WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Apr 11, 2023 – 03:22 pm 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)

The following versions of software and data (see references (i)) were used in the production of this report:

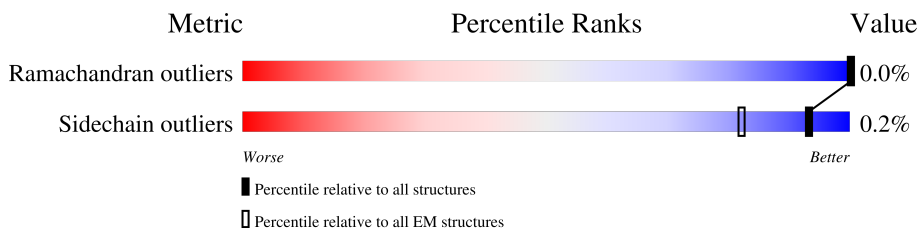|		
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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.
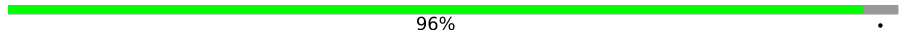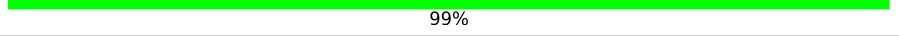
Metric	Percentile Ranks	Value
Ramachandran outliers		0.0%
Sidechain outliers		0.2%

Worse   *Better*

▌ Percentile relative to all structures

▯ Percentile relative to all EM structures
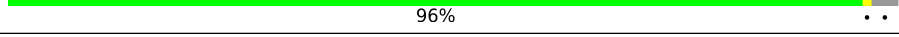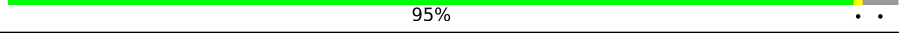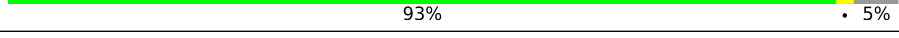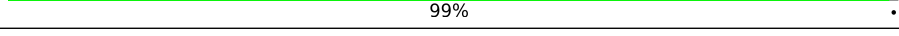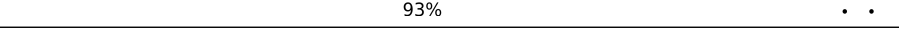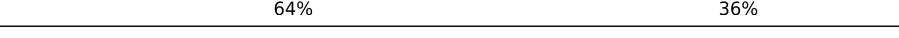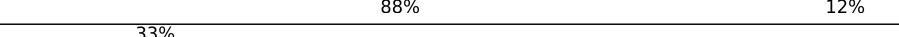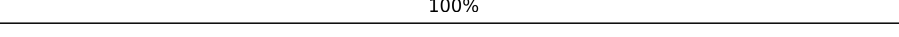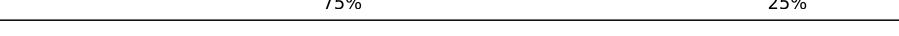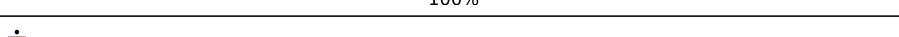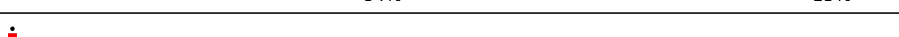
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	96%
11	C	347	76% 23%
12	D	221	76% 24%
13	E	215	99%
14	F	155	76% 24%
15	G	177	96%
16	H	146	95%
17	I	122	93% 5%
18	J	70	99%
19	K	120	93%
20	L	70	64% 36%
21	M	352	88% 12%
22	N	209	33% 100%
23	O	240	75% 25%
24	Q	735	30% 70%
25	R	400	67% 33%
26	T	209	33% 100%
27	U	286	36% 63%
28	V	122	84% 15%
29	W	492	62% 38%
30	X	328	64% 36%
31	a	295	60% 40%
32	b	223	77% 23%
33	c	115	96%
34	d	687	72% 27%

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Mol	Chain	Length	Quality of chain
35	e	307	83% 17%
36	f	210	98%
37	g	121	84% 16%
38	h	284	58% 40%
39	i	222	82% 18%
40	j	149	7% 66% 32%
41	k	157	100%
42	l	1082	49% 51%
43	m	220	59% 41%
44	n	140	96%
45	o	127	87% 13%
46	p	566	18% 40% 60%
47	r	135	14% 72% 28%
47	v	135	73% 27%
48	s	102	12% 80% 20%
48	w	102	78% 22%
49	t	129	17% 84% 16%
49	x	129	5% 82% 18%
50	u	125	19% 78% 22%
50	y	125	75% 24%

2 Entry composition ⓘ

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 IIH helicase subunit XPD.

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

- Molecule 2 is a protein called TFB1 isoform 1.

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

- Molecule 3 is a protein called RNA polymerase II transcription factor B subunit 2.

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

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

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

- 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 2338	C 1492	N 390	O 442	S 14	0	0

- 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 514	C 326	N 90	O 95	S 3	0	0

- 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 2379	C 1504	N 408	O 449	S 18	0	0

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 4263	C 2035	N 761	O 1259	P 208	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	209	Total 4300	C 2045	N 802	O 1245	P 208	0	0

- Molecule 27 is a protein called TOA1 isoform 1.

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

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

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

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

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

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 1708	C 1089	N 293	O 320	S 6	0	0

- 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 1394	C 884	N 234	O 271	S 5	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Histone H3.2.

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

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 653	C 412	N 127	O 113	S 1	0	0
48	w	80	Total 638	C 401	N 125	O 111	S 1	0	0

- Molecule 49 is a protein called Histone H2A.

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

- Molecule 50 is a protein called Histone H2B.

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

- Molecule 51 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
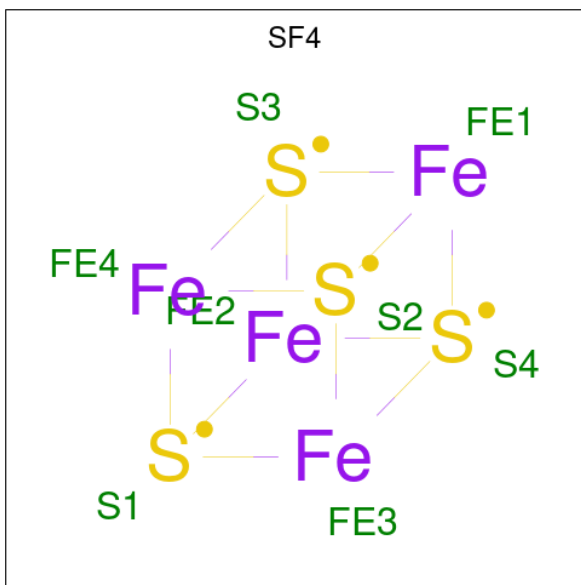
Mol	Chain	Residues	Atoms			AltConf
51	0	1	Total 8	Fe 4	S 4	0

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

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

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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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 0:
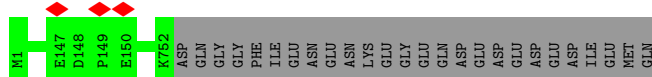
• Molecule 2: TFB1 isoform 1

Chain 1:

• Molecule 3: RNA polymerase II transcription factor B subunit 2

Chain 2:

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

Chain 3:

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

Chain 4:   89%   11%

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

Chain 5:   88%   10%

• Molecule 7: General transcription and DNA repair factor IIH

Chain 6:   83%   17%

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

Chain 7:   73%   27%

ASP ALA ASP ASN SER VAL GLY ARG GLY SER ASN GLY HIS LYS ARG PHE LYS SER LYS ALA VAL ARG GLY GLU SER LEU SER GLY LEU ALA GLY ASP MET ALA TYR MET GLU TYR SER THR ASN LYS ASN LYS GLU LEU LYS GLU HIS **H830** **Y837** TYR LYS ASN LEU LYS

LYS

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

Chain A: 87% 13%

MET V2 **D188** ARG ALA THR GLY ASP ALA ASP GLU P197 **K217** M1079 THR LEU ASN THR PHE HIS PHE ALA GLY VAL ALA SER LYS K1093 L1177 ASP GLU ALA GLU GLN GLN S1184 M1454 PRO GLU GLN LYS ILE GLU ILE ASP GLY GLN ASP GLY VAL THR PRO

TYR SER ASN GLU SER GLY LEU VAL ASN ALA ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY ASN ASP SER ALA MET ALA GLY GLY PHE THR ALA TYR GLY GLY ALA ASP TYR GLU ALA THR SER PRO PHE GLY ALA TYR GLY GLU ALA PRO THR SER

PRO GLY PHE GLY VAL SER PRO GLY PHE SER PRO THR SER PRO THR TYR SER PRO THR SER PRO ALA TYR SER P1572 P1600 T1601 ASP S1653 TYR SER PRO THR S1665 T1678 SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER SER PRO ALA TYR SER PRO THR SER

PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO ASN TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO GLY TYR SER PRO SER SER PRO ALA TYR SER PRO LYS GLN GLU GLN LYS

HIS ASN GLU GLU ASN GLU SER ARG

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

Chain B: 96% .

MET SER ASP ALA ASN SER GLU LYS TYR TYR ASP GLU ASP PRO TYR GLY PHE F18 E157 ASP SER SER GLU SER G163 **R241** E468 GLN LYS LYS ALA MET SER SER R476 I502 GLY ARG ASP G506 I669 GLU GLY GLY PHE GLU D675 E714 ALA ASN GLU GLU ASN ASP

LEU D722 F1224

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

Chain C: 76% 23%

MET GLY SER HIS HIS HIS HIS HIS HIS SER ASN SER GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU ASP THR GLY SER S3 **K199** **D268** LYS VAL ASN PHE ALA SER GLY ASP ASN ASN THR ALA SER ASN MET LEU GLY SER ASN GLU ASP VAL MET MET

THR GLY ALA GLU GLN ASP PRO TYR SER ASN ALA SER GLN MET GLY ASN THR GLY SER GLY TYR ASP ASN ALA TRP

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

Chain D: 76% 24%

MET ASN VAL SER THR SER THR PHE GLN THR R11 S73 GLN LYS LYS HIS LYS LYS LYS LYS HIS LEU LYS HIS GLU ASN ALA ASN ASP GLU THR THR ALA VAL GLU GLU GLY ASP ASP ASP LEU ASP ASP GLU ASP VAL ASN ALA ASP ASP ASP PHE MET HIS SER E117 L220 TYR

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

Chain E:

99%

MET D2 D41 M215

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

Chain F:

76% 24%

MET SER ASP TYR GLU GLU ALA PHE ASN ASP GLY N12 E21 H22 F23 F35 LYS ASP GLY GLU THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN GLN HIS E62 L155

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

Chain G:

96%

M1 D50 I171 HIS HIS HIS HIS HIS HIS

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

Chain H:

95%

MET S2 K37 P69 ALA ASN ASP SER SER A75 R130 R146

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

Chain I:

93% 5%

MET T2 Q90 K93 D94 K117 ARG THR GLN PHE SER

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

Chain J:

99%

M1 R69 ASP

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

Chain K:

93%

M1 D24 R54 D82 A115 ALA ASP ASP ALA PHE

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

Chain L:

64% 36%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA T26 R70

• Molecule 21: Transcription initiation factor IIB

Chain M:

88% 12%

MET MET THR ARG GLU SER ILE ASP LYS ARG ALA GLY ARG R14 D58 THR ARG SER GLU TRP ARG THR PHE SER ASN ASP ASP HIS ASN GLY ASP ASP PRO SER R78 V342 GLU LYS LYS LYS HIS HIS HIS HIS HIS HIS

• Molecule 22: Nontemplate DNA (209-MER)

33%

Chain N:

100%

A-73 A1 T2 A3 T11 G12 C13 G14 T21 G22 G23 T24 C25 G26 T27 A30 C31 A32 G33 C34 T35 C36 T37 C40 A41 C42 C43 G44 C45 T46 T47 A48 A49 A50 C51 G52 C53 A54 C55 G56 T57 A58 C59 T104 C105 T106 C107 C108 A109 G110 A113 C114 G115

T116 G117 T118 C119 T123 A124 T125 A126 T127 A128 C129 A130 T131 C132 G133 A134 T135

• Molecule 23: TATA-binding protein

Chain O:

75% 25%

MET ALA ASP GLU GLU ARG LEU LYS GLU PHE LYS GLU ALA ASN LYS ILE VAL PHE ASP PRO ASN THR ARG GLN VAL TRP GLU ASN GLN ASN ARG ASP GLY THR LYS PRO ALA THR THR PHE GLN SER GLU GLU ASP ILE LYS ARG ALA ALA PRO GLU SER GLU LYS ASP THR SER ALA T60

D165 M240

• Molecule 24: Transcription initiation factor IIF subunit alpha

Chain Q:

30% 70%

MET SER ARG ARG ASN PRO PRO GLY SER ARG ASN GLY GLY PRO THR N17 R35 MET GLY GLN ASN GLY SER ASN SER SER PRO GLY VAL PRO ASN GLY ASP ASN SER ARG GLY SER LEU VAL LYS LYS ASP PRO GLU TYR ALA GLU GLU GLU ARG GLU GLU LYS MET LEU LEU GLN

ILE GLY VAL GLU ALA ASP GLY ARG SER ASN VAL LYS VAL LYS ASP GLU D94 P95 N96 K168 LYS ALA GLU GLN GLU GLU ARG SER THR PRO VAL SER ALA VAL GLU VAL GLU SER ASN GLY LEU SER ASN GLY SER THR SER VAL SER LEU ASN ASN THR VAL LYS ASP GLY SER GLN THR PRO THR VAL ASP SER VAL

THR LYS ASP ASN THR ALA ASN GLY VAL ASN SER SER ILE PRO THR VAL THR GLY SER VAL PRO PRO ALA SER PRO THR VAL SER ALA VAL GLU SER ASN GLY LEU SER ASN GLY SER THR SER ALA ALA ASN GLY LEU ASP GLY ASN ALA SER THR ALA ASN LEU ALA ASN GLY

ARG PRO LEU VAL THR LYS LEU GLU GLU ASP ALA GLY PRO ALA GLU ASP THR LYS VAL GLY MET VAL LYS TYR ASP GLY LYS VAL THR ASN GLU GLU PHE GLU GLU GLY THR MET ASP PRO LEU ALA ASP VAL ALA PRO ASP GLY GLY ARG ALA LYS ARG GLY ASN L325

• Molecule 25: Transcription initiation factor IIF subunit beta

Chain R:

• Molecule 26: Template DNA (209-MER)

Chain T:

• Molecule 27: TOA1 isoform 1

Chain U:

GLU LEU ASP SER ASP ASP **D228** **S232** GLU GLY GLU GLU ASP GLY **P239** **K250** **R253** **N272** **V286**

• Molecule 28: Transcription initiation factor IIA subunit 2

Chain V: 84% • 15%

MET ALA VAL PRO **G5** **D24** **E88** ASP SER HIS ARG ASP ALA SER GLN ASN GLY SER GLY ASP SER **Q103** **E122**

• Molecule 29: Transcription initiation factor IIE subunit alpha

Chain W: 62% 38%

MET **D2** **M227** PHE ARG PRO GLY ASP SER ALA PRO LEU PRO ASN MET GLY THR ALA LEU GLY ASN ASP SER ARG ARG ALA GLY ALA ASN SER GLN **A258** **R306** LEU ASP ASN GLU GLU GLU PHE ASP PRO VAL VAL THR ALA SER ALA MET ASP SER ILE ASN PRO ASP ASN

GLU PRO ALA GLU GLU THR SER TYR GLN ASN ASN ARG THR LEU THR GLU GLN GLU MET **E349** **K366** **K367** **Q368** **A369** LYS LEU ASN LYS GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU GLU GLU MET GLU ASP VAL MET ASP ASN ASP GLU THR ALA

ARG GLU ASN ALA **L409** **E410** **V416** THR ASP THR ALA GLY THR ALA LYS THR GLU SER ASN THR SER ASN ASP VAL LYS GLN GLU SER ILE ASN ASP LYS THR GLU ASP ALA VAL ASN ALA THR ALA THR ALA SER GLY PRO SER ALA ASN ALA LYS PRO ASN ASP GLY ASP ASP ASP

ASP ASP ASP ASP ASP GLU MET ASP ILE GLU PHE GLU ASP VAL ALA ALA LEU GLU HIS HIS HIS HIS

• Molecule 30: Transcription initiation factor IIE subunit beta

Chain X: 64% 36%

MET SER LYS ASN ARG ASP PRO LEU LEU ALA ASN LEU ALA PHE LYS SER LYS VAL LYS SER ALA PRO VAL ILE ALA PRO ALA LYS VAL GLY GLN LYS LYS THR ASN ASP THR VAL ILE THR ILE ASP GLY ASN THR ARG ARG THR ALA SER GLU ALA GLN GLN ASN THR LEU

ASN SER ALA LYS ASN PRO VAL LEU VAL ASP ILE LYS GLU ALA GLY SER ASN SER ASN ALA ILE SER LEU ASP ASP ASP ASP GLU GLU PHE GLY SER SER PRO SER LYS LYS VAL ARG PRO GLY **S106** **L143** **Q296** THR LYS ARG VAL GLU VAL LYS LYS ARG

GLN **R308** **R327** VAL

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

Chain a: 60% 40%

MET ASN **V3** **F52** SER GLN LEU ASN ASP PRO ASN ALA ALA VAL ASN MET THR GLN ASN ILE MET THR LEU PRO ASP GLY LYS ASN GLY ASN LEU LEU GLU GLU **E82** **N135** ASN SER GLY VAL GLY SER ALA LYS GLY **P145** **L150** **T206** ASP THR SER THR THR ALA THR ALA

THR ASN GLY ASN ALA GLY GLY GLY SER ASN LYS SER VAL ARG PRO THR GLY GLN ALA ASN MET ALA THR VAL PRO SER THR ASN VAL ASN MET THR VAL ASN THR MET GLY THR GLY GLY GLN THR ILE ASP ASN GLY THR GLY ARG THR ASN GLY ASN MET GLY ILE

THR I277 I288 ARG SER THR PRO ASN TYR ILE

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

Chain b:

77%   23%

MET SER GLN SER THR ALA SER LEU VAL PRO GLU GLY ASN GLN GLY SER LEU GLN GLU ASP VAL S22 K147 F172 LYS ASN GLU GLU SER LEU SER GLU GLU HIS ALA SER LEU LEU VAL ARG ASP SER LYS PRO S193 I213 THR GLY SER SER THR SER SER ASN

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

Chain c:

96%   ..

M1 K53 P111 SER LYS SER LYS

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

Chain d:

72%   27%

MET THR THR GLU ASP PRO ASP SER ASN HIS LEU SER SER SER GLU T15 A29 LEU SER ASN PRO ASN SER SER SER LEU HIS SER PRO THR SER ASP GLU PRO VAL PRO GLU GLU SER ALA GLY LYS ALA ASP THR SER ILE ARG LEU GLU LEU GLY ASP LEU GLU LEU GLU ASN LYS THR LYS LYS ASP

ASN ASP LYS ASN LEU LYS PHE LEU LEU LYS ASN LYS ASP GLY LYS THR ASP S85 L107 Q130 LEU GLY SER ASP SER SER ASP GLY HIS ASN SER GLU LYS LYS ASP THR ASP GLY ALA ASP GLU GLN ASN VAL GLN ILE GLY GLU ASP PHE MET GLU VAL ASP TYR GLU GLU ASP LYS ASP ASN PRO VAL ASP SER

ARG ASN GLU GLU THR ASP HIS LYS THR ASN GLU GLU ASN GLY GLU THR ASP ASP ASN ILE GLU T193 D327 ARG THR SER G331 HIS H371 SER SER SER VAL PHE LYS GLY THR ASP PHE VAL HIS SER V385 L389 M411 ASP ARG ASP SER GLU SER GLU GLU ALA GLU THR K423 L481

ASP ASP ASP SER ILE VAL ASN HIS GLU GLN ASP L493 P571 R582 E583 GLN PRO GLN GLU ASN LYS N590 L623 THR GLU HIS LYS S628 T653 GLU ALA ASN A657 Q683 GLN LYS LYS VAL

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

Chain e:

83%   17%

M1 R55 N56 T112 VAL PRO GLN VAL THR ASN PHE ASN SER THR ASN GLU ASP GLN GLN ASN ASN SER LYS HIS THR GLU ASP THR VAL ASN GLU SER ARG ASN SER ASP ILE ILE ASP VAL ASP MET ASP ALA SER PRO ALA PRO SER ASN E159 H302 GLY ASN ILE LEU ILE

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

Chain f:

98%   .

MET G2 D52 G190 PRO ASP THR S194 L210

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

Chain g: 84% 16%

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

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

Chain h: 58% 40%

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

THR VAL PRO PRO SER GLN SER GLU GLU GLN GLN LYS GLY GLN GLN MET ALA LYS LYS GLU GLU GLY THR GLY THR ALA PRO LYS THR ASP SER PHE ILE PHE ASP GLY THR ALA LYS GLU VAL GLY VAL ASP GLU ALA ASN THR LYS ASP LYS LYS GLU GLU LYS GLU GLU ASN ASN ASP ASP ALA LEU ASP LEU ASP LEU ASP

LEU PHE ASP PRO ASP ASP PHE

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

Chain i: 82% 18%

MET SER ASN ASP PRO GLY ASN GLU V9 K37 LYS ALA ALA SER ALA LYS GLN THR ALA PRO ASN ASN SER ASN GLY GLY SER E55 K102 LYS SER THR GLU ASN GLU SER THR N111 S214 GLN SER PRO PRO SER SER GLN

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

7%

Chain j: 66% 32%

MET ASN LEU Q4 L15 T18 ASN PRO THR LEU ASP LYS PRO ASN GLU ALA GLU THR LYS GLU GLU PHE SER SER ALA GLU ASN ARG ASP GLU LYS ASP TYR LEU THR ASN GLN GLN PRO LYS ASN LEU SER THR PRO SER THR SER SER N62 G63 K78 D79 L90 L100

L104 E107 D138 D141 Q148 ARG

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

Chain k: 100%

M1 N2 T42 P43 E44 A45 T46 K47 H157

• Molecule 42: Mediator of RNA polymerase II transcription subunit 14

Chain l: 49% 51%

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

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

Chain m:

59%　　　41%

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

Chain n:

96%

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

Chain o:

87%　　　13%

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

Chain p:

18%

40% 60%

MET VAL GLU ASP S6 E9 L28 T32 Q36 T37 L38 G39 L40 E41 S42 F43 T44 E45 E46 L47 S48 N49 L54 S55 T56 A57 S58 K59 I60 I61 V62 I63 K69 K70 Q71 A82 S83 N84 F85 D86 N87 R94 D95 G96 E97 H98 E99 K100 K110

H118 N119 K122 S131 HIS ILE GLU ASP SER ASP SER THR SER HIS ASN ASN GLY SER SER ASP LYS SER LEU ASP SER SER ASN ALA SER PHE ASN ASN GLN GLY K161 Q177 C178 F179 Q180 D181 N182 C183 C184 D185 N193 Q203 G204 I205 N206 G207 K208 E209 V210 P211 E218

E219 N220 K221 S222 D223 S224 Q225 Y226 R227 F228 Y229 E230 Y231 I232 Y233 S234 Q235 E236 T237 K238 S239 W240 I241 N242 E243 S244 A245 E246 N247 F248 S249 N250 G251 E257 I258 V259 ALA ASN ALA LYS GLU SER ASN TYR THR ASP LEU ILE TRP PHE PRO GLU ASP PHE ILE SER PRO GLU LEU

ILE ILE ASP LYS VAL THR CYS SER SER ASN SER SER SER PRO PRO ILE ILE ASP PHE SER ASN ASN TYR ASN SER ARG ILE LEU GLN LEU MET ASN ASP PHE THR LYS LEU ILE ASN ILE LYS LYS PHE ASP ILE SER ASN ASP ASN LEU ASP LEU ILE SER GLU ILE LEU

LYS TRP VAL VAL GLN TRP SER ARG ILE VAL LEU GLN ASN VAL LYS LEU LEU ASN VAL LYS SER ARG THR PRO SER SER ASN SER SER GLU LEU GLU PRO ASP TYR GLN ALA PRO PHE SER THR SER THR LYS ASP LYS ASN SER SER ASN THR GLU GLU PRO ILE PRO ARG SER ASN ARG HIS

GLY SER VAL VAL GLU ALA SER ARG ARG ARG SER SER THR ASN LYS SER LYS ARG PRO SER ILE THR GLU ALA MET LEU LYS GLU GLU GLY LEU GLN PHE ASN LEU HIS GLU ILE LEU LEU SER GLU GLU PRO ALA ILE GLU GLU ASN GLY ASP SER ILE LYS GLU HIS SER THR

THR MET ASP GLY ALA ASN ASP LEU GLY PHE THR ALA SER VAL SER ASN GLN GLU ASN ALA GLY THR ASP ILE VAL MET GLU HIS GLY VAL LEU GLN GLY THR SER GLN ASN TYR GLY THR ALA THR ALA ASP ASP ALA ASP ILE GLU GLU GLU ASN GLY ASP SER ILE LYS ASP VAL SER SER LYS PRO SER LYS

PRO GLU SER SER VAL LEU GLN LEU ILE VAL SER GLU ASP HIS ILE ILE LEU ASP ILE LEU SER GLU CYS ASN LEU TYR ASP ASP VAL LYS CYS TRP SER PHE LYS ILE LEU GLU LYS PHE GLN ASP VAL ILE VAL SER

• Molecule 47: Histone H3.2

Chain r:

14%

72% 28%

ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR GLY GLY VAL LYS LYS P38 H39 R40 Y41 R42 P43 G44 T45 V46 A47 L48 R49 E50 R69 E73 Q76 D77 T80 D81

R134 ALA

• Molecule 47: Histone H3.2

Chain v:

73% 27%

ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR GLY GLY VAL LYS K37 P38 R134 ALA

• Molecule 48: Histone H4

Chain s:

12%

80% 20%

SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS V21 L22 R23 D24 N25 I26 Q27 K31 G48 L49 I50 Y51 E52 G102

• Molecule 48: Histone H4

Chain w:

• Molecule 49: Histone H2A

Chain t:

• Molecule 49: Histone H2A

Chain x:

• Molecule 50: Histone H2B

Chain u:

• Molecule 50: Histone H2B

Chain y:

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 $(e^-/\text{Å}^2)$	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: ZN, MG, SF4

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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
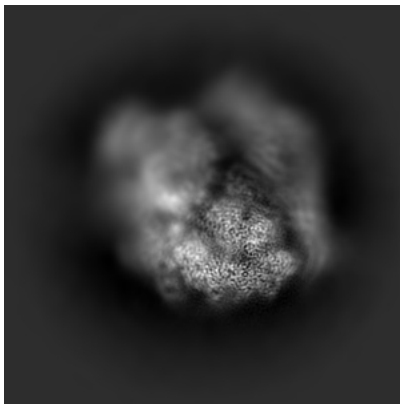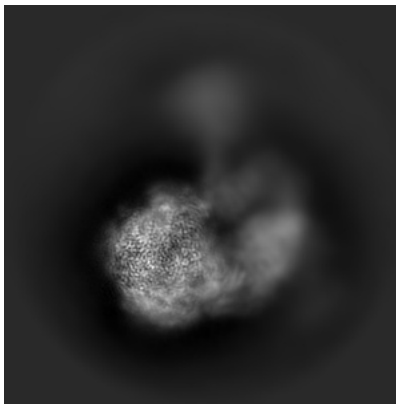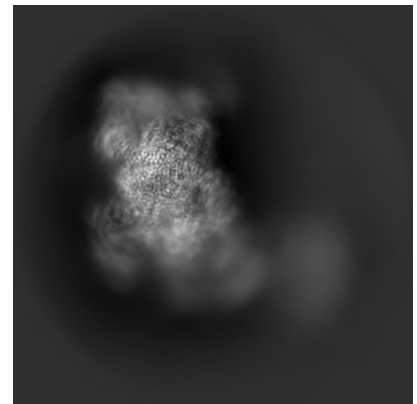
X   Y   Z

6.1.2   Raw map

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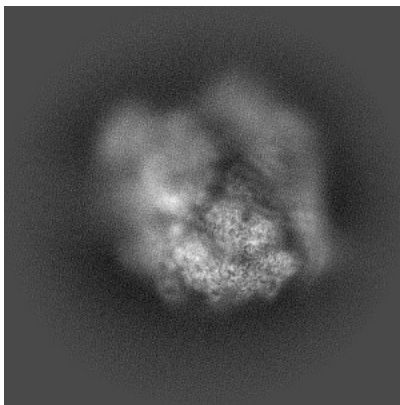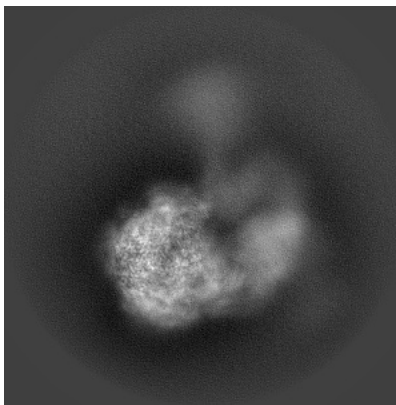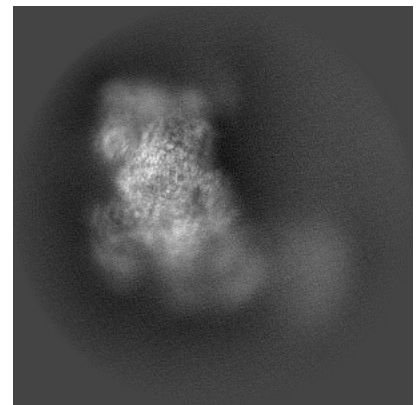
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
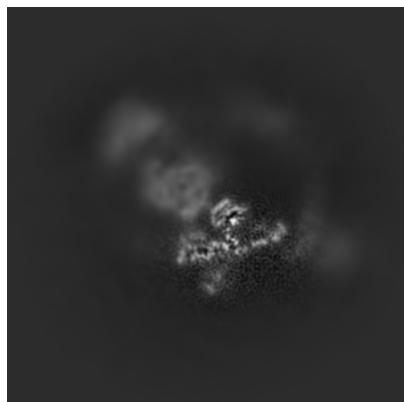
6.2.1 Primary map
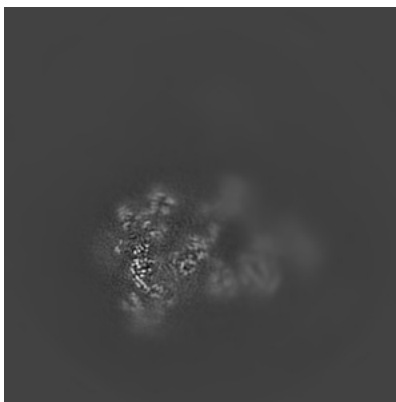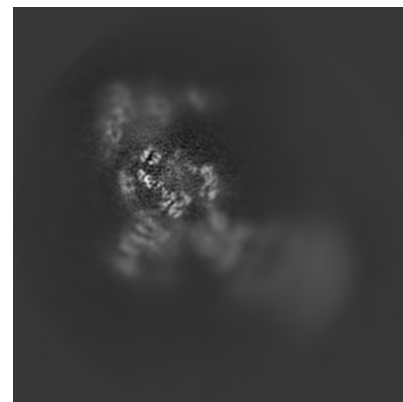
X Index: 200   Y Index: 200   Z Index: 200

6.2.2 Raw map
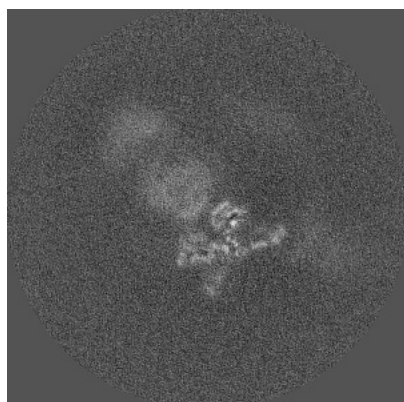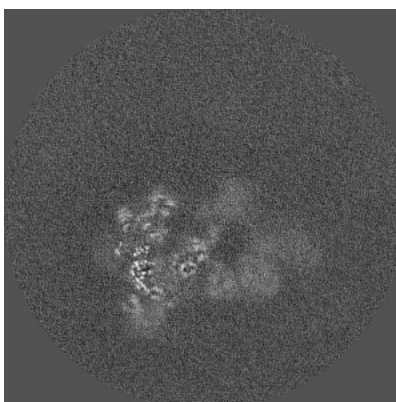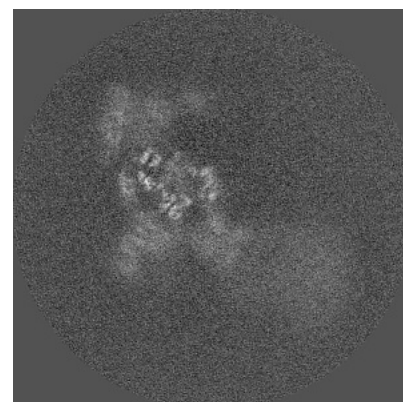
X Index: 200   Y Index: 200   Z Index: 200

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
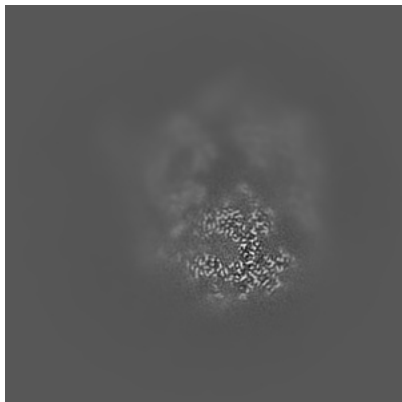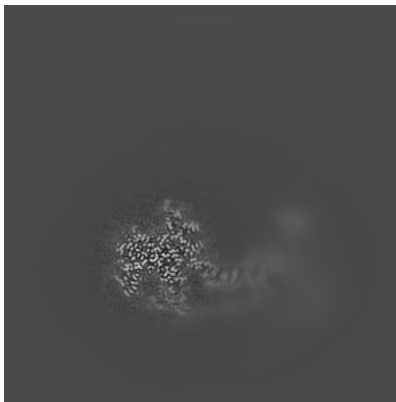
X Index: 145	Y Index: 248	Z Index: 138
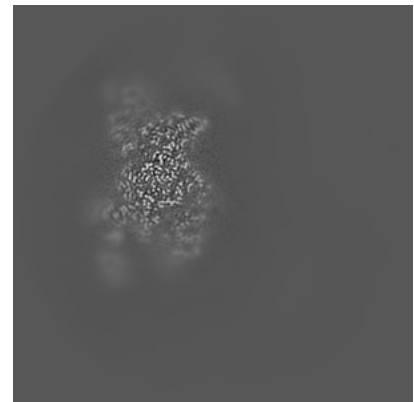
6.3.2 Raw map
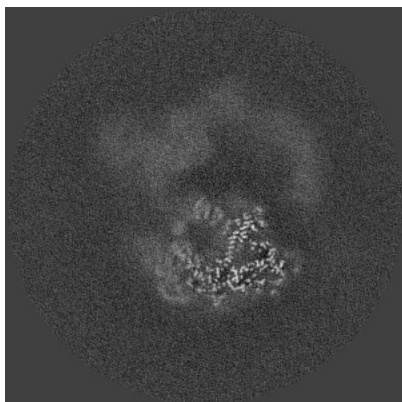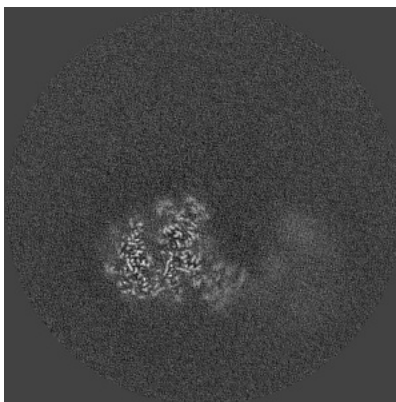
X Index: 163	Y Index: 232	Z Index: 138
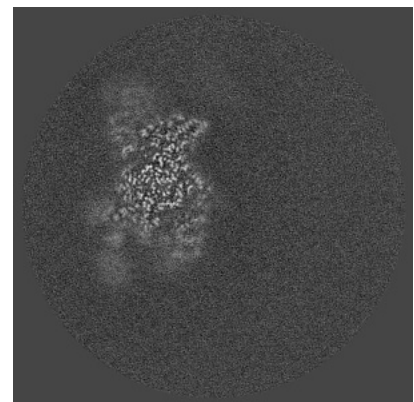
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
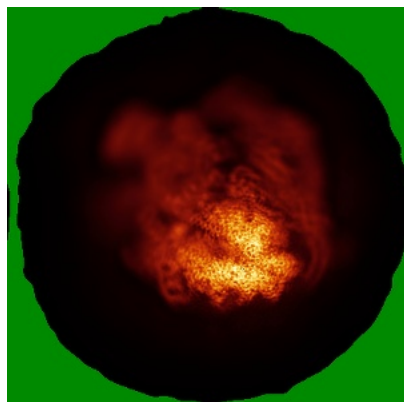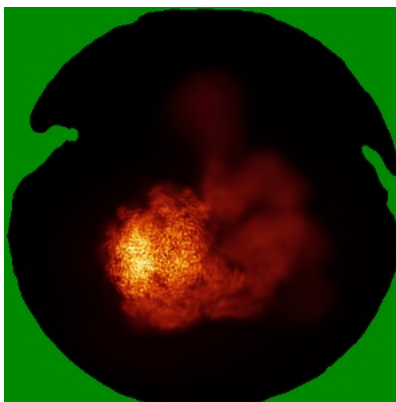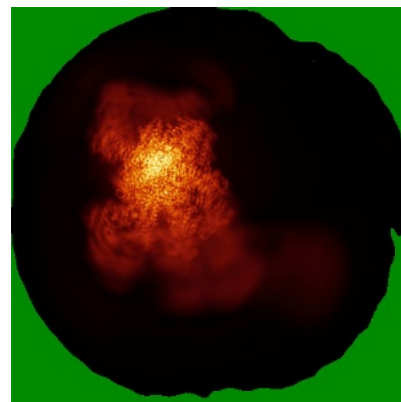
X Y Z

6.4.2 Raw map

X Y Z
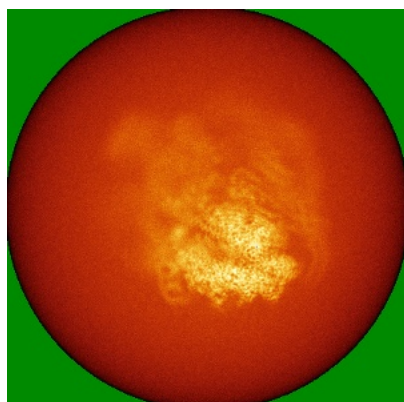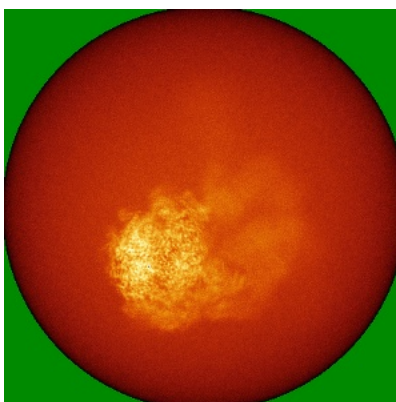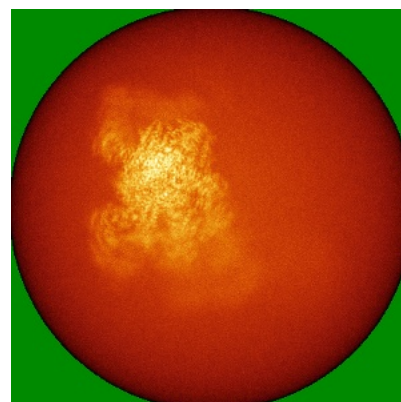
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
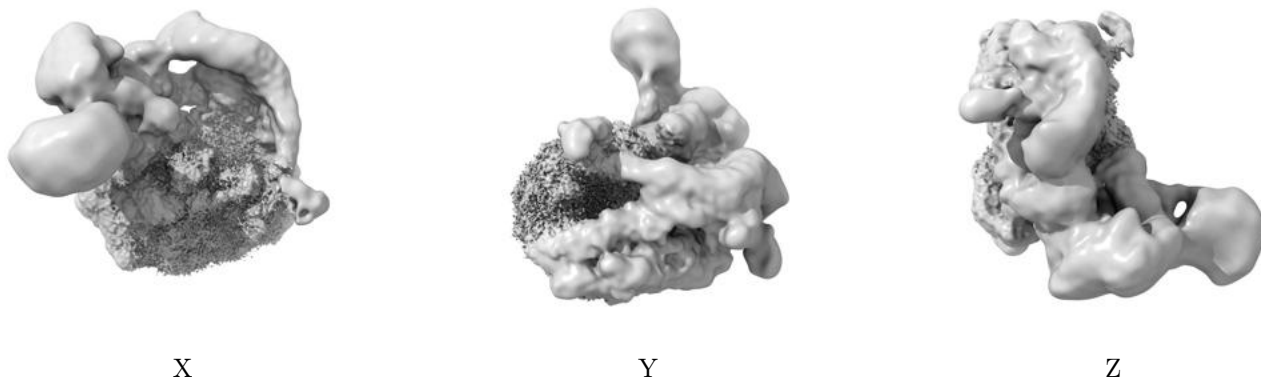
The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X   Y   Z
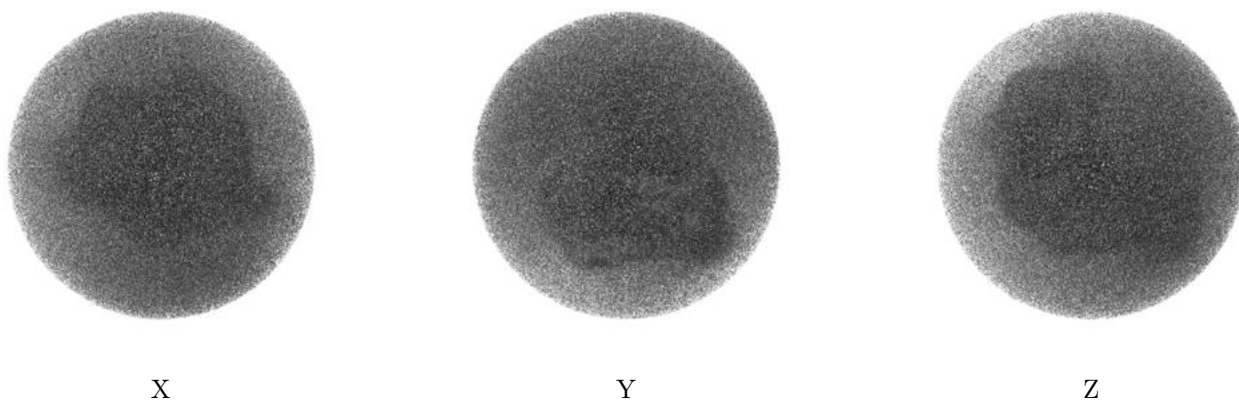
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
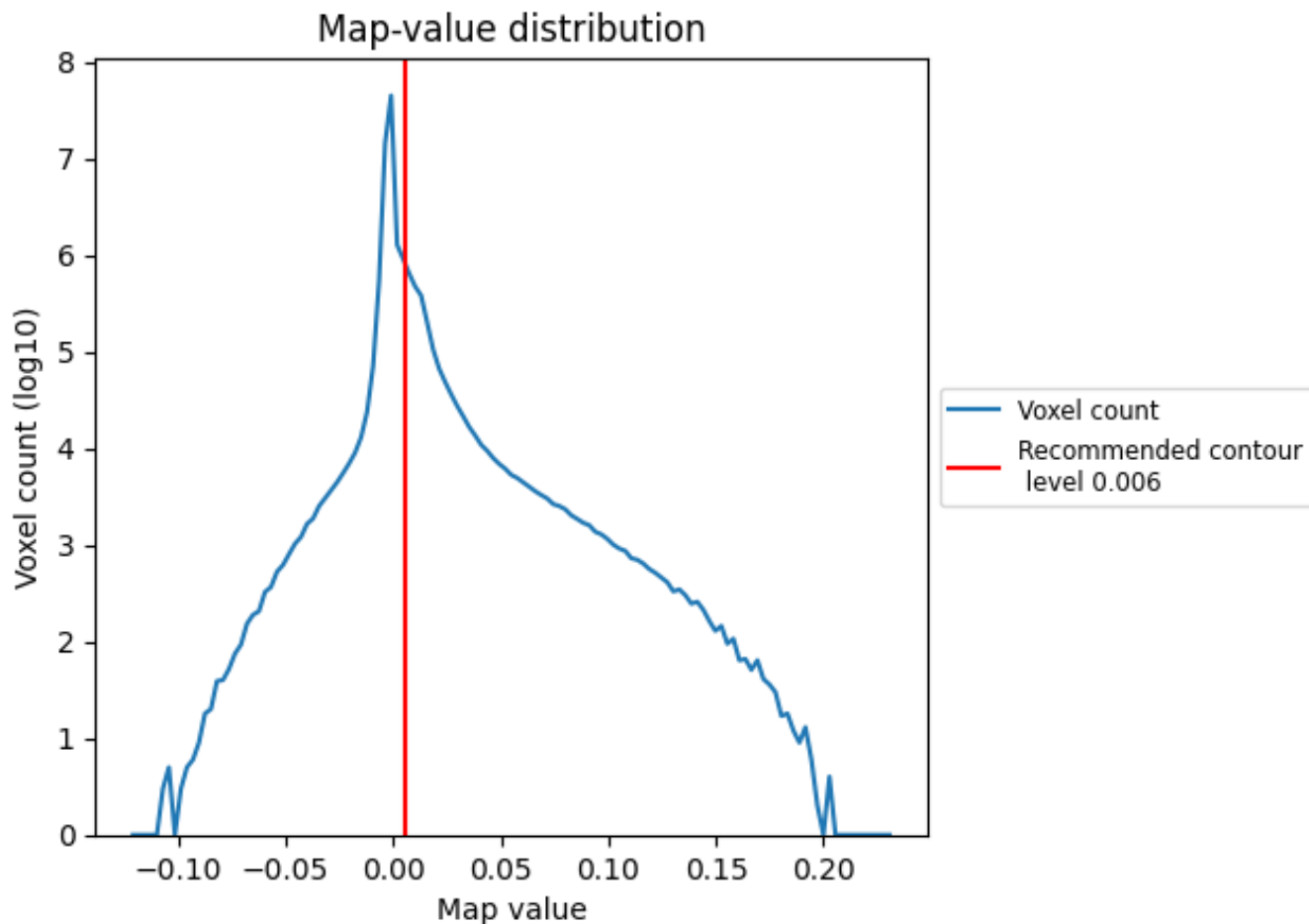
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
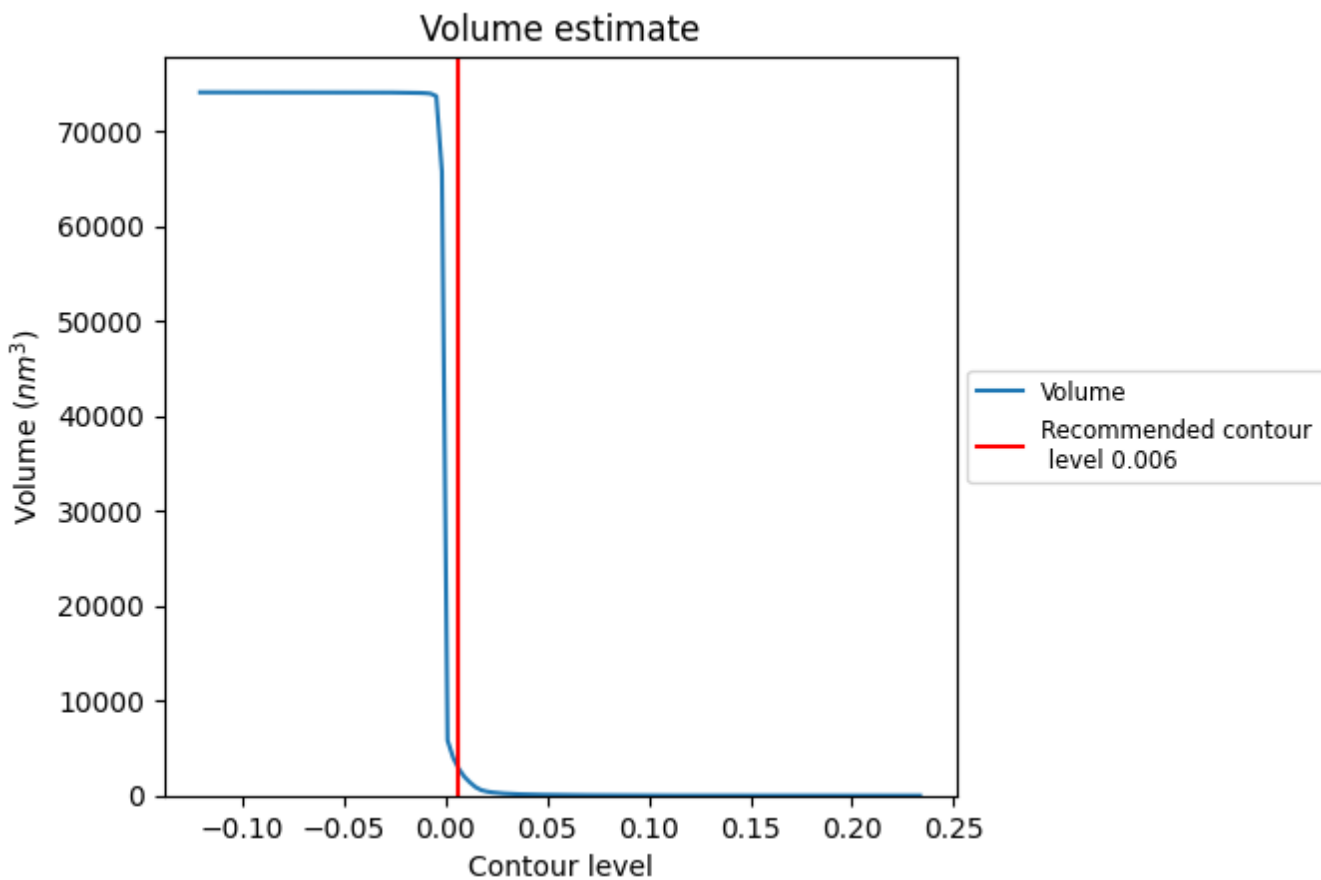
The volume at the recommended contour level is 2978 nm^3; this corresponds to an approximate mass of 2690 kDa.

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　ⓘ
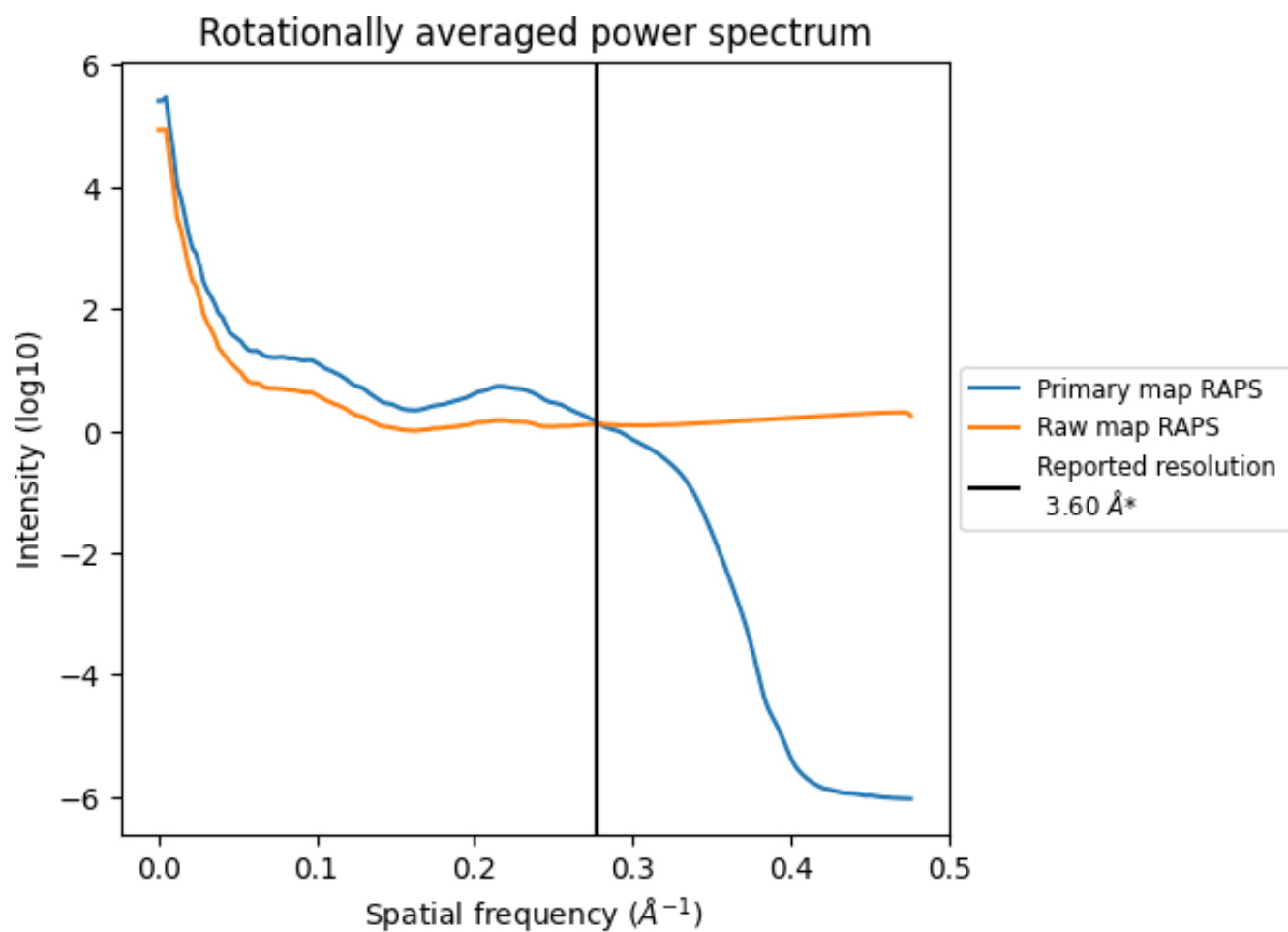
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ
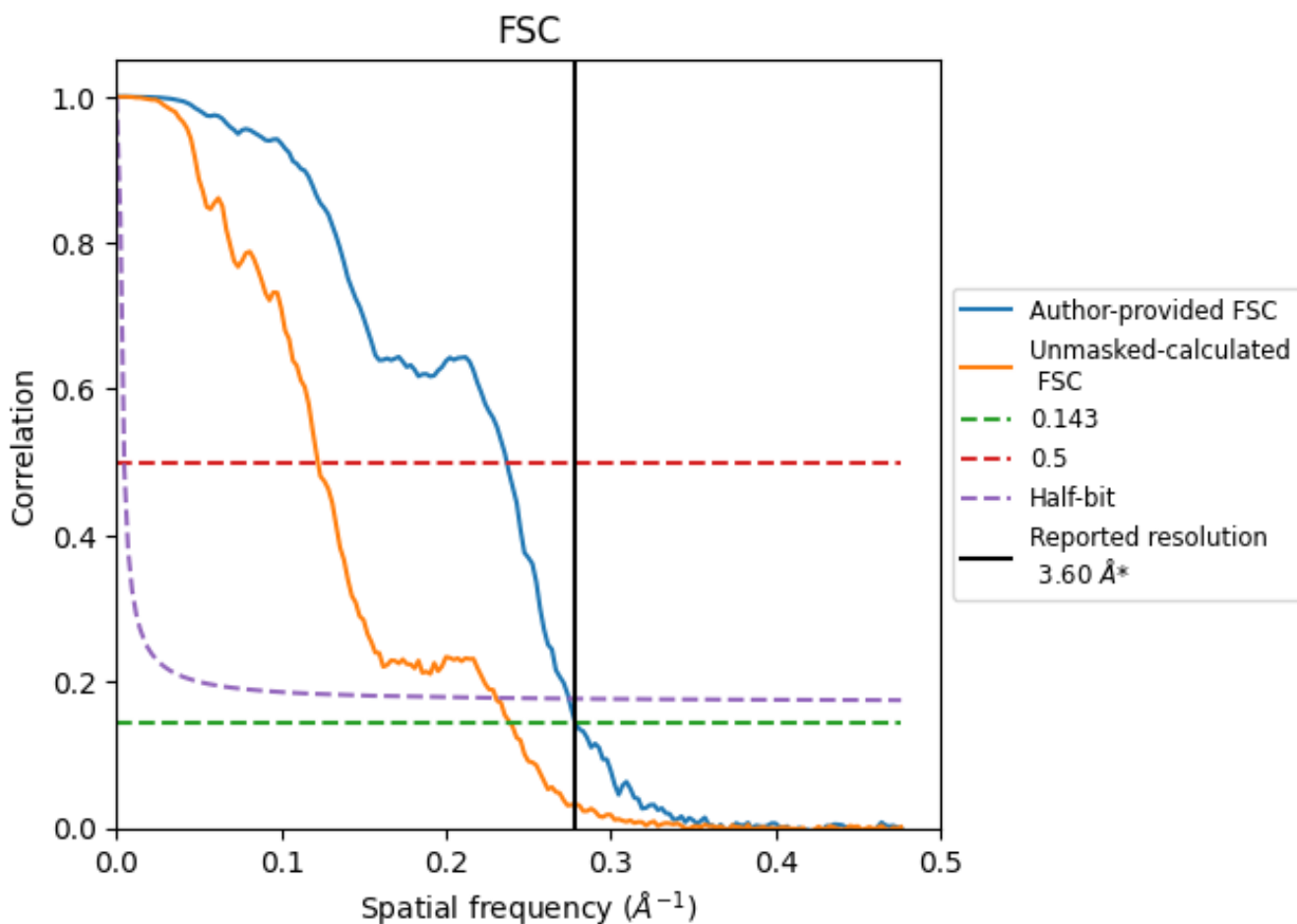
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
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 ⓘ

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 ⓘ

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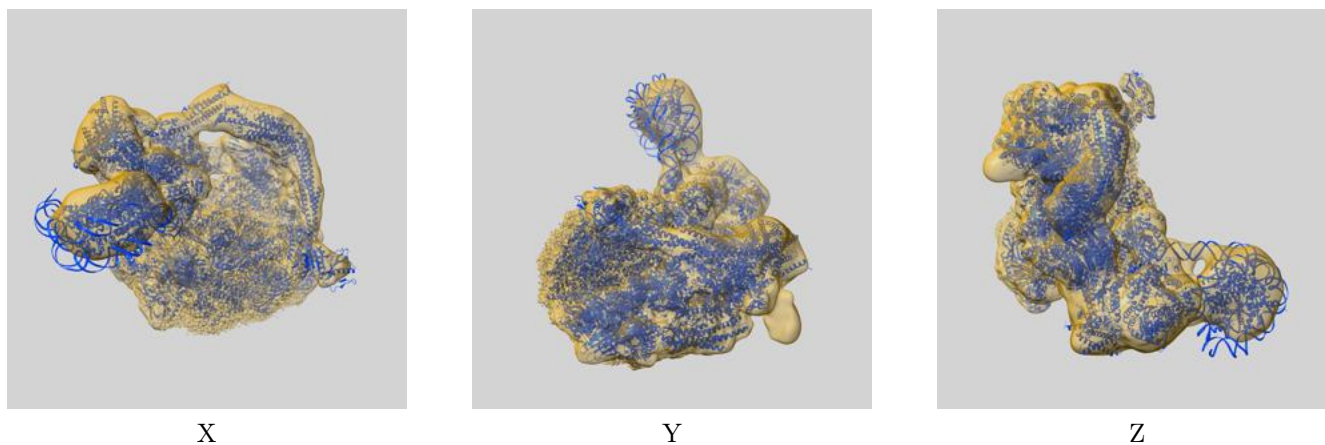
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X Y Z
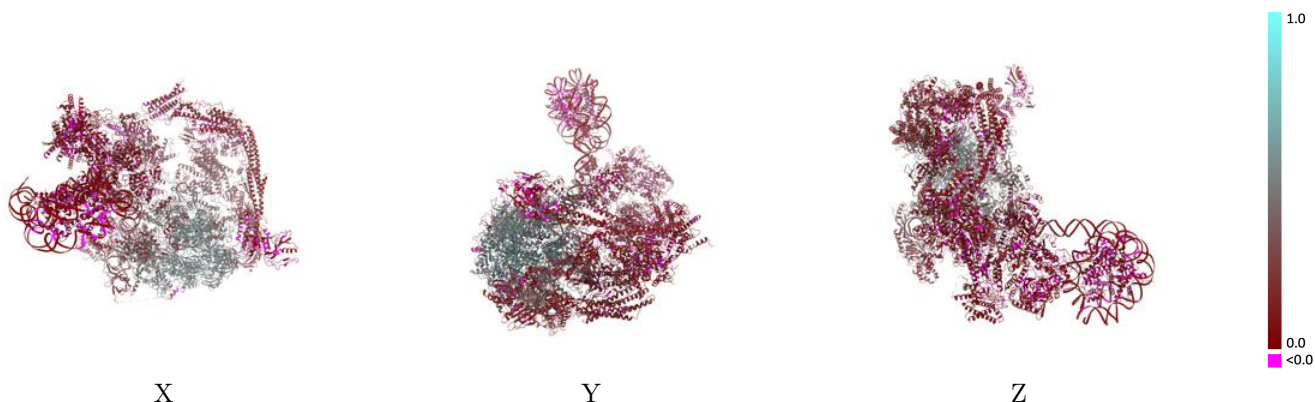
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ

X Y Z
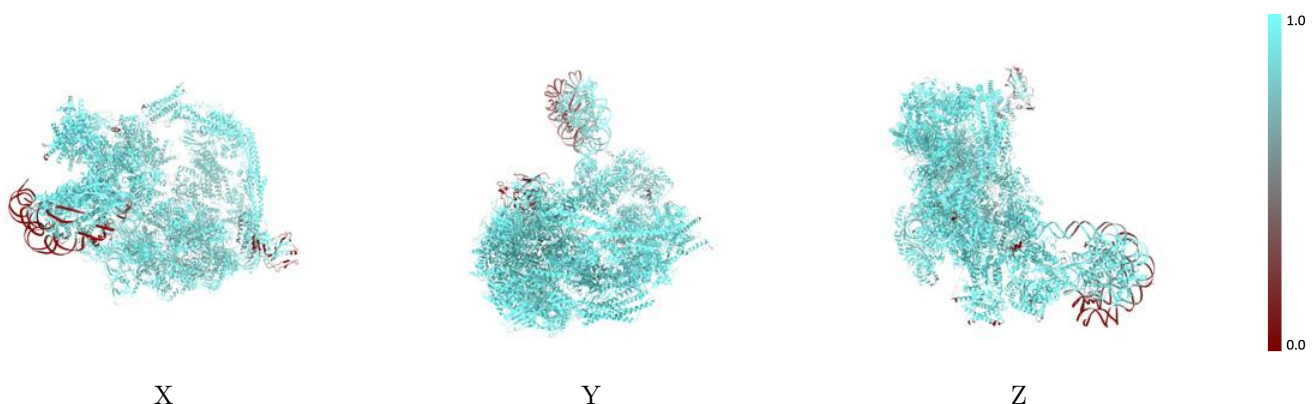
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4　Atom inclusion　ⓘ
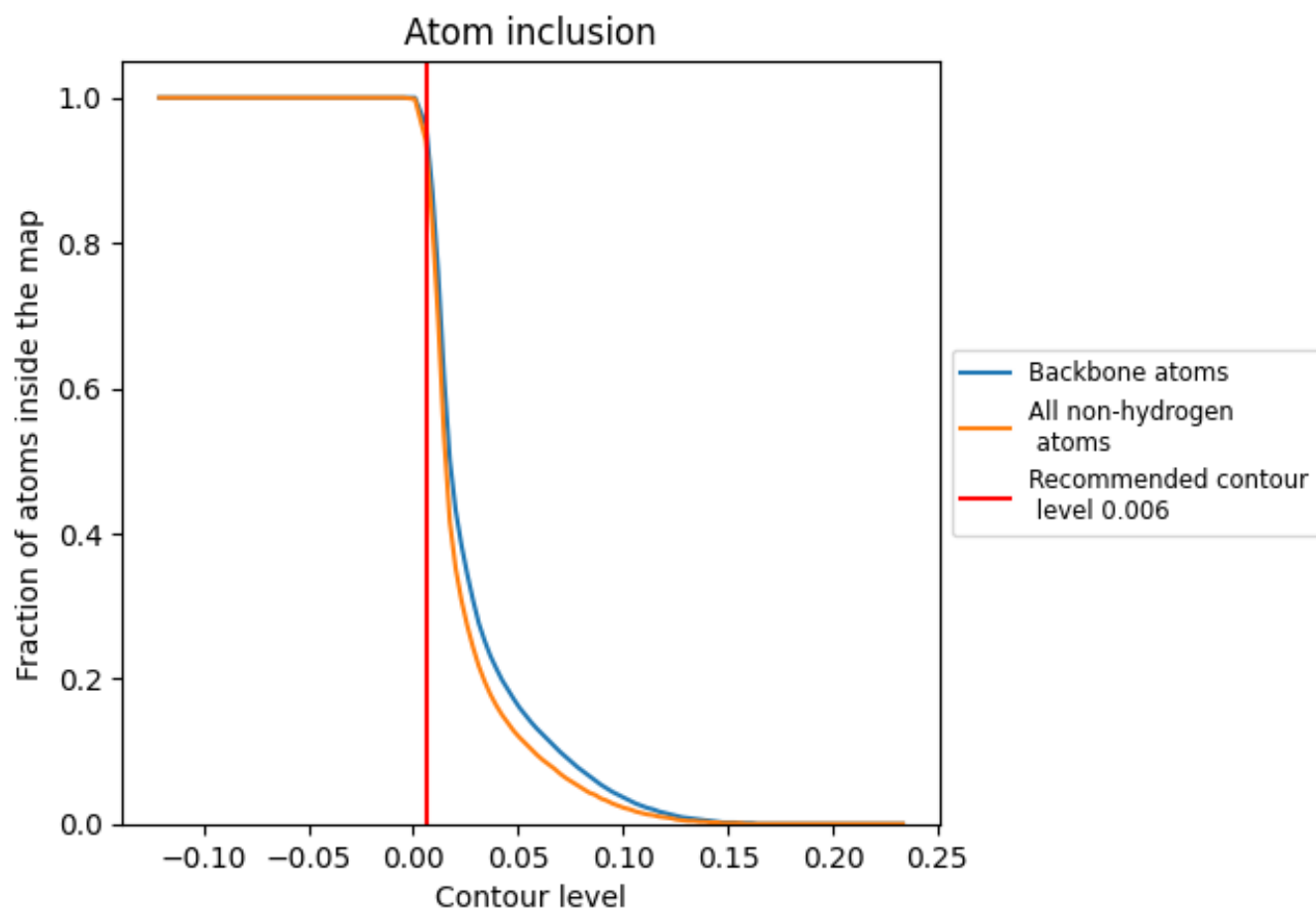
At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

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

1.0

0.0
<0.0

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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