



Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 08:37 am BST

PDB ID : 8CEO
EMDB ID : EMD-16611
Title : Yeast RNA polymerase II transcription pre-initiation complex with core Mediator and the +1 nucleosome
Authors : Wang, H.; Cramer, P.
Deposited on : 2023-02-02
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

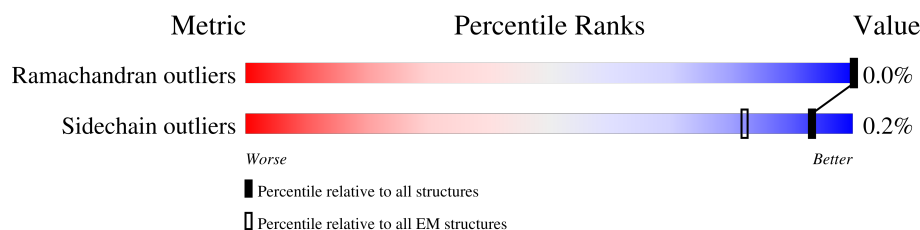
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



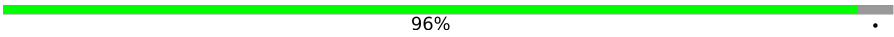


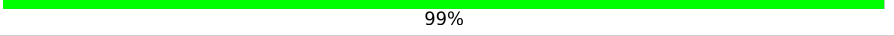

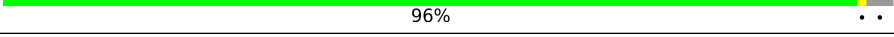
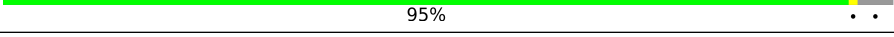
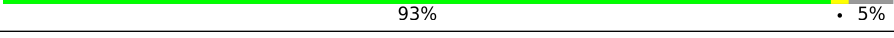
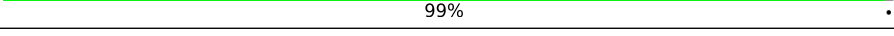
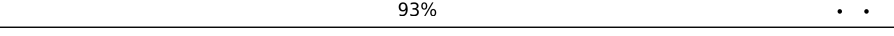
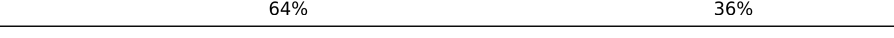
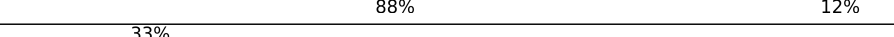
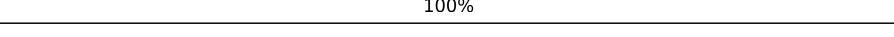
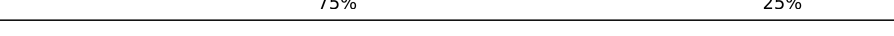


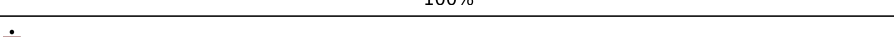

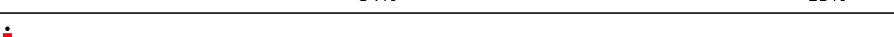






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	97% .
2	1	642	81% 19%
3	2	513	88% 12%
4	3	321	41% 59%
5	4	338	89% 11%
6	5	72	88% . 10%
7	6	461	83% 17%
8	7	843	73% 27%
9	A	1733	87% 13%


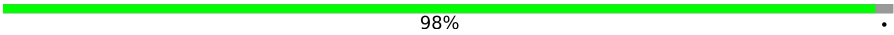







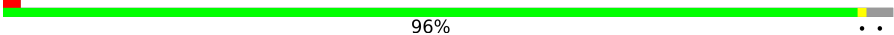










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Mol	Chain	Length	Quality of chain
10	B	1224	
11	C	347	
12	D	221	
13	E	215	
14	F	155	
15	G	177	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	352	
22	N	209	
23	O	240	
24	Q	735	
25	R	400	
26	T	209	
27	U	286	
28	V	122	
29	W	492	
30	X	328	
31	a	295	
32	b	223	
33	c	115	
34	d	687	

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Mol	Chain	Length	Quality of chain
35	e	307	
36	f	210	
37	g	121	
38	h	284	
39	i	222	
40	j	149	
41	k	157	
42	l	1082	
43	m	220	
44	n	140	
45	o	127	
46	p	566	
47	r	135	
47	v	135	
48	s	102	
48	w	102	
49	t	129	
49	x	129	
50	u	125	
50	y	125	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 113584 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 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 TFB1 isoform 1.

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 RNA polymerase II transcription factor B subunit 2.

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 IIIH 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 IIIH 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.

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	209	Total	C	N	O	P	0	0
			4263	2035	761	1259	208		

- 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	209	Total	C	N	O	P	0	0
			4300	2045	802	1245	208		

- Molecule 27 is a protein called TOA1 isoform 1.

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	172	Total	C	N	O	S	0	0
			1407	895	240	269	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 a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	97	Total	C	N	O	S	0	0
			801	506	155	138	2		
47	v	98	Total	C	N	O	S	0	0
			810	512	157	139	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	102	ALA	GLY	conflict	UNP P84233
r	110	ALA	CYS	engineered mutation	UNP P84233
v	102	ALA	GLY	conflict	UNP P84233
v	110	ALA	CYS	engineered mutation	UNP P84233

- Molecule 48 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
48	w	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

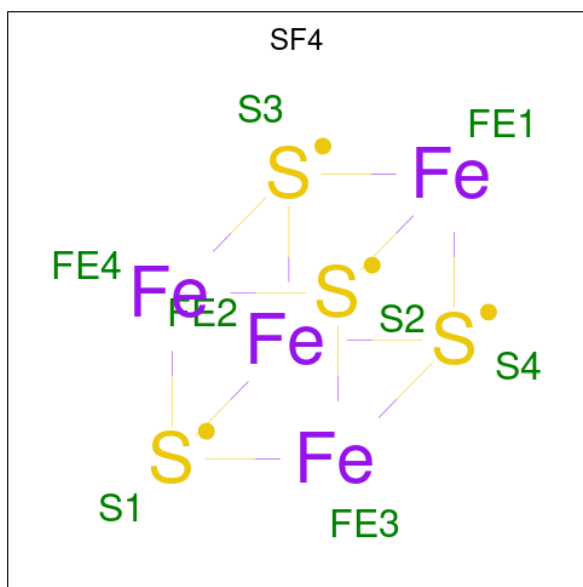
- Molecule 49 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	t	109	Total	C	N	O	0	0
			843	531	167	145		
49	x	106	Total	C	N	O	0	0
			818	516	160	142		

- Molecule 50 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	97	Total	C	N	O	S	0	0
			767	481	142	142	2		
50	y	95	Total	C	N	O	S	0	0
			745	469	134	140	2		

- Molecule 51 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
51	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	2	Total	Zn	0
			2	2	
52	4	1	Total	Zn	0
			1	1	
52	6	4	Total	Zn	0
			4	4	
52	A	2	Total	Zn	0
			2	2	
52	B	1	Total	Zn	0
			1	1	
52	C	1	Total	Zn	0
			1	1	
52	I	2	Total	Zn	0
			2	2	

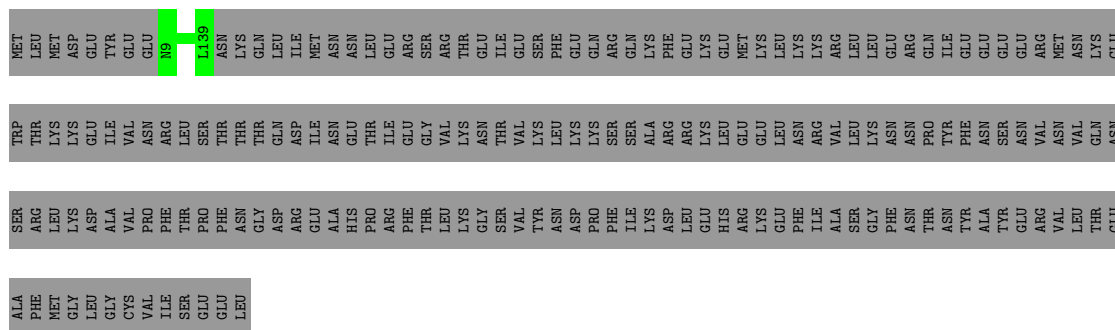
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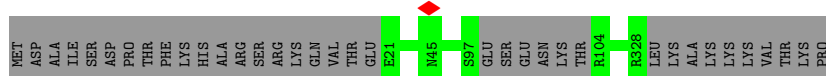
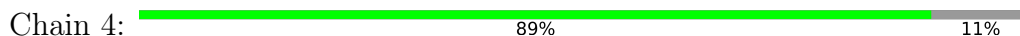
Mol	Chain	Residues	Atoms		AltConf
52	J	1	Total 1	Zn 1	0
52	L	1	Total 1	Zn 1	0
52	M	1	Total 1	Zn 1	0
52	W	1	Total 1	Zn 1	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

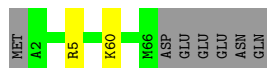
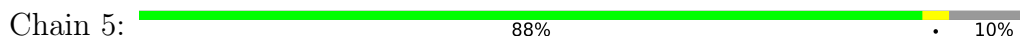
Mol	Chain	Residues	Atoms		AltConf
53	A	1	Total 1	Mg 1	0



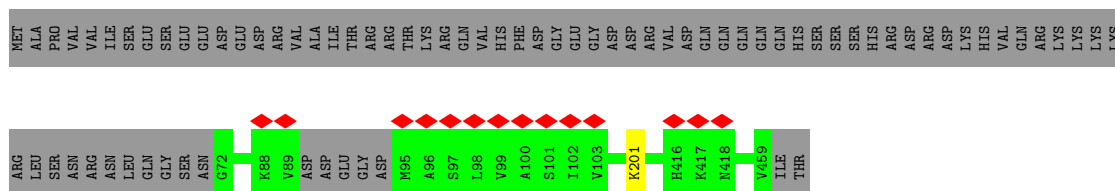
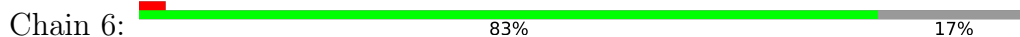
- Molecule 5: General transcription and DNA repair factor IIH subunit TFB4



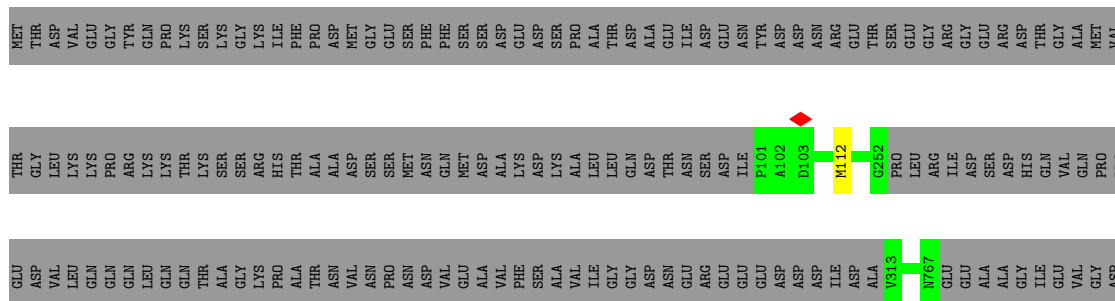
- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

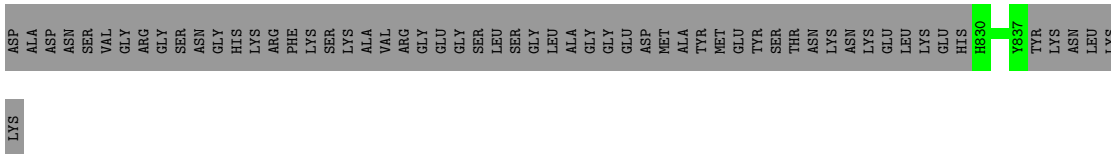


- Molecule 7: General transcription and DNA repair factor IIH

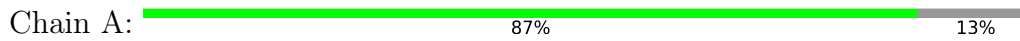


- Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

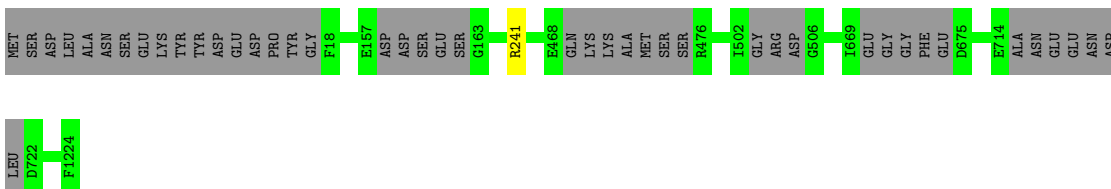




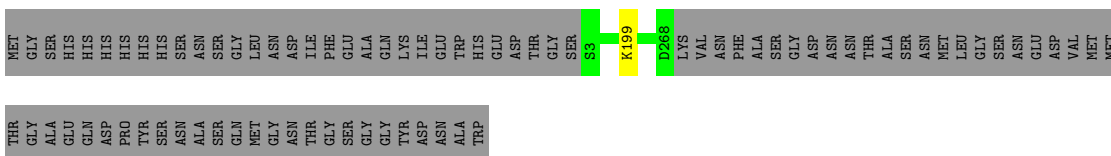
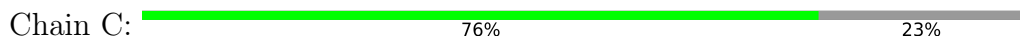
- Molecule 9: DNA-directed RNA polymerase II subunit RPB1



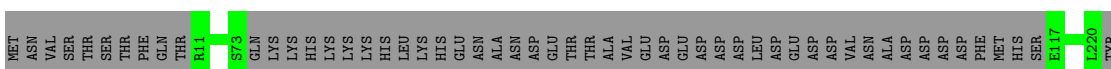
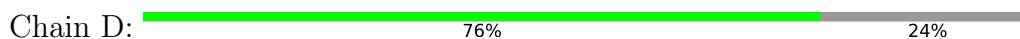
- Molecule 10: DNA-directed RNA polymerase II subunit RPB2



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



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



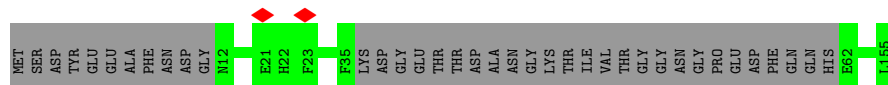
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  99%



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

Chain F:  76%  24%



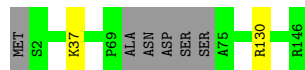
- Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G:  96%  ..



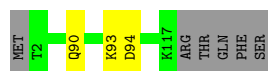
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  95%  ..



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

Chain I:  93%  5%



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

Chain J:  99%  .



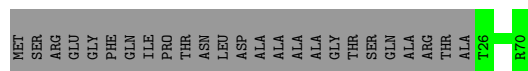
- Molecule 19: DNA-directed RNA polymerase II subunit RPB11

Chain K:  93%  ..




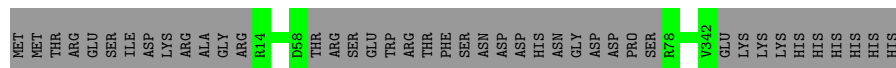
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  64% 36%



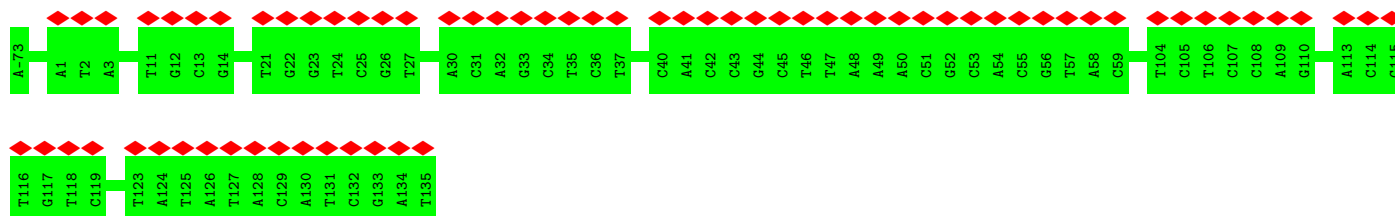
- Molecule 21: Transcription initiation factor IIB

Chain M:  88% 12%



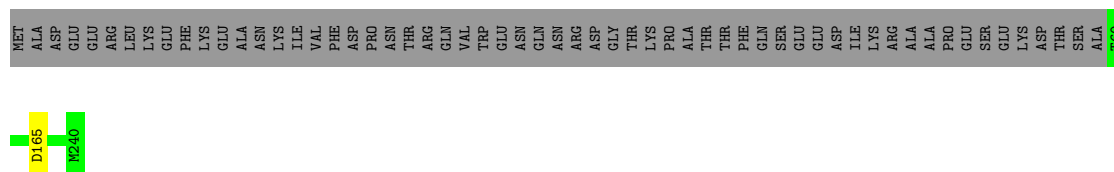
- Molecule 22: Nontemplate DNA (209-MER)

Chain N:  33% 100%



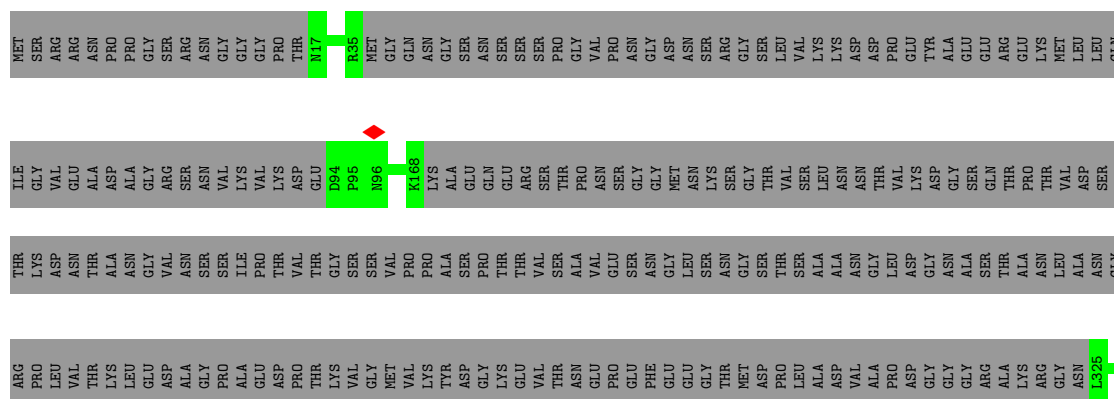
- Molecule 23: TATA-binding protein

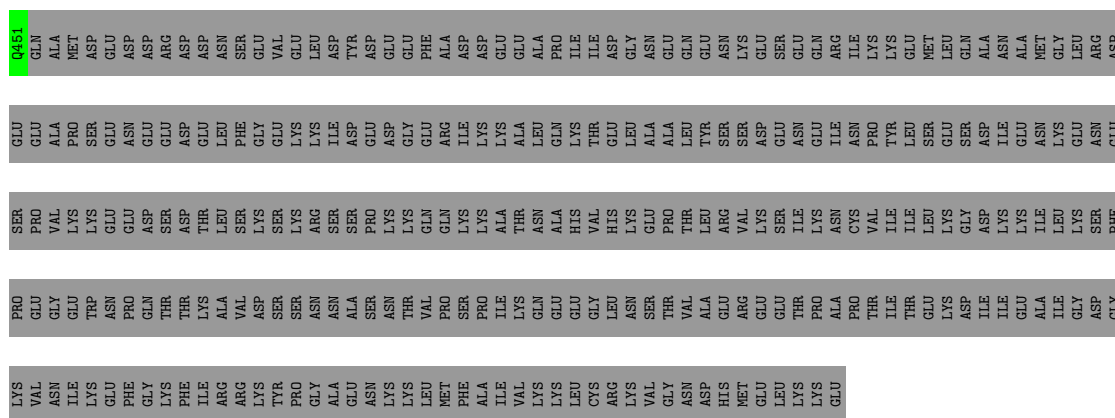
Chain O:  75% 25%



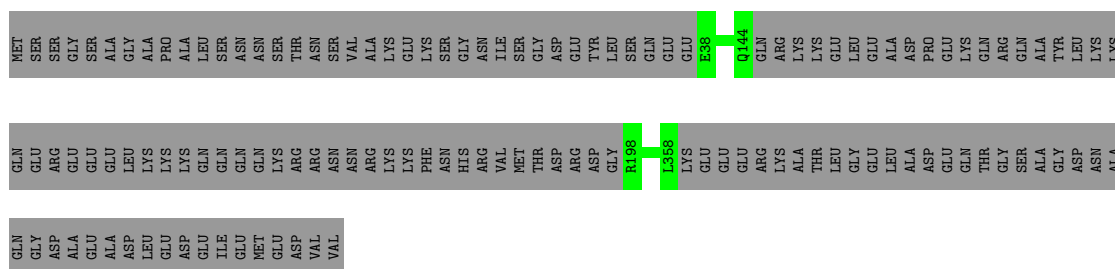
- Molecule 24: Transcription initiation factor IIF subunit alpha

Chain Q:  30% 70%

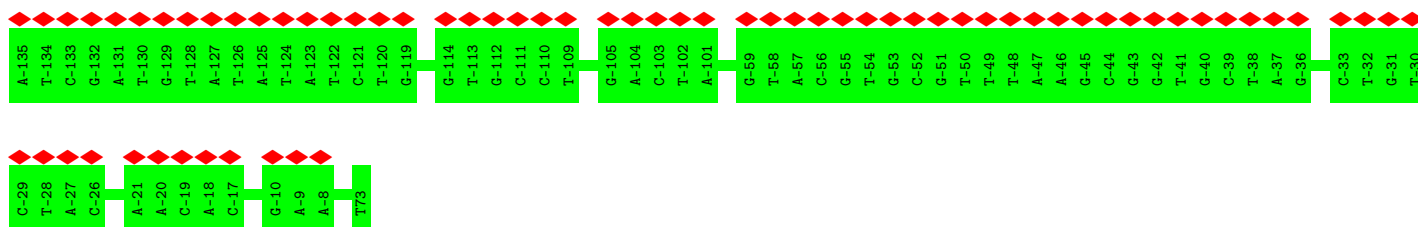




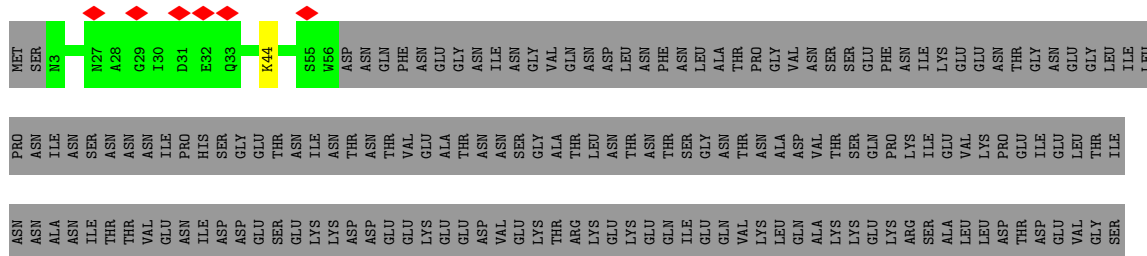
- Molecule 25: Transcription initiation factor IIF subunit beta




- Molecule 26: Template DNA (209-MER)

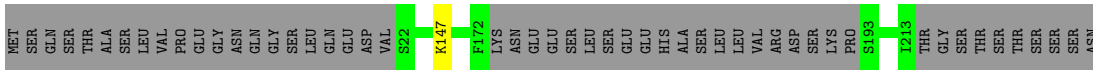


- Molecule 27: TOA1 isoform 1



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

Chain b:  77% 23%



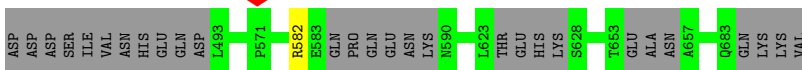
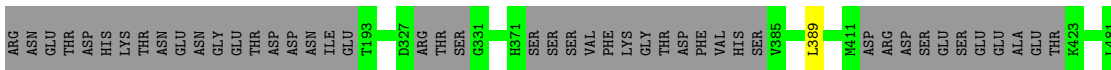
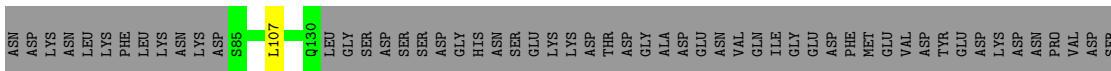
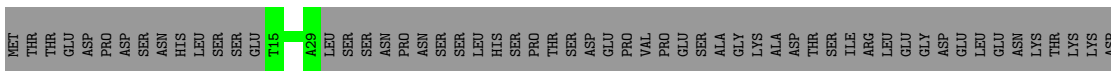
- Molecule 33: Mediator of RNA polymerase II transcription subunit 11

Chain c: 96% ..




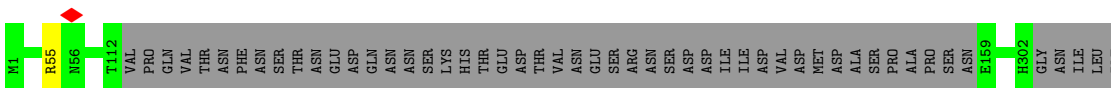
- Molecule 34: Mediator of RNA polymerase II transcription subunit 17

Chain d: 72% 27%



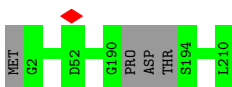
- Molecule 35: Mediator of RNA polymerase II transcription subunit 18

Chain e:  83% 17%



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

Chain f: 98% .



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

MET	S2	D32	ARG	ASN	ASP	ASP	ASP	GLU	GLY	SER	PHE	A42	V90	THR	GLU	HIS	SER	LYS	VAL	T97	E118	LYS	THR	THR
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----

- Chain h:  58% 40%

LEU	THR	MET
PHE	VAL	SER
ASP	PRO	VAL
PRO	PRO	GLN
ASP	SER	ASP
ASP	GLN	THR
PHE	SER	LYS
	GLU	ALA
	GLU	VAL
	GLN	GLU
	LYS	PHE
	GLY	SER
	GLN	MET
	MET	GLY
	ALA	HIS
	LYS	ILE
	LYS	ARG
	GLU	SER
	GLY	SER
	THR	SER
	PRO	VAL
	LYS	SER
	THR	LEU
	ASP	VAL
	SER	ALA
	PHE	GLU
	ILE	ALA
	PHE	THR
	ASP	SER
	GLY	ASN
	THR	THR
	ALA	ASN
	LYS	SER
	GLU	GLU
	VAL	ASP
	GLY	LYS
	ASP	L37
	GLU	S38
	ALA	
	ASP	L46
	ASN	
	THR	D103
	LYS	
	ASP	K113
	LYS	
	GLU	N119
	LYS	
	GLU	I181
	GLU	
	ASN	P207
	ASN	GLY
	ASP	GLU
	ASP	GLU
	ALA	VAL
	LEU	GLU
	ASP	GLU
	LEU	THR
	ASP	GLU
	LEU	VAL
	ASP	

- Chain i: 82% 18%

NET	SER	ASN	ASP	PRO	GLY	ASN	GLU	V9	K37	ALA	ALA	ALA	ALA	ALA	LYS	GLN	THR	PRO	PRO	ASN	ASN	SER	SER	ASN	GLY	GLY	SER	E55	K62	LYS	SER	THR	GLU	ASN	GLU	GLU	SER	THR	M11	S214	GLN	SER	PRO	PRO	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----

- Chain j: 

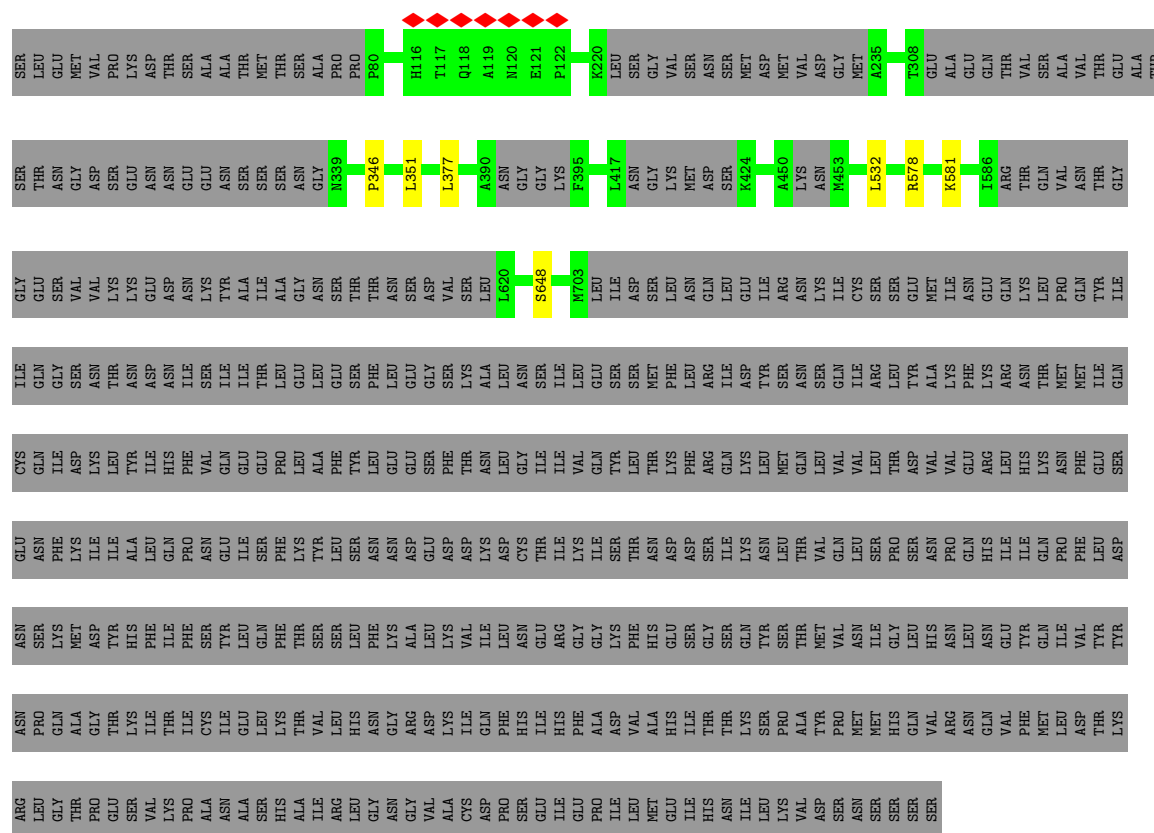
Sequence logo for the 100th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis lists amino acids. MET, ASN, LEU, Q4, L15, T18, and ASN are highlighted in green. PRO, THR, LEU, ASP, LYS, PRO, ASN, ALA, GLU, THR, LYS, GLU, PHE, SER, SER, ALA, GLU, ASN, ARG, ASP, GLU, LYS, ASP, TTR, LEU, THR, THR, ASN, GLN, GLN, PRO, LYS, ASN, LEU, SER, THR, THR, PRO, SER, THR, SER, SER, SER, N62, G63, K78, D79, L90, and L100 are in grey. Red diamonds indicate positions with high information content.

- Chain k: 100%

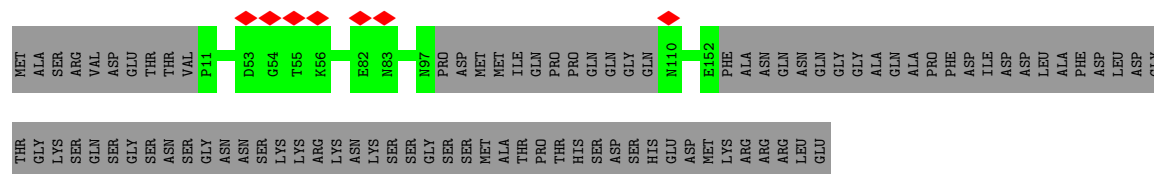
Diagram illustrating a 1D lattice structure with 15 sites. The sites are labeled M1, N2, T42, P43, E44, A45, T46, K47, and H157. The lattice is composed of blue diamonds representing sites, with some sites (M1, N2, T42, P43, E44, A45, T46, K47, H157) highlighted in red.

- Chain 1:  49% 51%

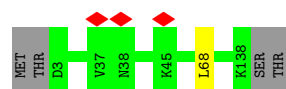
MET	THR	THR	THR	ILE	GLY	SER	PRO	PRO	GLN	MET	MET	LEU	LEU	ALA	ASN	ASN	GLU	GLU	GLY	MET	MET	HIS	HIS	ALA	ALA	LEU	LEU	LYS	ASN	ASN	GLY	GLN	GLN	GLY	GLY	PRO	VAL	VAL	LYS	ASN	ASN	THR	THR	THR	GLN	LEU	HIS	GLY	HIS	GLY	PRO	PRO	GLU	GLU	GLY	THR	THR	THR	ALA	ALA	GLN	GLN	LYS	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



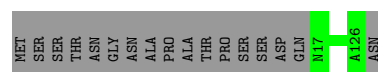
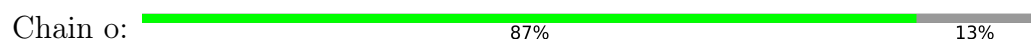
• Molecule 43: Mediator of RNA polymerase II transcription subunit 19



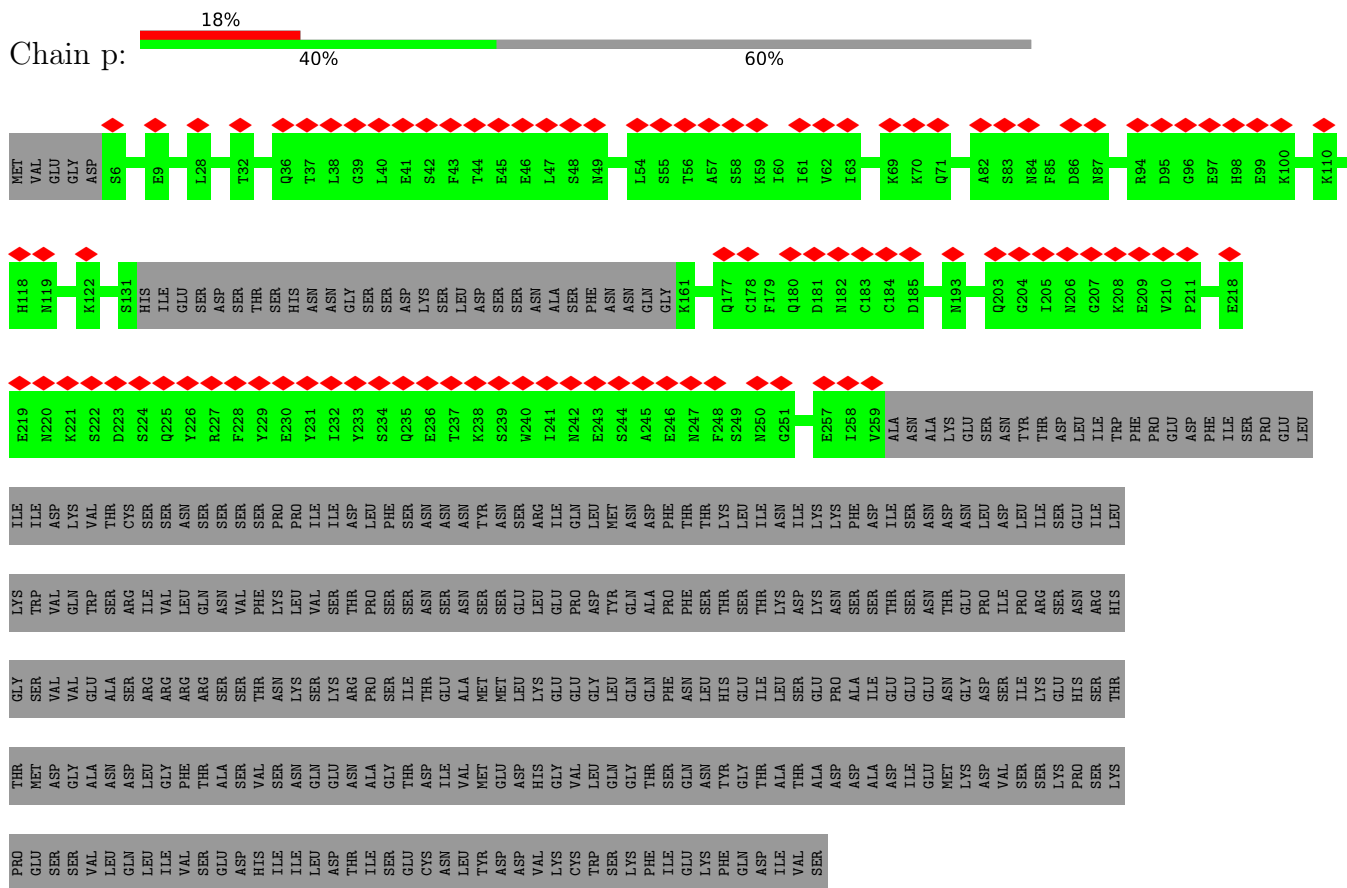
• Molecule 44: Mediator of RNA polymerase II transcription subunit 21



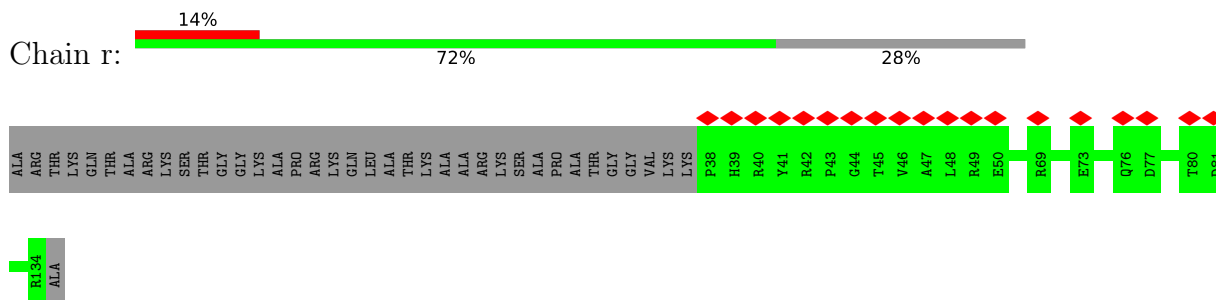
• Molecule 45: Mediator of RNA polymerase II transcription subunit 31



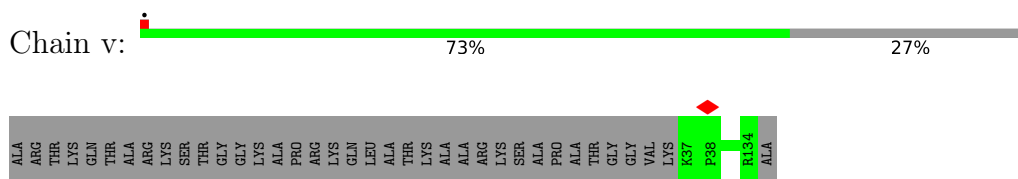
• Molecule 46: Mediator of RNA polymerase II transcription subunit 1



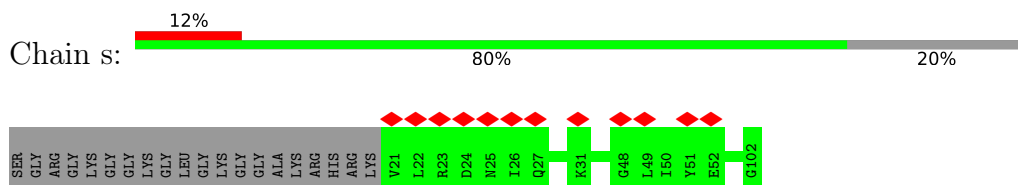
- Molecule 47: Histone H3.2




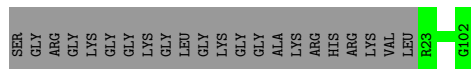
- Molecule 47: Histone H3.2




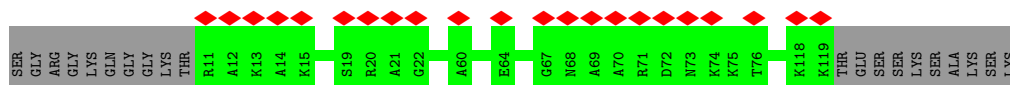
- Molecule 48: Histone H4




• Molecule 48: Histone H4

Chain w:  78% 22%


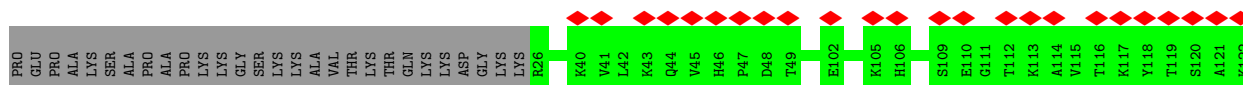
• Molecule 49: Histone H2A

Chain t:  17% 84% 16%

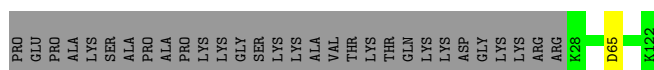
• Molecule 49: Histone H2A

Chain x:  5% 82% 18%

• Molecule 50: Histone H2B

Chain u:  19% 78% 22%

• Molecule 50: Histone H2B

Chain y:  75% 24%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50715	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	0.234	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	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: MG, SF4, ZN

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	0.27	0/6209	0.50	0/8384
2	1	0.25	0/4277	0.48	0/5755
3	2	0.28	0/3717	0.54	0/5028
4	3	0.27	0/1109	0.51	0/1492
5	4	0.28	0/2377	0.50	0/3216
6	5	0.28	0/520	0.64	0/701
7	6	0.28	0/3082	0.52	0/4165
8	7	0.28	0/5059	0.52	0/6841
9	A	0.29	0/12048	0.51	0/16321
10	B	0.32	0/9589	0.53	0/12934
11	C	0.32	0/2130	0.50	0/2887
12	D	0.25	0/1351	0.54	0/1811
13	E	0.30	0/1788	0.59	1/2406 (0.0%)
14	F	0.31	0/1001	0.58	0/1347
15	G	0.29	0/1367	0.60	1/1844 (0.1%)
16	H	0.33	0/1139	0.62	0/1544
17	I	0.33	0/962	0.63	1/1295 (0.1%)
18	J	0.35	0/578	0.60	0/775
19	K	0.32	0/942	0.62	2/1272 (0.2%)
20	L	0.34	0/361	0.70	0/478
21	M	0.27	0/2408	0.52	0/3241
22	N	0.55	0/4776	0.95	0/7366
23	O	0.31	0/1449	0.60	1/1952 (0.1%)
24	Q	0.28	0/1907	0.57	0/2556
25	R	0.26	0/2270	0.54	0/3052
26	T	0.54	0/4830	0.91	0/7457
27	U	0.28	0/898	0.57	0/1212
28	V	0.28	0/822	0.63	1/1109 (0.1%)
29	W	0.25	0/2513	0.51	0/3388
30	X	0.25	0/1739	0.53	1/2339 (0.0%)
31	a	0.26	0/1531	0.56	1/2072 (0.0%)
32	b	0.26	0/1436	0.56	0/1947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.29	0/913	0.58	0/1228
34	d	0.27	0/4118	0.55	2/5532 (0.0%)
35	e	0.29	0/2054	0.54	1/2782 (0.0%)
36	f	0.29	0/1602	0.53	0/2169
37	g	0.29	0/818	0.56	0/1104
38	h	0.31	0/1415	0.71	3/1907 (0.2%)
39	i	0.25	0/1543	0.54	0/2084
40	j	0.28	0/865	0.79	3/1166 (0.3%)
41	k	0.28	0/1277	0.59	0/1727
42	l	0.28	0/4468	0.61	5/6048 (0.1%)
43	m	0.28	0/1093	0.54	0/1481
44	n	0.28	0/1106	0.65	1/1488 (0.1%)
45	o	0.28	0/949	0.57	0/1294
46	p	0.27	0/1898	0.55	0/2559
47	r	0.29	0/813	0.70	0/1091
47	v	0.28	0/822	0.61	0/1103
48	s	0.32	0/660	0.73	0/883
48	w	0.28	0/645	0.69	0/862
49	t	0.31	0/853	0.64	0/1149
49	x	0.30	0/828	0.60	0/1117
50	u	0.30	0/778	0.63	0/1043
50	y	0.31	0/756	0.66	1/1015 (0.1%)
All	All	0.32	0/116459	0.60	25/159019 (0.0%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	l	346	PRO	CA-N-CD	-11.19	95.84	111.50
42	l	532	LEU	CA-CB-CG	7.13	131.70	115.30
42	l	351	LEU	CA-CB-CG	7.00	131.39	115.30
15	G	50	ASP	CB-CG-OD1	6.71	124.34	118.30
50	y	65	ASP	CB-CG-OD1	6.64	124.27	118.30
38	h	103	ASP	CB-CG-OD1	6.52	124.17	118.30
42	l	377	LEU	CA-CB-CG	6.46	130.16	115.30
19	K	24	ASP	CB-CG-OD1	6.42	124.07	118.30
38	h	46	LEU	CA-CB-CG	6.36	129.93	115.30
40	j	138	ASP	CB-CG-OD1	6.23	123.91	118.30
40	j	15	LEU	CA-CB-CG	6.14	129.43	115.30
34	d	107	LEU	CA-CB-CG	6.07	129.25	115.30
35	e	55	ARG	CA-CB-CG	6.04	126.69	113.40
30	X	143	LEU	CA-CB-CG	5.96	129.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	82	ASP	CB-CG-OD1	5.81	123.53	118.30
28	V	24	ASP	CB-CG-OD1	5.75	123.47	118.30
17	I	94	ASP	CB-CG-OD1	5.68	123.42	118.30
13	E	41	ASP	CB-CG-OD1	5.66	123.39	118.30
40	j	141	ASP	CB-CG-OD1	5.44	123.19	118.30
42	l	346	PRO	N-CD-CG	-5.39	95.11	103.20
44	n	68	LEU	CA-CB-CG	5.37	127.65	115.30
34	d	389	LEU	CA-CB-CG	5.08	126.99	115.30
23	O	165	ASP	CB-CG-OD1	5.07	122.86	118.30
38	h	181	ILE	CG1-CB-CG2	-5.07	100.24	111.40
31	a	150	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	750/778 (96%)	735 (98%)	15 (2%)	0	100	100
2	1	508/642 (79%)	504 (99%)	4 (1%)	0	100	100
3	2	448/513 (87%)	434 (97%)	14 (3%)	0	100	100
4	3	129/321 (40%)	127 (98%)	2 (2%)	0	100	100
5	4	298/338 (88%)	288 (97%)	10 (3%)	0	100	100
6	5	63/72 (88%)	61 (97%)	2 (3%)	0	100	100
7	6	379/461 (82%)	367 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	609/843 (72%)	584 (96%)	25 (4%)	0	100	100
9	A	1494/1733 (86%)	1449 (97%)	45 (3%)	0	100	100
10	B	1168/1224 (95%)	1131 (97%)	37 (3%)	0	100	100
11	C	264/347 (76%)	258 (98%)	6 (2%)	0	100	100
12	D	163/221 (74%)	160 (98%)	3 (2%)	0	100	100
13	E	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
14	F	114/155 (74%)	111 (97%)	3 (3%)	0	100	100
15	G	169/177 (96%)	161 (95%)	8 (5%)	0	100	100
16	H	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
17	I	114/122 (93%)	109 (96%)	5 (4%)	0	100	100
18	J	67/70 (96%)	67 (100%)	0	0	100	100
19	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
20	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
21	M	306/352 (87%)	295 (96%)	11 (4%)	0	100	100
23	O	179/240 (75%)	170 (95%)	9 (5%)	0	100	100
24	Q	215/735 (29%)	205 (95%)	10 (5%)	0	100	100
25	R	264/400 (66%)	255 (97%)	9 (3%)	0	100	100
27	U	101/286 (35%)	96 (95%)	5 (5%)	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%)	200 (97%)	7 (3%)	0	100	100
31	a	170/295 (58%)	161 (95%)	9 (5%)	0	100	100
32	b	168/223 (75%)	162 (96%)	6 (4%)	0	100	100
33	c	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
34	d	481/687 (70%)	468 (97%)	13 (3%)	0	100	100
35	e	252/307 (82%)	244 (97%)	8 (3%)	0	100	100
36	f	202/210 (96%)	194 (96%)	8 (4%)	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%)	93 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	155/157 (99%)	154 (99%)	1 (1%)	0	100	100
42	l	521/1082 (48%)	503 (96%)	17 (3%)	1 (0%)	47	79
43	m	126/220 (57%)	120 (95%)	6 (5%)	0	100	100
44	n	134/140 (96%)	132 (98%)	2 (2%)	0	100	100
45	o	108/127 (85%)	108 (100%)	0	0	100	100
46	p	221/566 (39%)	207 (94%)	14 (6%)	0	100	100
47	r	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
47	v	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
48	s	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
48	w	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
49	t	107/129 (83%)	103 (96%)	4 (4%)	0	100	100
49	x	104/129 (81%)	104 (100%)	0	0	100	100
50	u	95/125 (76%)	91 (96%)	4 (4%)	0	100	100
50	y	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
All	All	12842/17410 (74%)	12464 (97%)	377 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	480 (99%)	3 (1%)	86	94
3	2	414/468 (88%)	413 (100%)	1 (0%)	93	98
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%)	57 (97%)	2 (3%)	37	69
7	6	346/418 (83%)	345 (100%)	1 (0%)	92	97
8	7	547/737 (74%)	546 (100%)	1 (0%)	93	98
9	A	1330/1520 (88%)	1329 (100%)	1 (0%)	93	98
10	B	1024/1061 (96%)	1023 (100%)	1 (0%)	93	98
11	C	234/299 (78%)	233 (100%)	1 (0%)	91	97
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%)	152 (100%)	0	100	100
16	H	123/128 (96%)	121 (98%)	2 (2%)	62	83
17	I	110/116 (95%)	108 (98%)	2 (2%)	59	81
18	J	64/65 (98%)	64 (100%)	0	100	100
19	K	99/102 (97%)	98 (99%)	1 (1%)	76	88
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%)	204 (100%)	0	100	100
25	R	252/363 (69%)	252 (100%)	0	100	100
27	U	99/260 (38%)	95 (96%)	4 (4%)	31	65
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	161/207 (78%)	160 (99%)	1 (1%)	86	94
33	c	104/108 (96%)	103 (99%)	1 (1%)	76	88
34	d	469/642 (73%)	468 (100%)	1 (0%)	93	98
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	158/258 (61%)	156 (99%)	2 (1%)	69	86
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	505/1001 (50%)	503 (100%)	2 (0%)	91	97
43	m	119/195 (61%)	119 (100%)	0	100	100
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%)	212 (100%)	0	100	100
47	r	84/109 (77%)	84 (100%)	0	100	100
47	v	85/109 (78%)	85 (100%)	0	100	100
48	s	67/78 (86%)	67 (100%)	0	100	100
48	w	65/78 (83%)	65 (100%)	0	100	100
49	t	86/101 (85%)	86 (100%)	0	100	100
49	x	84/101 (83%)	84 (100%)	0	100	100
50	u	83/105 (79%)	83 (100%)	0	100	100
50	y	81/105 (77%)	81 (100%)	0	100	100
All	All	11775/15543 (76%)	11748 (100%)	27 (0%)	93	98

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	94	ARG
2	1	105	GLN
2	1	539	LYS
3	2	409	ARG
6	5	5	ARG
6	5	60	LYS
7	6	201	LYS
8	7	112	MET
9	A	217	LYS
10	B	241	ARG
11	C	199	LYS
16	H	37	LYS
16	H	130	ARG
17	I	90	GLN

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Mol	Chain	Res	Type
17	I	93	LYS
19	K	54	ARG
27	U	44	LYS
27	U	250	LYS
27	U	253	ARG
27	U	272	ASN
32	b	147	LYS
33	c	53	LYS
34	d	582	ARG
38	h	113	LYS
38	h	119	ASN
42	l	578	ARG
42	l	581	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	573	GLN
3	2	206	GLN
9	A	171	GLN
10	B	776	GLN
10	B	1097	HIS
10	B	1178	ASN
15	G	96	GLN
19	K	89	ASN
21	M	303	GLN
25	R	43	ASN
37	g	4	GLN
39	i	27	ASN
42	l	339	ASN
43	m	29	ASN
50	u	92	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 monosaccharides 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	$\# Z > 2$
51	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
51	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	22.84

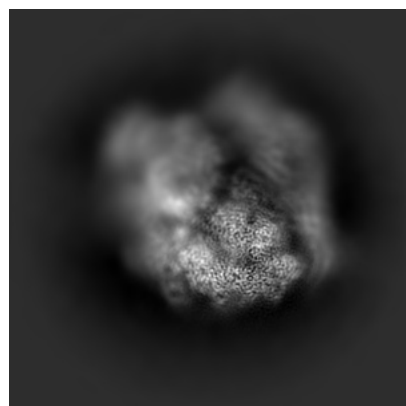
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16611. These allow visual inspection of the internal detail of the map and identification of artifacts.

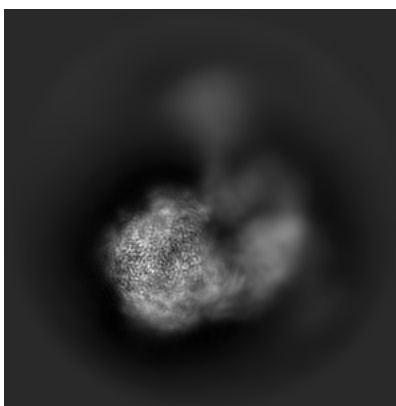
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

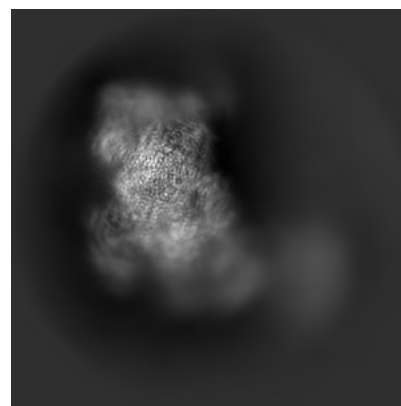
6.1.1 Primary map



X

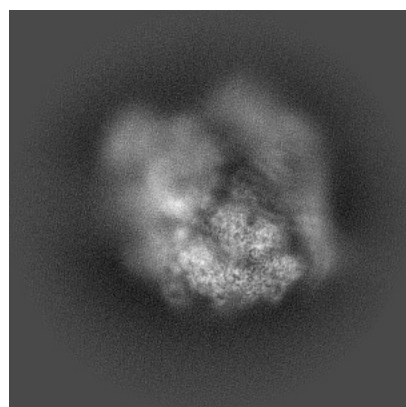


Y

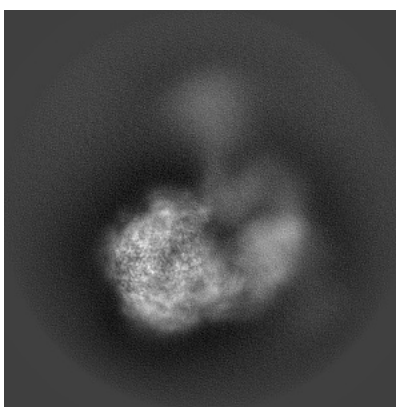


Z

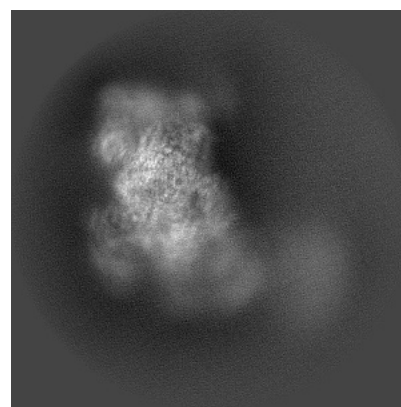
6.1.2 Raw map



X



Y

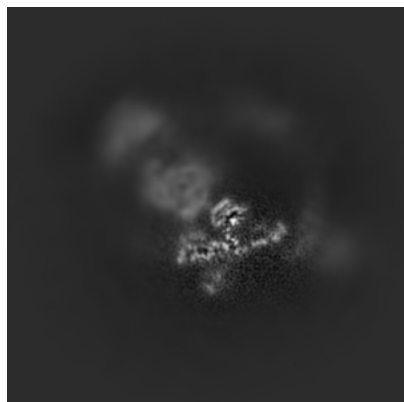


Z

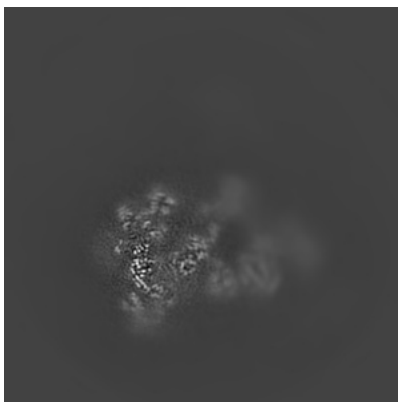
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

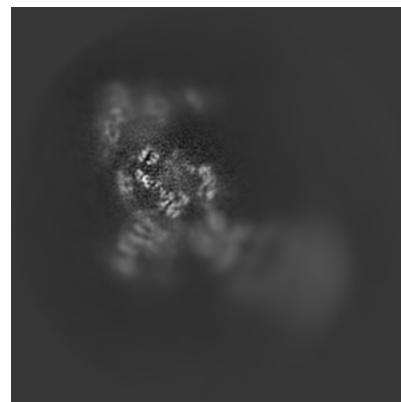
6.2.1 Primary map



X Index: 200

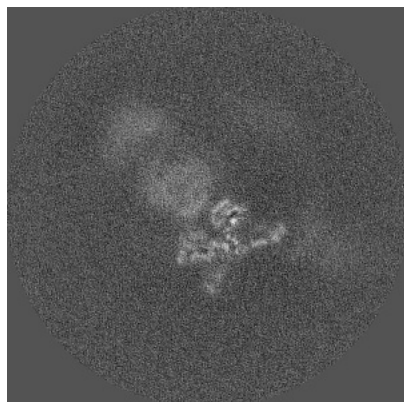


Y Index: 200

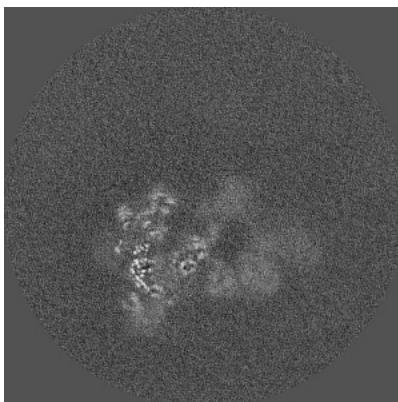


Z Index: 200

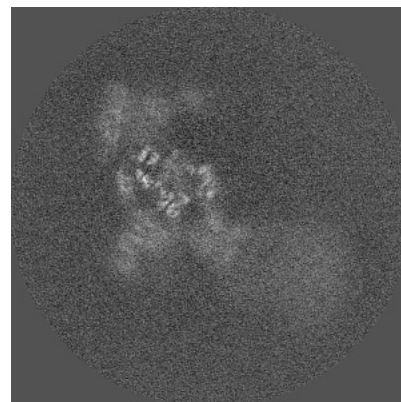
6.2.2 Raw map



X Index: 200



Y Index: 200

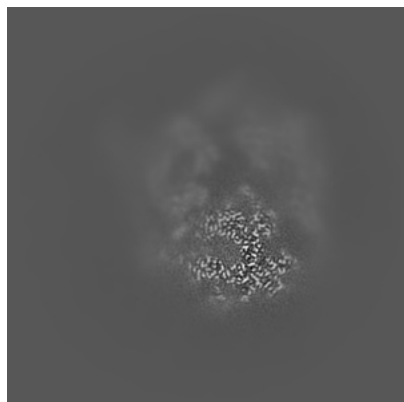


Z Index: 200

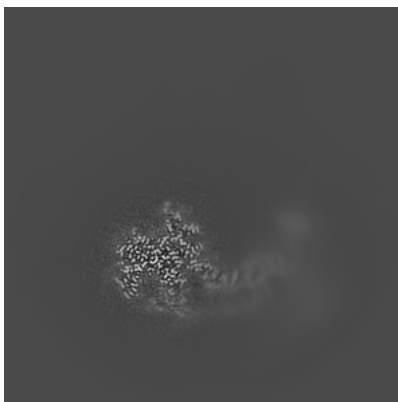
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

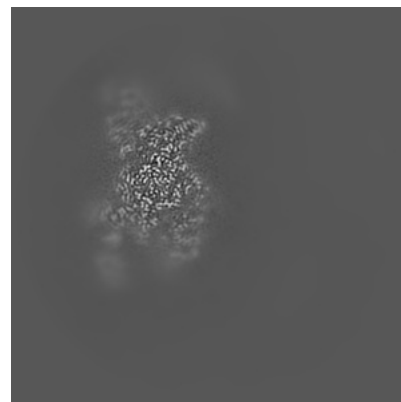
6.3.1 Primary map



X Index: 145

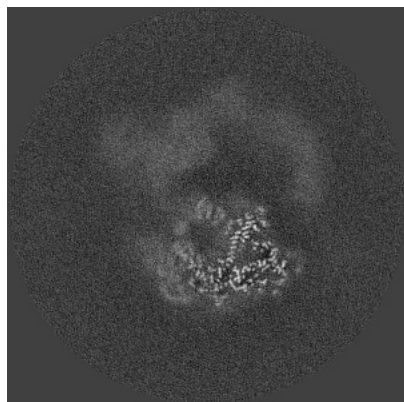


Y Index: 248

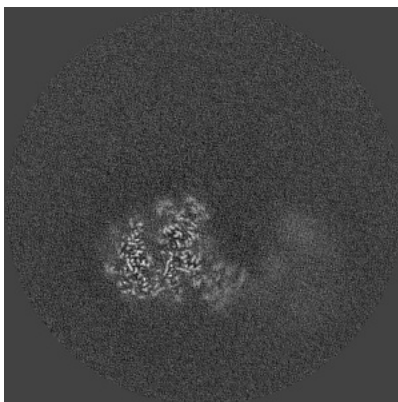


Z Index: 138

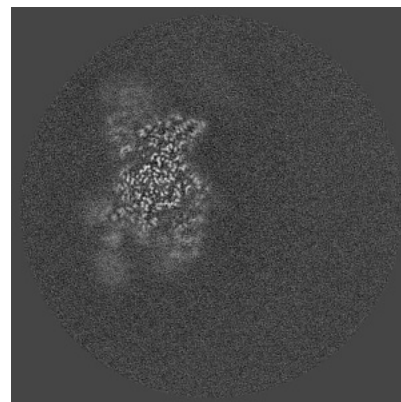
6.3.2 Raw map



X Index: 163



Y Index: 232

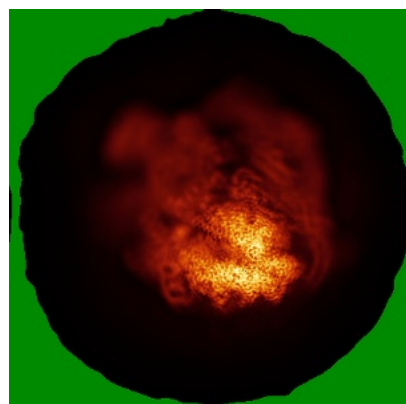


Z Index: 138

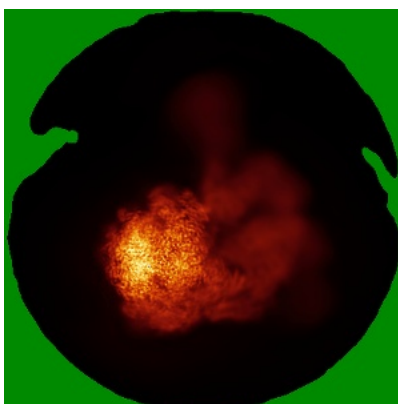
The images above show the largest variance slices of the map in three orthogonal directions.

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

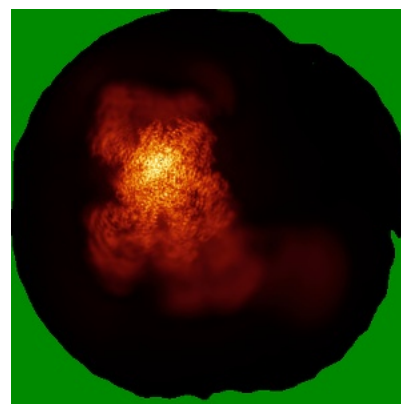
6.4.1 Primary map



X

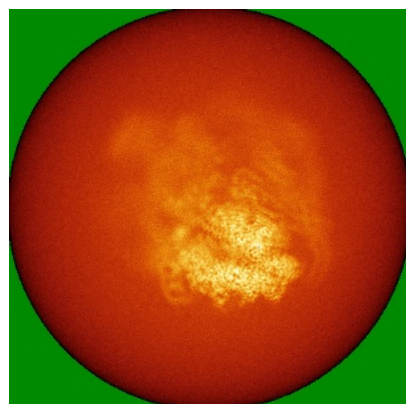


Y

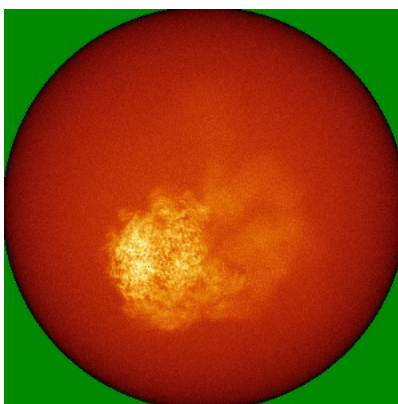


Z

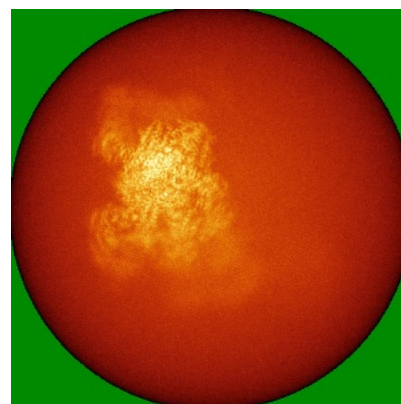
6.4.2 Raw map



X



Y

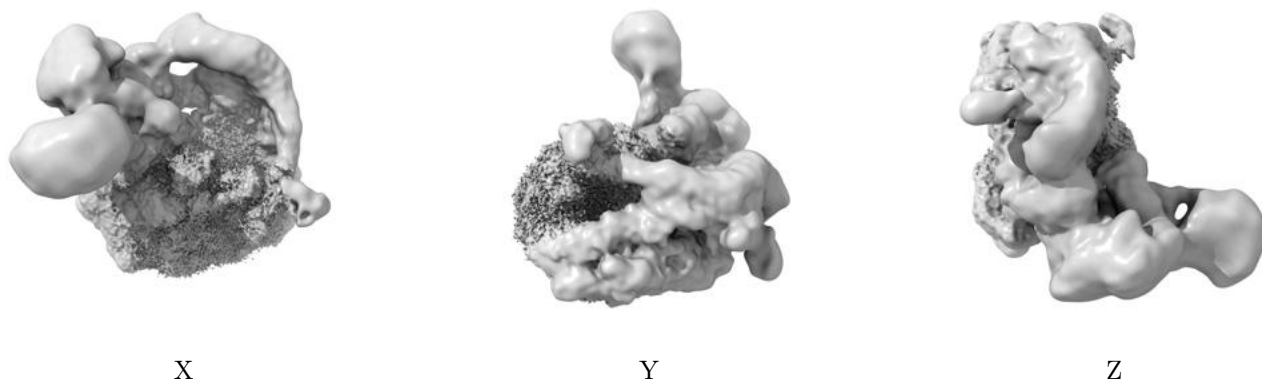


Z

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.

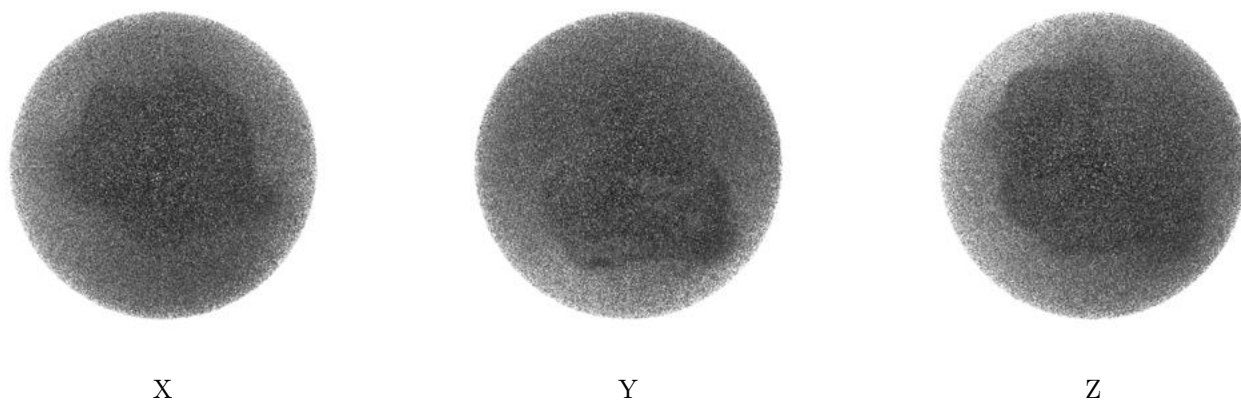
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

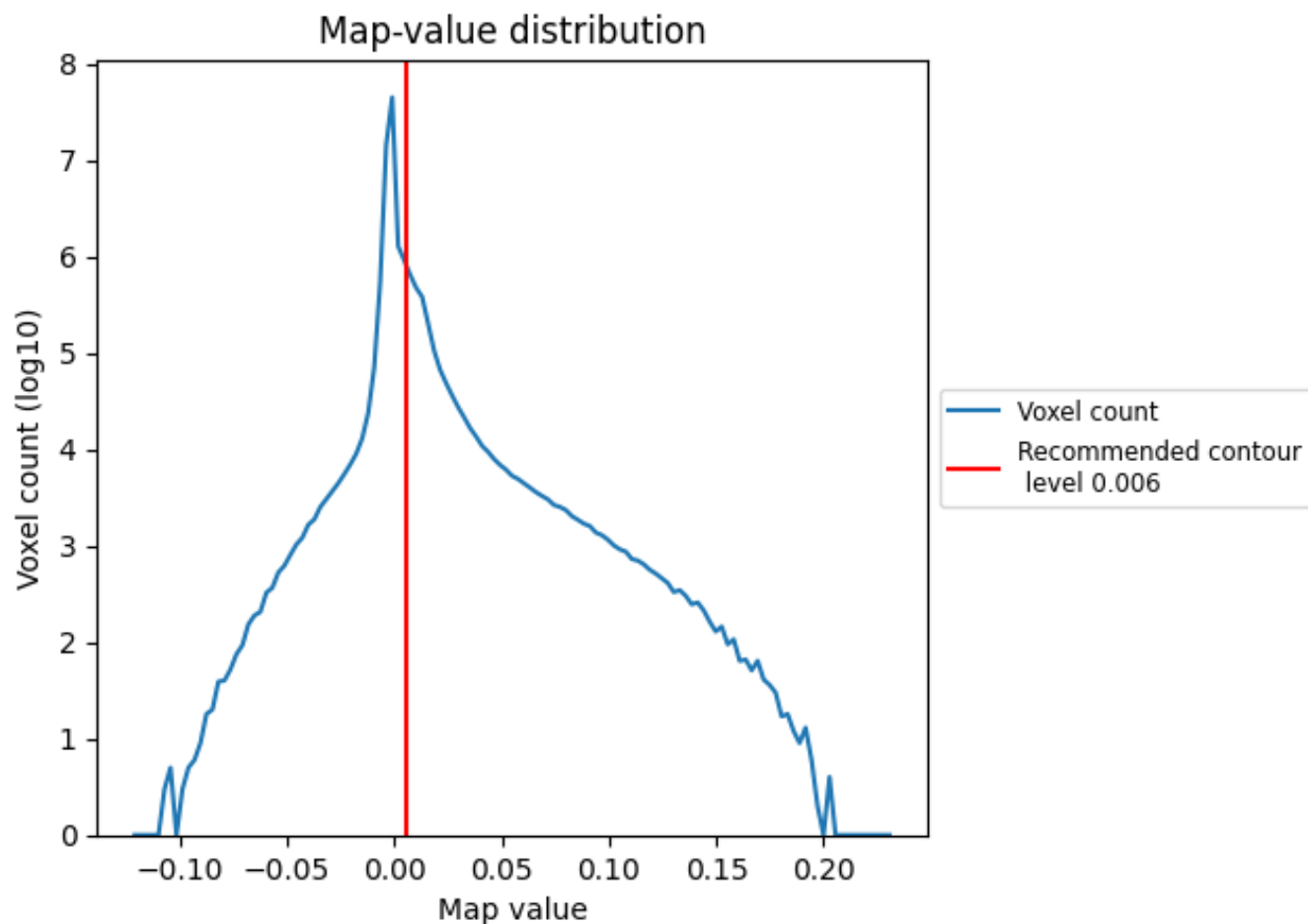
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

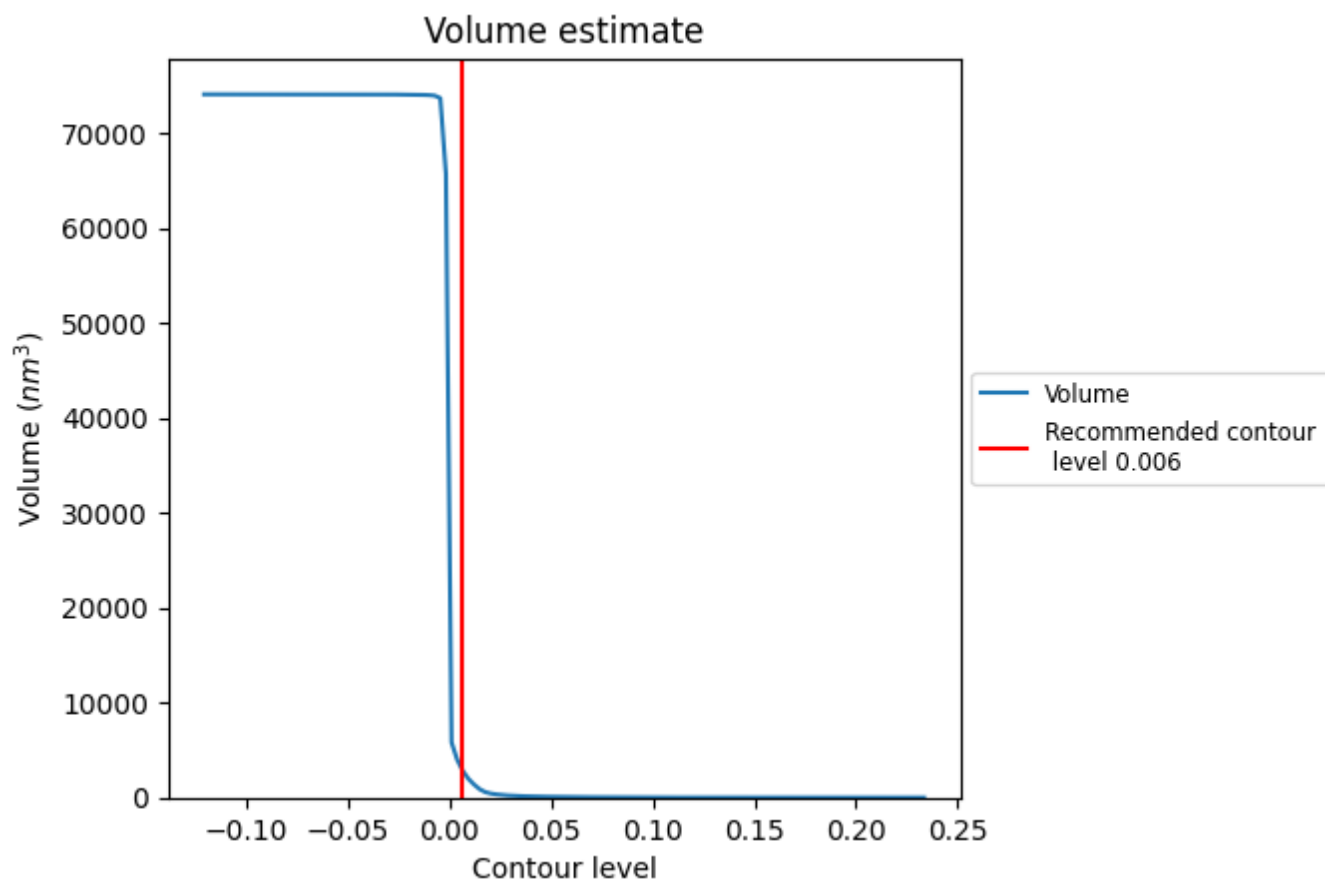
This section contains the results of statistical analysis of the map.

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.

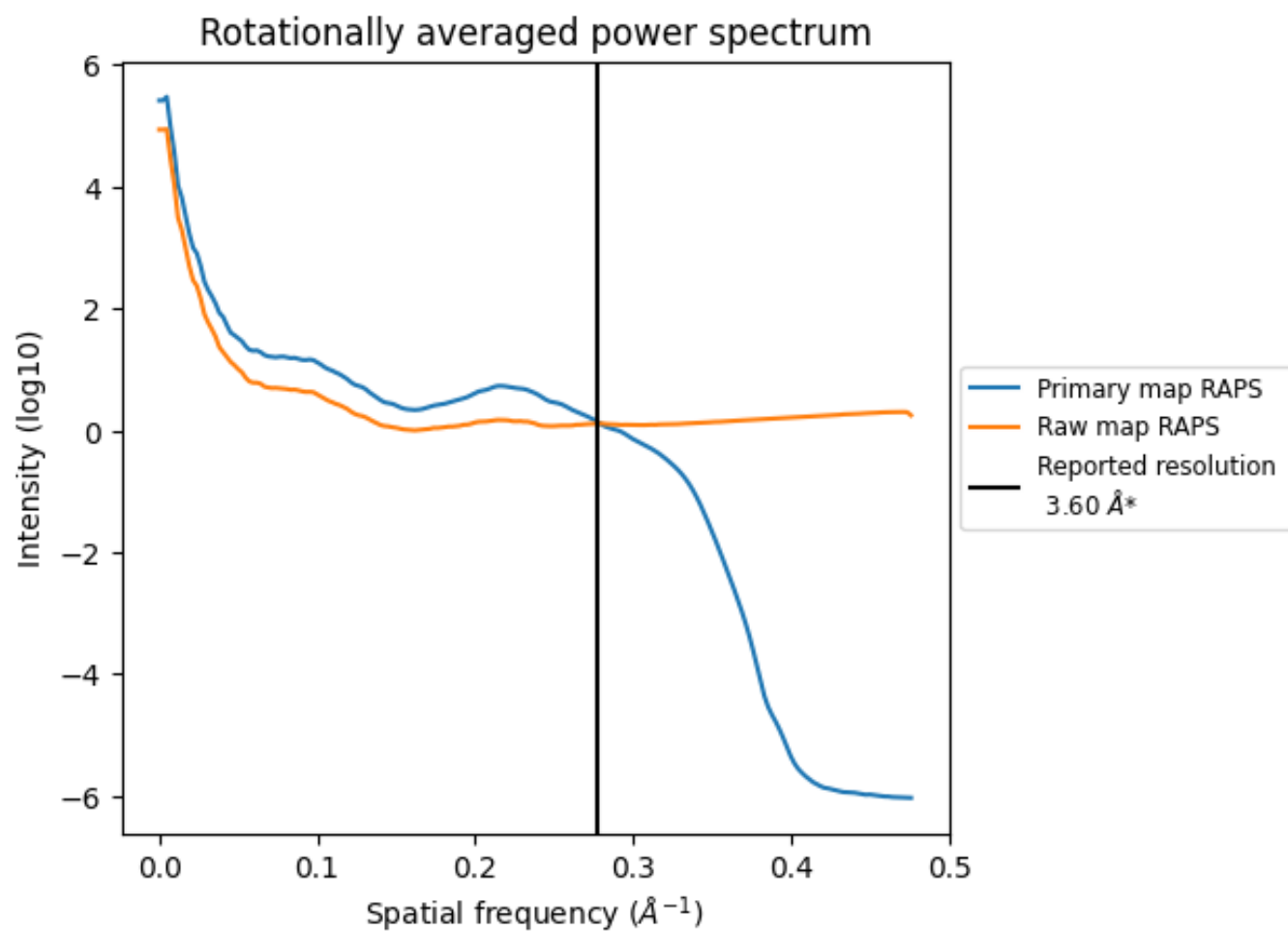
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2978 nm^3 ; this corresponds to an approximate mass of 2690 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 ⓘ

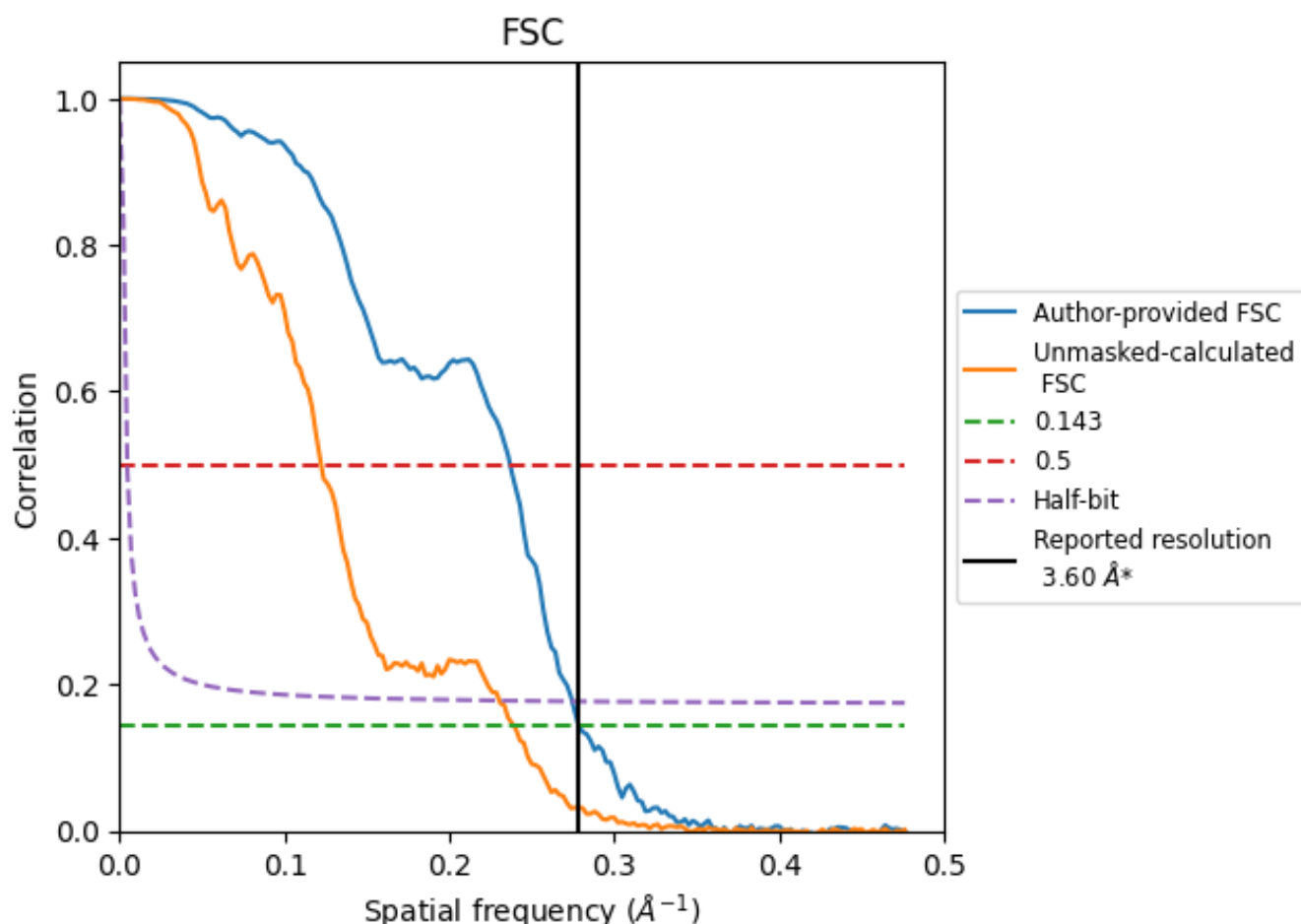


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

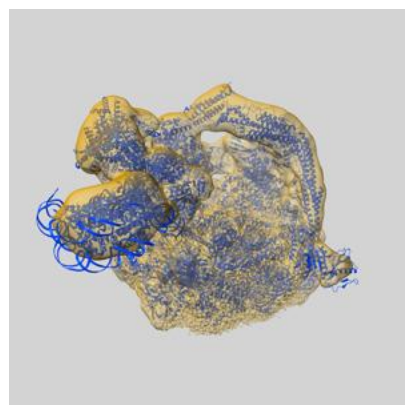
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.22	3.64
Unmasked-calculated*	4.18	8.18	4.34

*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 4.18 differs from the reported value 3.6 by more than 10 %

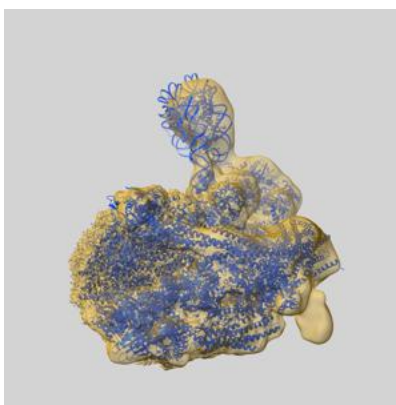
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16611 and PDB model 8CEO. Per-residue inclusion information can be found in section 3 on page 16.

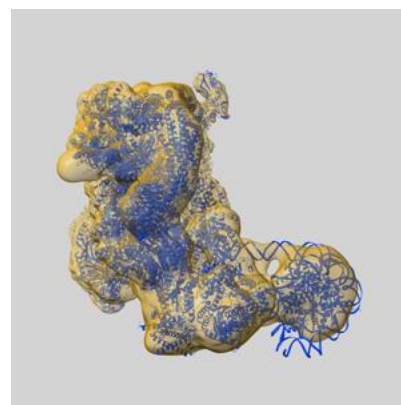
9.1 Map-model overlay [i](#)



X



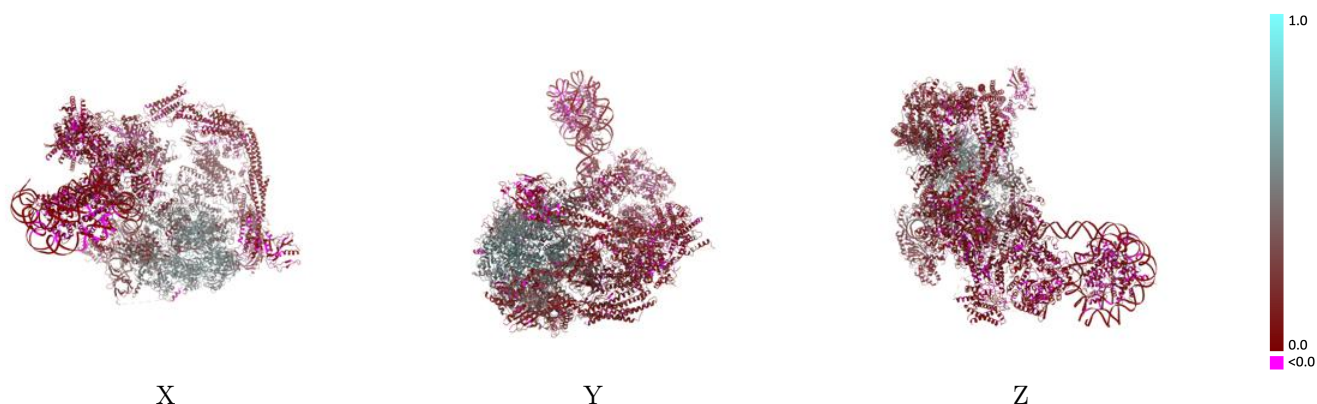
Y



Z

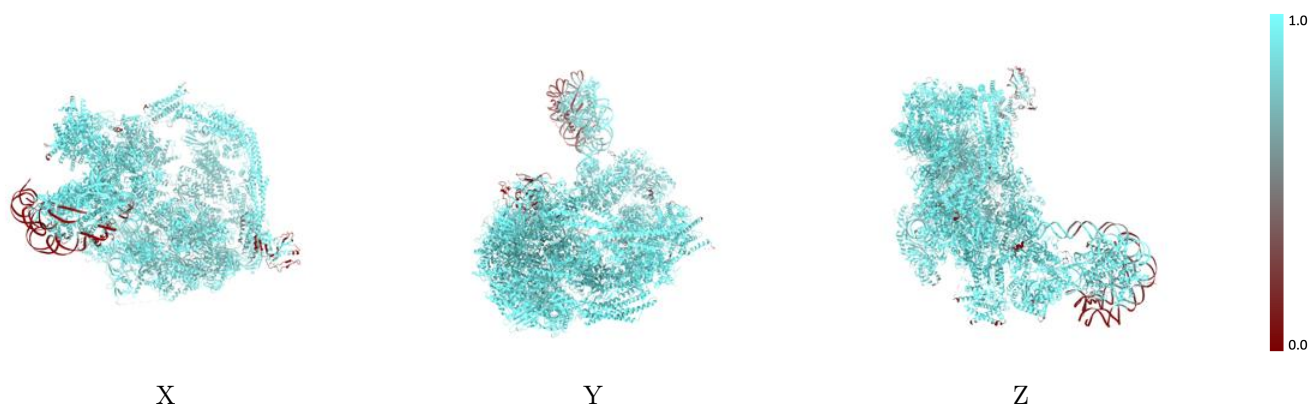
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



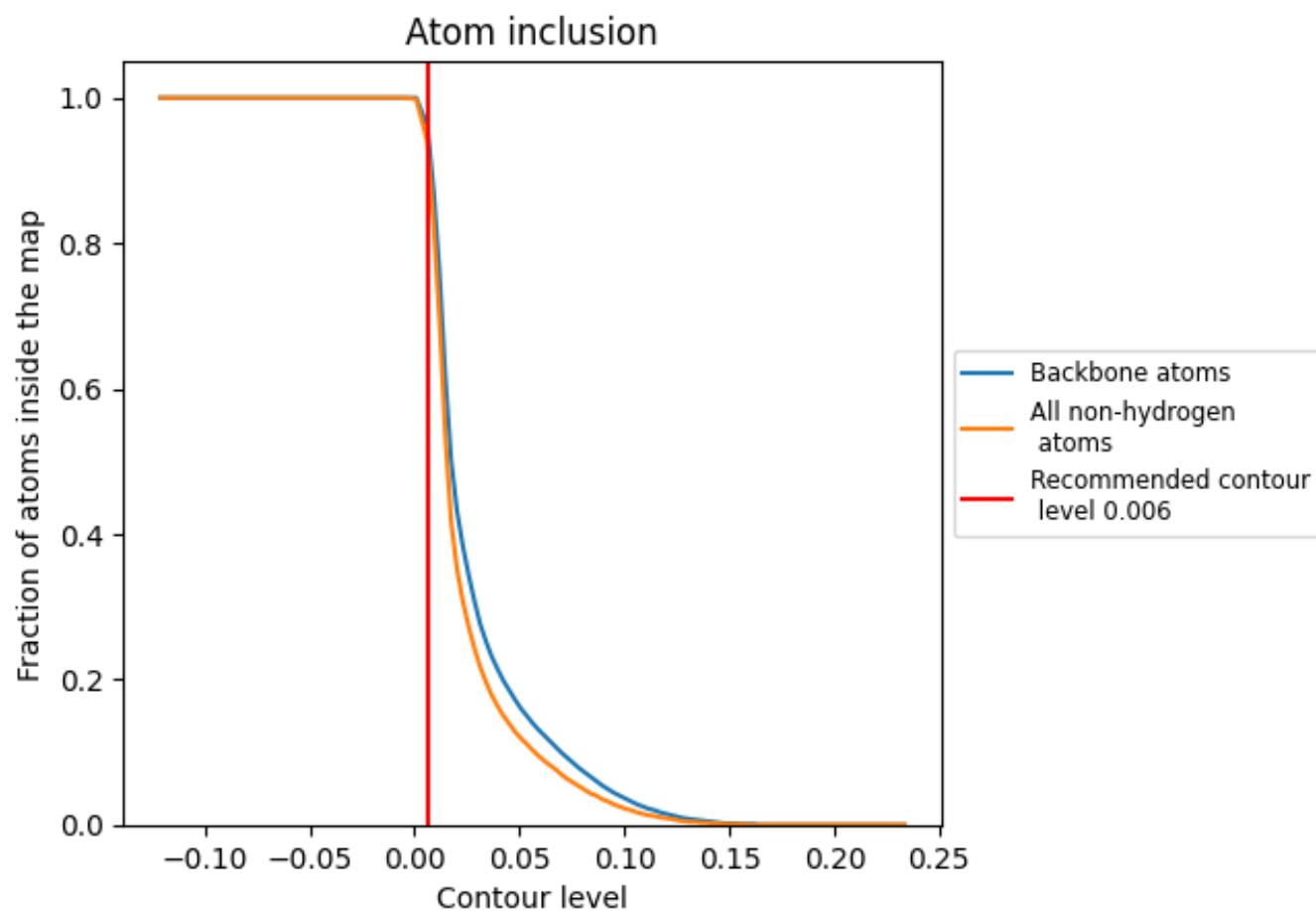
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.2220
0	 0.9880	 0.1100
1	 0.9590	 0.0830
2	 0.9790	 0.0750
3	 0.9880	 0.1710
4	 0.9970	 0.0610
5	 1.0000	 0.0720
6	 0.9640	 0.0820
7	 0.9890	 0.1030
A	 0.9860	 0.4510
B	 0.9850	 0.5000
C	 0.9890	 0.5120
D	 0.9670	 0.1990
E	 0.9900	 0.3850
F	 0.9220	 0.3790
G	 0.9840	 0.3480
H	 0.9780	 0.4460
I	 0.9910	 0.3480
J	 0.9910	 0.5340
K	 0.9770	 0.5050
L	 0.9860	 0.4710
M	 0.9770	 0.3570
N	 0.6520	 0.0940
O	 0.9940	 0.2260
Q	 0.9790	 0.2350
R	 0.9950	 0.2040
T	 0.6500	 0.0970
U	 0.9270	 0.1280
V	 0.9930	 0.1340
W	 0.9690	 0.1600
X	 0.9910	 0.1520
a	 0.9970	 0.1340
b	 0.9870	 0.1620
c	 0.9970	 0.1800
d	 0.9940	 0.1620



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Chain	Atom inclusion	Q-score
e	 0.9620	 0.3730
f	 0.9630	 0.3520
g	 0.9960	 0.1630
h	 0.9550	 0.1030
i	 0.9980	 0.1290
j	 0.8210	 0.1120
k	 0.9450	 0.0840
l	 0.9750	 0.1270
m	 0.9210	 0.0650
n	 0.9680	 0.0960
o	 0.9790	 0.1190
p	 0.5320	 0.0620
r	 0.7950	 0.0260
s	 0.7970	 0.0360
t	 0.7720	 0.0170
u	 0.7470	 0.0230
v	 0.9740	 0.0510
w	 1.0000	 0.0850
x	 0.9280	 0.0490
y	 0.9930	 0.0530