



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 02:05 pm BST

PDB ID : 29WD / pdb_000029wd
EMDB ID : EMD-57401
Title : RNA polymerase II pre-initiation complex bound to ADP-BeF3 in the presence of the +1 nucleosome
Authors : Zhan, Y.; Abril-Garrido, J.; Dienemann, C.; Cramer, P.
Deposited on : 2026-04-10
Resolution : 4.20 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

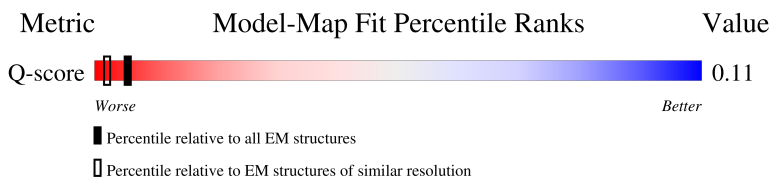
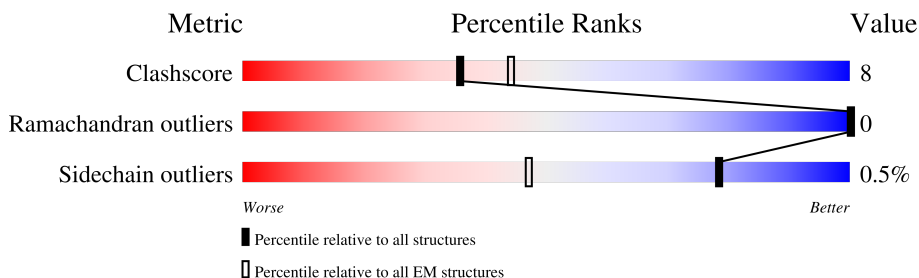
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



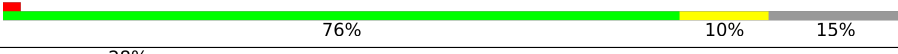
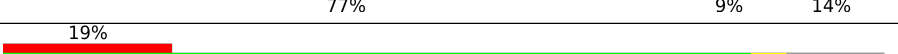
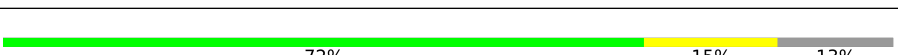
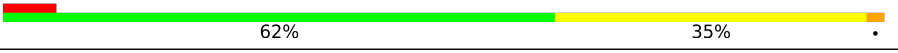
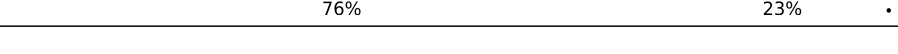
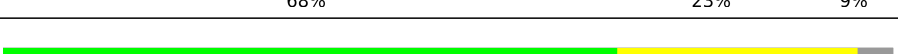
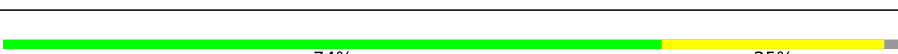
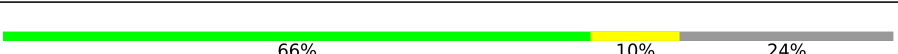
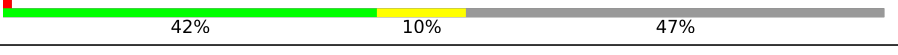
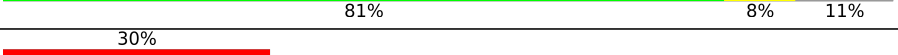
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	0	782	
2	1	760	
3	2	548	
4	3	462	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	8	346	
10	9	323	
11	A	1984	
12	B	1300	
13	C	275	
14	D	184	
15	E	210	
16	F	127	
17	G	172	
18	H	150	
19	I	125	
20	J	67	
21	K	117	
22	L	58	
23	M	316	
24	N	236	
25	O	339	
26	Q	517	
27	R	249	
28	T	236	
29	U	376	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	V	109	
31	W	439	
32	X	291	
33	a	136	
33	e	136	
34	b	103	
34	f	103	
35	c	130	
35	g	130	
36	d	126	
36	h	126	

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 85718 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 3 is a protein called General transcription factor IIIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 4 is a protein called General transcription factor IIIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	421	Total	C	N	O	S	0	0
			3338	2154	584	587	13		

- Molecule 5 is a protein called General transcription factor IIIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 6 is a protein called General transcription factor IIIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	69	Total	C	N	O	S	0	0
			549	352	88	106	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	217	Total	C	N	O	S	0	0
			1762	1107	302	341	12		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	299	Total	C	N	O	S	0	0
			2378	1535	406	426	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 14 is a protein called RNA polymerase II subunit D.

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

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

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 22 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	252	Total	C	N	O	S	0	0
			1954	1224	346	367	17		

- Molecule 24 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	227	Total	C	N	O	P	0	0
			4649	2202	867	1354	226		

- Molecule 25 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 26 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 27 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 28 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	227	Total	C	N	O	P	0	0
			4652	2205	855	1366	226		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	113	Total	C	N	O	S	0	0
			931	585	152	190	4		

- Molecule 30 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 31 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

- Molecule 32 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 33 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	97	Total	C	N	O	S	0	0
			801	505	155	138	3		
33	e	98	Total	C	N	O	S	0	0
			810	511	157	139	3		

- Molecule 34 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
34	f	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 35 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	109	Total	C	N	O	0	0
			843	531	167	145		
35	g	106	Total	C	N	O	0	0
			818	516	160	142		

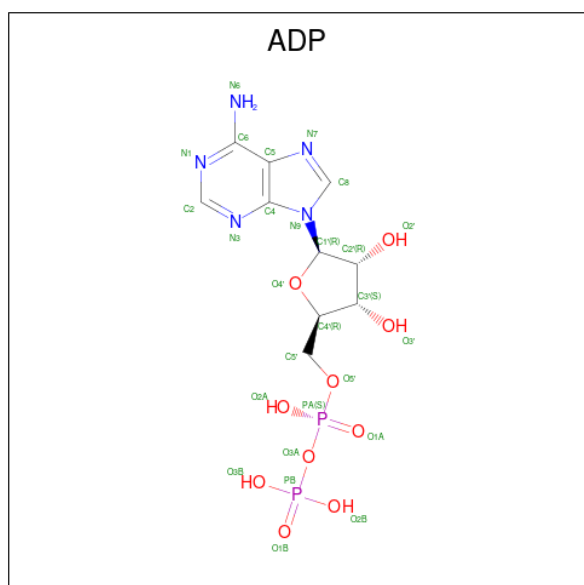
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 36 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
36	h	95	Total	C	N	O	S	0	0
			744	468	134	140	2		

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

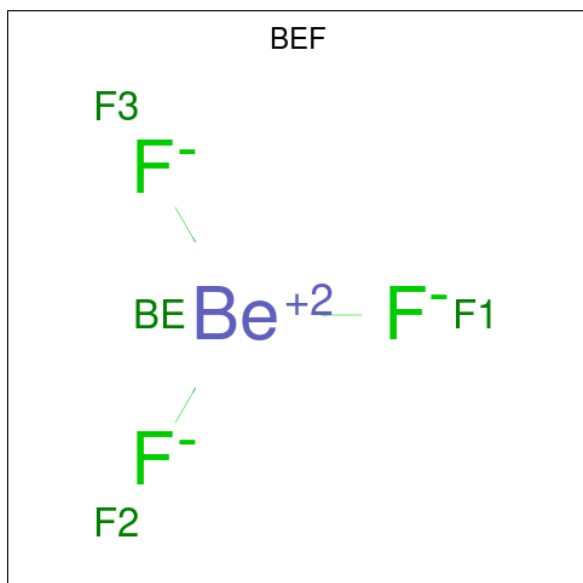


Mol	Chain	Residues	Atoms					AltConf
37	0	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	0	1	Total	Mg	0
			1	1	
38	A	1	Total	Mg	0
			1	1	

- Molecule 39 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).

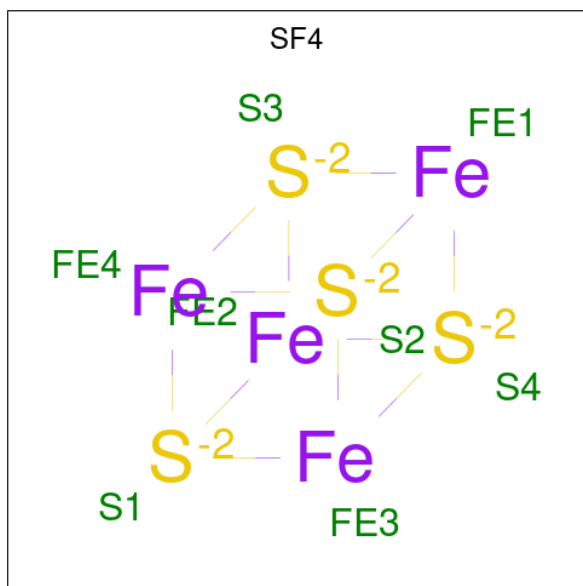


Mol	Chain	Residues	Atoms			AltConf
39	0	1	Total	Be	F	0
			4	1	3	

- Molecule 40 is UNKNOWN (CCD ID: UNK) (formula: C₄H₉NO₂).

Mol	Chain	Residues	Atoms				AltConf
40	0	16	Total	C	N	O	0
			81	48	16	17	
40	2	2	Total	C	N	O	0
			10	6	2	2	
40	A	2	Total	C	N	O	0
			11	6	2	3	
40	N	4	Total	C	N	O	0
			20	12	4	4	
40	T	1	Total	C	N	O	0
			5	3	1	1	
40	W	2	Total	C	N	O	0
			10	6	2	2	

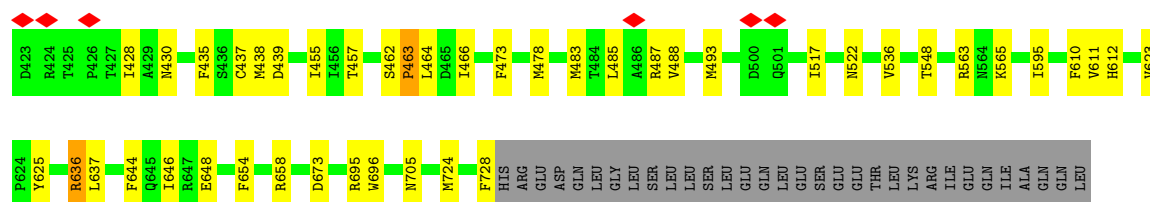
- Molecule 41 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



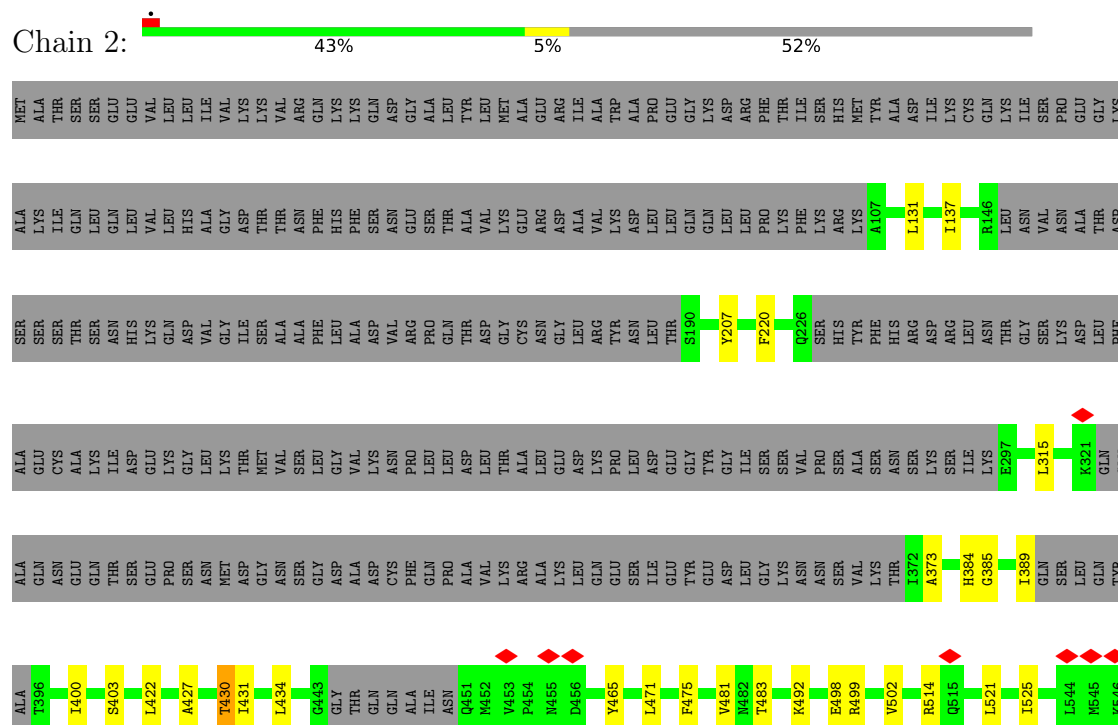
Mol	Chain	Residues	Atoms			AltConf
41	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 42 is ZINC ION (CCD ID: ZN) (formula: Zn).

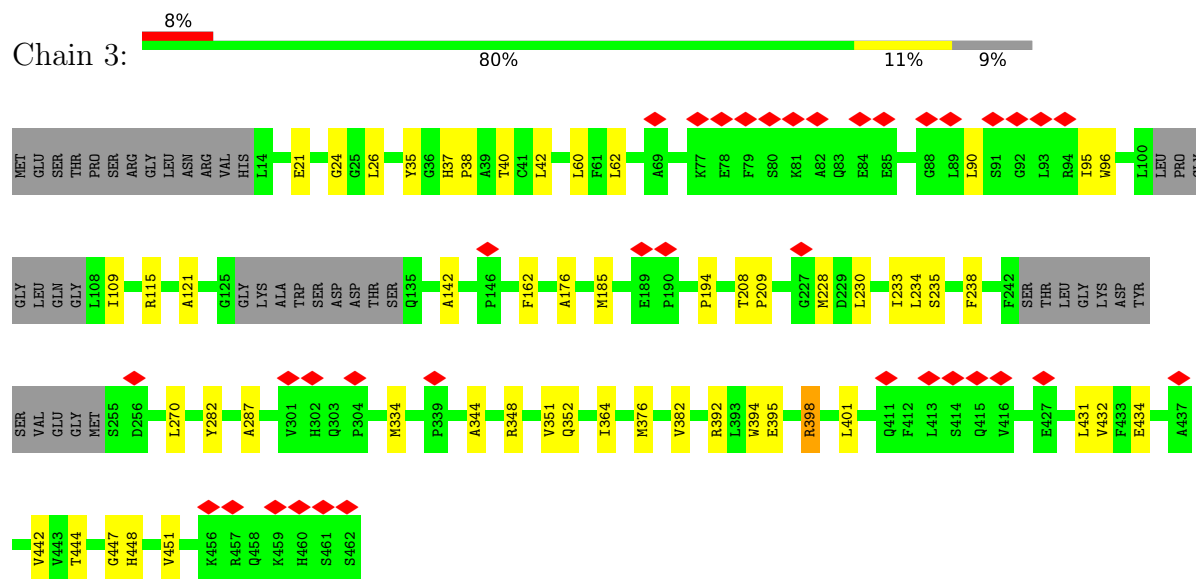
Mol	Chain	Residues	Atoms		AltConf
42	4	3	Total	Zn	0
			3	3	
42	5	2	Total	Zn	0
			2	2	
42	7	2	Total	Zn	0
			2	2	
42	A	3	Total	Zn	0
			3	3	
42	B	1	Total	Zn	0
			1	1	
42	C	1	Total	Zn	0
			1	1	
42	I	2	Total	Zn	0
			2	2	
42	J	1	Total	Zn	0
			1	1	
42	L	1	Total	Zn	0
			1	1	
42	W	1	Total	Zn	0
			1	1	



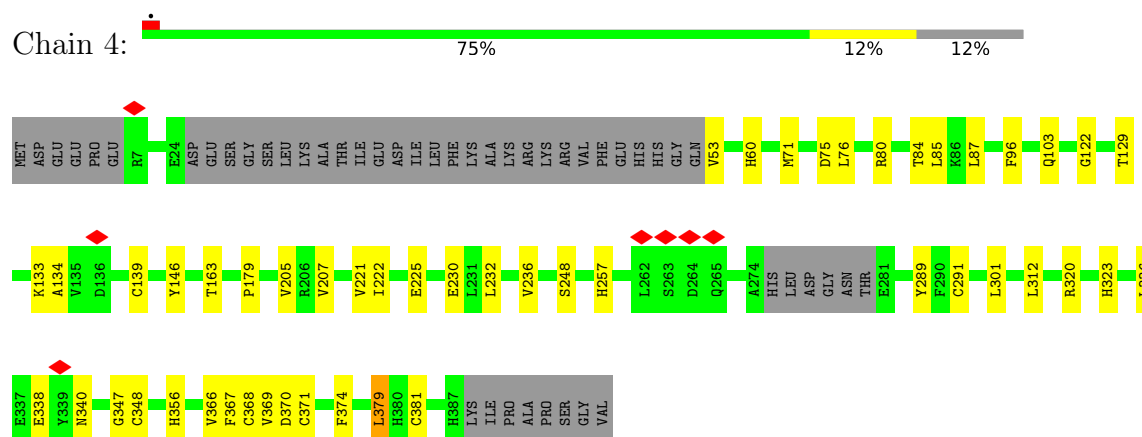
• Molecule 3: General transcription factor IIH subunit 1



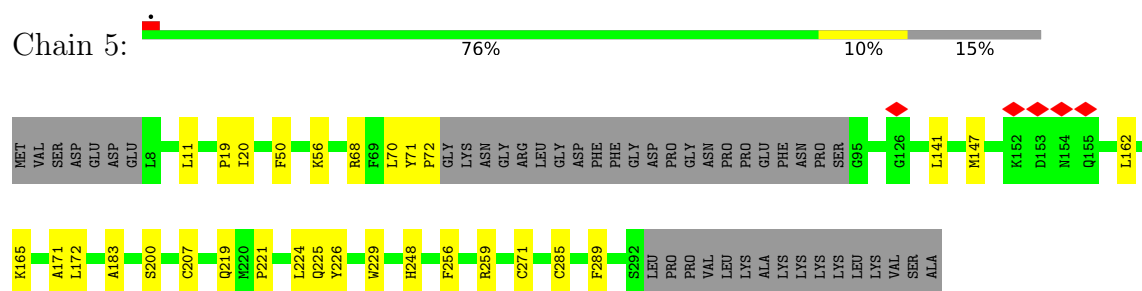
• Molecule 4: General transcription factor IIH subunit 4



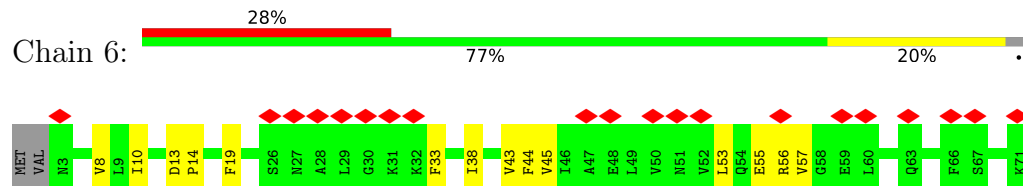
• Molecule 5: General transcription factor IIH subunit 2



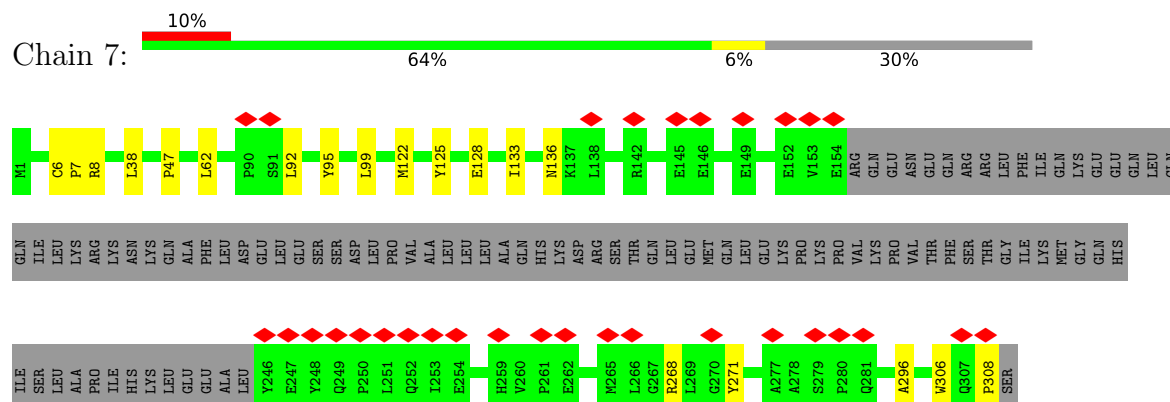
- Molecule 6: General transcription factor IIH subunit 3



- Molecule 7: General transcription factor IIH subunit 5

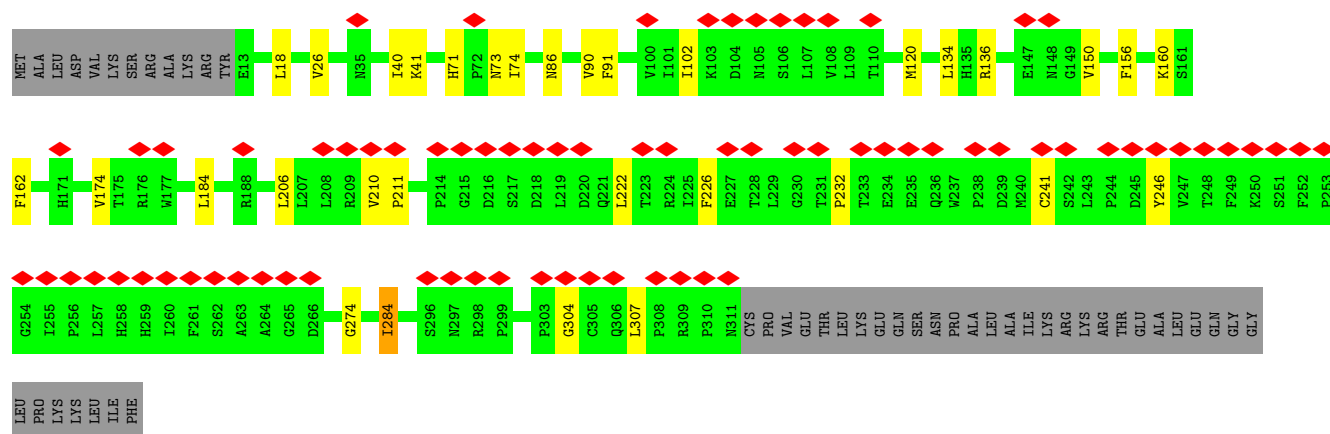


- Molecule 8: CDK-activating kinase assembly factor MAT1

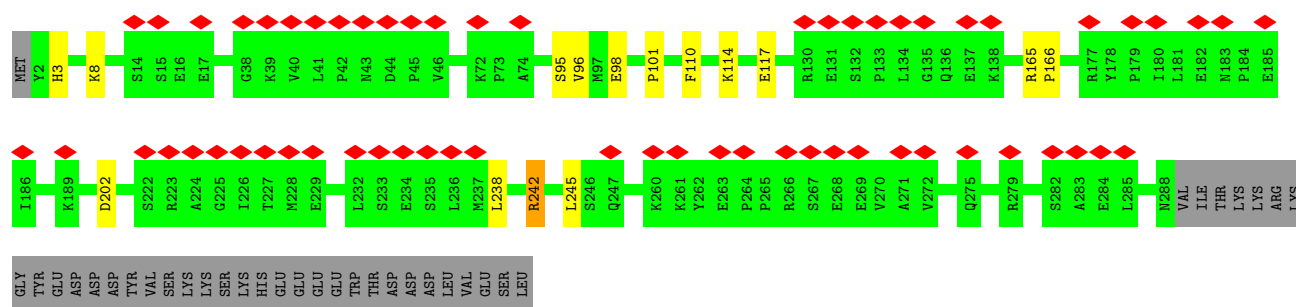
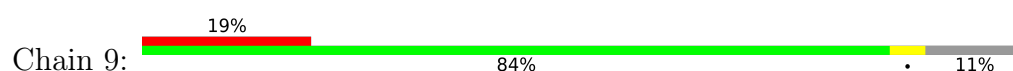


- Molecule 9: Cyclin-dependent kinase 7

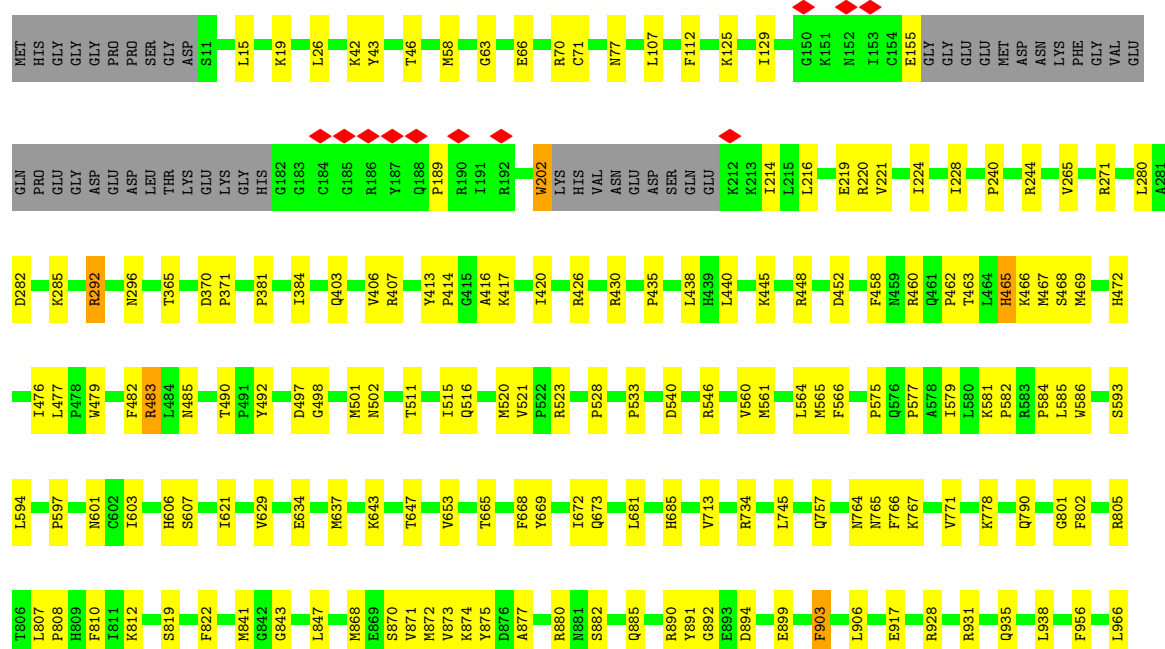


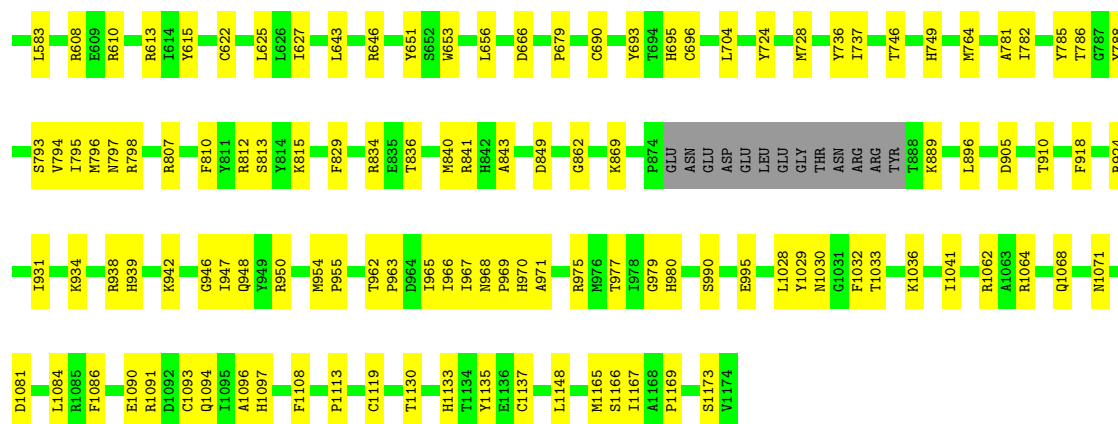


• Molecule 10: Cyclin-H



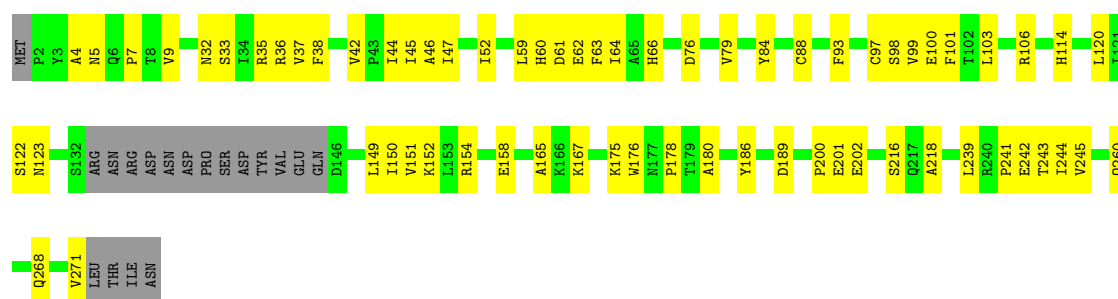
• Molecule 11: DNA-directed RNA polymerase subunit





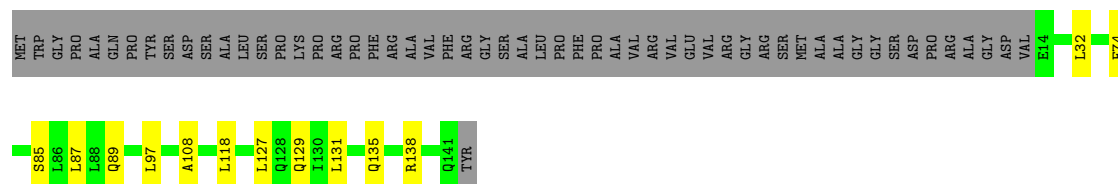
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain C: 69% 24% 7%



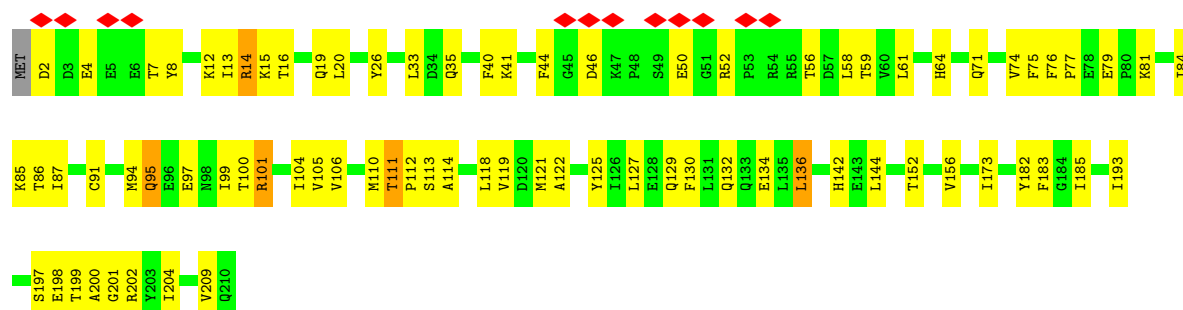
• Molecule 14: RNA polymerase II subunit D

Chain D: 62% 7% 30%

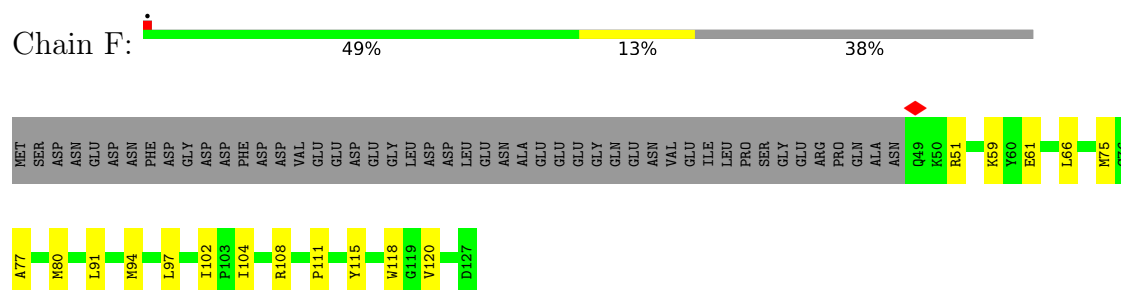


• Molecule 15: DNA-directed RNA polymerase II subunit E

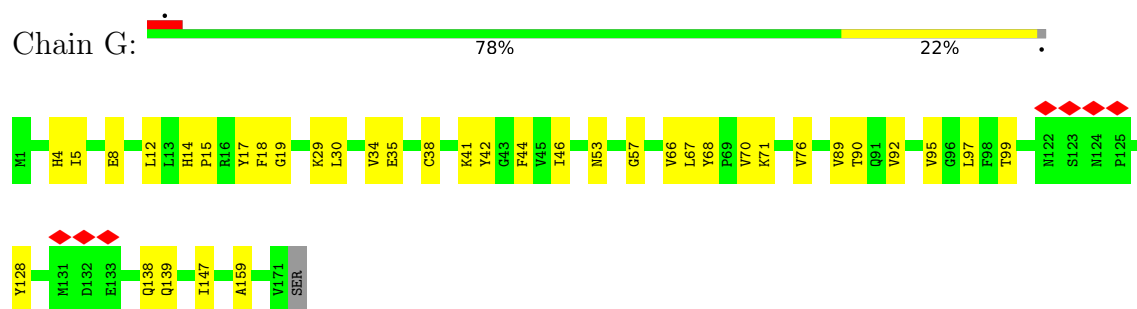
Chain E: 6% 62% 35%



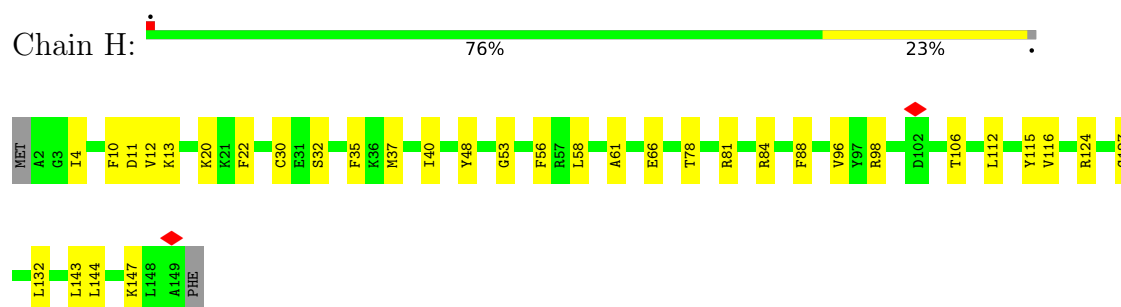
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC2



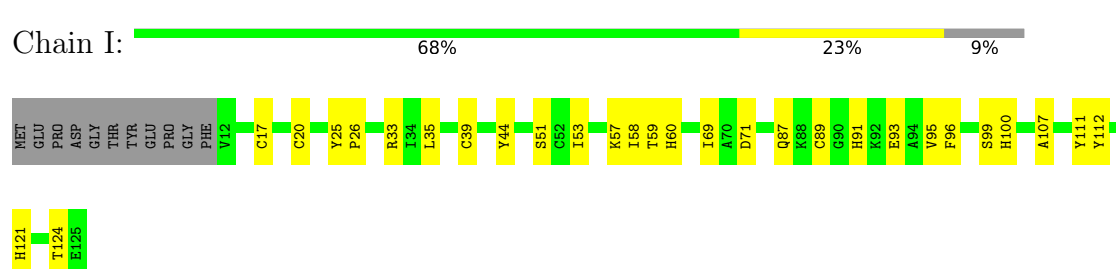
- Molecule 17: DNA-directed RNA polymerase II subunit RPB7



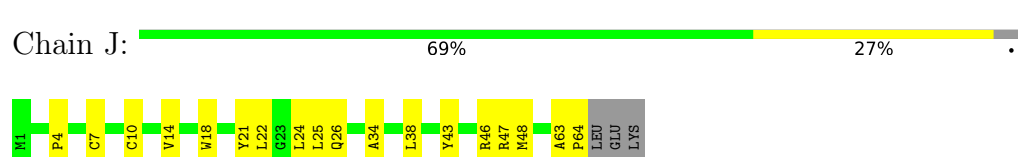
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 19: DNA-directed RNA polymerase II subunit RPB9

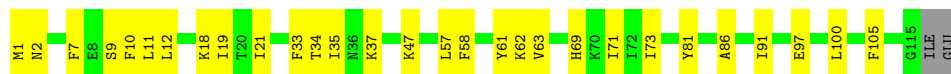


- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5



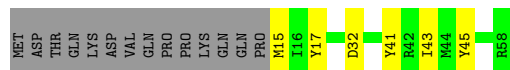
- Molecule 21: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  74% 25%



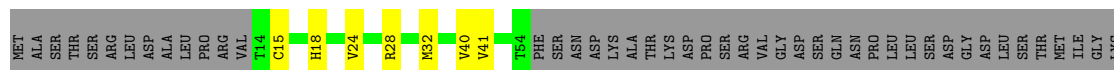
- Molecule 22: RNA polymerase II subunit K

Chain L:  66% 10% 24%



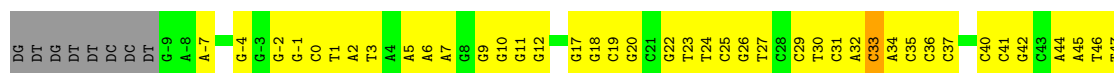
- Molecule 23: Transcription initiation factor IIB

Chain M:  72% 7% 20%

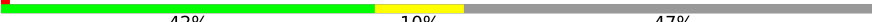


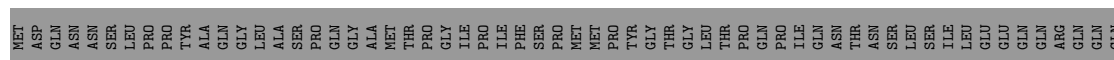
- Molecule 24: DNA (227-MER)

Chain N:  27% 25% 68%

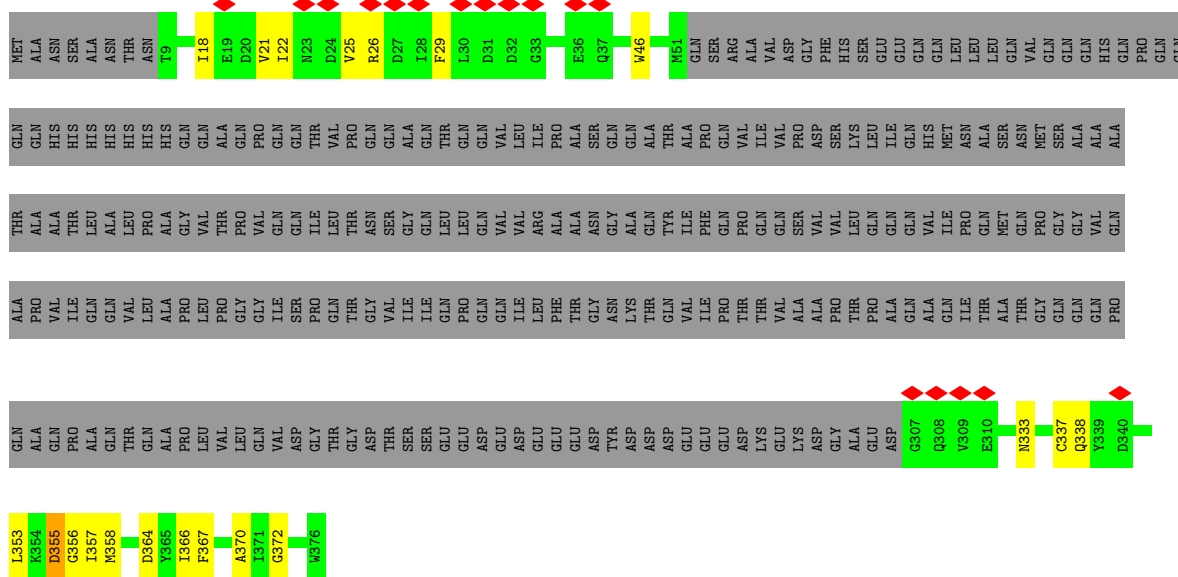


- Molecule 25: TATA-box-binding protein

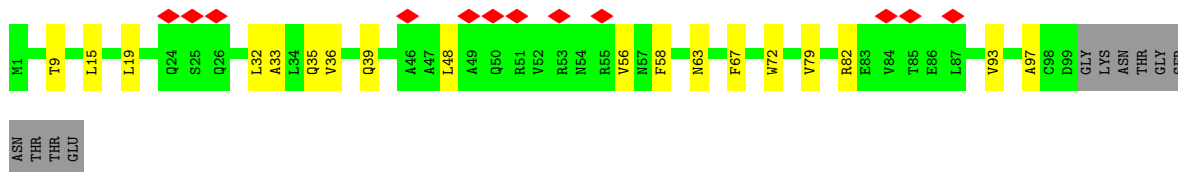
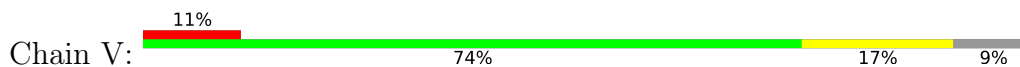
Chain O:  42% 10% 47%



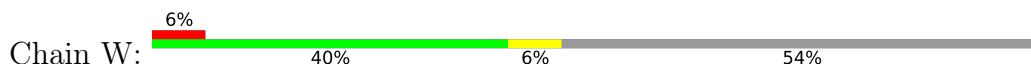
- Molecule 29: Transcription initiation factor IIA subunit 1

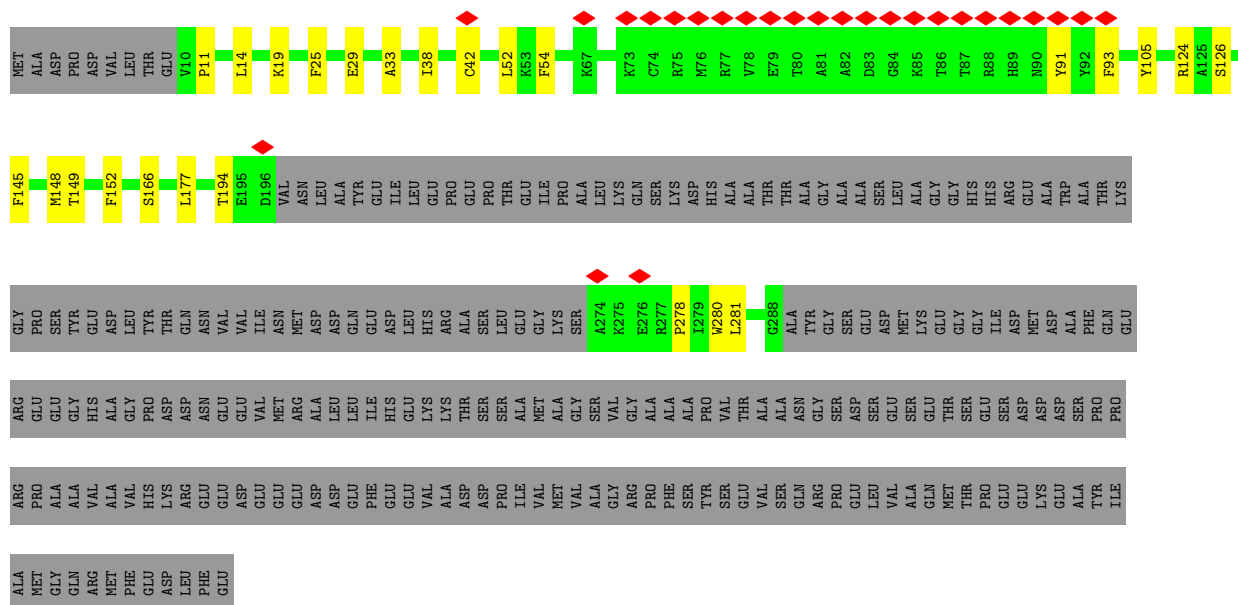


- Molecule 30: Transcription initiation factor IIA subunit 2

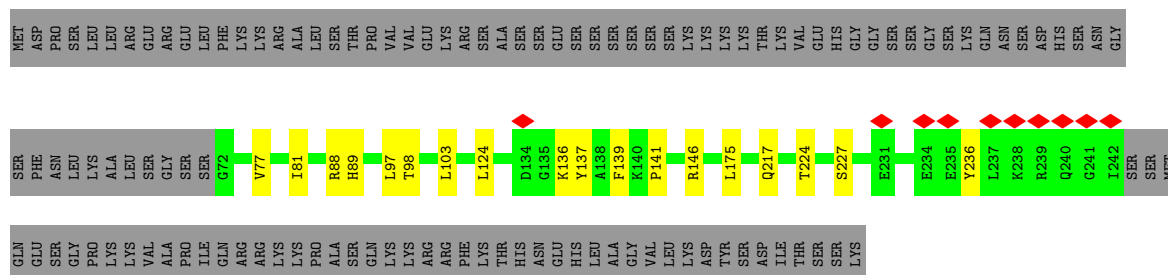


- Molecule 31: General transcription factor IIE subunit 1

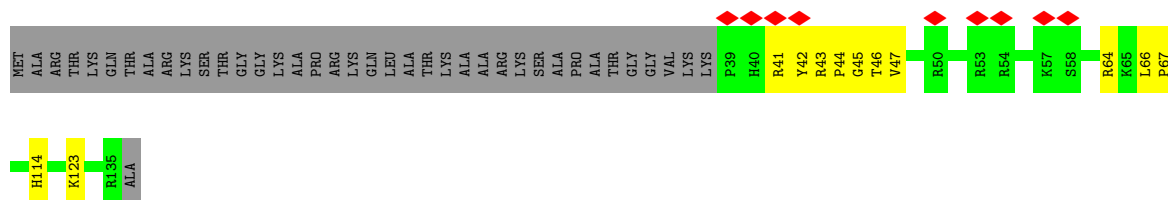




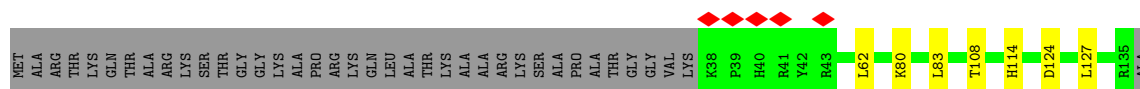
• Molecule 32: Transcription initiation factor IIE subunit beta



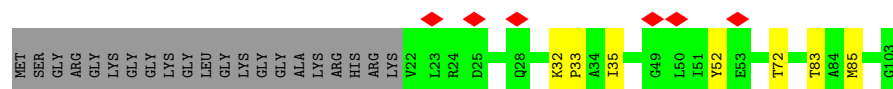
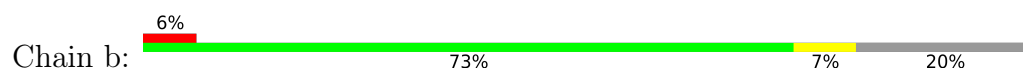
• Molecule 33: Histone H3.2



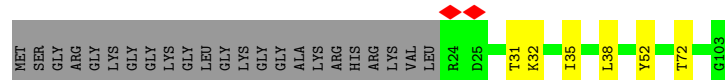
• Molecule 33: Histone H3.2



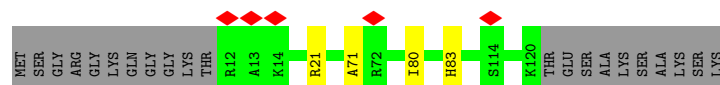
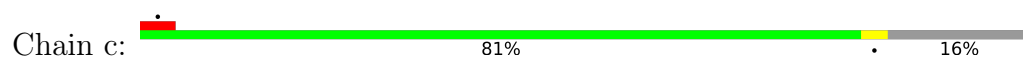
• Molecule 34: Histone H4



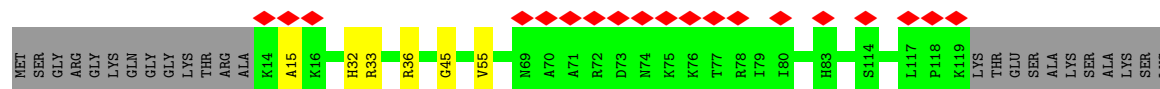
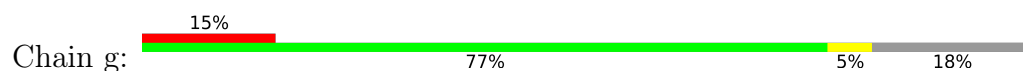
- Molecule 34: Histone H4



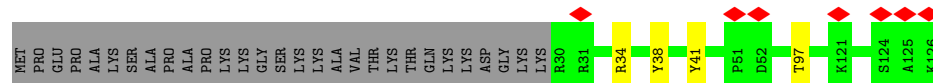
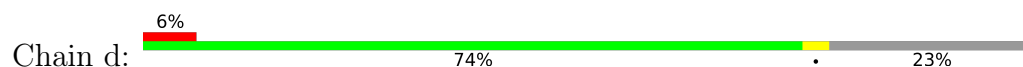
- Molecule 35: Histone H2A type 1



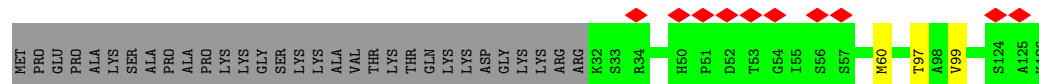
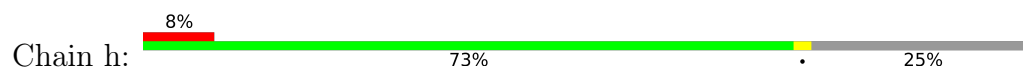
- Molecule 35: Histone H2A type 1



- Molecule 36: Histone H2B 1.1



- Molecule 36: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19577	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.014	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, ADP, MG, BEF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.25	0/4994	0.74	3/6745 (0.0%)
2	1	0.25	0/5875	0.74	2/7955 (0.0%)
3	2	0.24	0/2210	0.71	0/2975
4	3	0.26	0/3412	0.71	0/4622
5	4	0.25	0/2793	0.74	0/3780
6	5	0.22	0/2103	0.66	0/2846
7	6	0.28	0/555	0.85	0/747
8	7	0.25	0/1794	0.72	0/2419
9	8	0.21	0/2437	0.63	0/3306
10	9	0.25	0/2384	0.67	0/3220
11	A	0.34	0/11479	0.83	0/15496
12	B	0.34	0/9257	0.79	2/12493 (0.0%)
13	C	0.42	0/2102	0.84	0/2857
14	D	0.19	0/1064	0.59	0/1428
15	E	0.38	0/1752	0.96	3/2366 (0.1%)
16	F	0.41	0/646	0.78	0/871
17	G	0.28	0/1382	0.76	0/1874
18	H	0.37	0/1207	0.76	0/1628
19	I	0.35	0/949	0.77	0/1284
20	J	0.38	0/516	0.87	0/696
21	K	0.42	0/939	0.82	0/1271
22	L	0.35	0/378	0.78	0/500
23	M	0.25	0/1984	0.65	0/2679
24	N	0.46	0/5217	0.99	7/8049 (0.1%)
25	O	0.26	0/1448	0.66	0/1948
26	Q	0.22	0/1167	0.69	0/1576
27	R	0.23	0/1817	0.63	0/2445
28	T	0.50	4/5217 (0.1%)	0.96	15/8052 (0.2%)
29	U	0.20	0/946	0.71	2/1274 (0.2%)
30	V	0.19	0/816	0.65	0/1105
31	W	0.31	0/1686	0.83	4/2266 (0.2%)
32	X	0.23	0/1427	0.69	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.26	0/813	0.68	0/1090
33	e	0.22	0/822	0.63	0/1102
34	b	0.19	0/660	0.62	0/883
34	f	0.21	0/645	0.68	0/862
35	c	0.21	0/853	0.68	0/1149
35	g	0.25	0/828	0.74	0/1117
36	d	0.21	0/777	0.63	0/1041
36	h	0.22	0/755	0.63	0/1013
All	All	0.32	4/88106 (0.0%)	0.78	38/120946 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	5
2	1	0	5
3	2	0	1
4	3	0	1
6	5	0	1
10	9	0	1
11	A	0	3
12	B	0	4
15	E	0	1
18	H	0	1
19	I	0	1
23	M	0	1
24	N	0	1
33	a	0	1
35	c	0	1
35	g	0	1
All	All	0	29

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	-45	DT	C5'-C4'	7.86	1.68	1.52
28	T	-45	DT	O5'-C5'	7.13	1.64	1.42
28	T	-46	DA	C3'-O3'	5.92	1.60	1.42
28	T	-45	DT	P-O5'	5.65	1.71	1.60

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	T	-45	DT	O5'-C5'-C4'	11.01	127.32	110.80
1	0	609	LYS	CG-CD-CE	10.09	134.51	111.30
1	0	611	GLY	N-CA-C	8.08	125.98	113.86
28	T	-46	DA	O3'-P-O5'	7.49	115.23	104.00
1	0	609	LYS	CD-CE-NZ	6.84	133.78	111.90

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	ARG	Sidechain
1	0	391	ARG	Sidechain
1	0	472	ARG	Sidechain
1	0	645	ARG	Sidechain
1	0	676	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4890	0	4949	97	0
2	1	5751	0	5796	50	0
3	2	2167	0	2175	24	0
4	3	3338	0	3343	36	0
5	4	2732	0	2708	31	0
6	5	2066	0	2101	24	0
7	6	549	0	558	11	0
8	7	1762	0	1734	13	0
9	8	2378	0	2397	18	0
10	9	2334	0	2357	9	0
11	A	11274	0	11411	220	0
12	B	9076	0	9116	139	0
13	C	2059	0	2009	52	0
14	D	1050	0	1033	7	0
15	E	1721	0	1737	65	0
16	F	636	0	665	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1351	0	1358	28	0
18	H	1186	0	1147	26	0
19	I	928	0	859	28	0
20	J	507	0	523	14	0
21	K	920	0	942	27	0
22	L	373	0	381	5	0
23	M	1954	0	1990	15	0
24	N	4649	0	2543	203	0
25	O	1422	0	1514	26	0
26	Q	1138	0	1103	15	0
27	R	1788	0	1819	15	0
28	T	4652	0	2549	156	0
29	U	931	0	888	13	0
30	V	806	0	818	14	0
31	W	1659	0	1666	16	0
32	X	1403	0	1428	12	0
33	a	801	0	839	14	0
33	e	810	0	851	5	0
34	b	653	0	696	4	0
34	f	638	0	676	5	0
35	c	843	0	908	2	0
35	g	818	0	877	4	0
36	d	766	0	797	4	0
36	h	744	0	771	3	0
37	0	27	0	12	2	0
38	0	1	0	0	0	0
38	A	1	0	0	0	0
39	0	4	0	0	0	0
40	0	81	0	48	0	0
40	2	10	0	6	0	0
40	A	11	0	6	0	0
40	N	20	0	12	0	0
40	T	5	0	3	0	0
40	W	10	0	6	0	0
41	1	8	0	0	0	0
42	4	3	0	0	0	0
42	5	2	0	0	0	0
42	7	2	0	0	0	0
42	A	3	0	0	0	0
42	B	1	0	0	0	0
42	C	1	0	0	0	0
42	I	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	J	1	0	0	0	0
42	L	1	0	0	0	0
42	W	1	0	0	0	0
All	All	85718	0	82125	1273	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 8.

The worst 5 of 1273 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)
28:T:-45:DT:O5'	28:T:-45:DT:C5'	1.64	1.43
1:0:609:LYS:HD3	28:T:-45:DT:C6	1.80	1.16
1:0:609:LYS:HE3	28:T:-46:DA:H1'	1.46	0.97
24:N:109:DT:H2''	24:N:110:DA:C8	2.06	0.90
28:T:-136:DT:H4'	33:a:42:TYR:HB2	1.56	0.87

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	0	601/782 (77%)	581 (97%)	20 (3%)	0	100	100
2	1	710/760 (93%)	678 (96%)	32 (4%)	0	100	100
3	2	253/548 (46%)	246 (97%)	7 (3%)	0	100	100
4	3	413/462 (89%)	401 (97%)	12 (3%)	0	100	100
5	4	341/395 (86%)	321 (94%)	20 (6%)	0	100	100
6	5	259/308 (84%)	250 (96%)	9 (4%)	0	100	100
7	6	67/71 (94%)	65 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	213/309 (69%)	196 (92%)	17 (8%)	0	100	100
9	8	297/346 (86%)	286 (96%)	11 (4%)	0	100	100
10	9	285/323 (88%)	279 (98%)	6 (2%)	0	100	100
11	A	1413/1984 (71%)	1359 (96%)	54 (4%)	0	100	100
12	B	1130/1300 (87%)	1097 (97%)	33 (3%)	0	100	100
13	C	253/275 (92%)	242 (96%)	11 (4%)	0	100	100
14	D	126/184 (68%)	120 (95%)	6 (5%)	0	100	100
15	E	207/210 (99%)	194 (94%)	13 (6%)	0	100	100
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
17	G	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
18	H	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
19	I	112/125 (90%)	107 (96%)	5 (4%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
22	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
23	M	248/316 (78%)	241 (97%)	7 (3%)	0	100	100
25	O	177/339 (52%)	168 (95%)	9 (5%)	0	100	100
26	Q	134/517 (26%)	128 (96%)	6 (4%)	0	100	100
27	R	218/249 (88%)	214 (98%)	4 (2%)	0	100	100
29	U	109/376 (29%)	105 (96%)	4 (4%)	0	100	100
30	V	97/109 (89%)	92 (95%)	5 (5%)	0	100	100
31	W	198/439 (45%)	195 (98%)	3 (2%)	0	100	100
32	X	169/291 (58%)	163 (96%)	6 (4%)	0	100	100
33	a	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
33	e	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
34	b	80/103 (78%)	79 (99%)	1 (1%)	0	100	100
34	f	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
35	c	107/130 (82%)	104 (97%)	3 (3%)	0	100	100
35	g	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
36	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
36	h	93/126 (74%)	93 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9387/12699 (74%)	9049 (96%)	338 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	536/688 (78%)	534 (100%)	2 (0%)	84	82
2	1	624/664 (94%)	616 (99%)	8 (1%)	61	71
3	2	241/484 (50%)	239 (99%)	2 (1%)	73	77
4	3	351/399 (88%)	351 (100%)	0	100	100
5	4	311/352 (88%)	309 (99%)	2 (1%)	78	80
6	5	234/272 (86%)	231 (99%)	3 (1%)	61	71
7	6	62/64 (97%)	62 (100%)	0	100	100
8	7	198/283 (70%)	198 (100%)	0	100	100
9	8	259/299 (87%)	257 (99%)	2 (1%)	73	77
10	9	259/296 (88%)	258 (100%)	1 (0%)	84	82
11	A	1254/1763 (71%)	1245 (99%)	9 (1%)	76	78
12	B	994/1127 (88%)	994 (100%)	0	100	100
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/160 (74%)	117 (99%)	1 (1%)	73	77
15	E	191/192 (100%)	188 (98%)	3 (2%)	55	69
16	F	69/111 (62%)	69 (100%)	0	100	100
17	G	152/153 (99%)	150 (99%)	2 (1%)	61	71
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	53 (100%)	0	100	100
21	K	104/106 (98%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	121 (100%)	0	100	100
27	R	196/218 (90%)	195 (100%)	1 (0%)	81	81
29	U	105/324 (32%)	104 (99%)	1 (1%)	68	75
30	V	90/98 (92%)	89 (99%)	1 (1%)	65	73
31	W	182/373 (49%)	181 (100%)	1 (0%)	81	81
32	X	154/261 (59%)	154 (100%)	0	100	100
33	a	85/111 (77%)	85 (100%)	0	100	100
33	e	86/111 (78%)	86 (100%)	0	100	100
34	b	67/79 (85%)	67 (100%)	0	100	100
34	f	65/79 (82%)	65 (100%)	0	100	100
35	c	86/101 (85%)	86 (100%)	0	100	100
35	g	84/101 (83%)	84 (100%)	0	100	100
36	d	83/106 (78%)	83 (100%)	0	100	100
36	h	81/106 (76%)	81 (100%)	0	100	100
All	All	8371/11096 (75%)	8332 (100%)	39 (0%)	78	81

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	A	1398	LEU
27	R	14	GLN
14	D	129	GLN
15	E	101	ARG
30	V	79	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
12	B	23	GLN
13	C	217	GLN
36	h	50	HIS
12	B	111	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	B	941	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 19 are monoatomic and 27 are unknown - leaving 3 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
39	BEF	0	903	37	0,3,3	-	-	-		
37	ADP	0	901	39	27,29,29	1.36	5 (18%)	42,45,45	2.02	14 (33%)
41	SF4	1	1000	2	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	0	901	39	-	5/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	SF4	1	1000	2	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	901	ADP	C5-C4	4.27	1.47	1.39
37	0	901	ADP	C5-C6	2.61	1.48	1.41
37	0	901	ADP	C8-N7	2.35	1.36	1.31
37	0	901	ADP	C4-N9	-2.31	1.32	1.37
37	0	901	ADP	C5-N7	-2.10	1.35	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	901	ADP	C5-C4-N3	-5.15	120.03	126.75
37	0	901	ADP	N3-C4-N9	4.44	134.39	127.08
37	0	901	ADP	C4-N9-C8	3.95	110.01	105.73
37	0	901	ADP	C2-N3-C4	3.49	119.99	111.75
37	0	901	ADP	N3-C2-N1	-3.11	123.74	128.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	0	901	ADP	C5'-O5'-PA-O1A
37	0	901	ADP	C4'-C5'-O5'-PA
37	0	901	ADP	O4'-C4'-C5'-O5'
37	0	901	ADP	C3'-C4'-C5'-O5'
37	0	901	ADP	C5'-O5'-PA-O3A

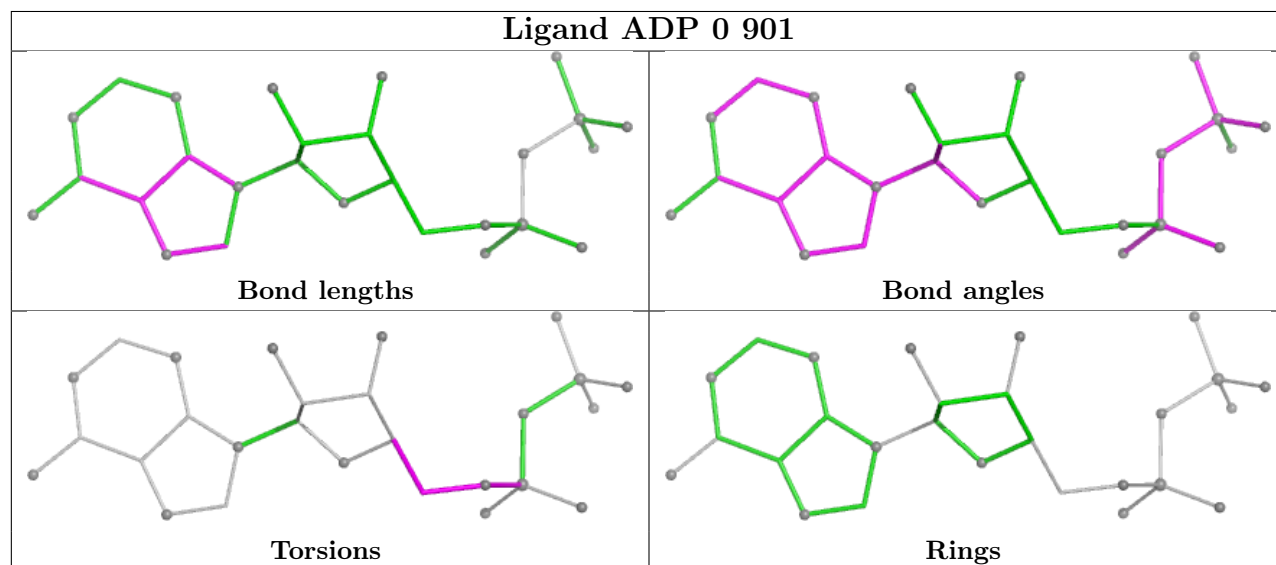
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	901	ADP	2	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.

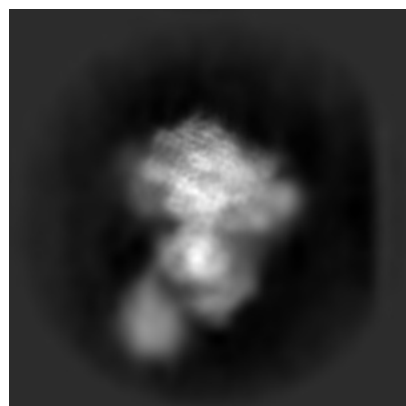
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57401. These allow visual inspection of the internal detail of the map and identification of artifacts.

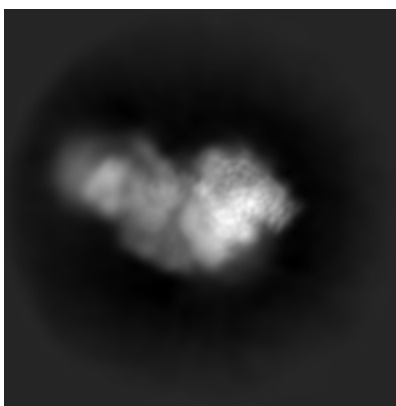
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

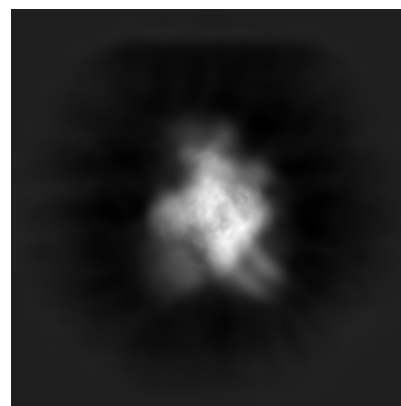
6.1.1 Primary map



X

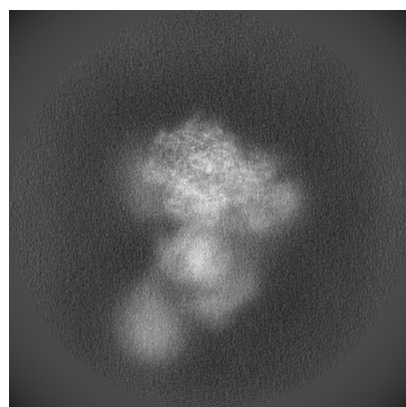


Y

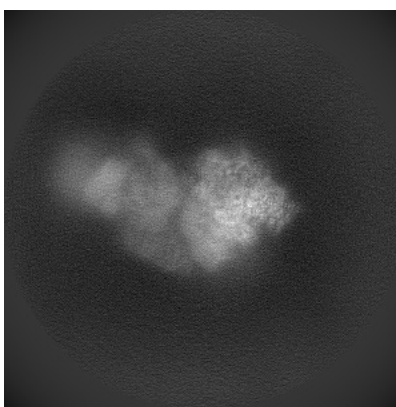


Z

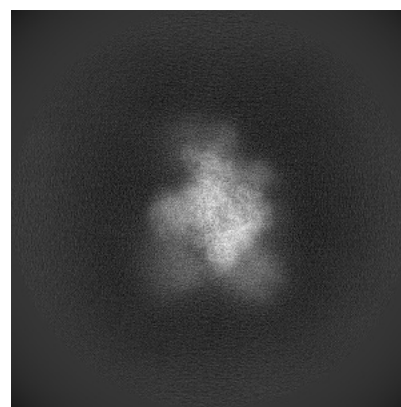
6.1.2 Raw map



X



Y

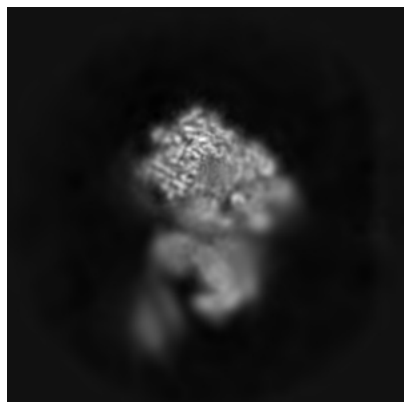


Z

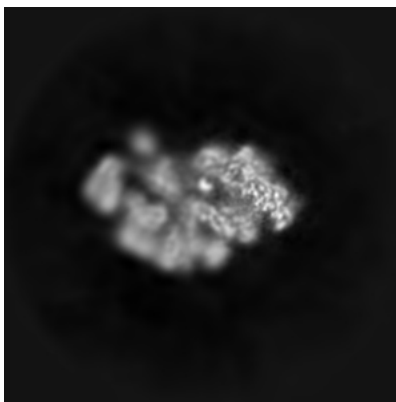
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

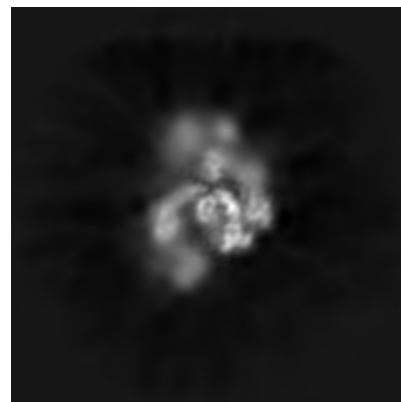
6.2.1 Primary map



X Index: 240

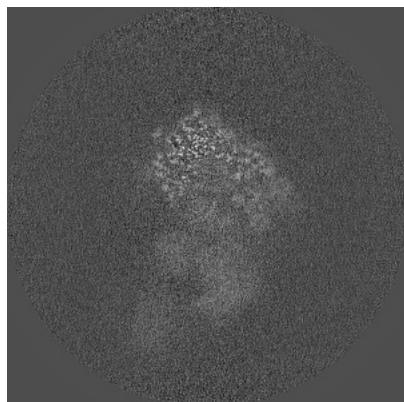


Y Index: 240

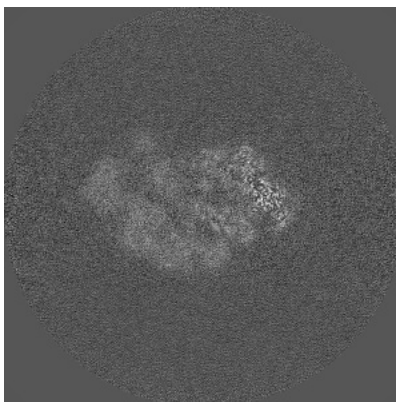


Z Index: 240

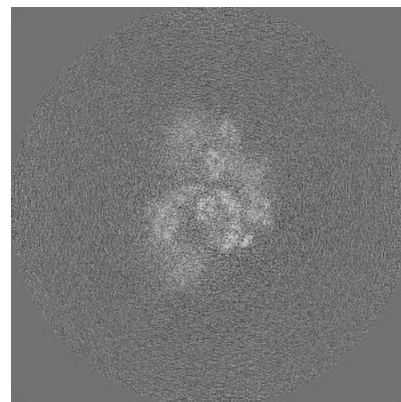
6.2.2 Raw map



X Index: 240



Y Index: 240

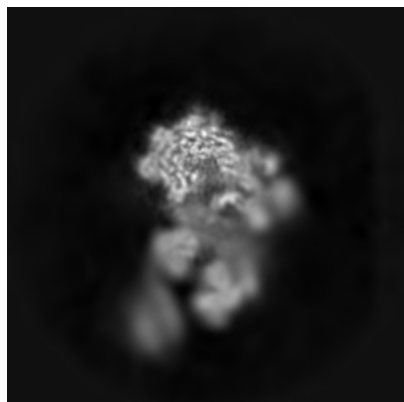


Z Index: 240

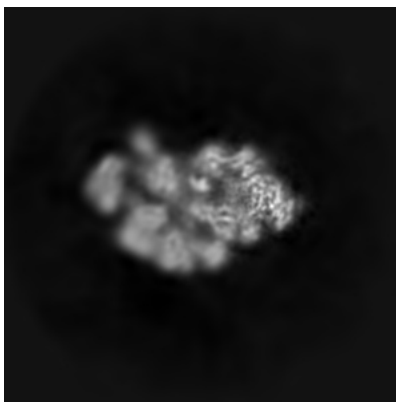
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

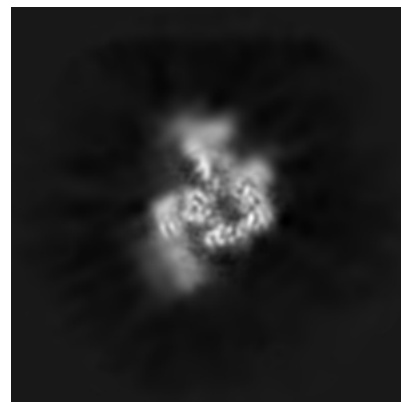
6.3.1 Primary map



X Index: 248

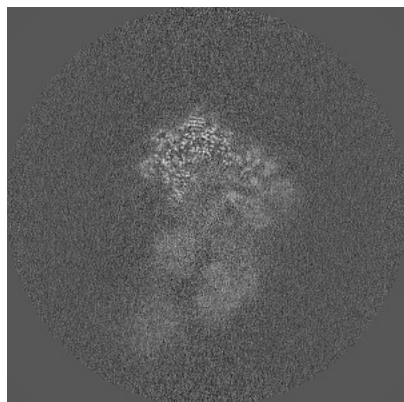


Y Index: 235

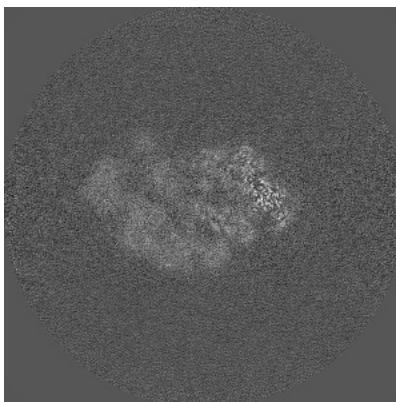


Z Index: 258

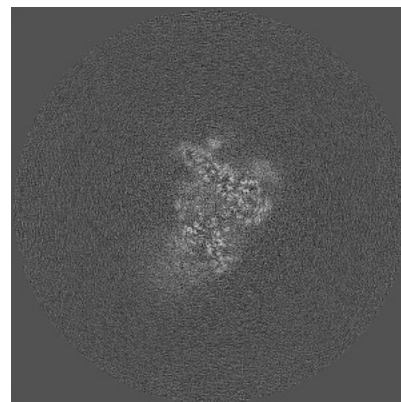
6.3.2 Raw map



X Index: 246



Y Index: 240

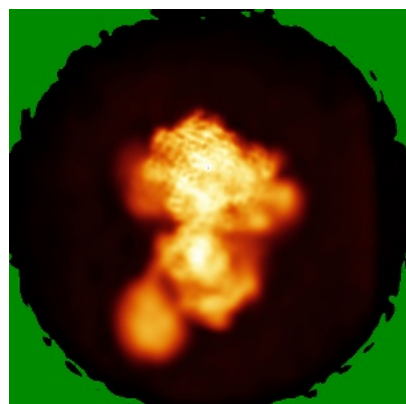


Z Index: 286

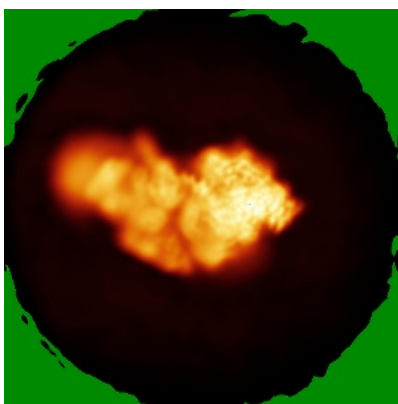
The images above show the largest variance slices of the map in three orthogonal directions.

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

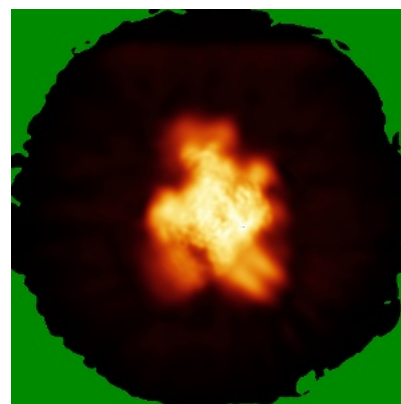
6.4.1 Primary map



X

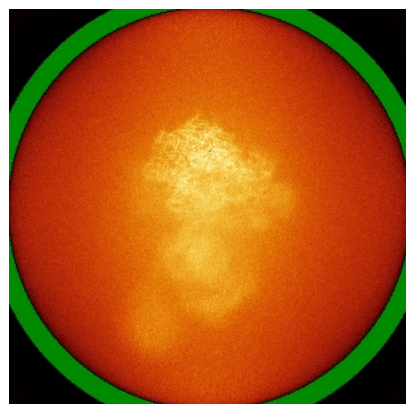


Y

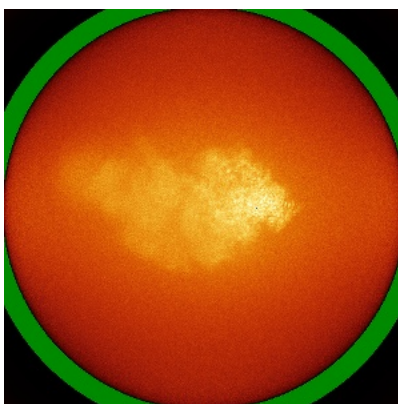


Z

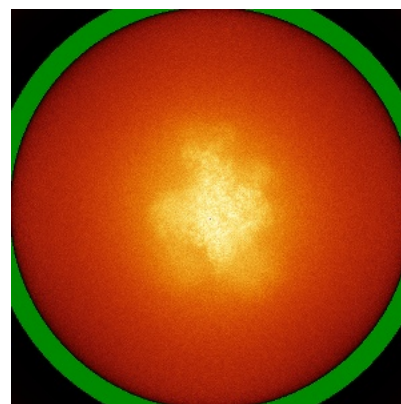
6.4.2 Raw map



X



Y

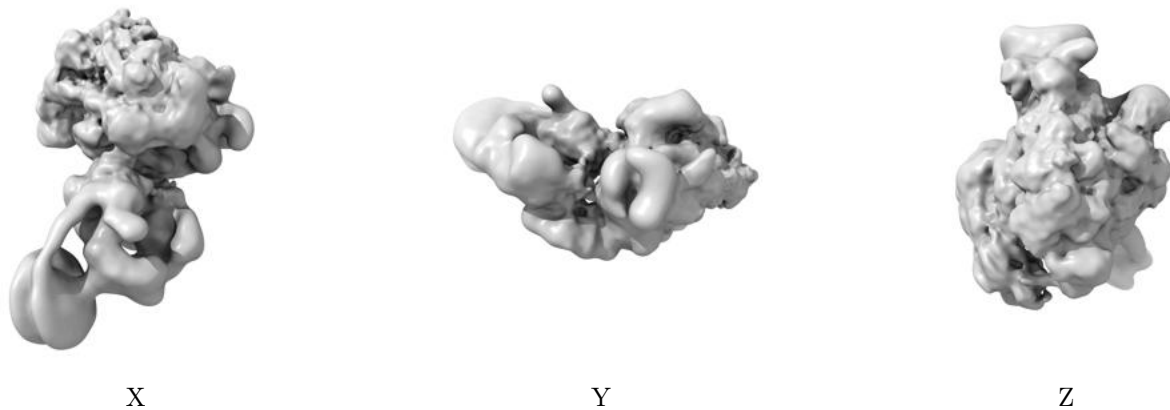


Z

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.

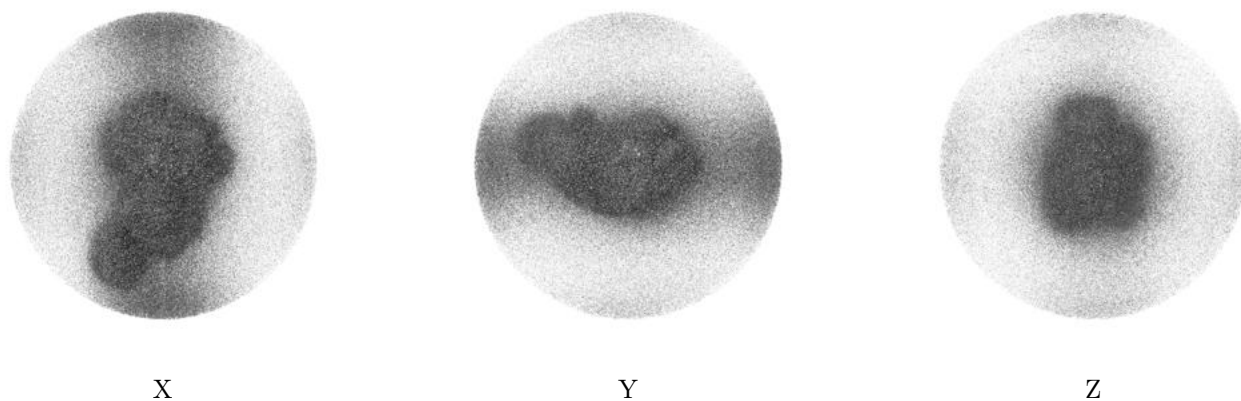
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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.

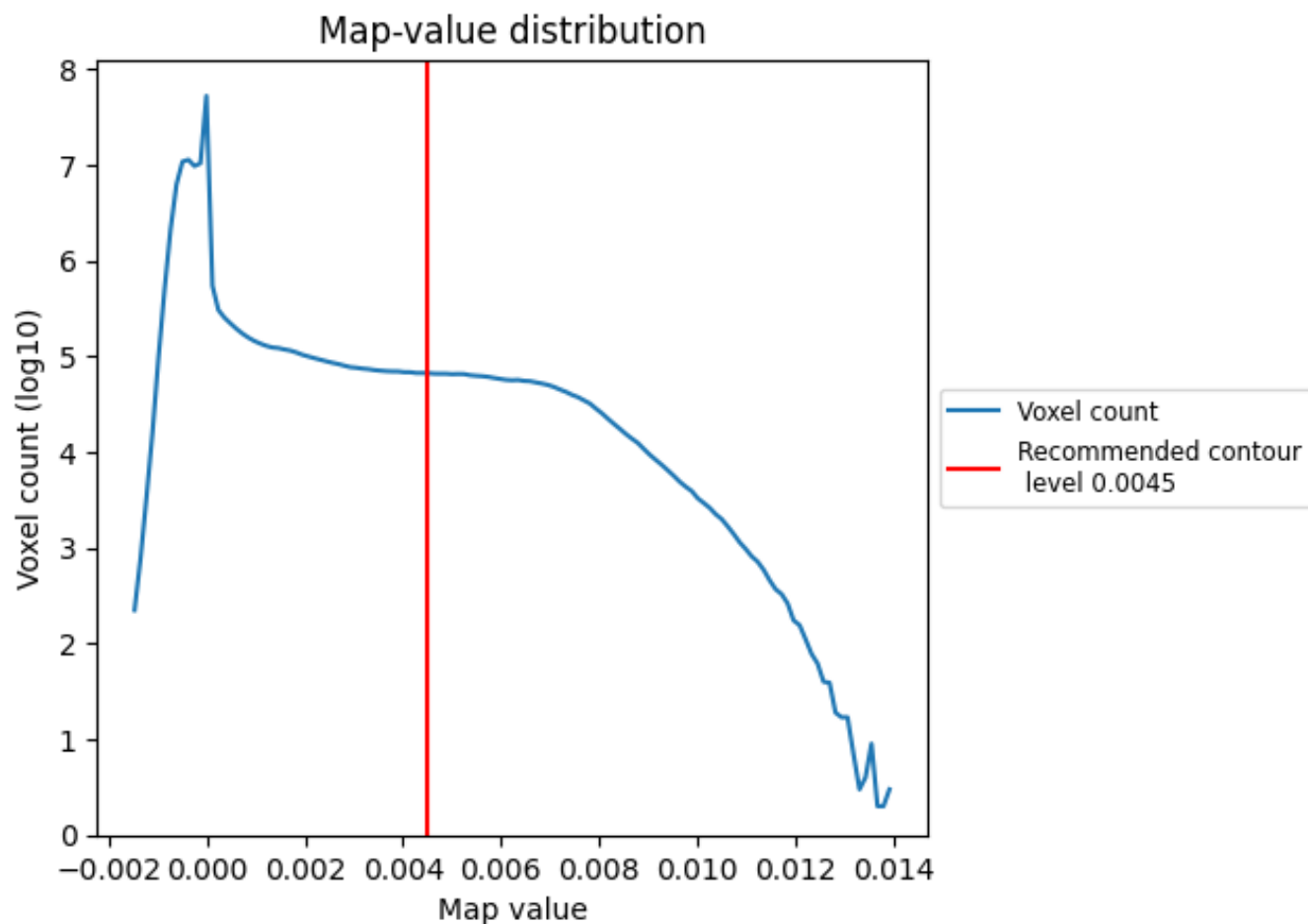
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

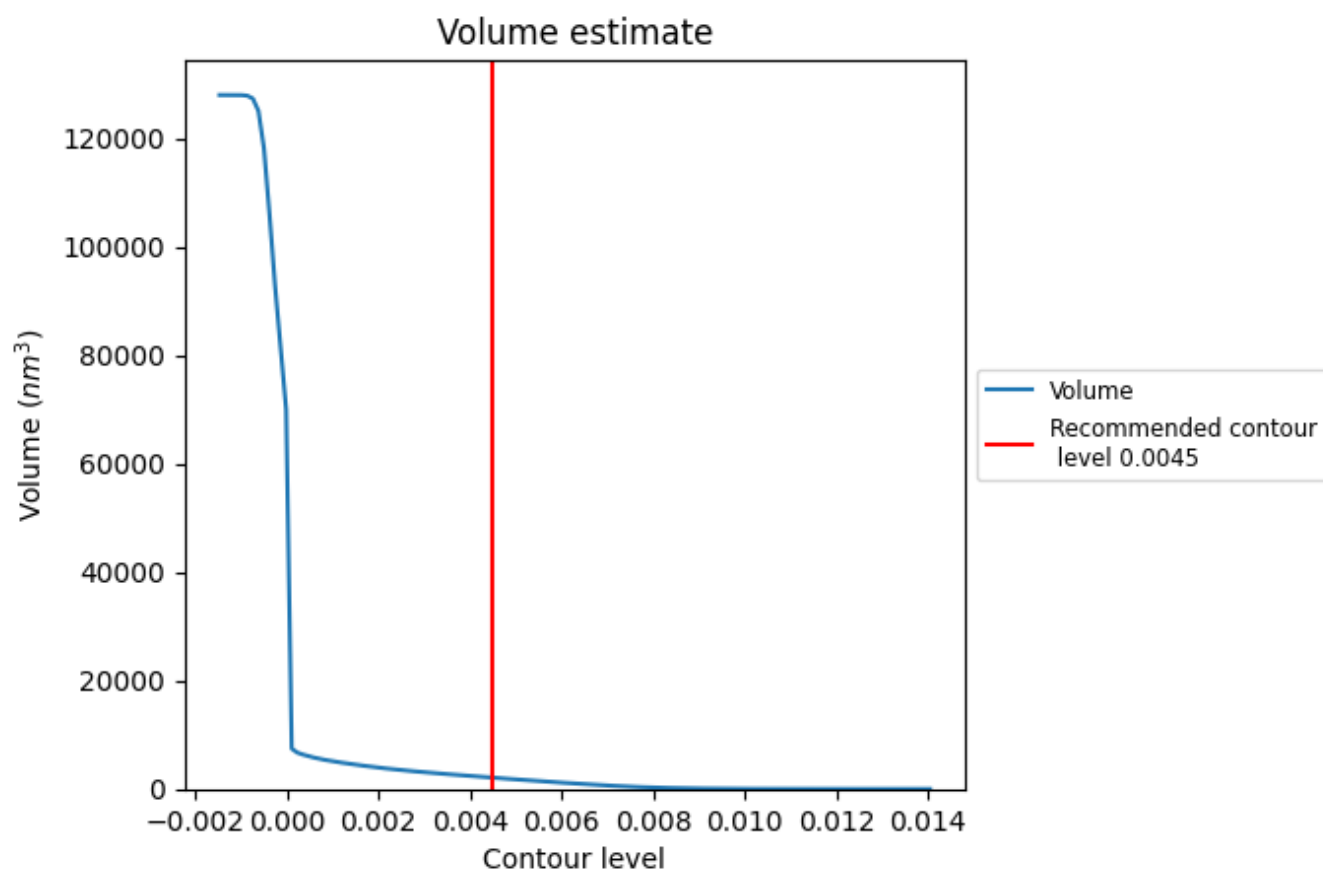
This section contains the results of statistical analysis of the map.

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.

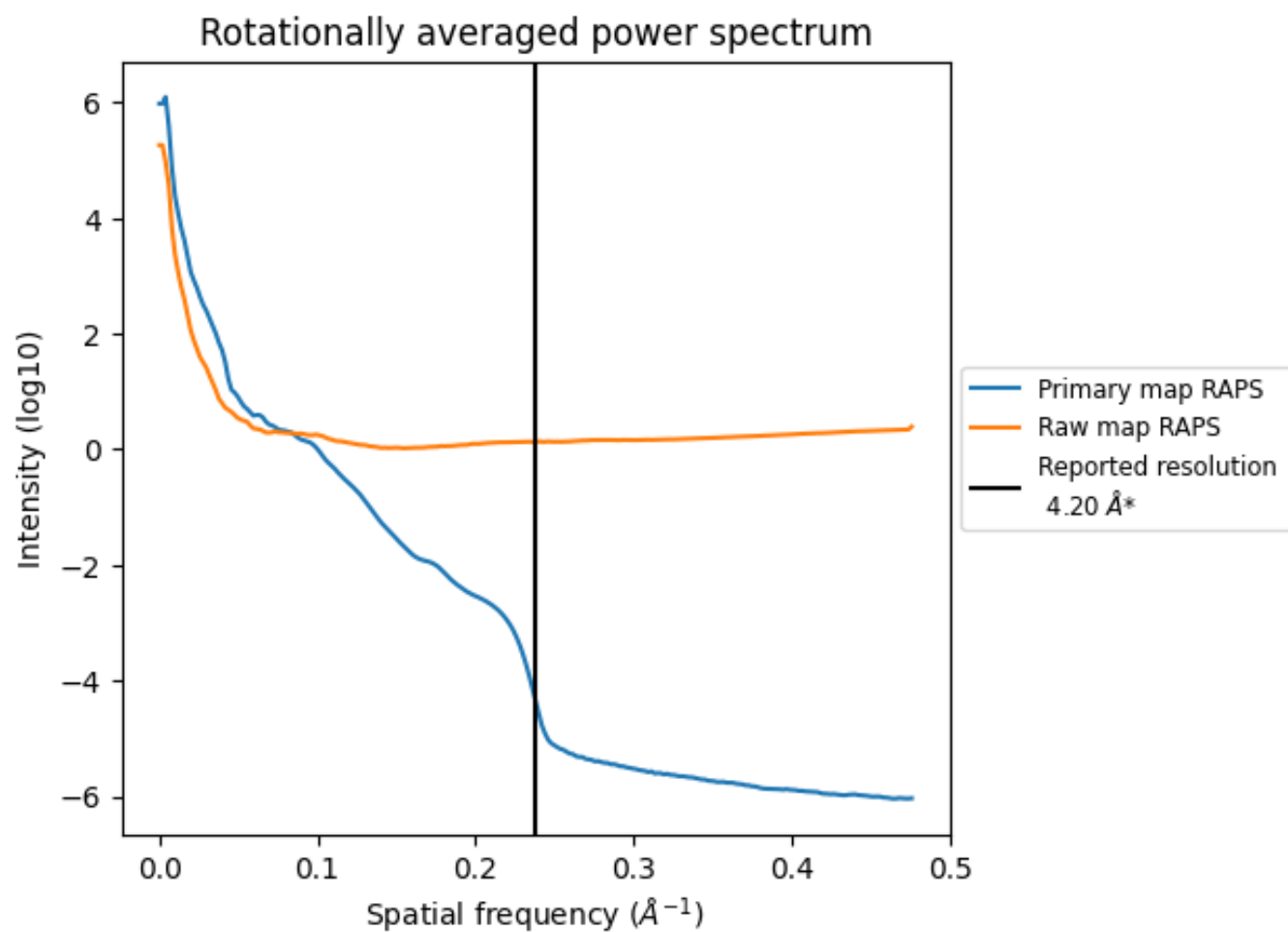
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2079 nm^3 ; this corresponds to an approximate mass of 1878 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 ⓘ

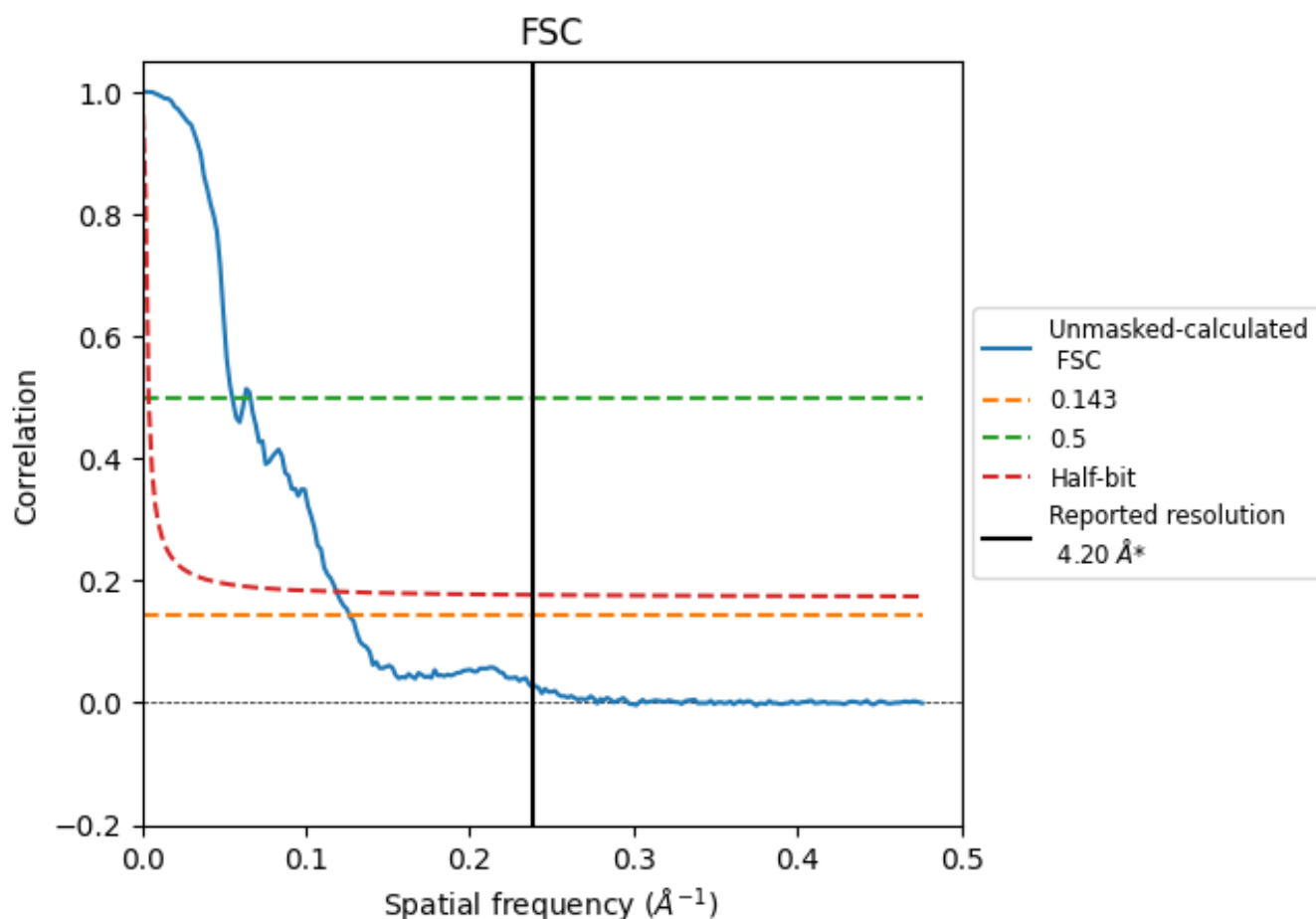


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

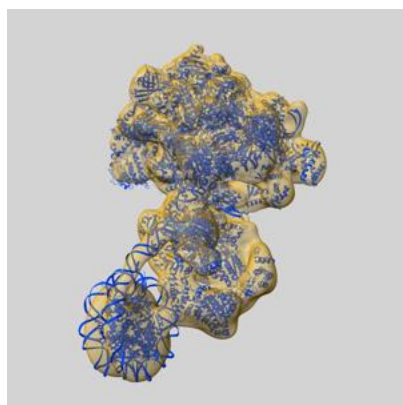
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.91	18.21	8.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.91 differs from the reported value 4.2 by more than 10 %

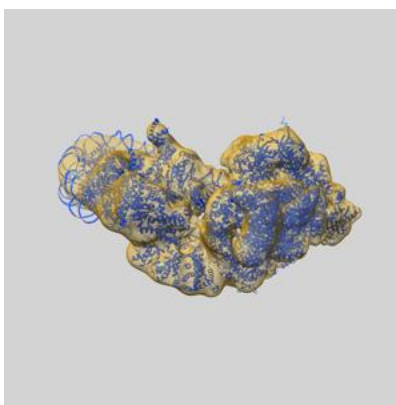
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57401 and PDB model 29WD. Per-residue inclusion information can be found in section [3](#) on page [13](#).

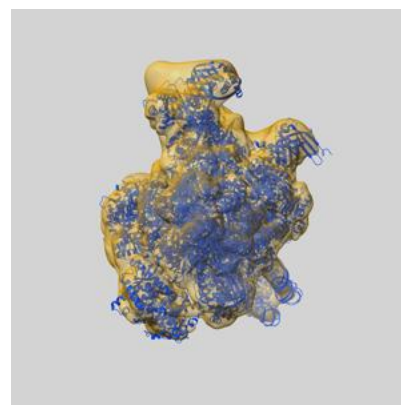
9.1 Map-model overlay [i](#)



X



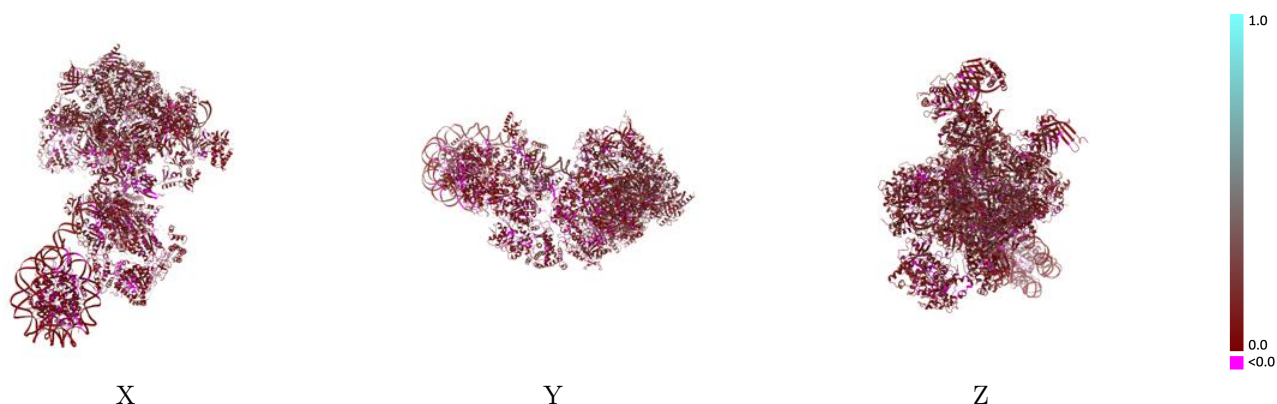
Y



Z

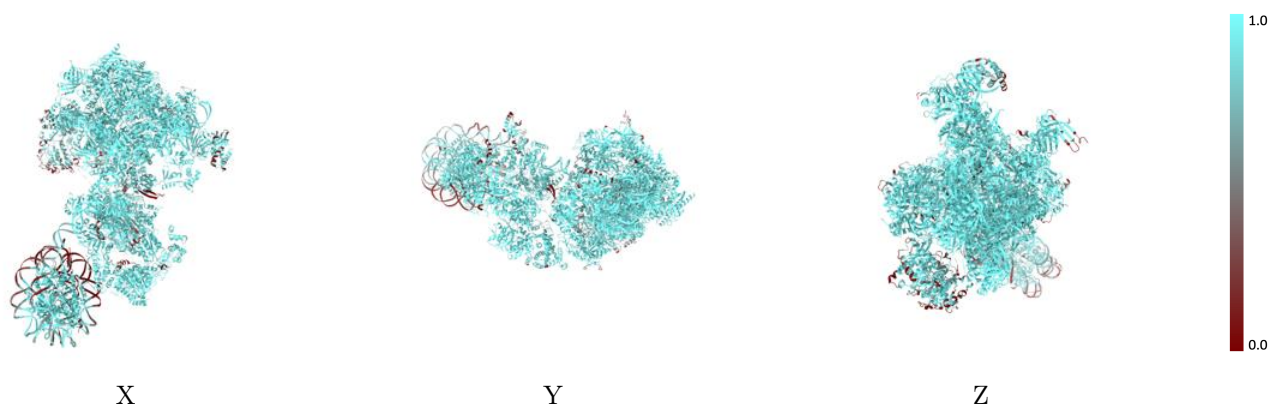
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



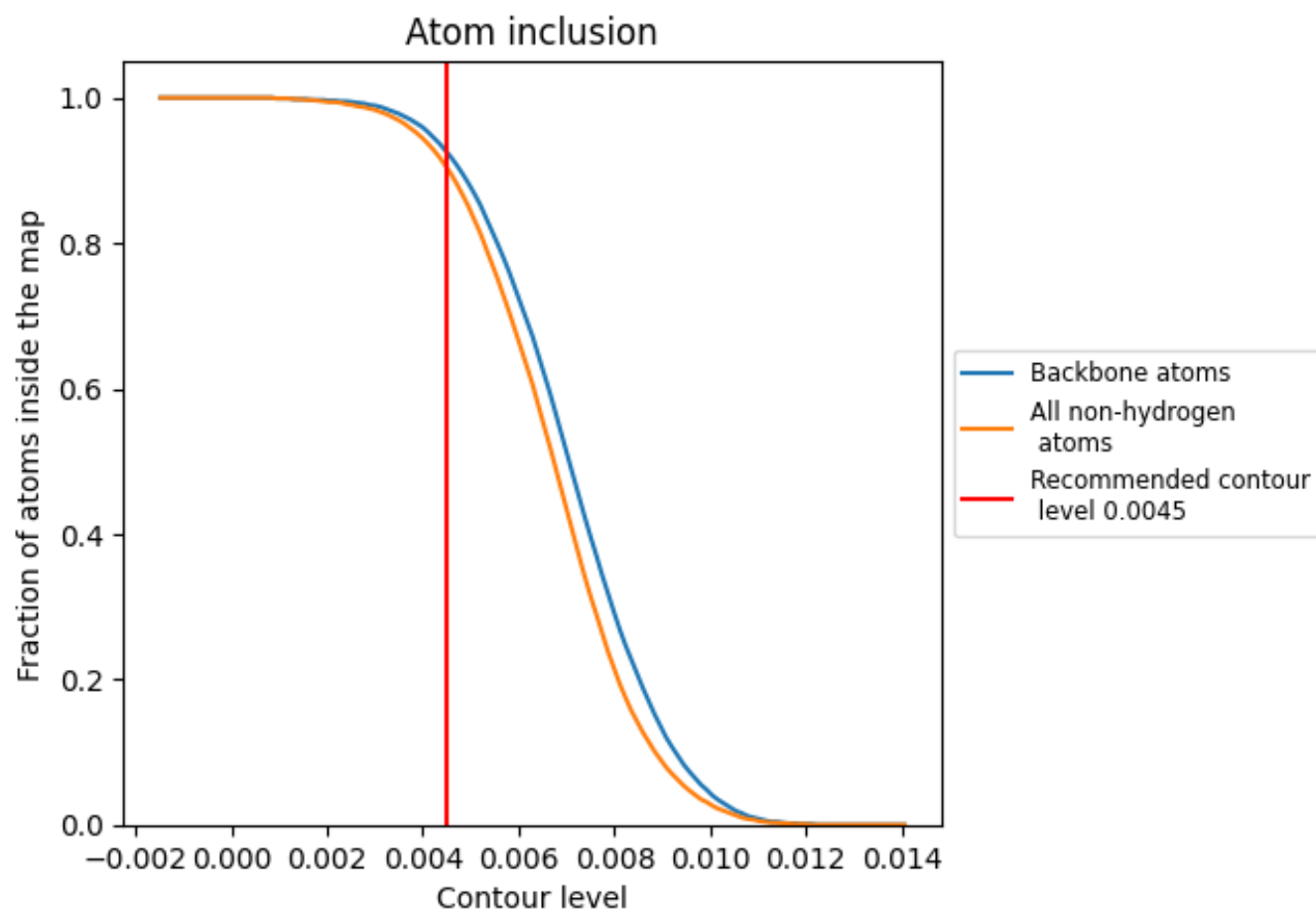
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.1100
0	 0.9820	 0.0950
1	 0.9750	 0.0840
2	 0.9320	 0.0720
3	 0.8890	 0.0850
4	 0.9620	 0.0740
5	 0.9660	 0.0670
6	 0.6740	 0.0180
7	 0.8340	 0.0920
8	 0.7340	 0.0620
9	 0.7540	 0.1020
A	 0.9800	 0.1550
B	 0.9940	 0.1720
C	 0.9760	 0.1870
D	 0.9870	 0.1200
E	 0.9260	 0.1180
F	 0.9640	 0.1640
G	 0.9510	 0.1200
H	 0.9550	 0.1260
I	 0.9810	 0.1390
J	 0.9880	 0.1780
K	 0.9810	 0.1850
L	 0.9890	 0.1730
M	 0.9690	 0.1400
N	 0.6480	 0.0960
O	 0.9730	 0.0980
Q	 0.9290	 0.0900
R	 0.9290	 0.0930
T	 0.6370	 0.0930
U	 0.8260	 0.0720
V	 0.8410	 0.0810
W	 0.8390	 0.0430
X	 0.9310	 0.0920
a	 0.8910	 0.0840
b	 0.9230	 0.0640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.9260	 0.0400
d	 0.9030	 0.0560
e	 0.9340	 0.0680
f	 0.9540	 0.0520
g	 0.8010	 0.0380
h	 0.8800	 0.0370