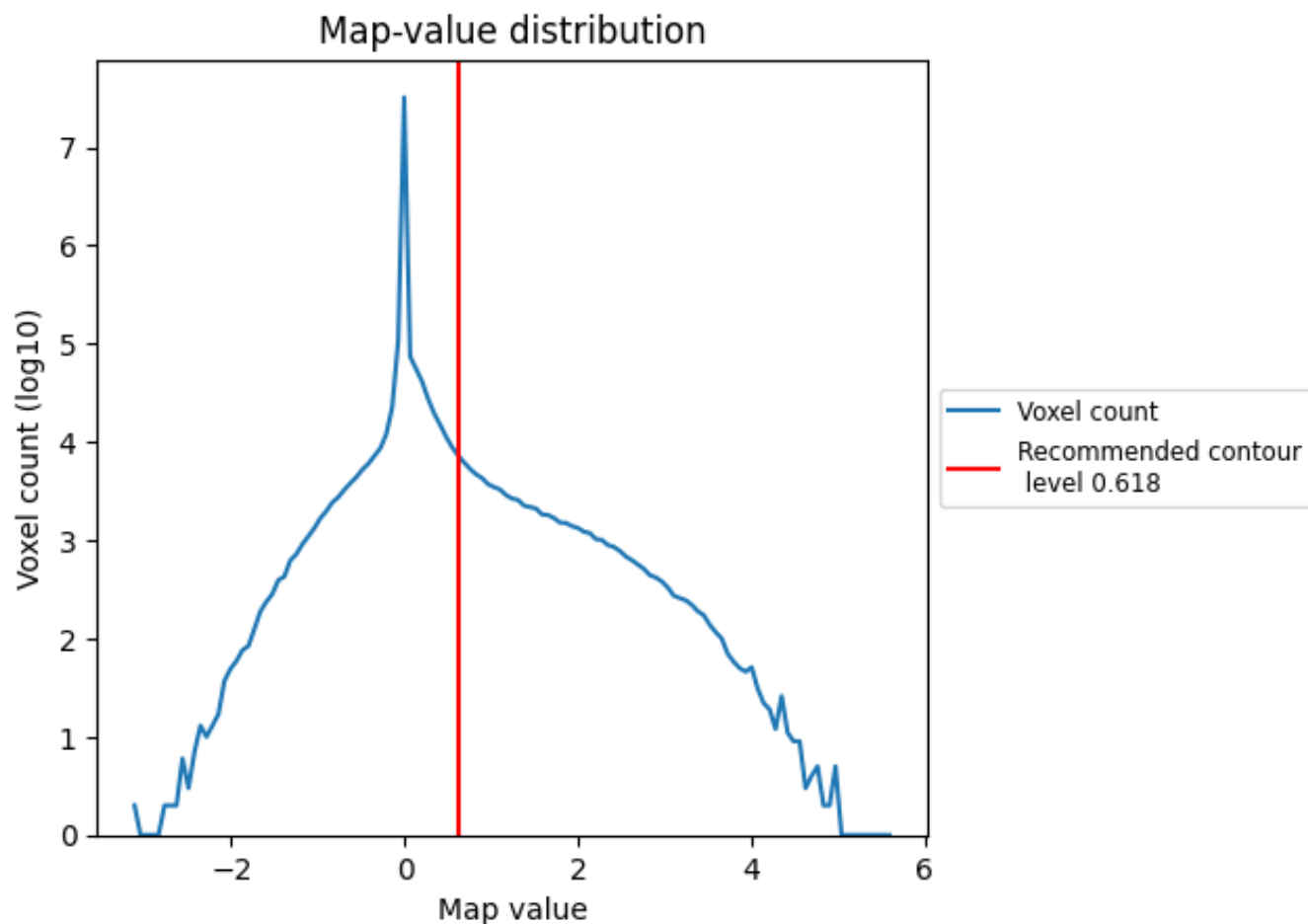
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

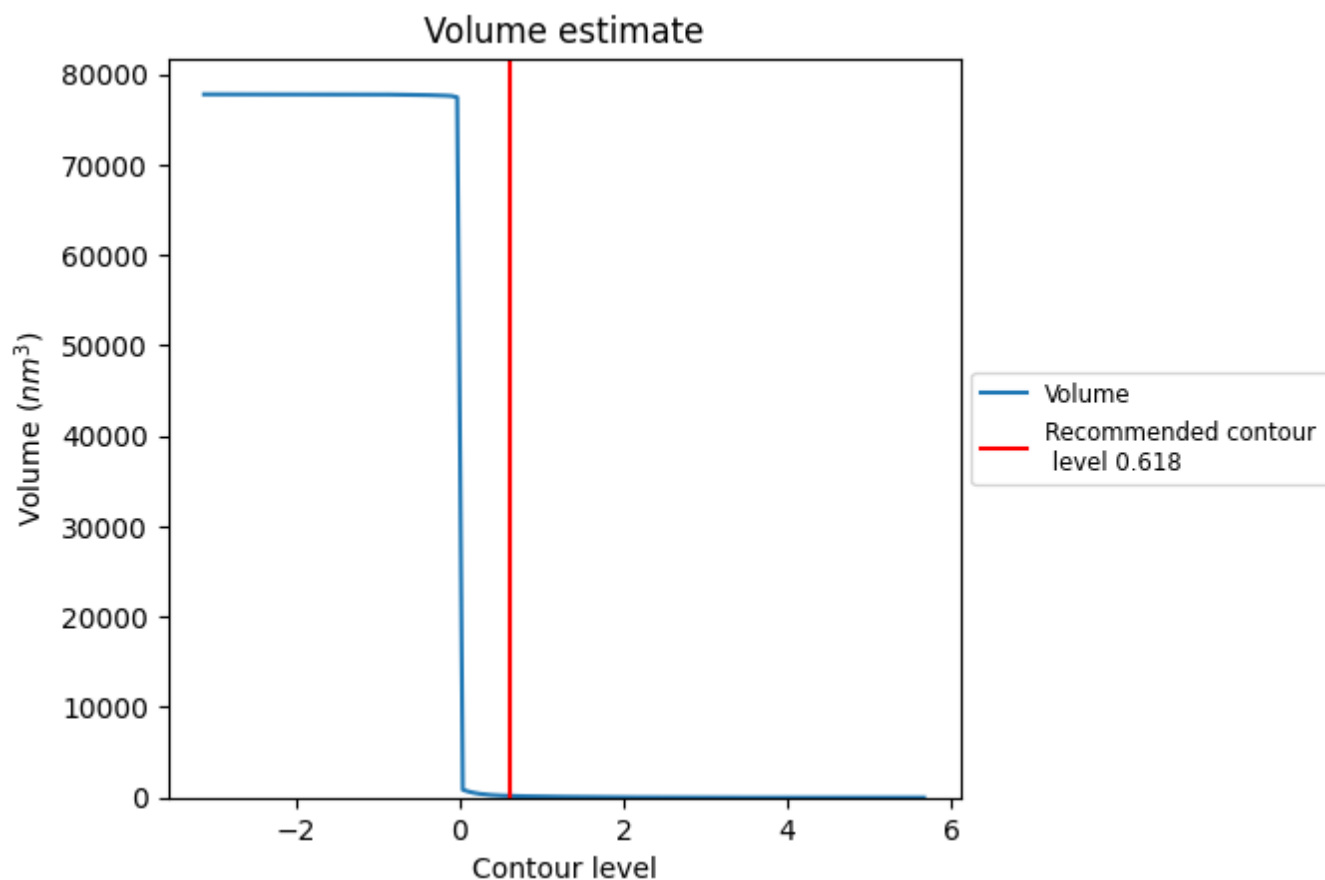
This section contains the results of statistical analysis of the map.

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.

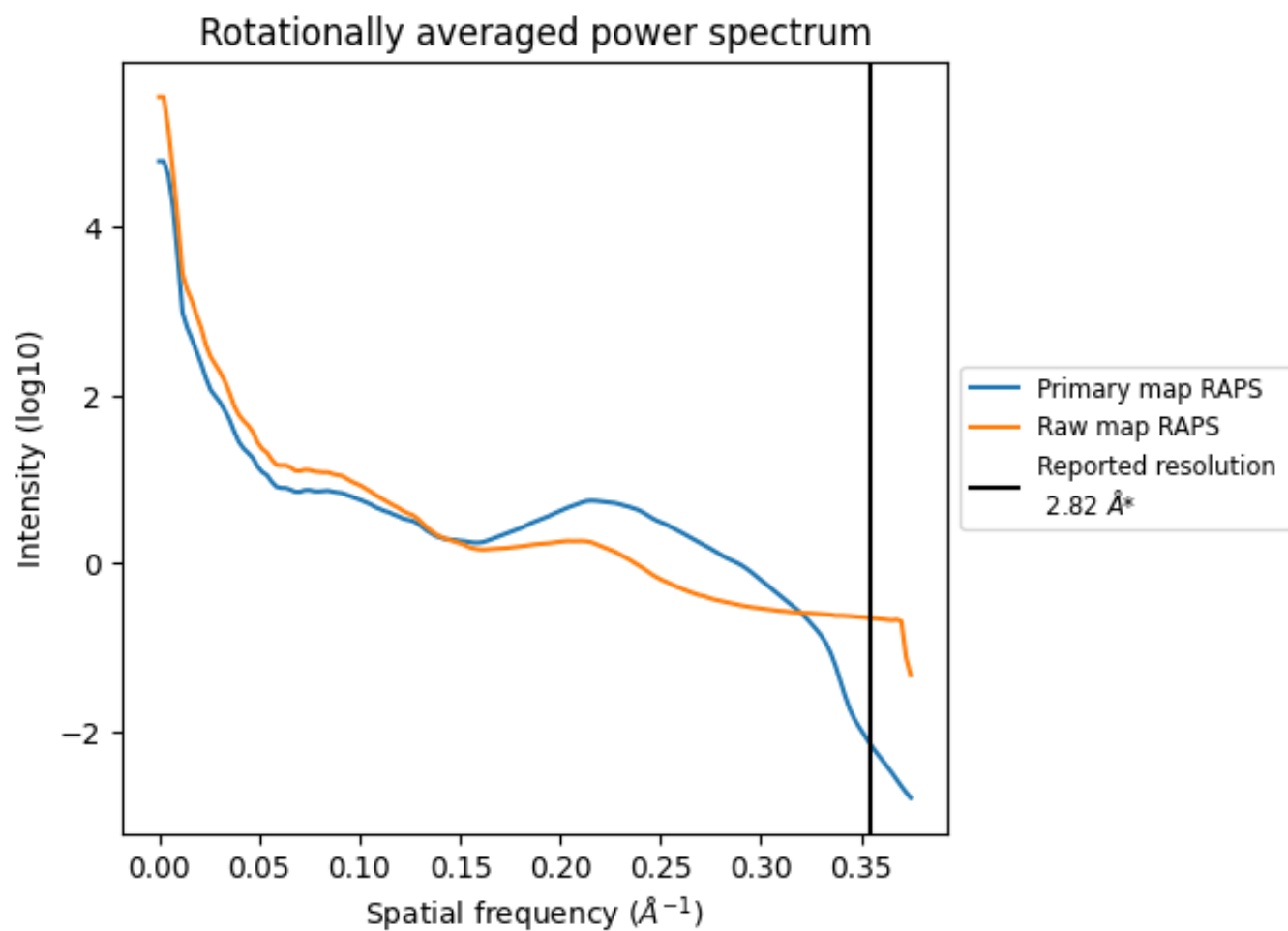
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm^3 ; this corresponds to an approximate mass of 166 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 ⓘ

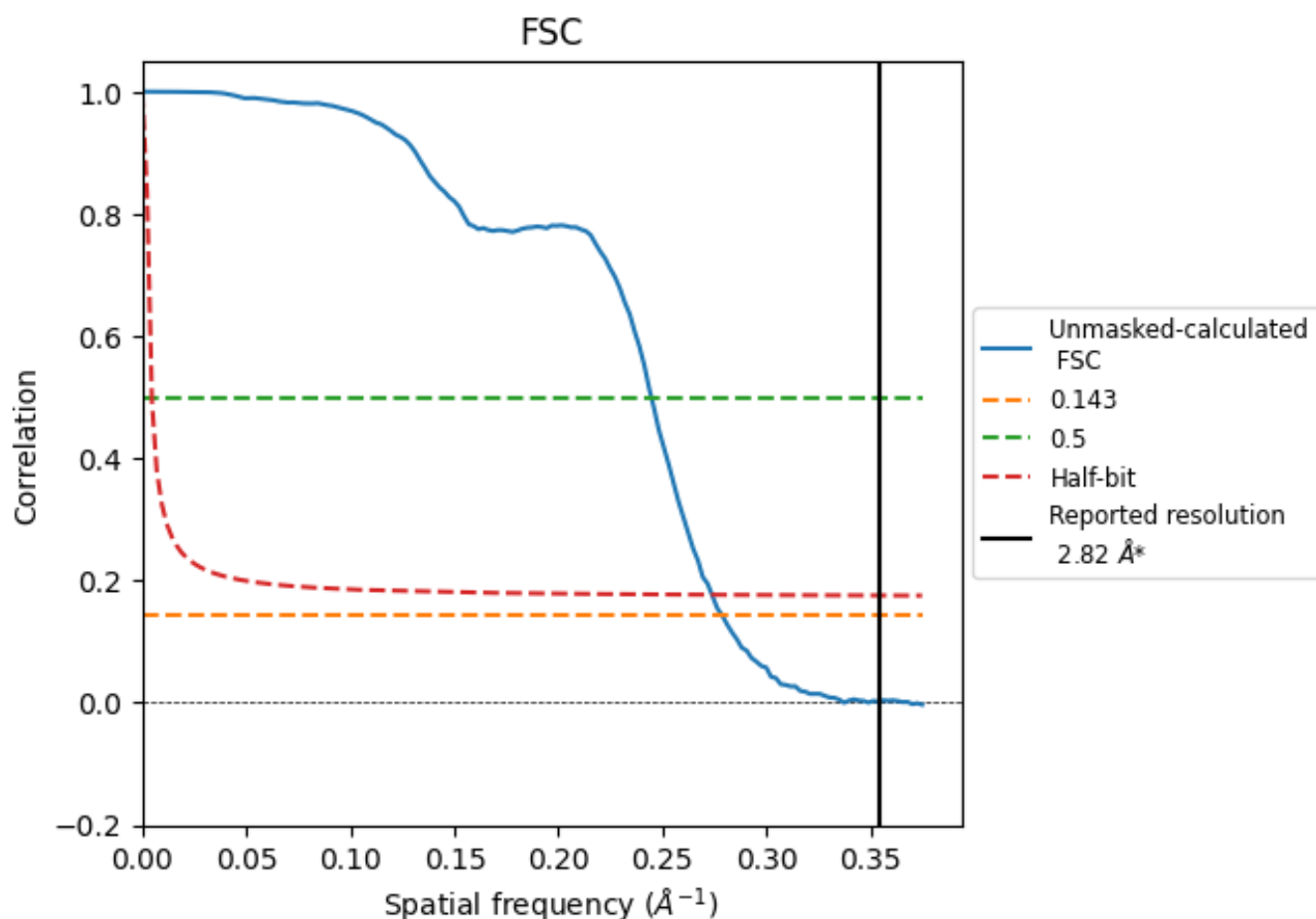


*Reported resolution corresponds to spatial frequency of 0.355 Å⁻¹

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 0.355 Å⁻¹

8.2 Resolution estimates [i](#)

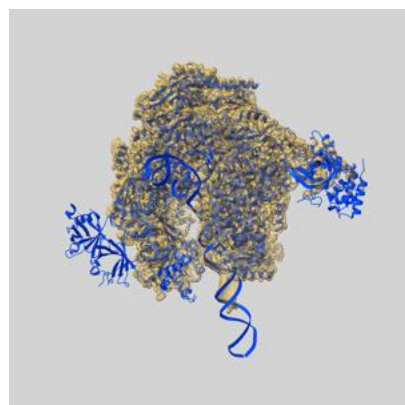
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.09	3.65

*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 3.59 differs from the reported value 2.82 by more than 10 %

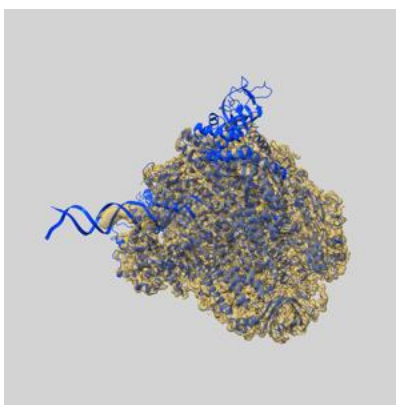
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37404 and PDB model 8WAT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

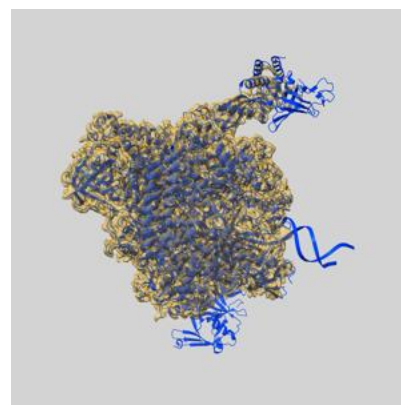
9.1 Map-model overlay [i](#)



X



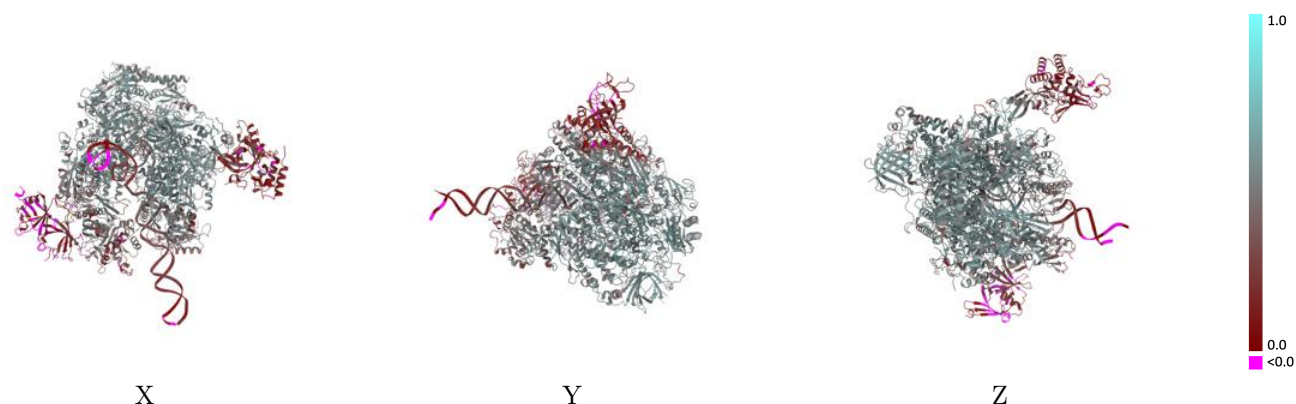
Y



Z

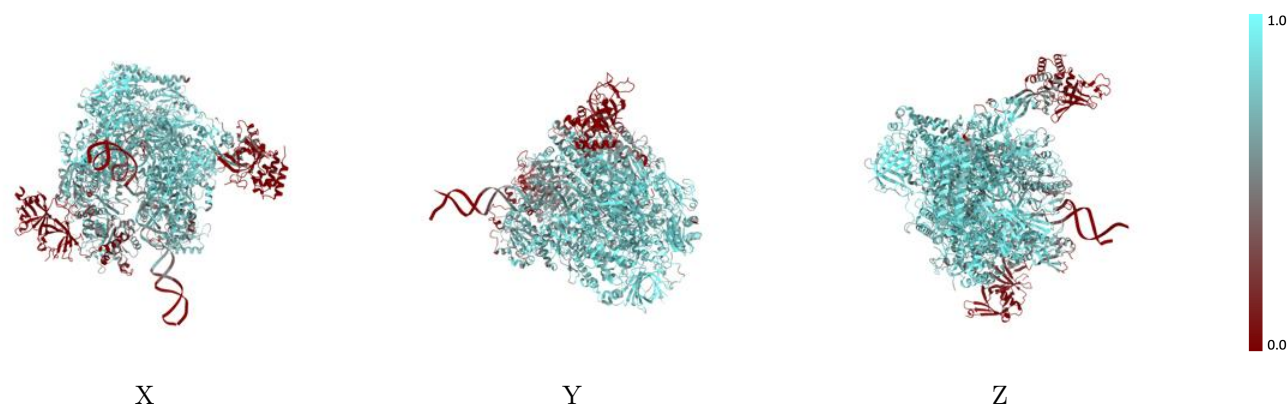
The images above show the 3D surface view of the map at the recommended contour level 0.618 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



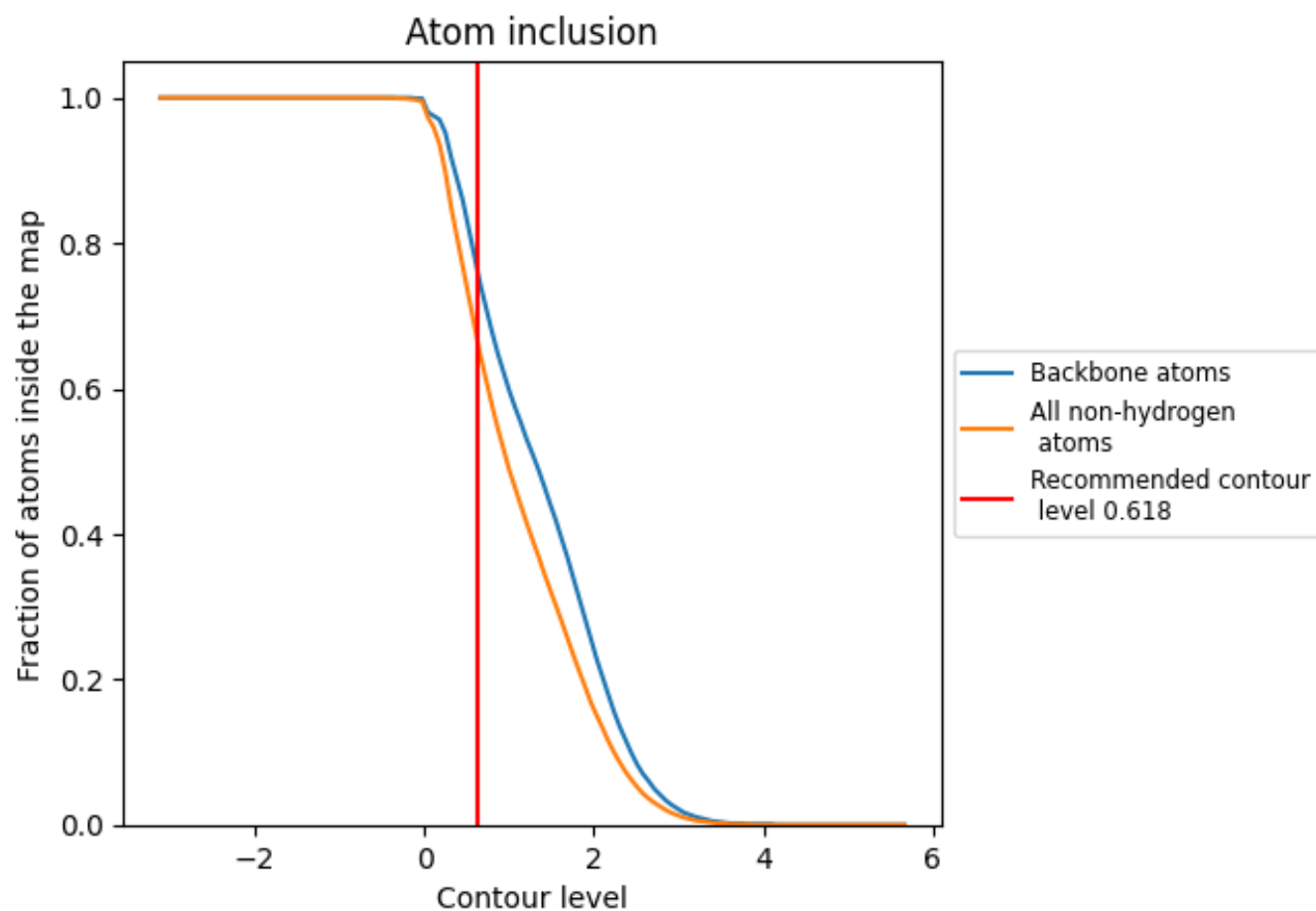
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.618).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.618) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6700	 0.4470
N	 0.8710	 0.5650
S	 0.0000	 0.1390
T	 0.0000	 0.0380
X	 0.2930	 0.2010
Y	 0.4500	 0.2850
Z	 0.8810	 0.5290
o	 0.7580	 0.4990
p	 0.7480	 0.4960
q	 0.8440	 0.5250
r	 0.1450	 0.1910
s	 0.7860	 0.4870
t	 0.7960	 0.5200
u	 0.3360	 0.2840
v	 0.8090	 0.5080
w	 0.6780	 0.4360
x	 0.8430	 0.5410
y	 0.8360	 0.5390
z	 0.7780	 0.4630

