



wwPDB EM Validation Summary Report ⓘ

Aug 23, 2026 – 12:48 pm BST

PDB ID : 8CEN / pdb_00008cen
EMDB ID : EMD-16610
Title : Yeast RNA polymerase II transcription pre-initiation complex with core Mediator
Authors : Wang, H.; Schilbach, S.; Cramer, P.
Deposited on : 2023-02-02
Resolution : 3.00 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
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

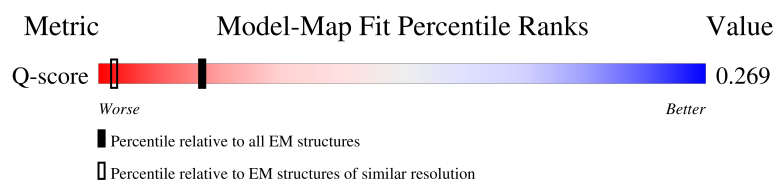
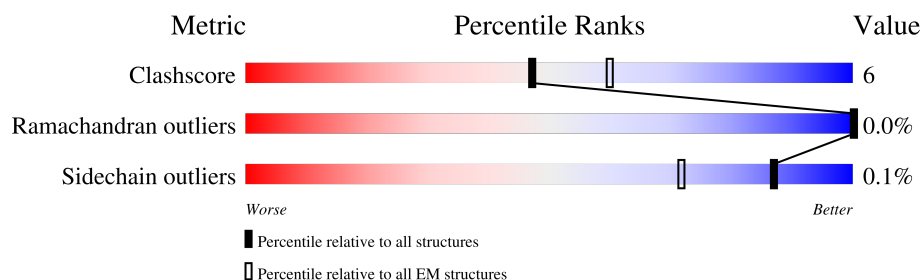
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	778	5% 79% 18% .
2	1	642	18% 70% 11% 19%
3	2	513	18% 75% 13% 12%
4	3	321	35% 6% 59%

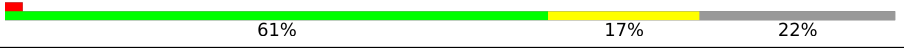
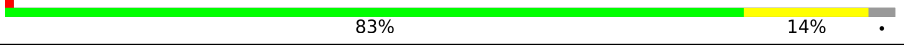
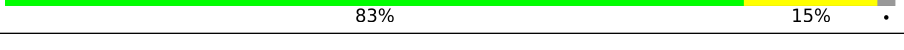
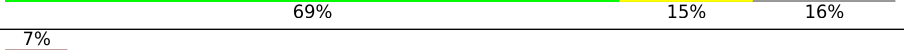
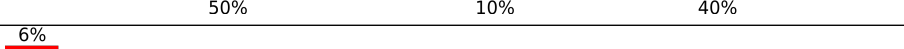
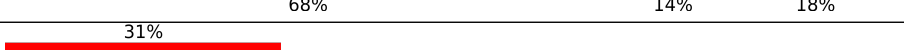
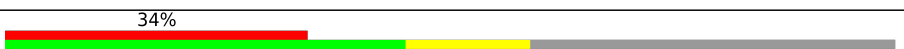
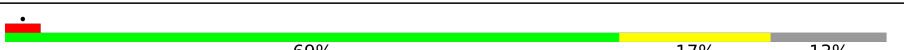
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Mol	Chain	Length	Quality of chain
5	4	338	
6	5	72	
7	6	461	
8	7	843	
9	A	1733	
10	B	1224	
11	C	347	
12	D	221	
13	E	215	
14	F	155	
15	G	177	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	352	
22	N	209	
23	O	240	
24	Q	735	
25	R	400	
26	T	209	
27	U	286	
28	V	122	
29	W	492	

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Mol	Chain	Length	Quality of chain
30	X	328	
31	a	295	
32	b	223	
33	c	115	
34	d	687	
35	e	307	
36	f	210	
37	g	121	
38	h	284	
39	i	222	
40	j	149	
41	k	157	
42	l	745	
43	m	220	
44	n	140	
45	o	127	
46	p	566	

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 101943 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 IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	522	Total	C	N	O	S	0	0
			4214	2660	734	798	22		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	452	Total	C	N	O	S	0	0
			3647	2354	600	677	16		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	302	Total	C	N	O	S	0	0
			2338	1492	390	442	14		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	383	Total	C	N	O	S	0	0
			3019	1915	523	552	29		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	615	Total	C	N	O	S	0	0
			4954	3153	860	914	27		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1508	Total	C	N	O	S	0	0
			11815	7442	2042	2269	62		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1180	Total	C	N	O	S	0	0
			9404	5946	1643	1760	55		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	266	Total	C	N	O	S	0	0
			2092	1315	348	416	13		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	initiating methionine	UNP P16370
C	-27	GLY	-	expression tag	UNP P16370
C	-26	SER	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	HIS	-	expression tag	UNP P16370
C	-19	SER	-	expression tag	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	ASN	-	expression tag	UNP P16370
C	-17	SER	-	expression tag	UNP P16370
C	-16	GLY	-	expression tag	UNP P16370
C	-15	LEU	-	expression tag	UNP P16370
C	-14	ASN	-	expression tag	UNP P16370
C	-13	ASP	-	expression tag	UNP P16370
C	-12	ILE	-	expression tag	UNP P16370
C	-11	PHE	-	expression tag	UNP P16370
C	-10	GLU	-	expression tag	UNP P16370
C	-9	ALA	-	expression tag	UNP P16370
C	-8	GLN	-	expression tag	UNP P16370
C	-7	LYS	-	expression tag	UNP P16370
C	-6	ILE	-	expression tag	UNP P16370
C	-5	GLU	-	expression tag	UNP P16370
C	-4	TRP	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	GLU	-	expression tag	UNP P16370
C	-1	ASP	-	expression tag	UNP P16370
C	0	THR	-	expression tag	UNP P16370
C	1	GLY	-	expression tag	UNP P16370
C	2	SER	-	expression tag	UNP P16370
C	3	SER	-	expression tag	UNP P16370

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	167	Total	C	N	O	S	0	0
			1343	829	242	270	2		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	118	Total	C	N	O	S	0	0
			983	623	164	193	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	HIS	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	310	Total	C	N	O	S	0	0
			2379	1504	408	449	18		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	346	LYS	-	expression tag	UNP P29055
M	347	HIS	-	expression tag	UNP P29055
M	348	HIS	-	expression tag	UNP P29055
M	349	HIS	-	expression tag	UNP P29055
M	350	HIS	-	expression tag	UNP P29055
M	351	HIS	-	expression tag	UNP P29055
M	352	HIS	-	expression tag	UNP P29055

- Molecule 22 is a DNA chain called NONTEMPLATE DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	73	Total	C	N	O	P	0	0
			1495	717	270	436	72		

- Molecule 23 is a protein called TATA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 24 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	221	Total	C	N	O	S	0	0
			1871	1179	346	339	7		

- Molecule 25 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	268	Total	C	N	O	S	0	0
			2230	1409	392	419	10		

- Molecule 26 is a DNA chain called TEMPLATE DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	73	Total	C	N	O	P	0	0
			1495	716	268	438	73		

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	304	Total	C	N	O	S	0	0
			2473	1558	431	477	7		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	483	ALA	-	expression tag	UNP P36100
W	484	ALA	-	expression tag	UNP P36100
W	485	ALA	-	expression tag	UNP P36100
W	486	LEU	-	expression tag	UNP P36100
W	487	GLU	-	expression tag	UNP P36100
W	488	HIS	-	expression tag	UNP P36100
W	489	HIS	-	expression tag	UNP P36100
W	490	HIS	-	expression tag	UNP P36100
W	491	HIS	-	expression tag	UNP P36100
W	492	HIS	-	expression tag	UNP P36100

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	211	Total	C	N	O	S	0	0
			1708	1089	293	320	6		

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	178	Total	C	N	O	S	0	0
			1495	970	240	278	7		

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	173	Total	C	N	O	S	0	0
			1414	900	241	270	3		

- Molecule 33 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	111	Total	C	N	O	S	0	0
			902	566	154	178	4		

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	501	Total	C	N	O	S	0	0
			4063	2613	684	752	14		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	256	Total	C	N	O	S	0	0
			2017	1280	336	390	11		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	206	Total	C	N	O	S	0	0
			1578	998	266	309	5		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	102	Total	C	N	O	S	0	0
			815	512	134	164	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	171	Total	C	N	O	S	0	0
			1394	884	234	271	5		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	181	Total	C	N	O	S	0	0
			1512	973	253	280	6		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	102	Total	C	N	O	S	0	0
			852	533	156	162	1		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	157	Total	C	N	O	S	0	0
			1259	777	222	257	3		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	535	Total	C	N	O	S	0	0
			4385	2846	759	763	17		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	130	Total	C	N	O	S	0	0
			1068	672	185	209	2		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	136	Total	C	N	O	S	0	0
			1095	685	185	220	5		

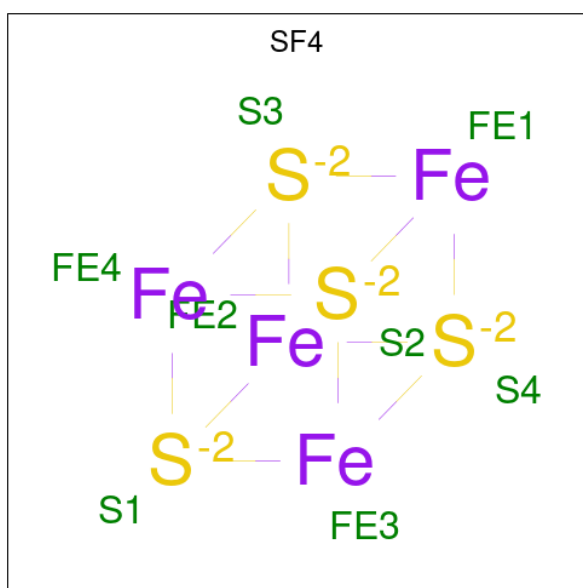
- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	110	Total	C	N	O	S	0	0
			922	607	143	166	6		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	225	Total	C	N	O	S	0	0
			1863	1193	298	366	6		

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
47	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	3	2	Total	Zn	0
			2	2	
48	4	1	Total	Zn	0
			1	1	
48	6	4	Total	Zn	0
			4	4	
48	A	2	Total	Zn	0
			2	2	

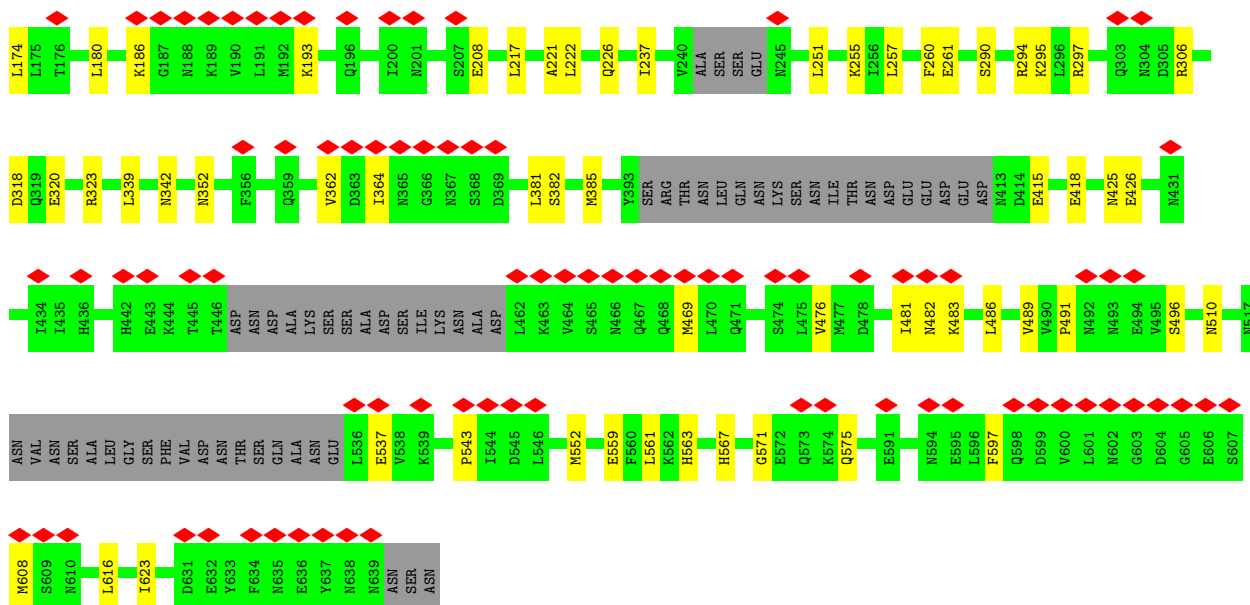
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Mol	Chain	Residues	Atoms		AltConf
48	B	1	Total 1	Zn 1	0
48	C	1	Total 1	Zn 1	0
48	I	2	Total 2	Zn 2	0
48	J	1	Total 1	Zn 1	0
48	L	1	Total 1	Zn 1	0
48	M	1	Total 1	Zn 1	0
48	W	1	Total 1	Zn 1	0

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

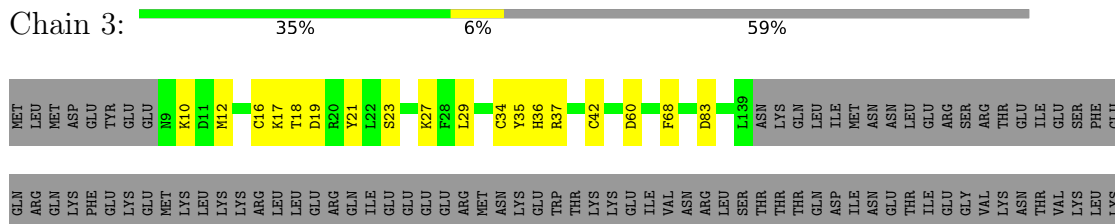
Mol	Chain	Residues	Atoms		AltConf
49	A	1	Total 1	Mg 1	0



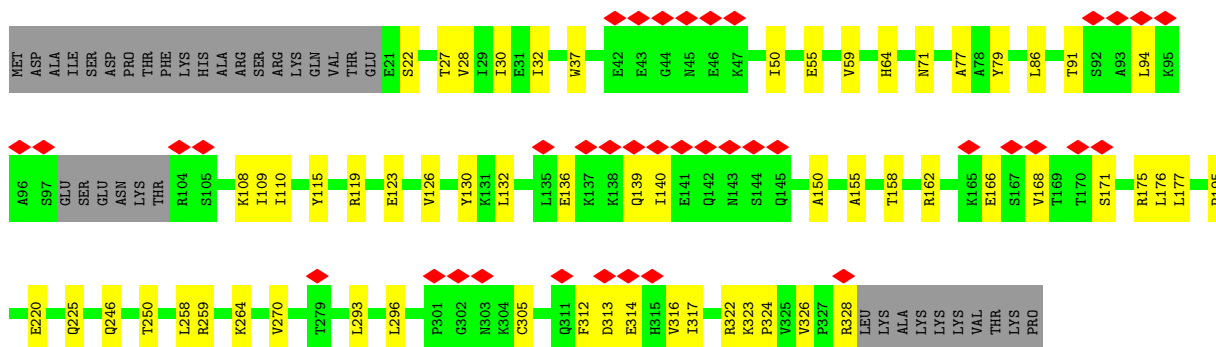
- Molecule 3: General transcription and DNA repair factor IIH subunit TFB2



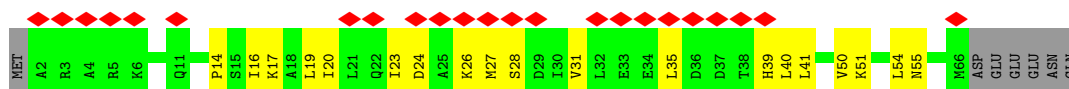
- Molecule 4: RNA polymerase II transcription factor B subunit 3



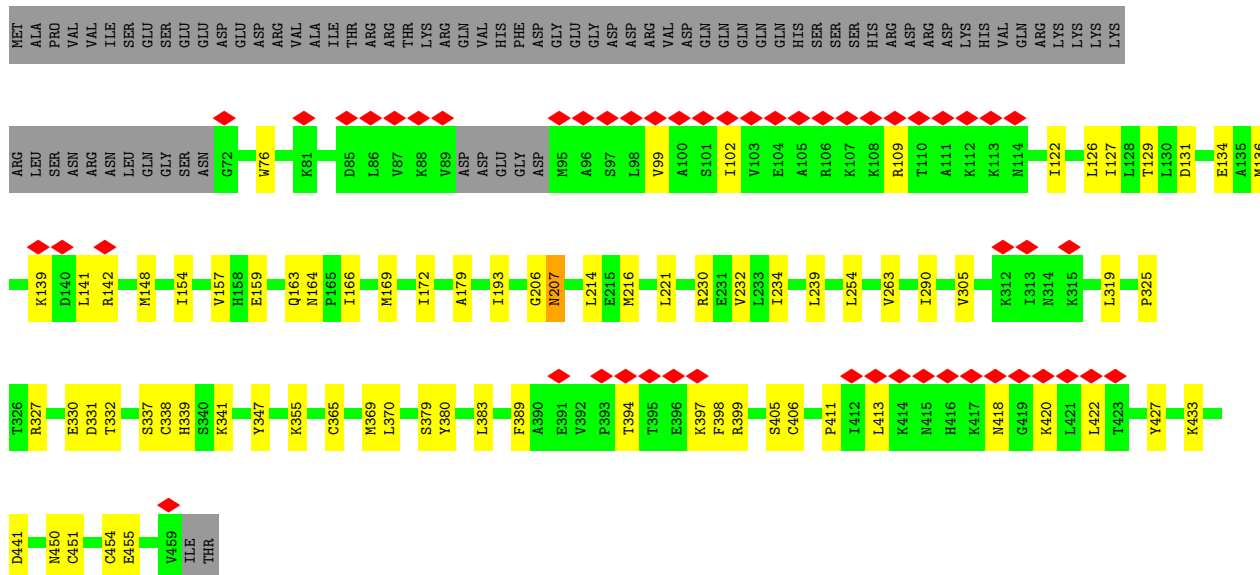
- Molecule 5: General transcription and DNA repair factor IIH subunit TFB4



- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5



- Molecule 7: General transcription and DNA repair factor IIH subunit SSL1



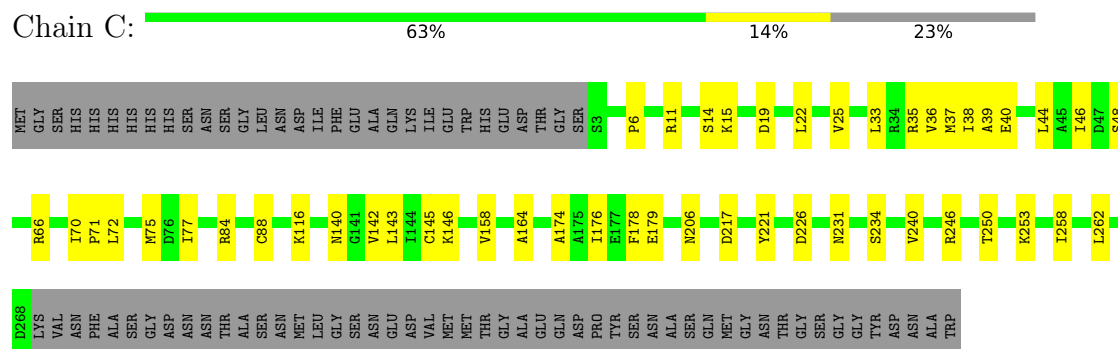
- Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB



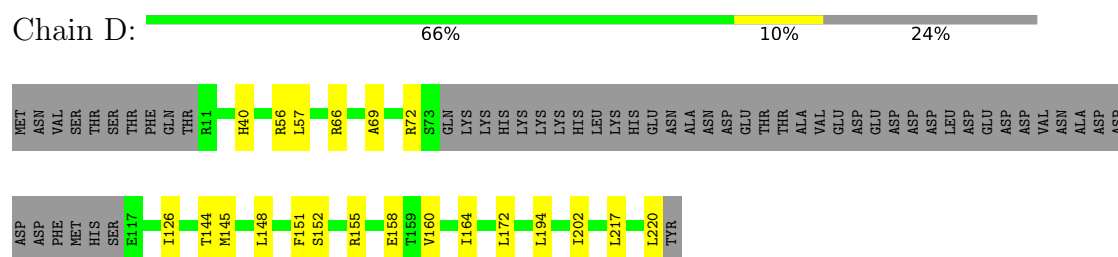


L1151	Q951	R728	F557	L387	R169	MET
M1152	V952	L729	R398	L170	ASP	
C1163	L953	R730	W561	Q415	LEU	
M1178	N957	I743	E567	L416	ALA	
M1187	L961	R747	V570	L420	ASN	
K1188	K962	P757	Q573	L424	GLU	
I1189	F963	F757	Q573	L424	LYS	
D1190	V966	D760	H590	T428	TVR	
H1195	I976	R766	L596	F429	TVR	
L1207	K979	Q770	L600	N443	ASP	
M1208	F980	S771	L600	N444	PRO	
R1220	H984	V787	L603	K445	TVR	
F1224	K987	T805	R604	L446	GLY	
	G988	M809	L608	L447	F18	
	G991	V825	M615	L448	E21	
	R996	M839	R617	L453	F38	
	P1000	B848	V633	L457	L69	
	I1001	K862	Y634	L461	I70	
	T1002	E883	K652	E468	L71	
	L1010	K864	Q656	GLN	I84	
	R1020	M868	Q667	LYS	K87	
	I1050	S869	V668	ALA	T98	
	S1056	E872	T669	MET	V102	
	S1066	L883	GLU	SER	N103	
	M1072	R884	D675	R476	L112	
	Q1093	D895	E691	Y486	L119	
	R1096	R904	D694	T498	R120	
	R1106	I911	E697	N499	N121	
	L1114	I912	Q706	T500	L122	
	R1124	E924	E714	F501	L128	
	M1133	R928	ALA	L502	Y137	
	E1134	T929	ASN	GLY	F138	
	R1135	D936	GLU	ARG	A139	
	D1136	A937	ASN	ASP	Y149	
	L1147	S938	ASP	S506	E157	
		T939	LEU	A509	ASP	
			FZ22	L521	ASP	
				V522	GLU	
				E526	GLU	
				K537	GLU	
				L541	GLU	
				Y412	GLU	
					G163	
					F165	

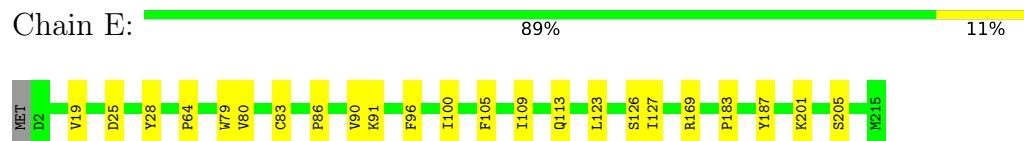
- Molecule 11: DNA-directed RNA polymerase II subunit RPB3



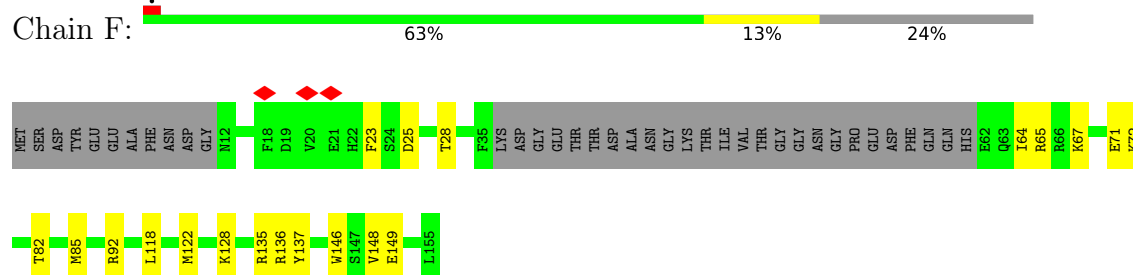
- Molecule 12: DNA-directed RNA polymerase II subunit RPB4



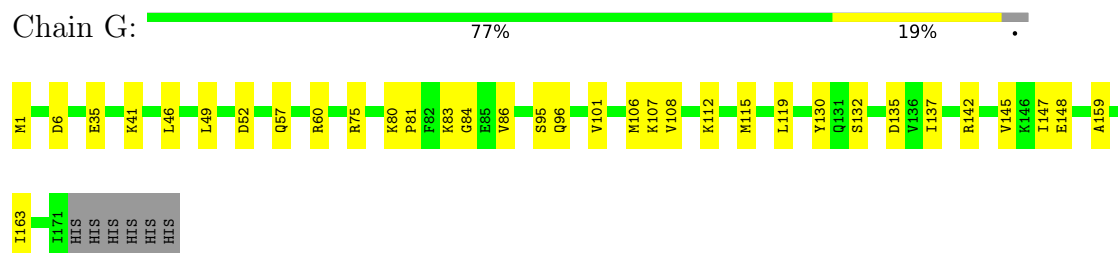
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

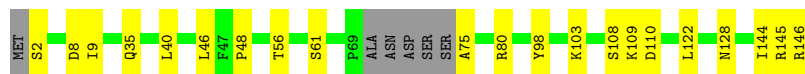


- Molecule 15: DNA-directed RNA polymerase II subunit RPB7



- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  82% 14% .



- Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I:  76% 19% 5%



- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  84% 14% .



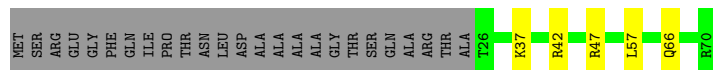
- Molecule 19: DNA-directed RNA polymerase II subunit RPB11

Chain K:  80% 16% .



- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  57% 7% 36%



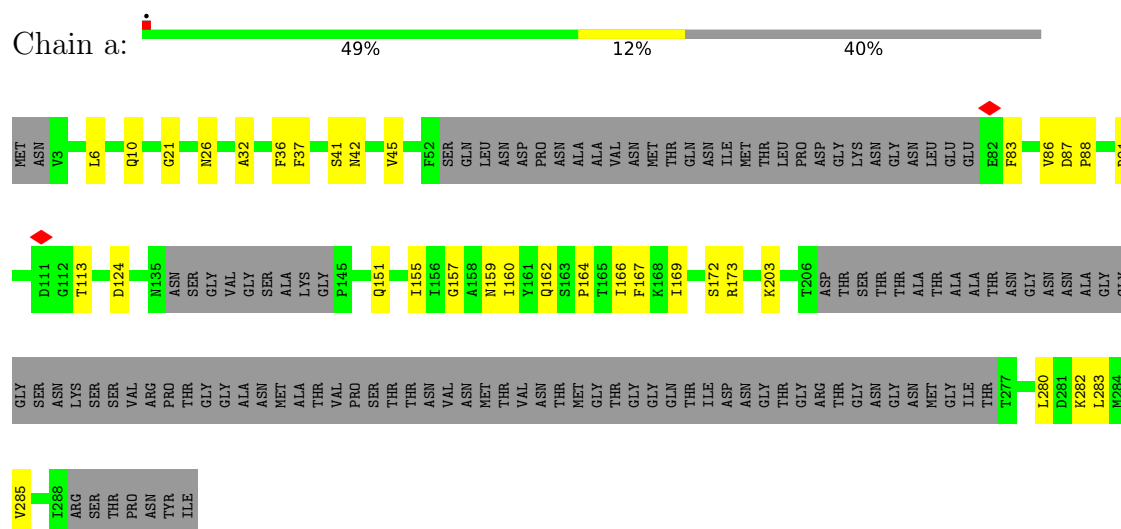
- Molecule 21: Transcription initiation factor IIB

Chain M:  73% 15% 12%

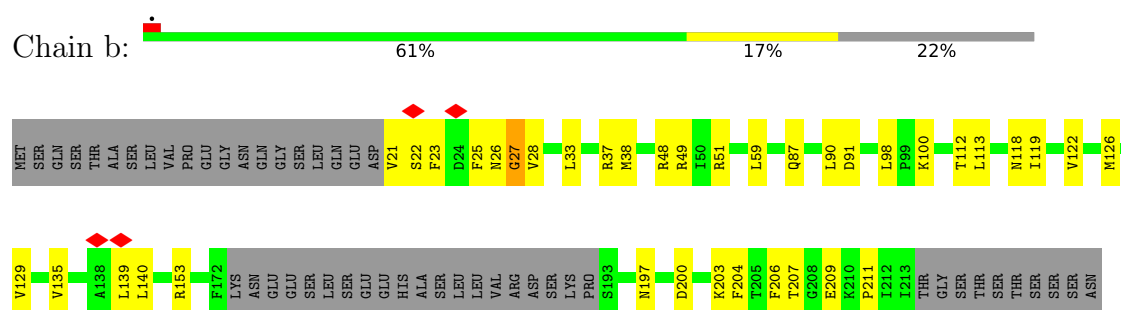


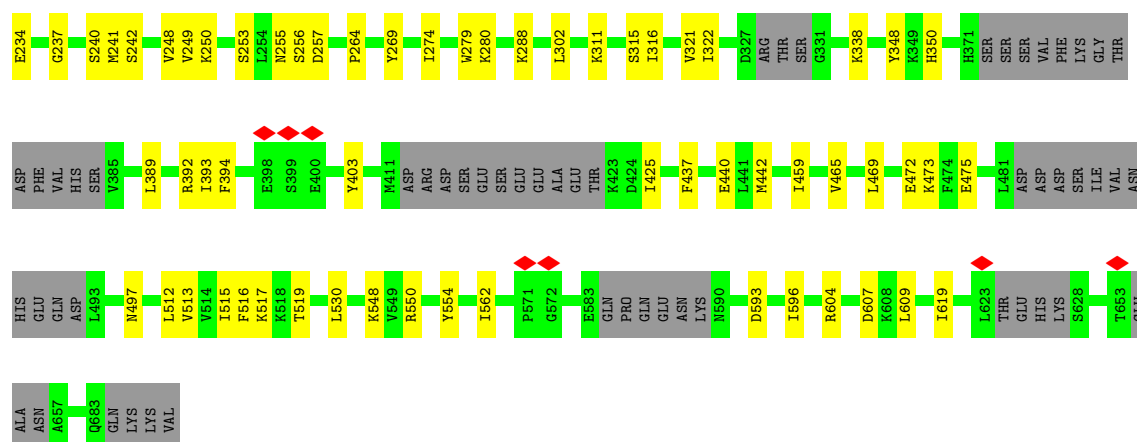
- Molecule 22: NONTEMPLATE DNA (209-MER)

- Molecule 31: Mediator of RNA polymerase II transcription subunit 6



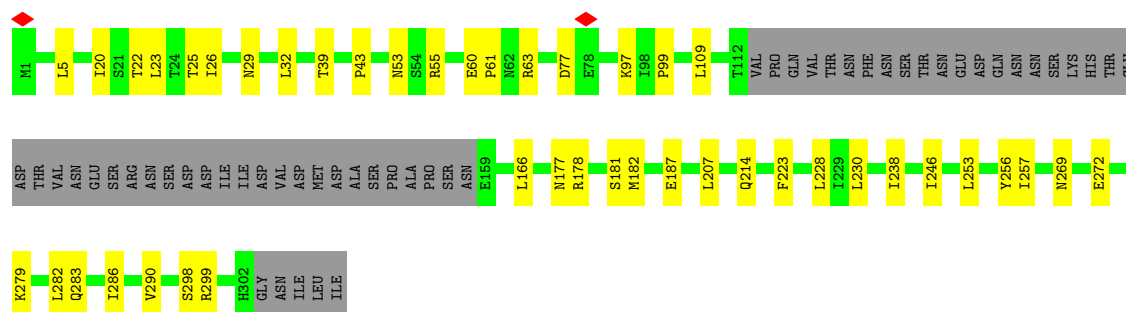
- Molecule 32: Mediator of RNA polymerase II transcription subunit 8





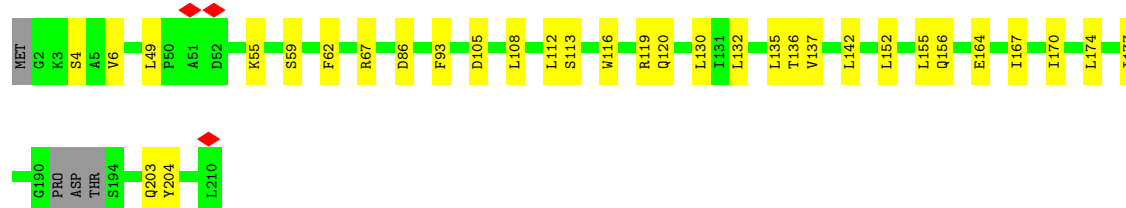
• Molecule 35: Mediator of RNA polymerase II transcription subunit 18

Chain e: 69% 14% 17%



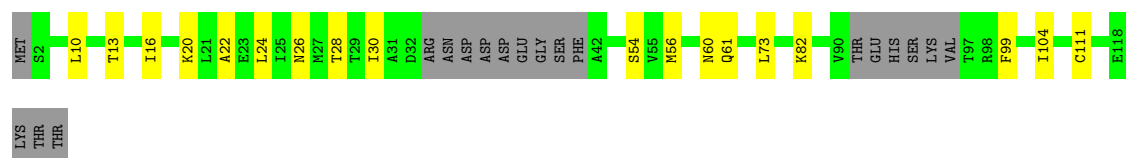
• Molecule 36: Mediator of RNA polymerase II transcription subunit 20

Chain f: 83% 15% .

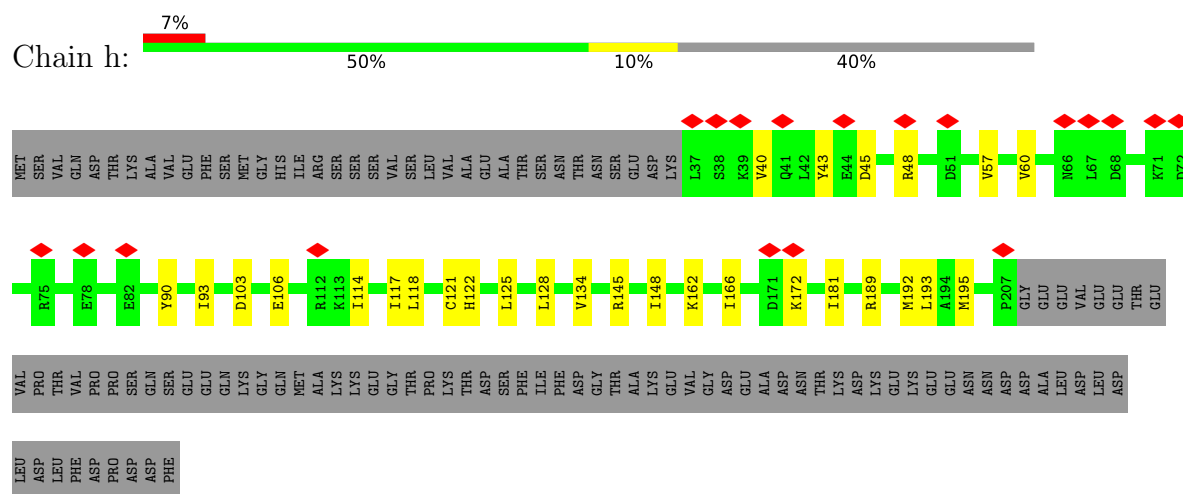


• Molecule 37: Mediator of RNA polymerase II transcription subunit 22

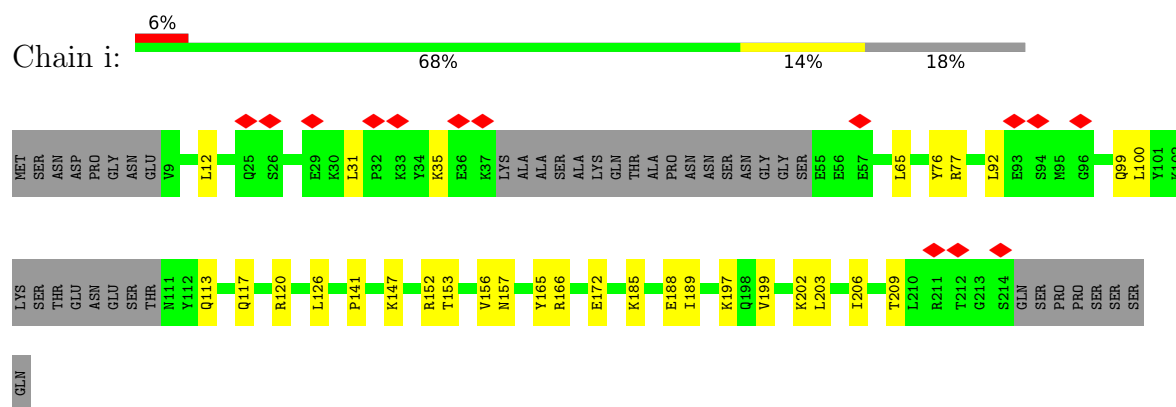
Chain g: 69% 15% 16%



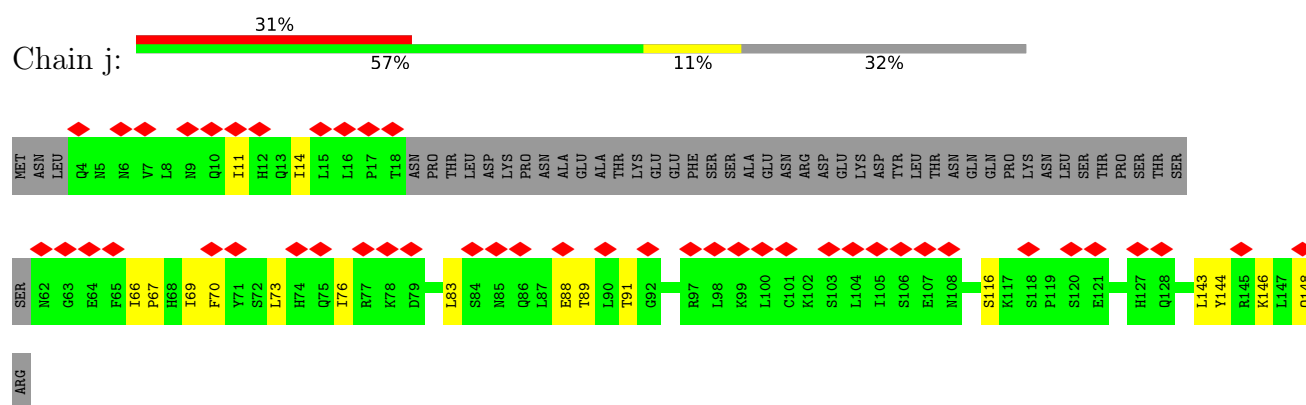
• Molecule 38: Mediator of RNA polymerase II transcription subunit 4



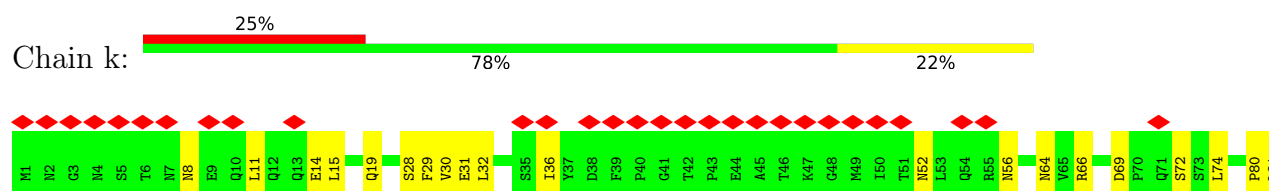
• Molecule 39: Mediator of RNA polymerase II transcription subunit 7



• Molecule 40: Mediator of RNA polymerase II transcription subunit 9



• Molecule 41: Mediator of RNA polymerase II transcription subunit 10



- Chain n:



Chain o:



Chain p:



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	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: ZN, SF4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.17	0/6209	0.44	0/8384
2	1	0.17	0/4277	0.43	1/5755 (0.0%)
3	2	0.19	0/3717	0.46	0/5028
4	3	0.14	0/1109	0.37	0/1492
5	4	0.17	0/2377	0.43	0/3216
6	5	0.20	0/520	0.48	0/701
7	6	0.17	0/3082	0.43	0/4165
8	7	0.16	0/5059	0.40	1/6841 (0.0%)
9	A	0.18	0/12048	0.42	0/16321
10	B	0.18	0/9589	0.41	0/12934
11	C	0.17	0/2130	0.39	0/2887
12	D	0.19	0/1351	0.50	0/1811
13	E	0.16	0/1788	0.42	0/2406
14	F	0.17	0/1001	0.40	0/1347
15	G	0.16	0/1367	0.40	0/1844
16	H	0.15	0/1139	0.36	0/1544
17	I	0.15	0/962	0.48	0/1295
18	J	0.19	0/578	0.42	0/775
19	K	0.17	0/942	0.38	0/1272
20	L	0.15	0/361	0.43	0/478
21	M	0.17	0/2408	0.44	0/3241
22	N	0.22	0/1677	0.40	0/2587
23	O	0.16	0/1449	0.41	0/1952
24	Q	0.16	0/1907	0.41	0/2556
25	R	0.15	0/2270	0.39	0/3052
26	T	0.21	0/1676	0.39	0/2584
27	U	0.21	0/898	0.54	0/1212
28	V	0.19	0/822	0.47	0/1109
29	W	0.19	0/2513	0.50	0/3388
30	X	0.17	0/1739	0.47	1/2339 (0.0%)
31	a	0.19	0/1531	0.49	0/2072
32	b	0.21	0/1443	0.48	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.20	0/913	0.54	0/1228
34	d	0.18	0/4118	0.44	0/5532
35	e	0.14	0/2054	0.40	0/2782
36	f	0.17	0/1602	0.44	0/2169
37	g	0.19	0/818	0.49	0/1104
38	h	0.23	0/1415	0.58	0/1907
39	i	0.18	0/1543	0.44	1/2084 (0.0%)
40	j	0.22	0/865	0.57	0/1166
41	k	0.27	0/1277	0.66	1/1727 (0.1%)
42	l	0.19	0/4468	0.47	0/6048
43	m	0.23	0/1093	0.65	5/1481 (0.3%)
44	n	0.21	0/1106	0.48	0/1488
45	o	0.18	0/949	0.41	0/1294
46	p	0.32	1/1898 (0.1%)	0.68	4/2559 (0.2%)
All	All	0.18	1/104058 (0.0%)	0.45	14/141114 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	p	211	PRO	CG-CD	-10.29	1.15	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	p	211	PRO	N-CD-CG	-16.42	78.57	103.20
46	p	211	PRO	CA-CB-CG	-14.28	77.37	104.50
8	7	106	PRO	CA-N-CD	-8.41	100.23	112.00
41	k	80	PRO	CA-N-CD	-7.78	101.10	112.00
46	p	211	PRO	N-CA-CB	-6.71	97.45	103.36

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	0	6091	0	6155	86	0
2	1	4214	0	4288	48	0
3	2	3647	0	3732	43	0
4	3	1089	0	1069	12	0
5	4	2338	0	2404	41	0
6	5	514	0	541	13	0
7	6	3019	0	3040	51	0
8	7	4954	0	4946	68	0
9	A	11815	0	11816	162	0
10	B	9404	0	9398	115	0
11	C	2092	0	2050	36	0
12	D	1343	0	1366	15	0
13	E	1752	0	1776	15	0
14	F	983	0	968	16	0
15	G	1339	0	1357	23	0
16	H	1120	0	1086	14	0
17	I	944	0	899	16	0
18	J	569	0	585	7	0
19	K	924	0	934	15	0
20	L	359	0	381	6	0
21	M	2379	0	2488	32	0
22	N	1495	0	828	7	0
23	O	1422	0	1500	25	0
24	Q	1871	0	1883	27	0
25	R	2230	0	2254	36	0
26	T	1495	0	827	6	0
27	U	885	0	866	14	0
28	V	815	0	822	22	0
29	W	2473	0	2476	40	0
30	X	1708	0	1761	17	0
31	a	1495	0	1476	22	0
32	b	1414	0	1413	36	0
33	c	902	0	918	12	0
34	d	4063	0	4247	58	0
35	e	2017	0	2024	31	0
36	f	1578	0	1595	21	0
37	g	815	0	839	15	0
38	h	1394	0	1420	22	0
39	i	1512	0	1544	26	0
40	j	852	0	857	12	0
41	k	1259	0	1241	27	0
42	l	4385	0	4612	60	0
43	m	1068	0	1021	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	1095	0	1116	24	0
45	o	922	0	907	15	0
46	p	1863	0	1819	32	0
47	0	8	0	0	0	0
48	3	2	0	0	0	0
48	4	1	0	0	0	0
48	6	4	0	0	0	0
48	A	2	0	0	0	0
48	B	1	0	0	0	0
48	C	1	0	0	0	0
48	I	2	0	0	0	0
48	J	1	0	0	0	0
48	L	1	0	0	0	0
48	M	1	0	0	0	0
48	W	1	0	0	0	0
49	A	1	0	0	0	0
All	All	101943	0	101545	1227	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 6.

The worst 5 of 1227 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)
4:3:16:CYS:HB3	4:3:42:CYS:SG	2.04	0.95
7:6:338:CYS:SG	7:6:339:HIS:CE1	2.75	0.79
29:W:127:CYS:HB3	29:W:152:CYS:SG	2.26	0.76
3:2:458:LEU:HD21	3:2:490:LYS:HD3	1.70	0.74
16:H:2:SER:N	16:H:61:SER:HG	1.86	0.74

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	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
2	1	508/642 (79%)	502 (99%)	6 (1%)	0	100	100
3	2	448/513 (87%)	441 (98%)	7 (2%)	0	100	100
4	3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
5	4	298/338 (88%)	289 (97%)	9 (3%)	0	100	100
6	5	63/72 (88%)	60 (95%)	3 (5%)	0	100	100
7	6	379/461 (82%)	366 (97%)	13 (3%)	0	100	100
8	7	609/843 (72%)	585 (96%)	24 (4%)	0	100	100
9	A	1494/1733 (86%)	1443 (97%)	51 (3%)	0	100	100
10	B	1168/1224 (95%)	1130 (97%)	38 (3%)	0	100	100
11	C	264/347 (76%)	257 (97%)	7 (3%)	0	100	100
12	D	163/221 (74%)	159 (98%)	4 (2%)	0	100	100
13	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
14	F	114/155 (74%)	108 (95%)	6 (5%)	0	100	100
15	G	169/177 (96%)	163 (96%)	6 (4%)	0	100	100
16	H	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
17	I	114/122 (93%)	110 (96%)	4 (4%)	0	100	100
18	J	67/70 (96%)	67 (100%)	0	0	100	100
19	K	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
20	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
21	M	306/352 (87%)	295 (96%)	11 (4%)	0	100	100
23	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
24	Q	215/735 (29%)	208 (97%)	7 (3%)	0	100	100
25	R	264/400 (66%)	259 (98%)	5 (2%)	0	100	100
27	U	101/286 (35%)	97 (96%)	4 (4%)	0	100	100
28	V	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
29	W	296/492 (60%)	290 (98%)	6 (2%)	0	100	100
30	X	207/328 (63%)	197 (95%)	10 (5%)	0	100	100
31	a	170/295 (58%)	163 (96%)	7 (4%)	0	100	100
32	b	169/223 (76%)	163 (96%)	5 (3%)	1 (1%)	21	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	c	109/115 (95%)	107 (98%)	2 (2%)	0	100	100
34	d	481/687 (70%)	470 (98%)	11 (2%)	0	100	100
35	e	252/307 (82%)	246 (98%)	6 (2%)	0	100	100
36	f	202/210 (96%)	196 (97%)	6 (3%)	0	100	100
37	g	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
38	h	169/284 (60%)	166 (98%)	3 (2%)	0	100	100
39	i	175/222 (79%)	173 (99%)	2 (1%)	0	100	100
40	j	98/149 (66%)	94 (96%)	4 (4%)	0	100	100
41	k	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
42	l	521/745 (70%)	506 (97%)	14 (3%)	1 (0%)	43	76
43	m	126/220 (57%)	122 (97%)	4 (3%)	0	100	100
44	n	134/140 (96%)	132 (98%)	2 (2%)	0	100	100
45	o	108/127 (85%)	107 (99%)	1 (1%)	0	100	100
46	p	221/566 (39%)	210 (95%)	11 (5%)	0	100	100
All	All	12095/16091 (75%)	11739 (97%)	354 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	b	27	GLY
42	l	648	SER

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	684/707 (97%)	684 (100%)	0	100	100
2	1	483/589 (82%)	483 (100%)	0	100	100
3	2	414/468 (88%)	414 (100%)	0	100	100
4	3	125/303 (41%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	267/300 (89%)	267 (100%)	0	100	100
6	5	59/66 (89%)	59 (100%)	0	100	100
7	6	346/418 (83%)	345 (100%)	1 (0%)	86	91
8	7	547/737 (74%)	547 (100%)	0	100	100
9	A	1330/1520 (88%)	1330 (100%)	0	100	100
10	B	1024/1061 (96%)	1023 (100%)	1 (0%)	88	93
11	C	234/299 (78%)	234 (100%)	0	100	100
12	D	149/200 (74%)	149 (100%)	0	100	100
13	E	196/197 (100%)	196 (100%)	0	100	100
14	F	108/137 (79%)	108 (100%)	0	100	100
15	G	152/158 (96%)	151 (99%)	1 (1%)	76	86
16	H	123/128 (96%)	123 (100%)	0	100	100
17	I	110/116 (95%)	110 (100%)	0	100	100
18	J	64/65 (98%)	64 (100%)	0	100	100
19	K	99/102 (97%)	99 (100%)	0	100	100
20	L	40/57 (70%)	40 (100%)	0	100	100
21	M	267/306 (87%)	267 (100%)	0	100	100
23	O	153/205 (75%)	153 (100%)	0	100	100
24	Q	204/641 (32%)	203 (100%)	1 (0%)	81	89
25	R	252/363 (69%)	252 (100%)	0	100	100
27	U	99/260 (38%)	99 (100%)	0	100	100
28	V	94/108 (87%)	94 (100%)	0	100	100
29	W	275/436 (63%)	275 (100%)	0	100	100
30	X	193/295 (65%)	193 (100%)	0	100	100
31	a	170/259 (66%)	170 (100%)	0	100	100
32	b	162/207 (78%)	162 (100%)	0	100	100
33	c	104/108 (96%)	104 (100%)	0	100	100
34	d	469/642 (73%)	469 (100%)	0	100	100
35	e	232/280 (83%)	232 (100%)	0	100	100
36	f	174/178 (98%)	174 (100%)	0	100	100
37	g	95/113 (84%)	95 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	158/258 (61%)	158 (100%)	0	100	100
39	i	174/208 (84%)	174 (100%)	0	100	100
40	j	100/144 (69%)	100 (100%)	0	100	100
41	k	145/145 (100%)	145 (100%)	0	100	100
42	l	505/688 (73%)	505 (100%)	0	100	100
43	m	119/195 (61%)	118 (99%)	1 (1%)	73	86
44	n	128/132 (97%)	128 (100%)	0	100	100
45	o	103/117 (88%)	103 (100%)	0	100	100
46	p	212/528 (40%)	211 (100%)	1 (0%)	81	89
All	All	11141/14444 (77%)	11135 (100%)	6 (0%)	87	93

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	Q	369	ASN
43	m	95	GLN
46	p	211	PRO
10	B	1178	ASN
7	6	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
16	H	133	ASN
45	o	45	GLN
27	U	40	ASN
44	n	135	ASN
42	l	89	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 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	$\# Z > 2$
47	SF4	0	801	1	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
47	SF4	0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1614:PRO	C	1629:THR	N	23.05

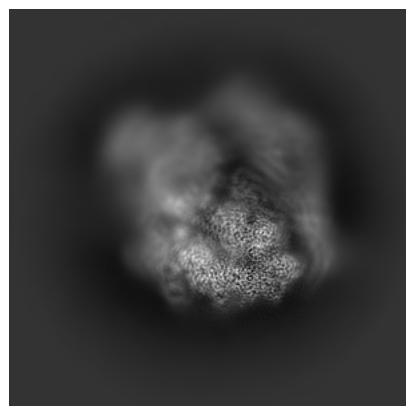
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16610. These allow visual inspection of the internal detail of the map and identification of artifacts.

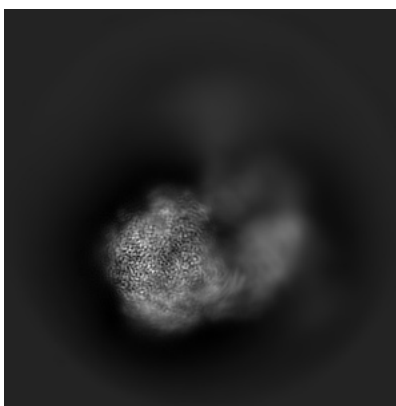
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

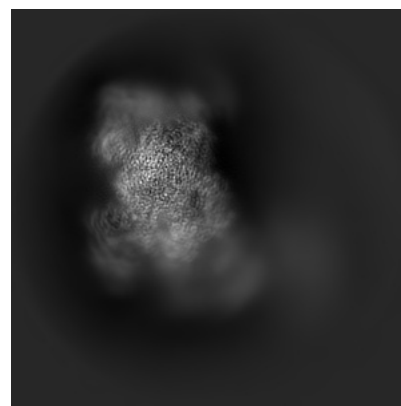
6.1.1 Primary map



X

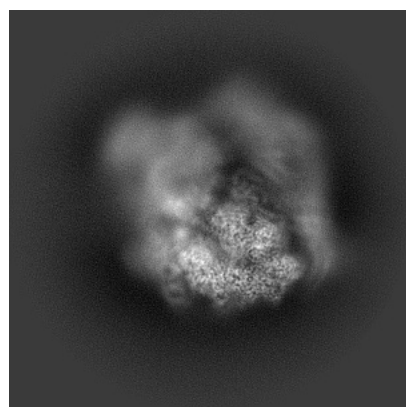


Y

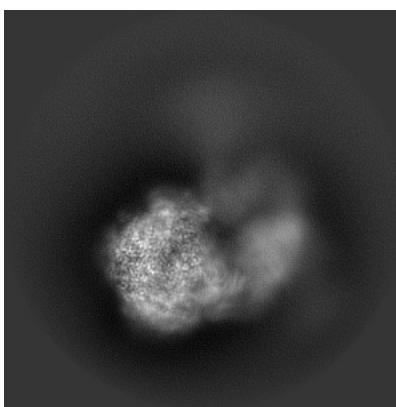


Z

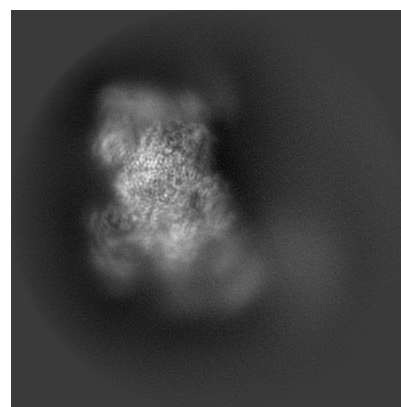
6.1.2 Raw map



X



Y



Z

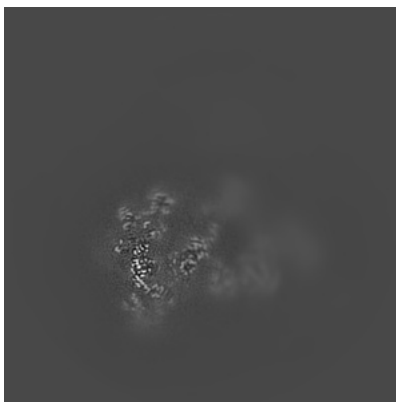
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

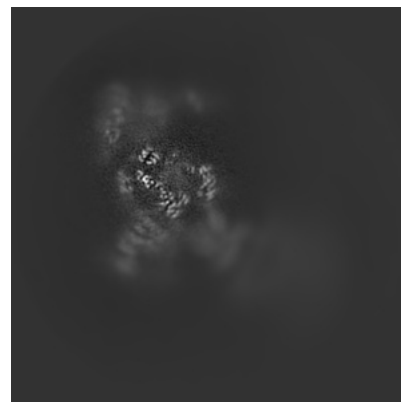
6.2.1 Primary map



X Index: 200

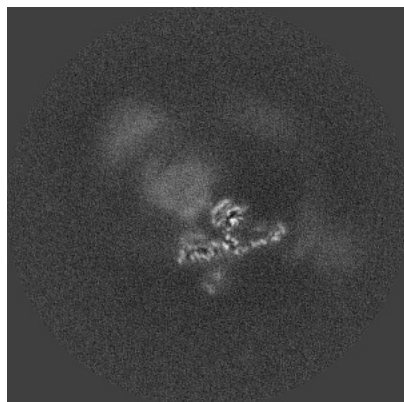


Y Index: 200

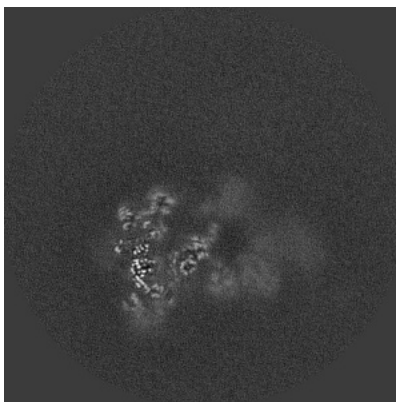


Z Index: 200

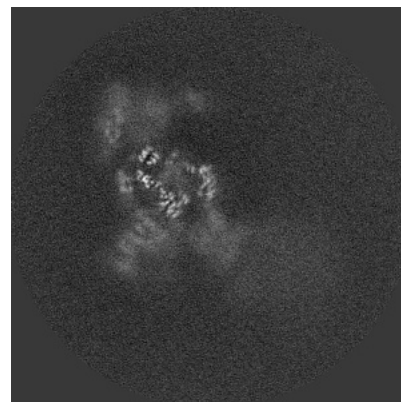
6.2.2 Raw map



X Index: 200



Y Index: 200

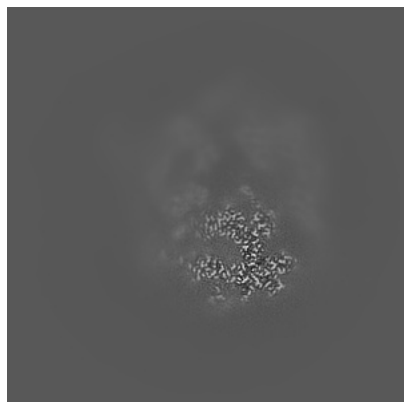


Z Index: 200

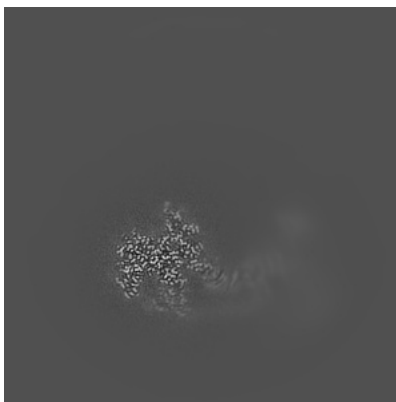
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

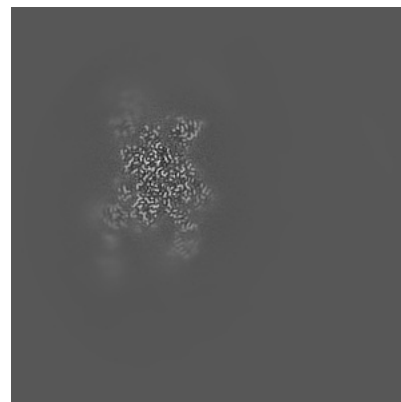
6.3.1 Primary map



X Index: 145

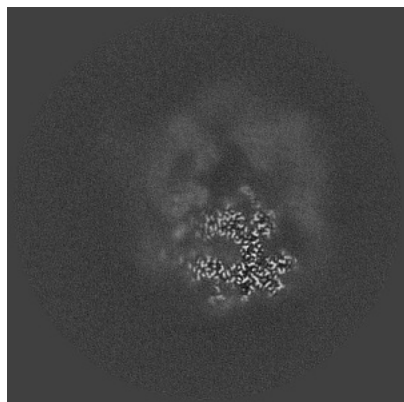


Y Index: 248

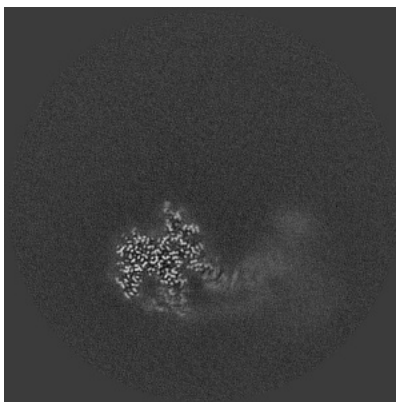


Z Index: 133

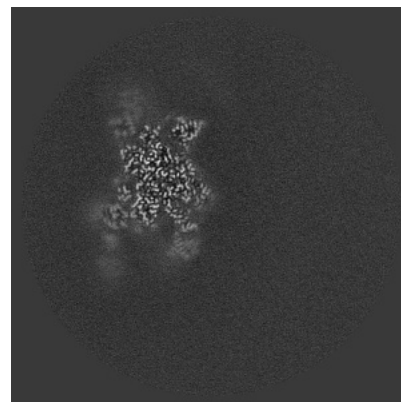
6.3.2 Raw map



X Index: 145



Y Index: 248

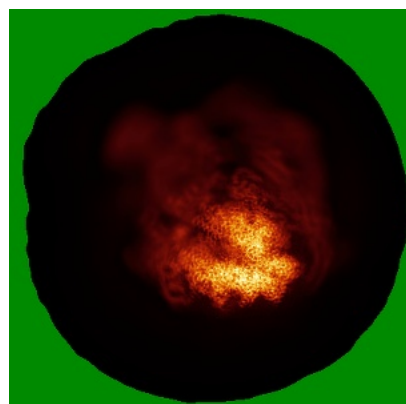


Z Index: 133

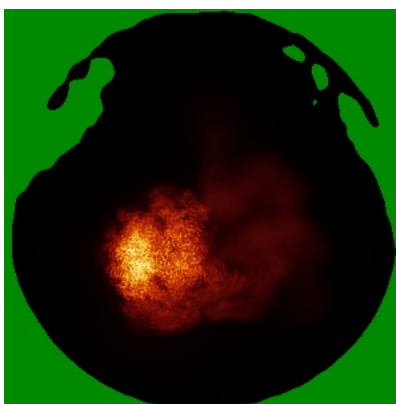
The images above show the largest variance slices of the map in three orthogonal directions.

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

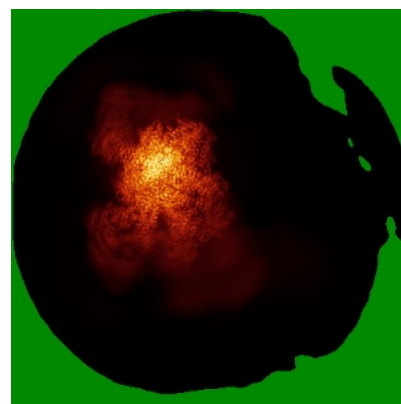
6.4.1 Primary map



X

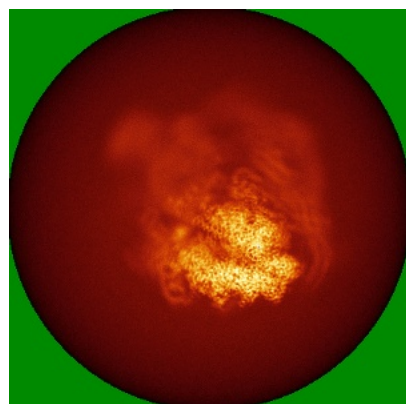


Y

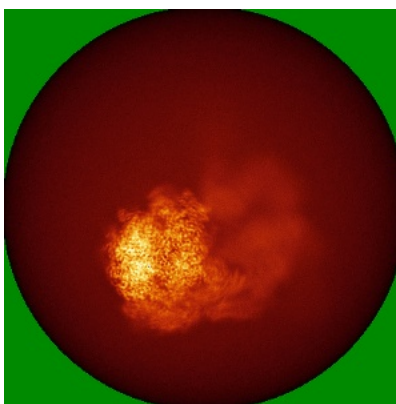


Z

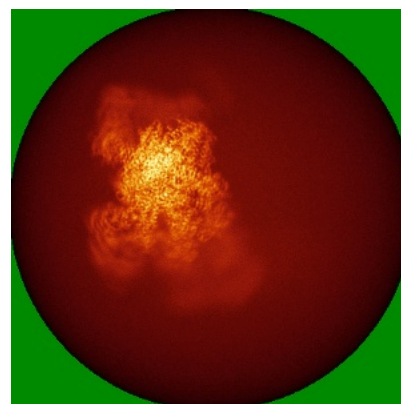
6.4.2 Raw map



X



Y

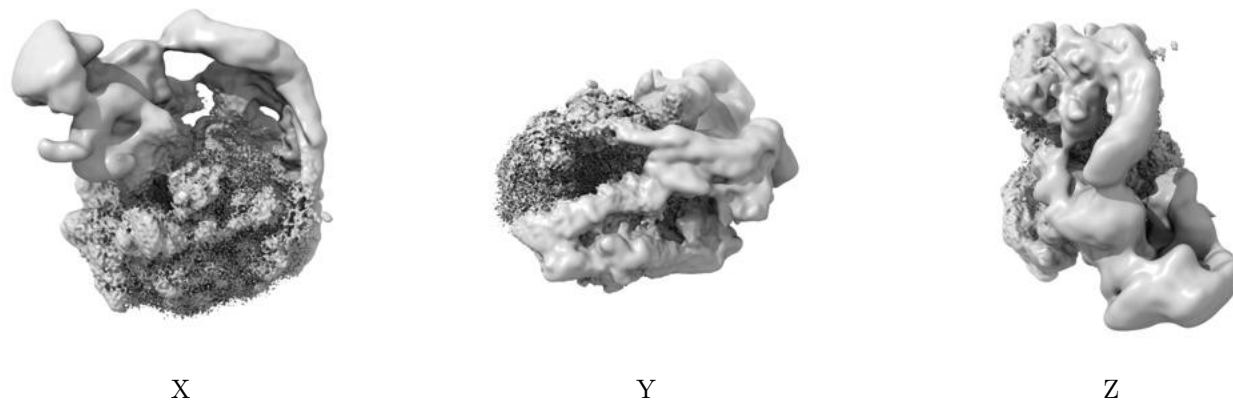


Z

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.

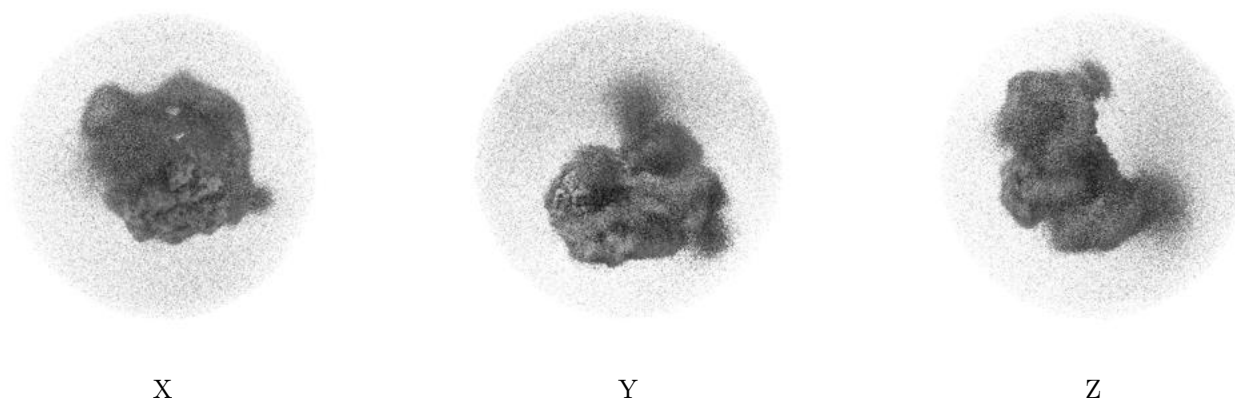
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

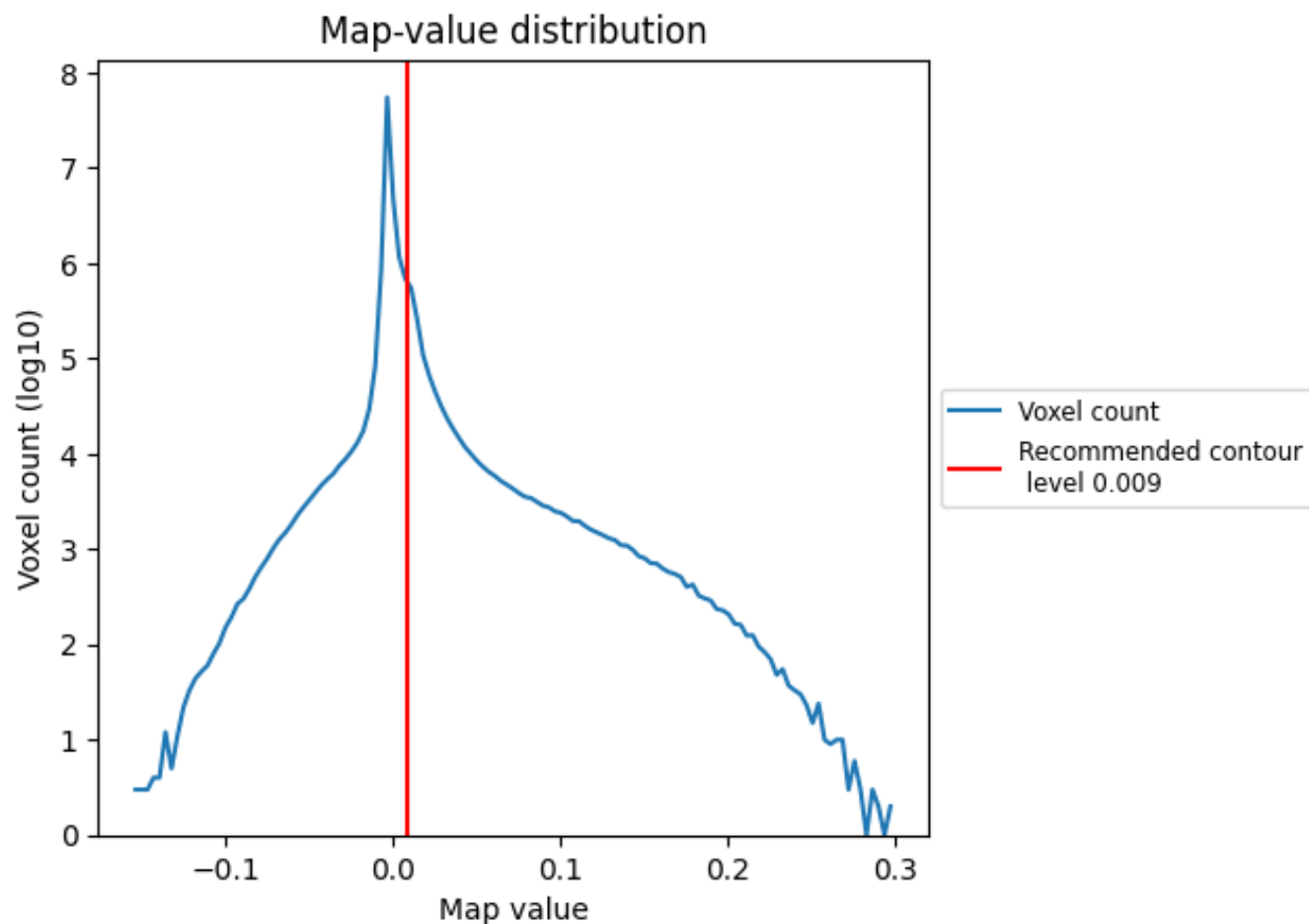
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

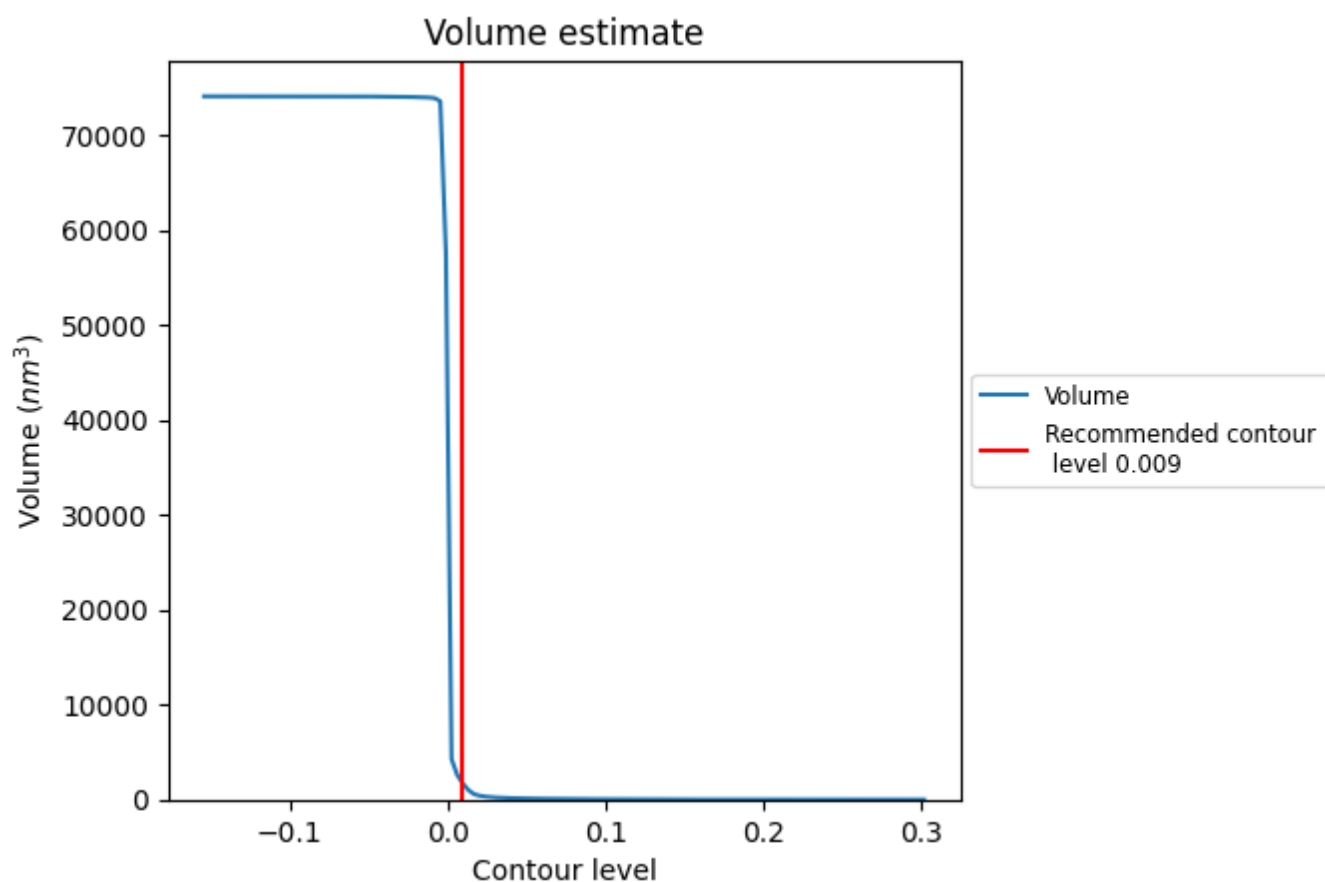
This section contains the results of statistical analysis of the map.

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.

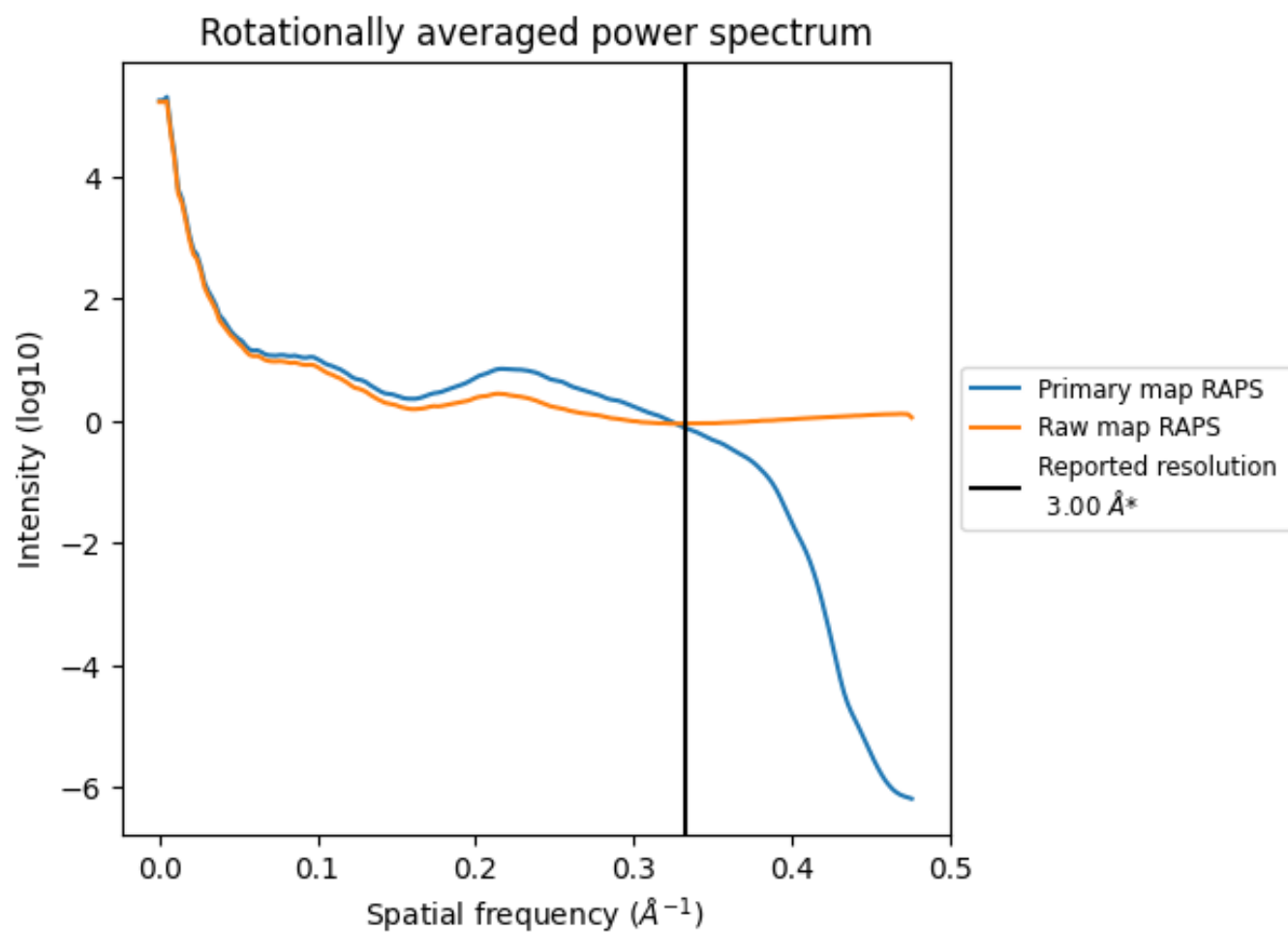
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1864 nm^3 ; this corresponds to an approximate mass of 1684 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 ⓘ

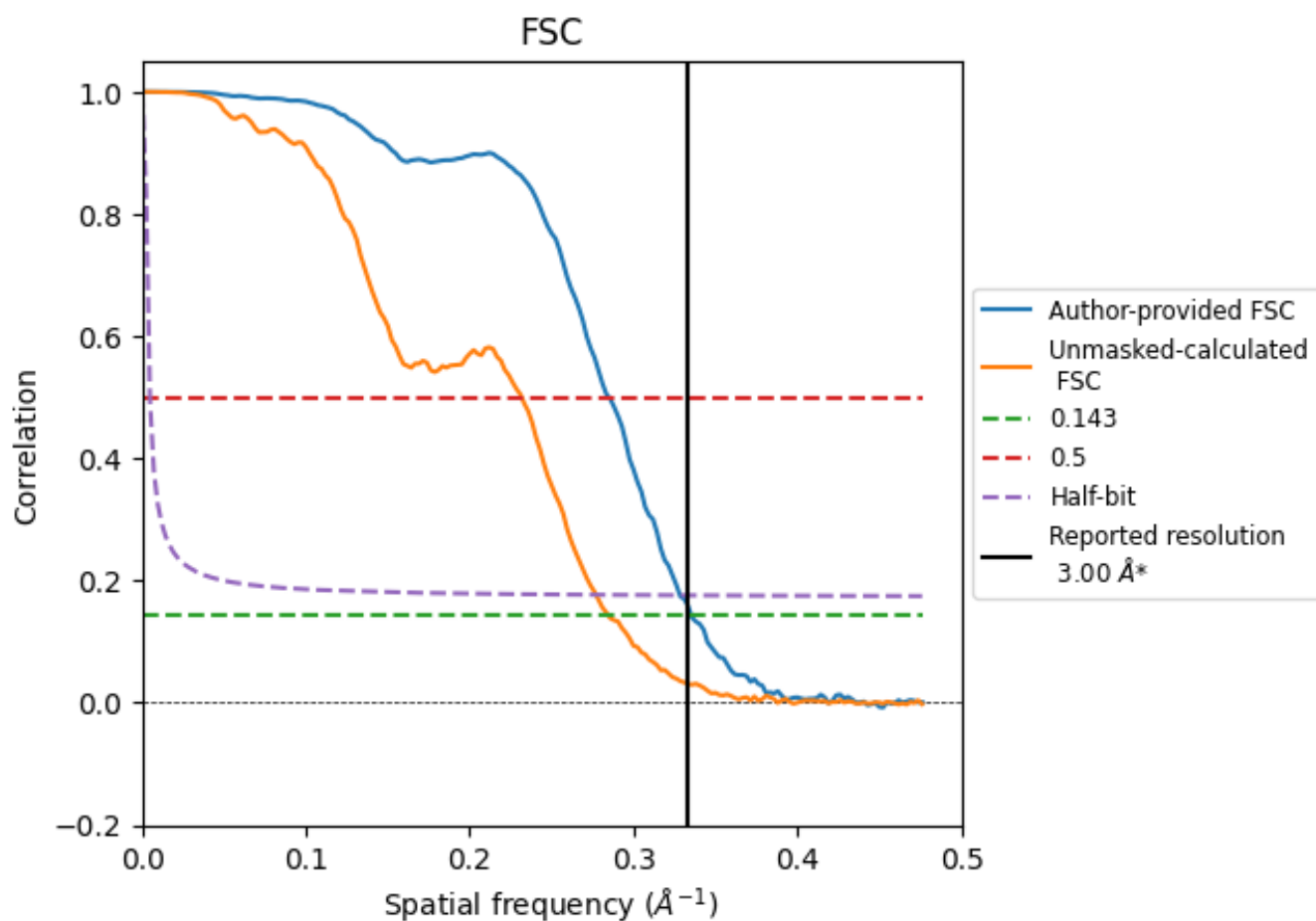


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

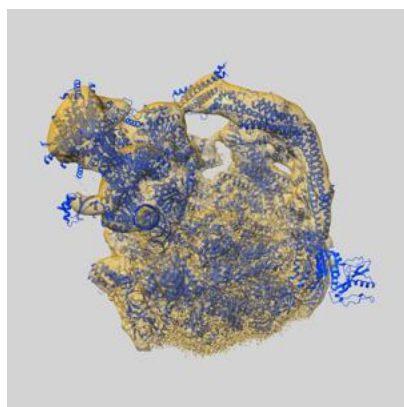
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.51	3.05
Unmasked-calculated*	3.51	4.32	3.61

*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 3.51 differs from the reported value 3.0 by more than 10 %

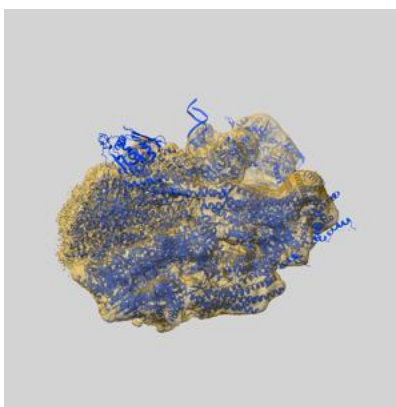
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16610 and PDB model 8CEN. Per-residue inclusion information can be found in section 3 on page 15.

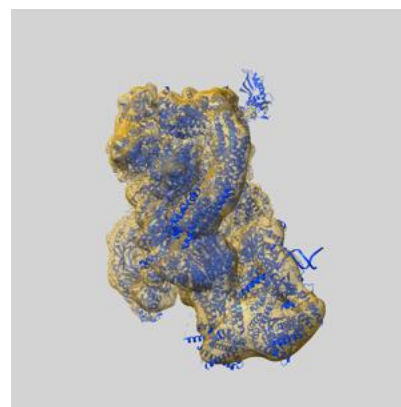
9.1 Map-model overlay [i](#)



X



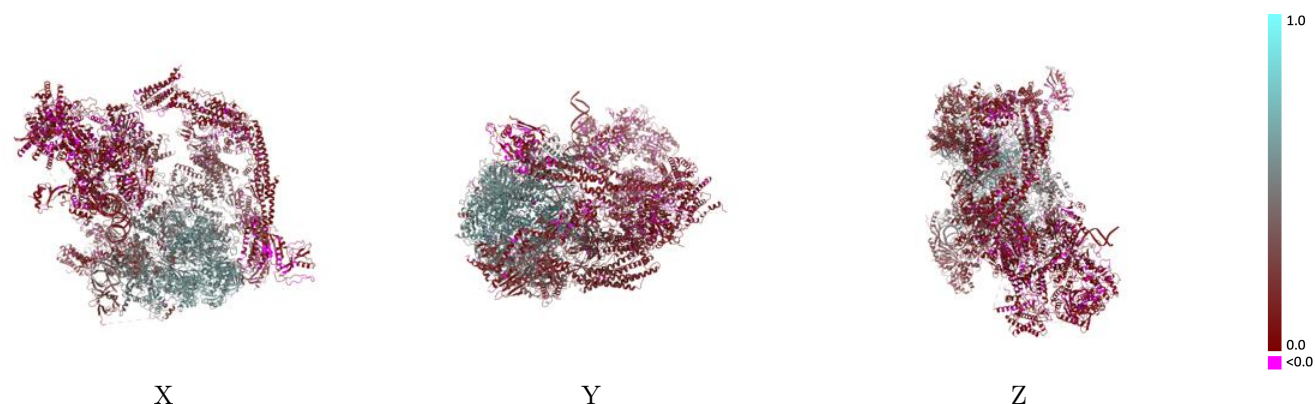
Y



Z

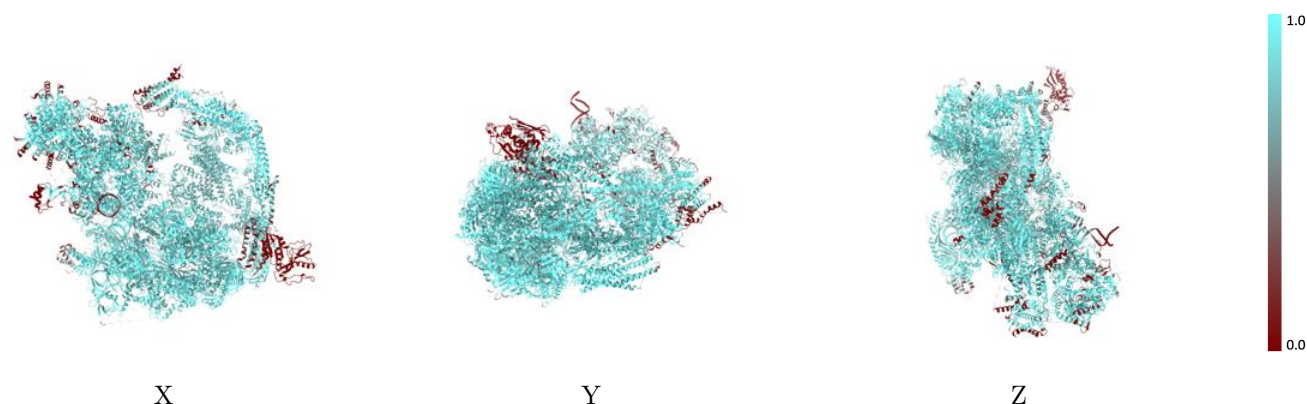
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



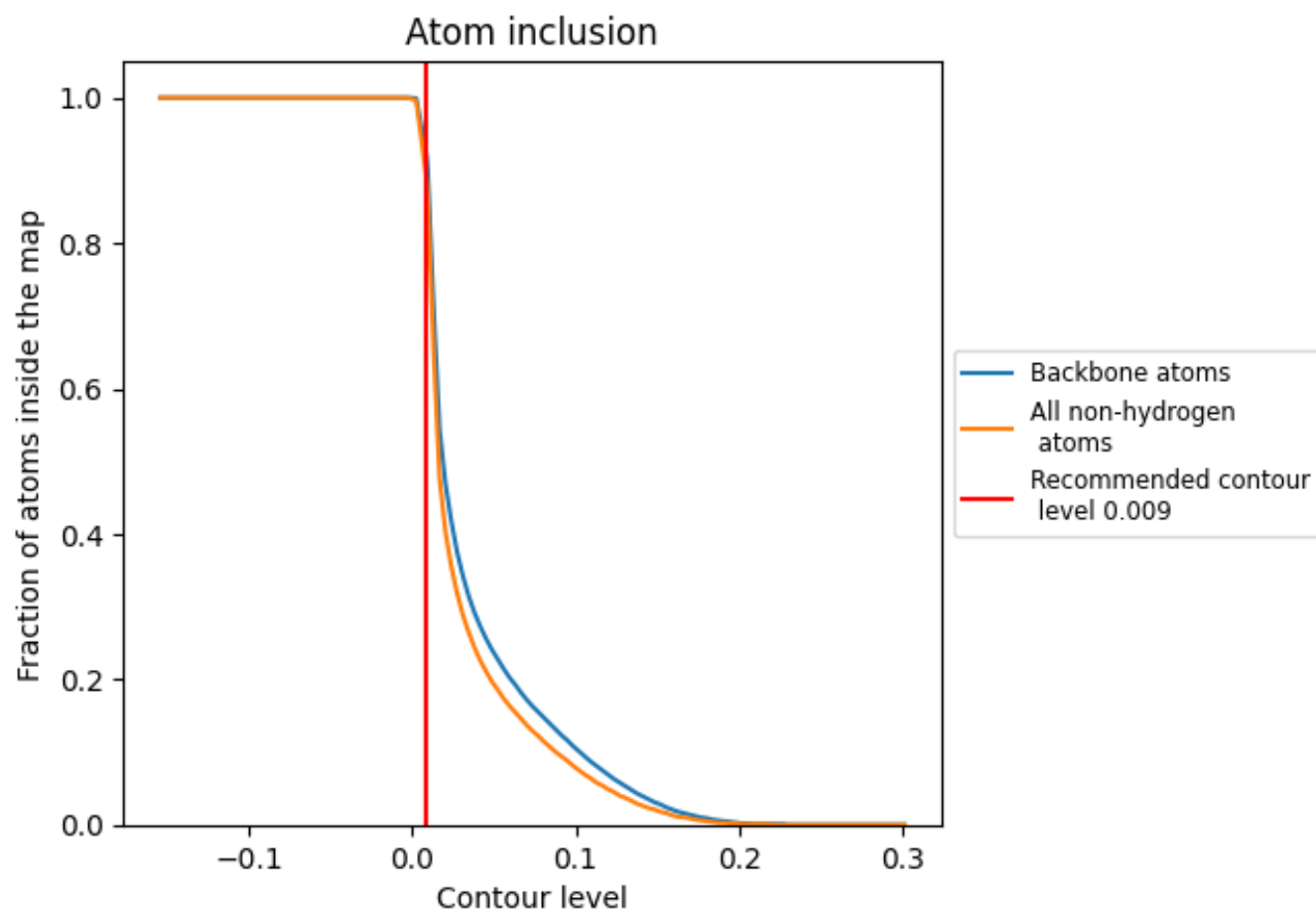
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.2690
0	 0.9110	 0.1000
1	 0.7380	 0.0770
2	 0.7750	 0.0740
3	 0.9280	 0.1710
4	 0.8560	 0.0600
5	 0.6250	 0.0530
6	 0.8420	 0.0690
7	 0.8850	 0.0880
A	 0.9700	 0.5110
B	 0.9810	 0.5560
C	 0.9810	 0.5870
D	 0.9060	 0.2590
E	 0.9770	 0.4580
F	 0.8920	 0.4250
G	 0.9560	 0.3940
H	 0.9770	 0.5400
I	 0.9700	 0.4300
J	 0.9840	 0.5910
K	 0.9860	 0.6000
L	 0.9860	 0.5190
M	 0.9510	 0.4190
N	 0.8850	 0.2060
O	 0.9740	 0.2610
Q	 0.9500	 0.3050
R	 0.9700	 0.2540
T	 0.8720	 0.2020
U	 0.7770	 0.1330
V	 0.8540	 0.1470
W	 0.8560	 0.1750
X	 0.9280	 0.1670
a	 0.9370	 0.1280
b	 0.9230	 0.1850
c	 0.9600	 0.2130
d	 0.9460	 0.1830



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Chain	Atom inclusion	Q-score
e	 0.9380	 0.4110
f	 0.9320	 0.4000
g	 0.9650	 0.1930
h	 0.8090	 0.1300
i	 0.9070	 0.1280
j	 0.4600	 0.0860
k	 0.7230	 0.0910
l	 0.8690	 0.1220
m	 0.4290	 0.0590
n	 0.8320	 0.1050
o	 0.9170	 0.1230
p	 0.0380	 0.0530