wwPDB EM Validation Summary Report (i)

Dec 19, 2022 – 11:14 am GMT

PDB ID	:	7NKY
EMDB ID	:	EMD-12450
Title	:	RNA Polymerase II-Spt4/5-nucleosome-FACT structure
Authors	:	Farnung, L.; Ochmann, M.; Engeholm, M.; Cramer, P.
Deposited on	:	2021-02-19
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

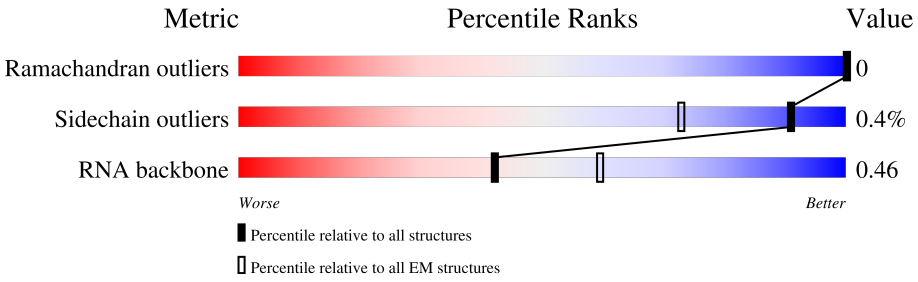
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



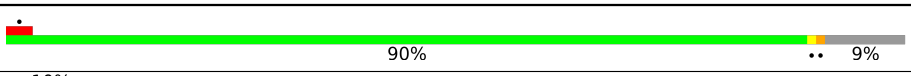
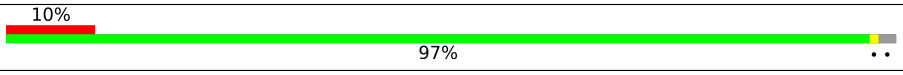
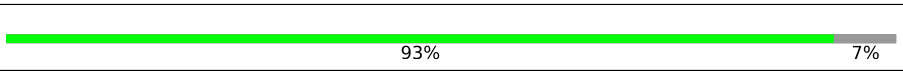
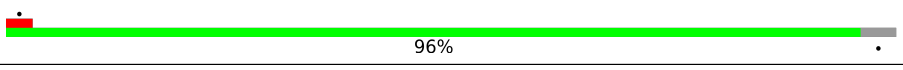
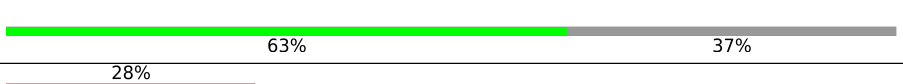
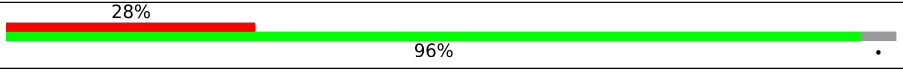
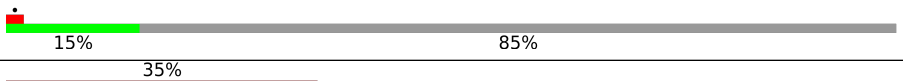
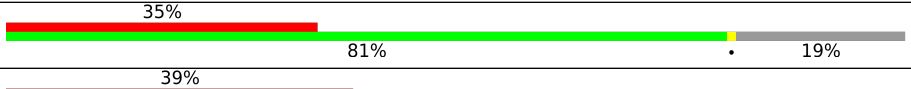
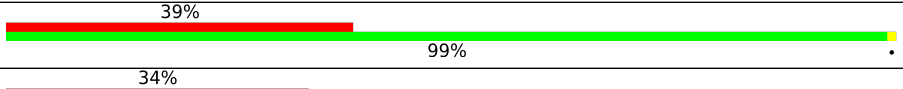
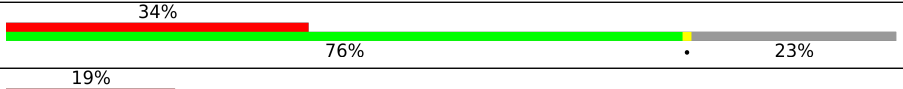
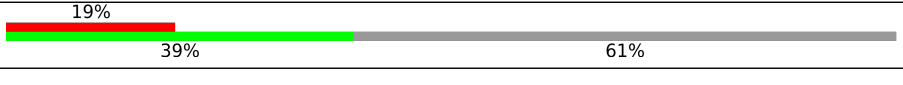
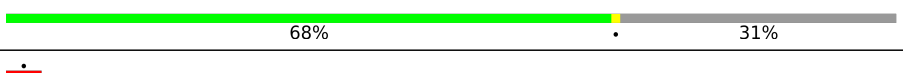
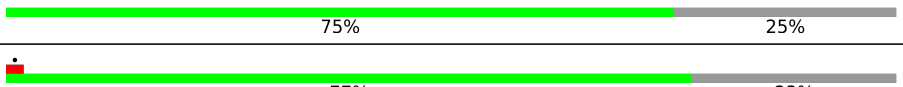
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	P	16	12% 62% 38%
2	N	138	99%
3	T	148	97%
4	A	1733	81% 19%
5	B	1224	91% 9%
6	C	318	82% 17%
7	E	215	99%
8	F	155	55% 44%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	
14	Y	102	
15	Z	1064	
16	D	221	
17	G	171	
18	O	552	
19	Q	1035	
20	a	136	
20	e	136	
21	b	103	
21	f	103	
22	c	130	
22	g	130	
23	d	123	
23	h	123	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 51842 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 RNA chain called RNA (5'-R(P*UP*CP*UP*UP*UP*UP*AP*UP*UP*UP *UP*UP*UP*CP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	P	16	325	146	40	123	16	0	0

- Molecule 2 is a DNA chain called DNA (138-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	N	138	2843	1346	526	833	138	0	0

- Molecule 3 is a DNA chain called DNA (148-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	T	148	3022	1434	567	874	147	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1410	11092	6987	1941	2102	62	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1116	8865	5611	1559	1640	55	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	265	2086	1312	347	414	13	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	44	Total	C	N	O	S	0	0
			351	217	70	60	4		

- Molecule 14 is a protein called Chromatin elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	98	Total	C	N	O	S	0	0
			739	461	126	142	10		

- Molecule 15 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	156	Total	C	N	O	S	0	0
			1252	804	224	221	3		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	18	PHE	VAL	conflict	UNP A0A6L0ZFJ2
Z	98	THR	SER	conflict	UNP A0A6L0ZFJ2
Z	176	GLU	ASP	conflict	UNP A0A6L0ZFJ2
Z	376	LEU	LYS	conflict	UNP A0A6L0ZFJ2
Z	1064	PHE	-	expression tag	UNP A0A6L0ZFJ2

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	180	Total	C	N	O	S	0	0
			1444	893	257	291	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 18 is a protein called FACT complex subunit POB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	427	Total	C	N	O	S	0	0
			3481	2204	606	665	6		

- Molecule 19 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	404	Total	C	N	O	S	0	0
			3264	2074	555	624	11		

- Molecule 20 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	88	Total	C	N	O	S	0	0
			720	456	135	126	3		
20	e	94	Total	C	N	O	S	0	0
			775	490	149	133	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	conflict	UNP P84233
e	102	ALA	GLY	conflict	UNP P84233

- Molecule 21 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
21	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 22 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	c	102	Total	C	N	O	0	0
			786	495	153	138		
22	g	97	Total	C	N	O	0	0
			747	468	148	131		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 23 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	95	Total	C	N	O	S	0	0
			745	469	134	140	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	conflict	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	conflict	UNP P02281

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Zn	0
			2	2	
24	B	1	Total	Zn	0
			1	1	
24	C	1	Total	Zn	0
			1	1	
24	I	2	Total	Zn	0
			2	2	
24	J	1	Total	Zn	0
			1	1	
24	L	1	Total	Zn	0
			1	1	
24	Y	1	Total	Zn	0
			1	1	

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

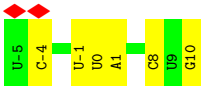
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

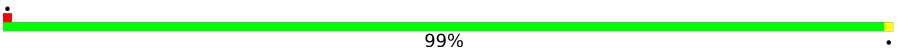
• Molecule 1: RNA (5'-R(P*UP*CP*UP*UP*UP*UP*AP*UP*UP*UP*UP*UP*UP*CP*UP*G)-3')

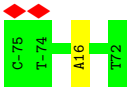
Chain P:



• Molecule 2: DNA (138-MER)

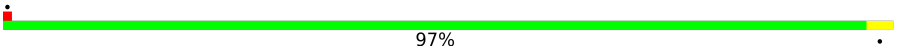
Chain N:

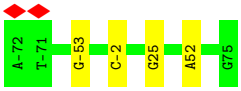




• Molecule 3: DNA (148-MER)

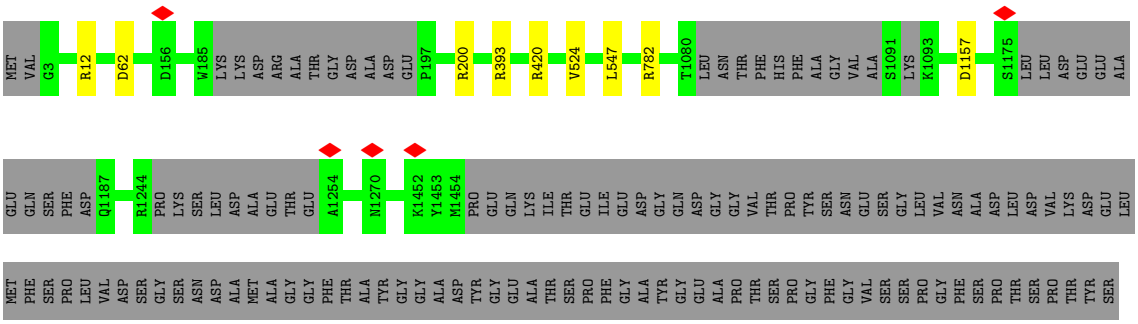
Chain T:

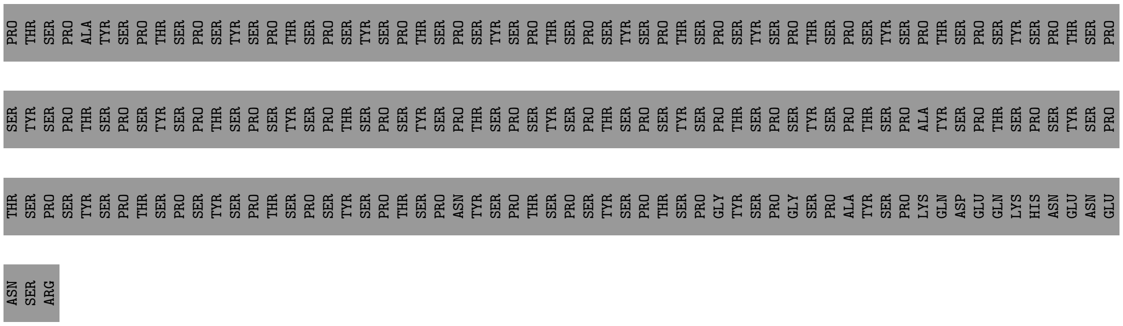




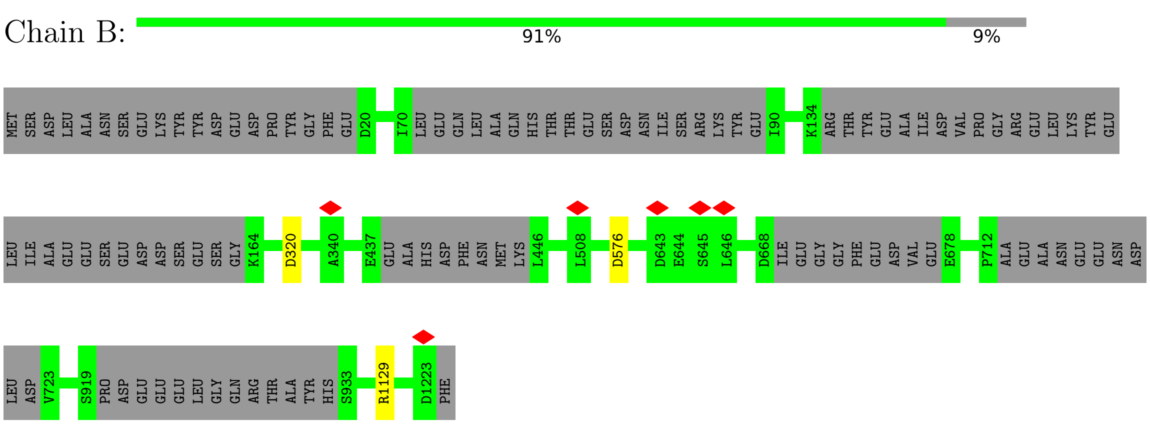
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A:

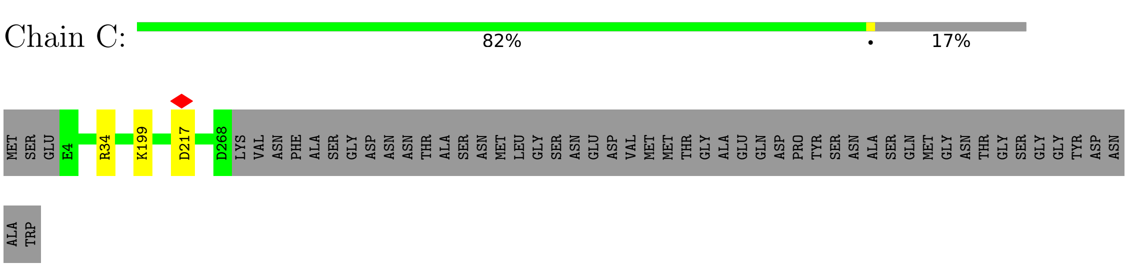




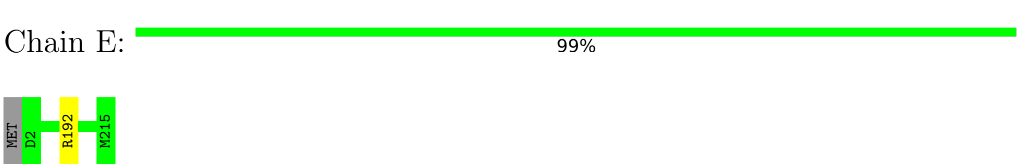
• Molecule 5: DNA-directed RNA polymerase II subunit RPB2



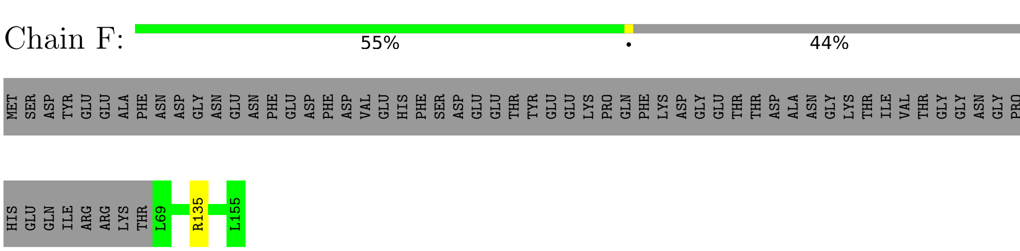
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

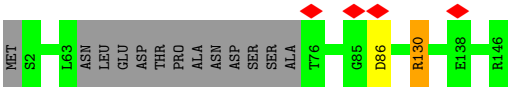


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



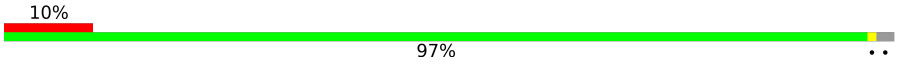
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

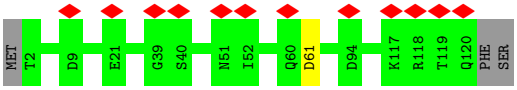
Chain H:



• Molecule 10: DNA-directed RNA polymerase II subunit RPB9

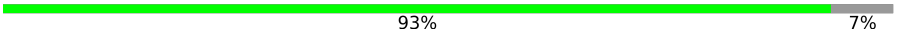
Chain I:





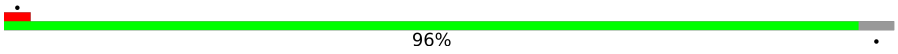
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

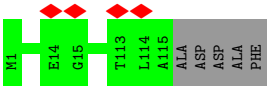
Chain J:



• Molecule 12: DNA-directed RNA polymerase II subunit RPB11

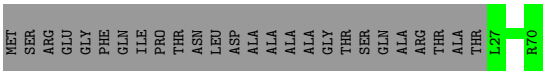
Chain K:





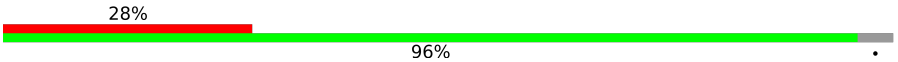
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

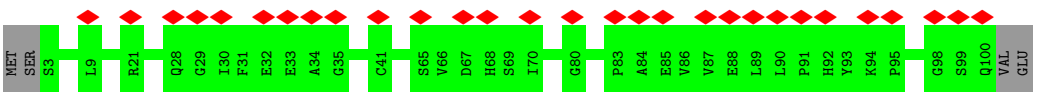
Chain L:



• Molecule 14: Chromatin elongation factor SPT4

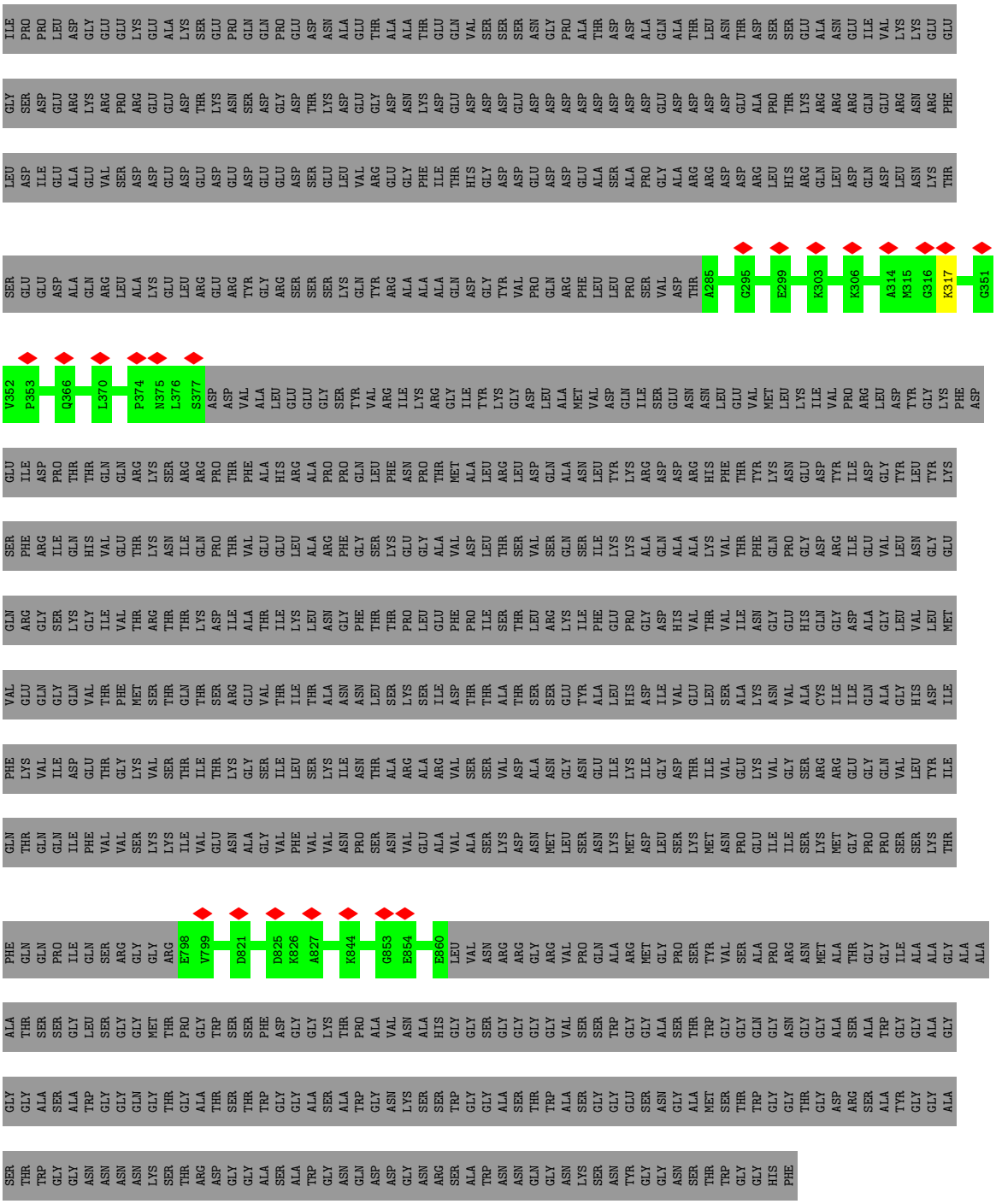
Chain Y:





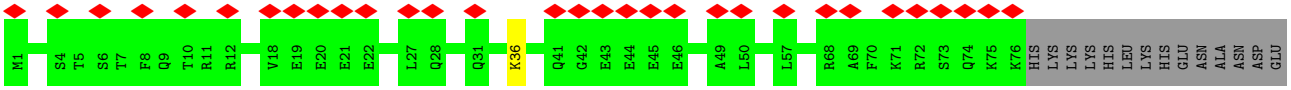
• Molecule 15: Transcription elongation factor SPT5

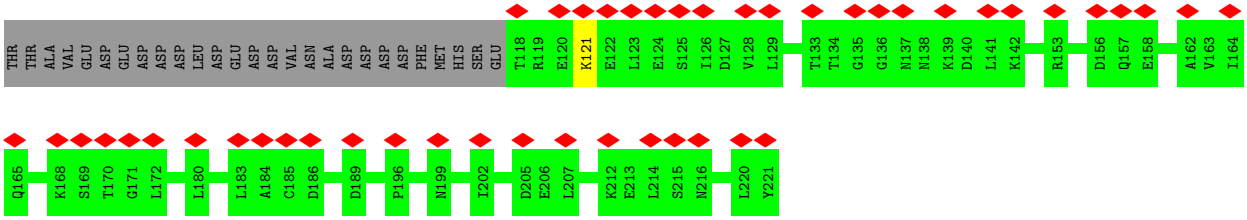
Chain Z:



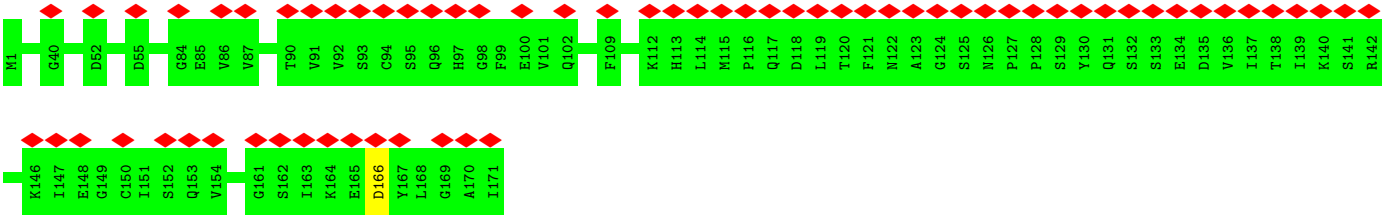
• Molecule 16: DNA-directed RNA polymerase II subunit RPB4

Chain D:

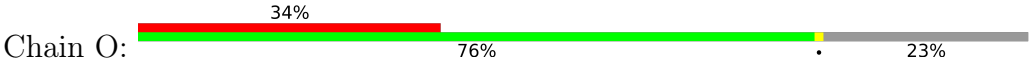


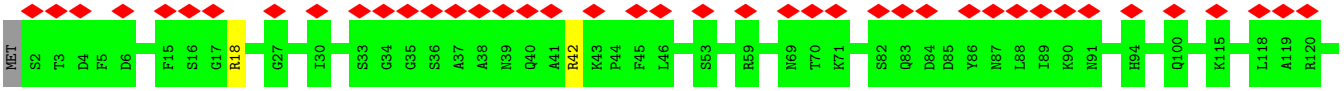


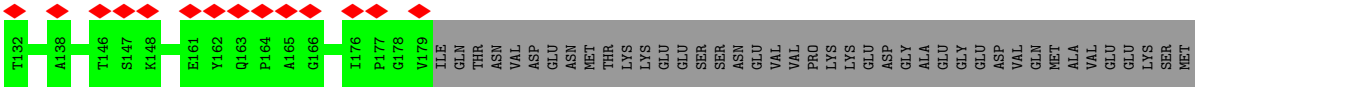
• Molecule 17: DNA-directed RNA polymerase II subunit RPB7

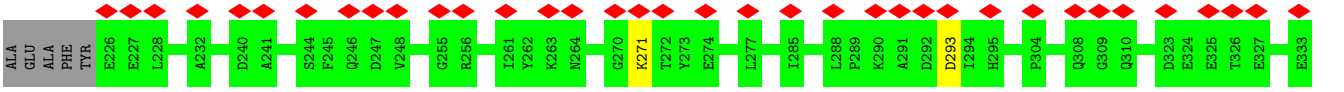


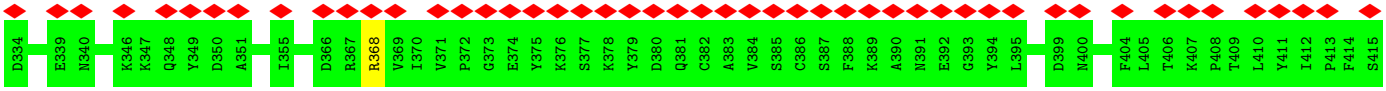
• Molecule 18: FACT complex subunit POB3

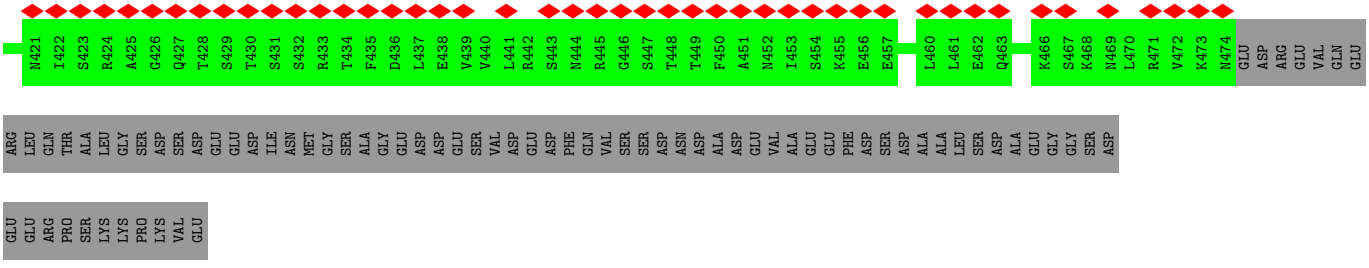




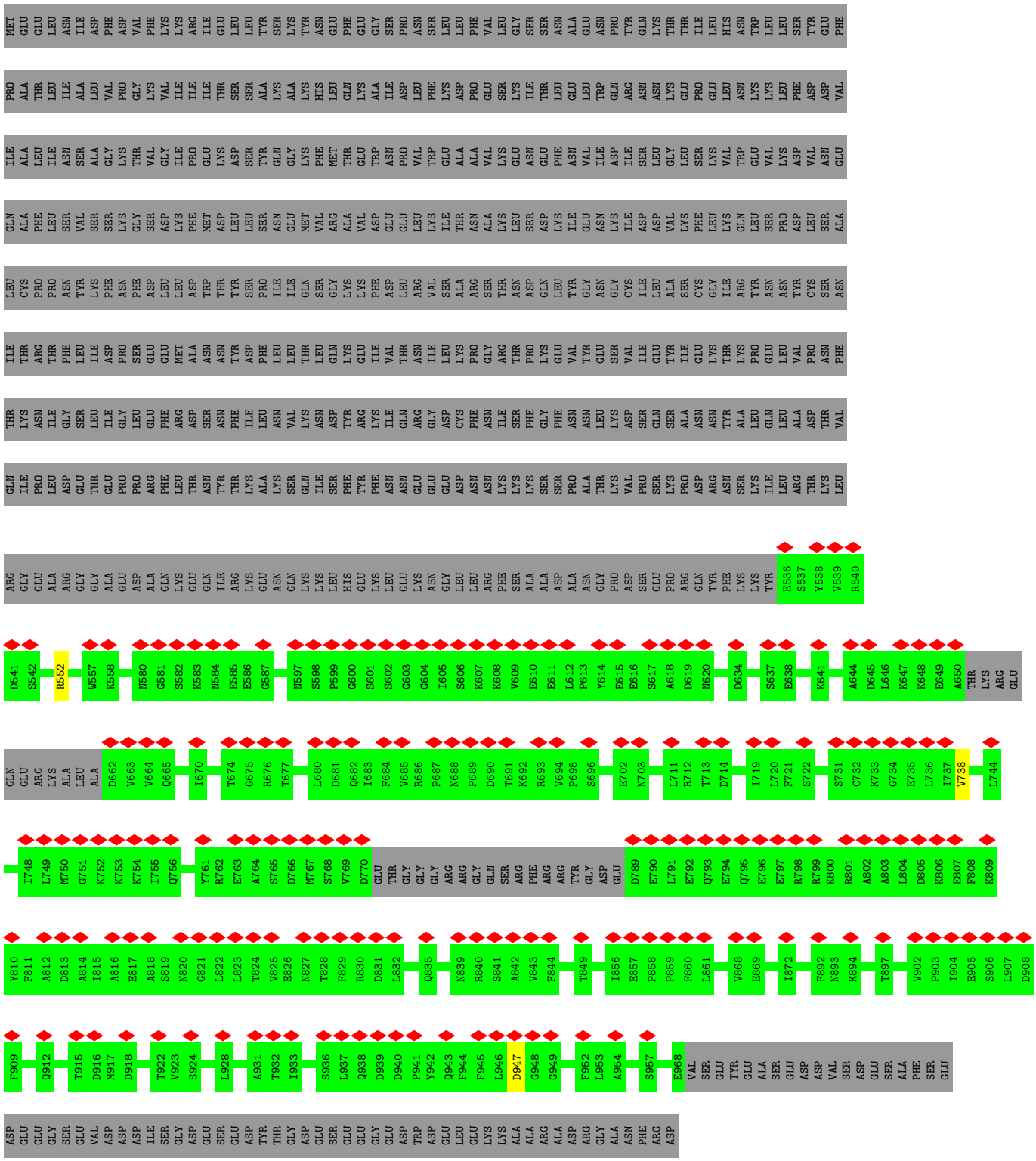






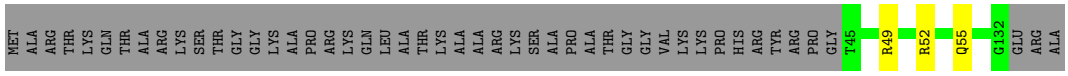


• Molecule 19: FACT complex subunit SPT16



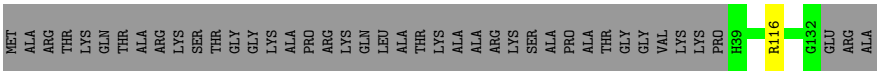
• Molecule 20: Histone H3.2

Chain a:



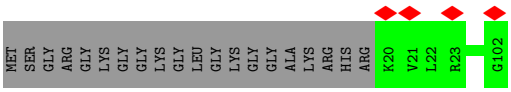
• Molecule 20: Histone H3.2

Chain e:



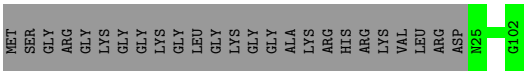
• Molecule 21: Histone H4

Chain b:



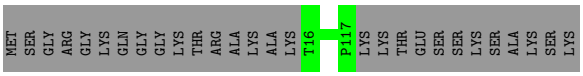
• Molecule 21: Histone H4

Chain f:



• Molecule 22: Histone H2A type 1

Chain c:

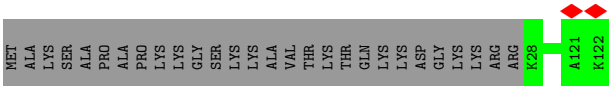


• Molecule 22: Histone H2A type 1

Chain g:

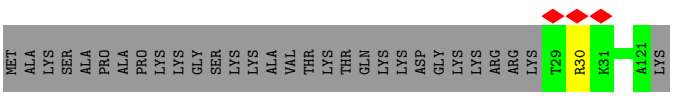
• Molecule 23: Histone H2B 1.1

Chain d:



• Molecule 23: Histone H2B 1.1

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47138	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 ($e^-/Å^2$)	40.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0023	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

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	P	0.25	0/358	0.79	0/552
2	N	0.75	0/3189	1.03	1/4922 (0.0%)
3	T	0.79	0/3392	1.02	4/5229 (0.1%)
4	A	0.32	0/11289	0.66	3/15263 (0.0%)
5	B	0.32	0/9037	0.67	2/12184 (0.0%)
6	C	0.34	0/2124	0.65	1/2879 (0.0%)
7	E	0.32	0/1788	0.67	0/2406
8	F	0.32	0/717	0.71	0/967
9	H	0.33	0/1086	0.72	1/1470 (0.1%)
10	I	0.34	0/989	0.80	1/1331 (0.1%)
11	J	0.36	0/541	0.71	0/727
12	K	0.33	0/938	0.68	0/1267
13	L	0.28	0/353	0.74	0/468
14	Y	0.31	0/755	0.68	0/1021
15	Z	0.34	0/1271	0.71	0/1702
16	D	0.36	0/1454	0.74	0/1949
17	G	0.31	0/1368	0.68	1/1844 (0.1%)
18	O	0.33	0/3550	0.70	1/4788 (0.0%)
19	Q	0.33	0/3329	0.70	1/4501 (0.0%)
20	a	0.36	0/728	0.76	0/977
20	e	0.30	0/786	0.70	0/1055
21	b	0.36	0/669	0.74	0/894
21	f	0.30	0/626	0.69	0/837
22	c	0.31	0/796	0.65	0/1077
22	g	0.29	0/756	0.68	0/1020
23	d	0.33	0/756	0.67	0/1015
23	h	0.31	0/737	0.61	0/993
All	All	0.41	0/53382	0.74	16/73338 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	3
6	C	0	1
8	F	0	1
9	H	0	1
19	Q	0	1
20	a	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	O	293	ASP	CB-CG-OD1	7.25	124.83	118.30
4	A	1157	ASP	CB-CG-OD1	6.65	124.29	118.30
2	N	16	DA	O4'-C1'-N9	6.08	112.25	108.00
19	Q	947	ASP	CB-CG-OD1	5.97	123.67	118.30
3	T	52	DA	O4'-C1'-N9	5.93	112.15	108.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	12	ARG	Sidechain
4	A	524	VAL	Peptide
4	A	782	ARG	Sidechain
6	C	34	ARG	Sidechain
8	F	135	ARG	Sidechain

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	
4	A	1399/1733 (81%)	1330 (95%)	69 (5%)	0	100	100
5	B	1102/1224 (90%)	1056 (96%)	46 (4%)	0	100	100
6	C	263/318 (83%)	248 (94%)	15 (6%)	0	100	100
7	E	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
8	F	85/155 (55%)	80 (94%)	5 (6%)	0	100	100
9	H	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
10	I	117/122 (96%)	105 (90%)	12 (10%)	0	100	100
11	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
12	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
13	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
14	Y	96/102 (94%)	92 (96%)	4 (4%)	0	100	100
15	Z	152/1064 (14%)	143 (94%)	9 (6%)	0	100	100
16	D	176/221 (80%)	162 (92%)	14 (8%)	0	100	100
17	G	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
18	O	419/552 (76%)	390 (93%)	29 (7%)	0	100	100
19	Q	398/1035 (38%)	367 (92%)	31 (8%)	0	100	100
20	a	86/136 (63%)	86 (100%)	0	0	100	100
20	e	92/136 (68%)	91 (99%)	1 (1%)	0	100	100
21	b	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
21	f	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
22	c	100/130 (77%)	97 (97%)	3 (3%)	0	100	100
22	g	95/130 (73%)	95 (100%)	0	0	100	100
23	d	93/123 (76%)	92 (99%)	1 (1%)	0	100	100
23	h	91/123 (74%)	90 (99%)	1 (1%)	0	100	100
All	All	5649/8302 (68%)	5373 (95%)	276 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	
4	A	1233/1520 (81%)	1230 (100%)	3 (0%)	93	98
5	B	967/1061 (91%)	966 (100%)	1 (0%)	93	98
6	C	233/274 (85%)	232 (100%)	1 (0%)	91	95
7	E	196/197 (100%)	195 (100%)	1 (0%)	88	95
8	F	77/137 (56%)	77 (100%)	0	100	100
9	H	117/128 (91%)	116 (99%)	1 (1%)	78	91
10	I	113/116 (97%)	113 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	39/57 (68%)	39 (100%)	0	100	100
14	Y	82/87 (94%)	82 (100%)	0	100	100
15	Z	136/877 (16%)	135 (99%)	1 (1%)	84	94
16	D	161/200 (80%)	159 (99%)	2 (1%)	71	88
17	G	152/152 (100%)	152 (100%)	0	100	100
18	O	382/489 (78%)	378 (99%)	4 (1%)	76	90
19	Q	365/935 (39%)	364 (100%)	1 (0%)	92	96
20	a	77/111 (69%)	75 (97%)	2 (3%)	46	76
20	e	82/111 (74%)	81 (99%)	1 (1%)	71	88
21	b	68/79 (86%)	68 (100%)	0	100	100
21	f	63/79 (80%)	63 (100%)	0	100	100
22	c	81/102 (79%)	81 (100%)	0	100	100
22	g	75/102 (74%)	75 (100%)	0	100	100
23	d	81/103 (79%)	81 (100%)	0	100	100
23	h	79/103 (77%)	78 (99%)	1 (1%)	69	87
All	All	5018/7187 (70%)	4999 (100%)	19 (0%)	91	95

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Q	552	ARG
20	e	116	ARG
23	h	30	ARG
20	a	55	GLN
16	D	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	1187	ASN
5	B	1205	GLN
19	Q	682	GLN
5	B	763	GLN
4	A	1011	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	15/16 (93%)	5 (33%)	1 (6%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	-4	C
1	P	0	U
1	P	1	A
1	P	8	C
1	P	10	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	P	-1	U

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

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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	O	3
2	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	-65:DG	O3'	-54:DT	P	30.81
1	O	241:ALA	C	242:ILE	N	5.38
1	O	239:GLY	C	240:ASP	N	5.32
1	O	237:VAL	C	238:ALA	N	3.21

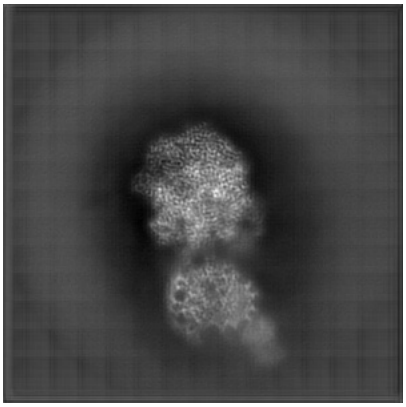
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12450. These allow visual inspection of the internal detail of the map and identification of artifacts.

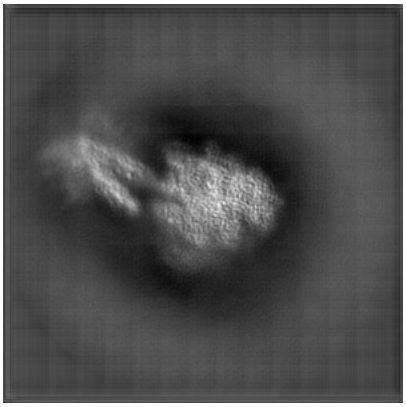
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

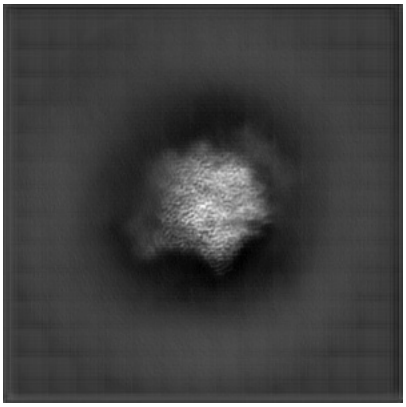
6.1.1 Primary map



X



Y

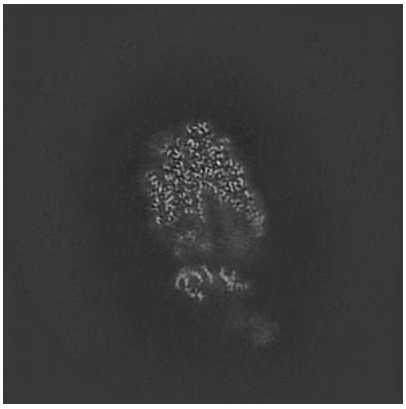


Z

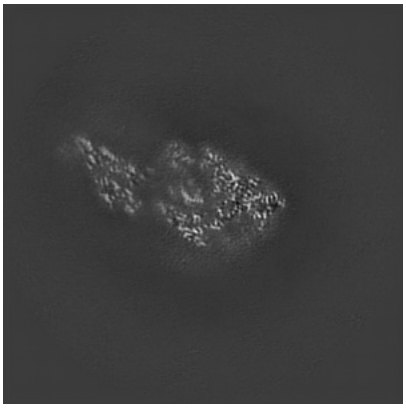
The images above show the map projected in three orthogonal directions.

6.2 Central slices

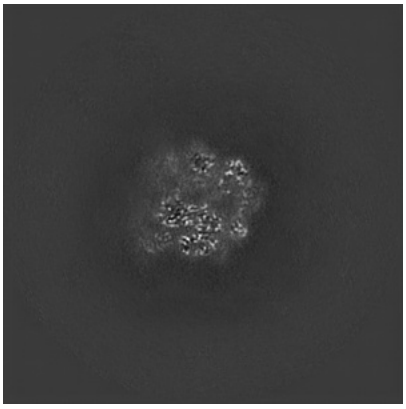
6.2.1 Primary map



X Index: 200



Y Index: 200

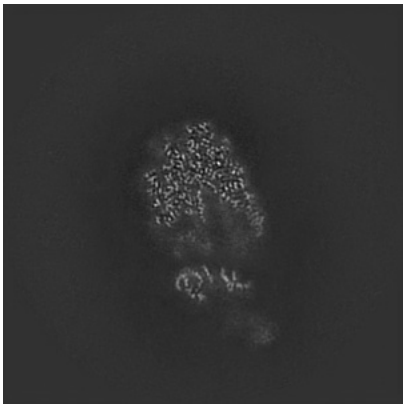


Z Index: 200

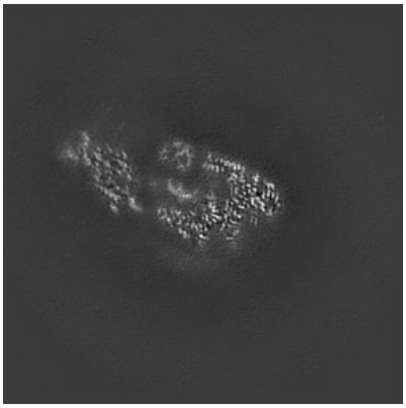
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

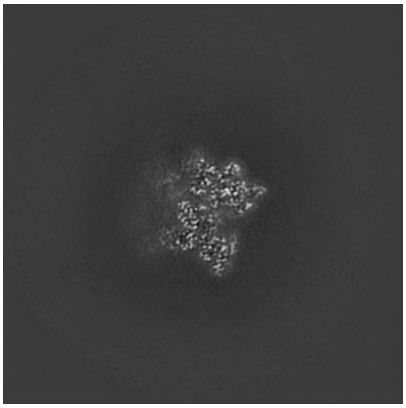
6.3.1 Primary map



X Index: 201



Y Index: 194



Z Index: 212

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

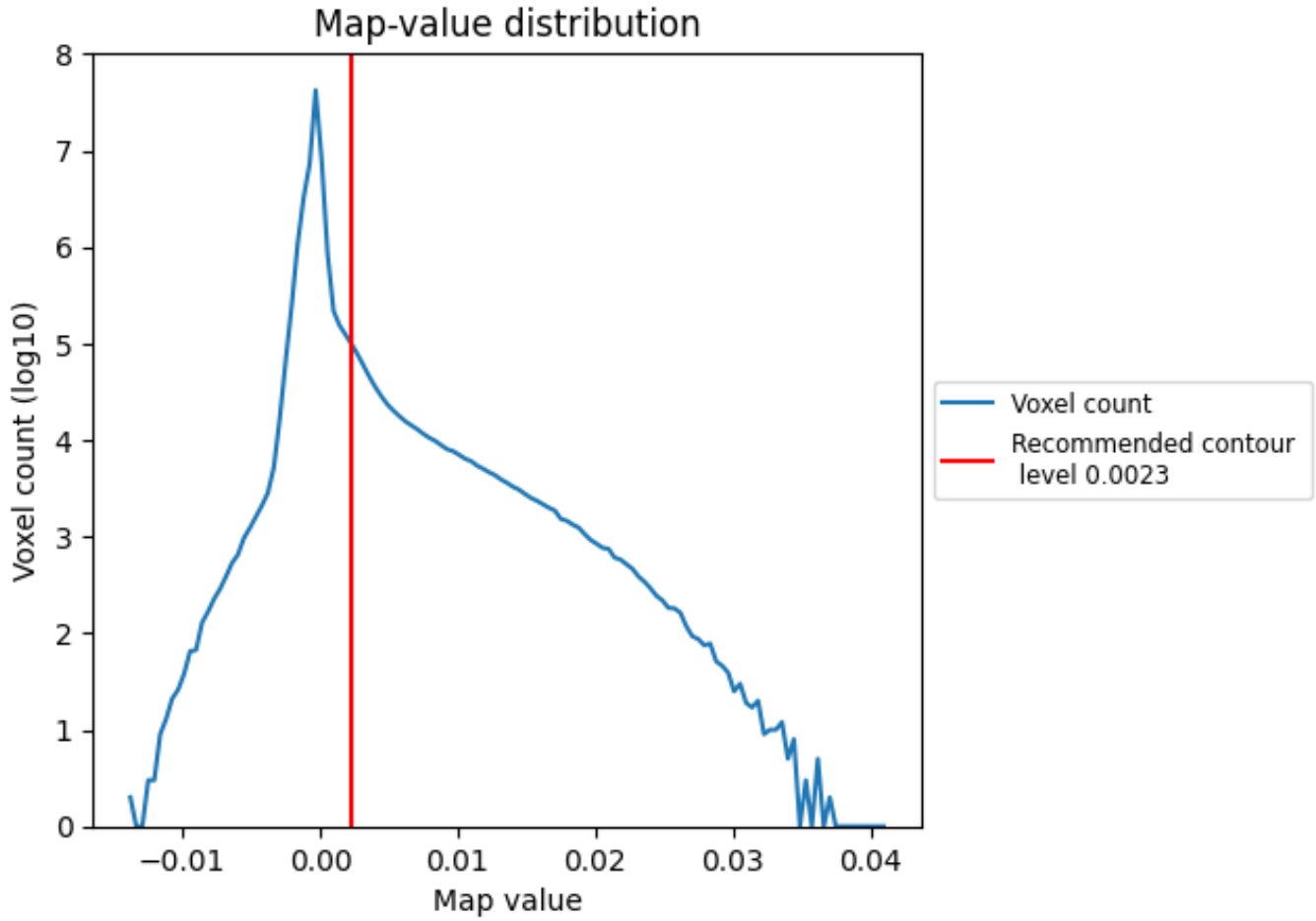
6.5 Mask visualisation (i)

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

7 Map analysis

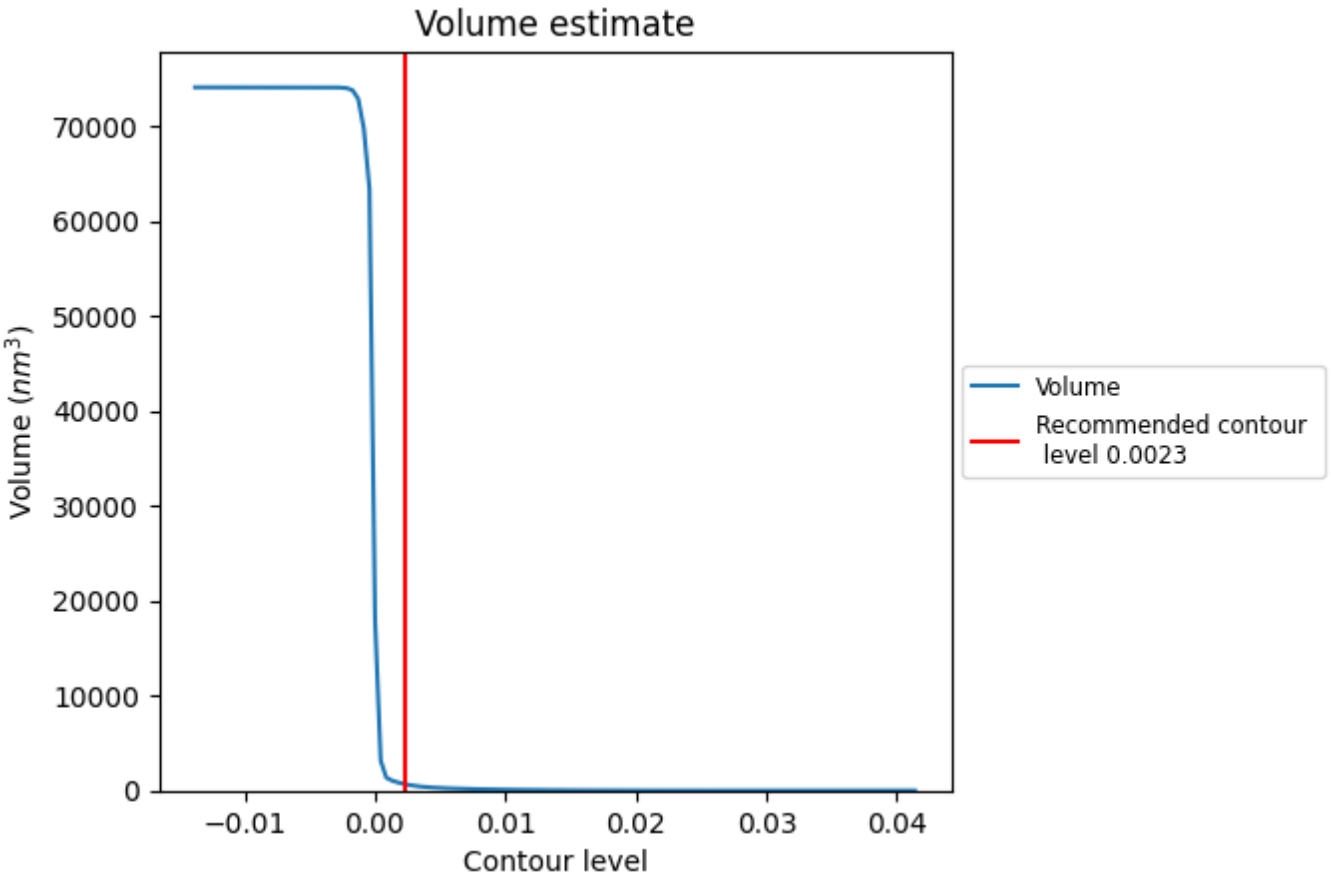
This section contains the results of statistical analysis of the map.

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.

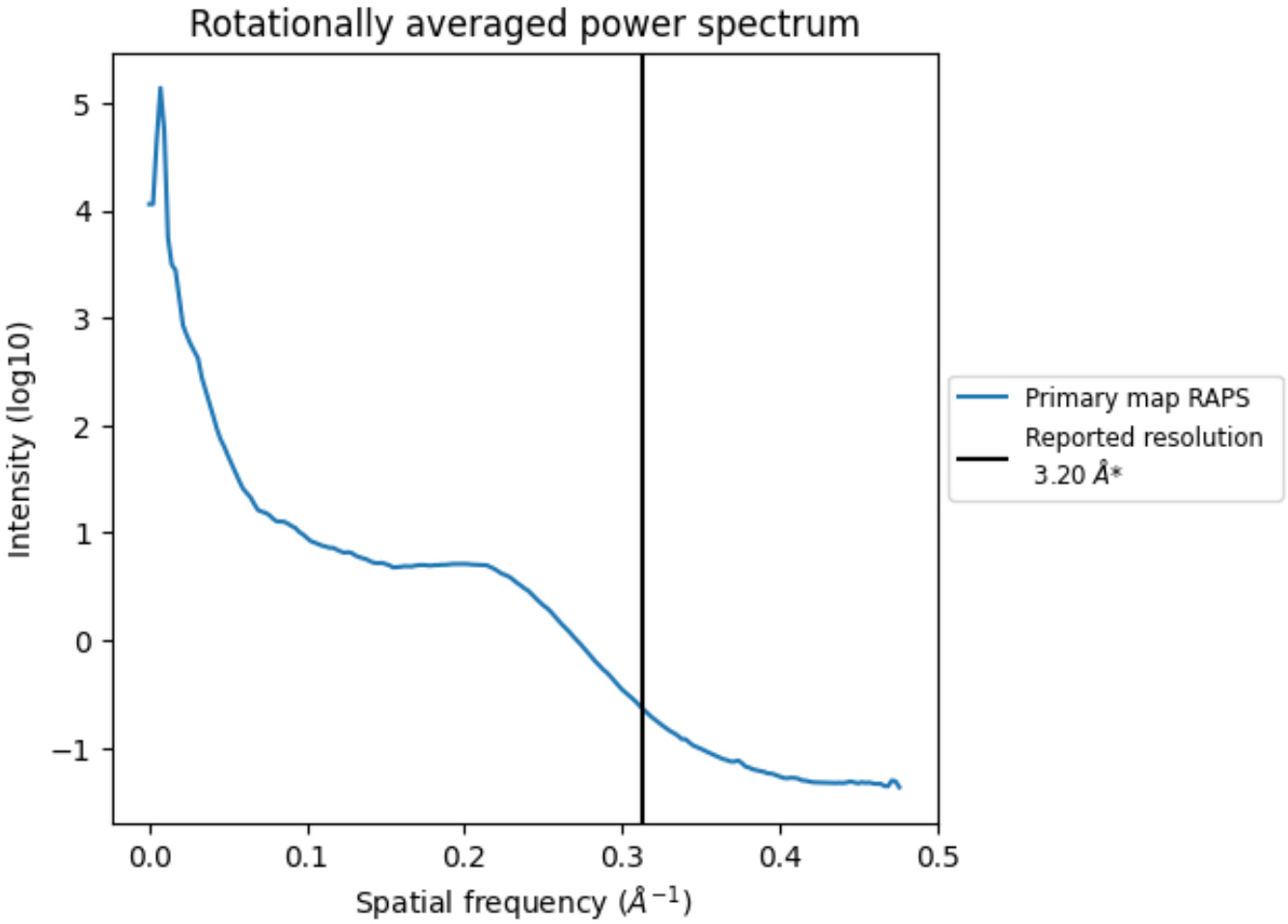
7.2 Volume estimate (i)



The volume at the recommended contour level is 679 nm^3; this corresponds to an approximate mass of 613 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

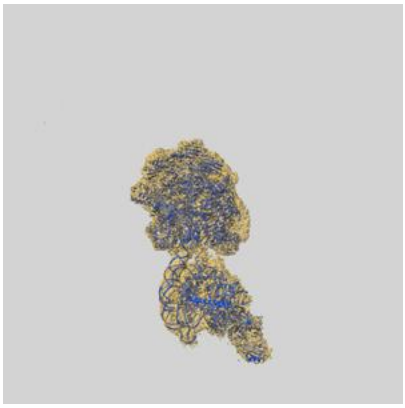
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

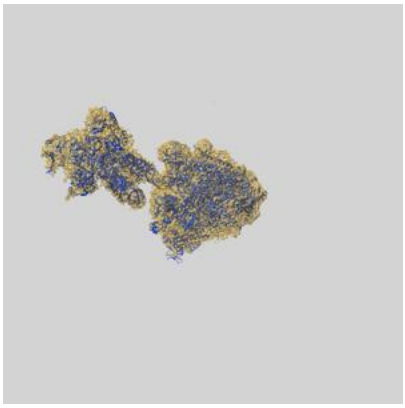
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12450 and PDB model 7NKY. Per-residue inclusion information can be found in section 3 on page 9.

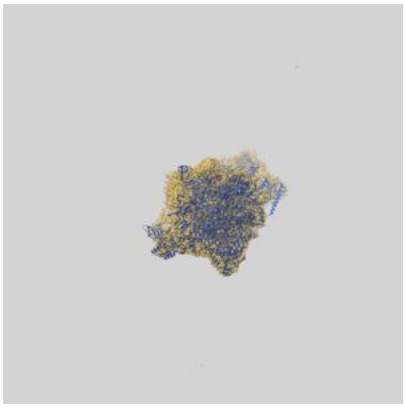
9.1 Map-model overlay



X



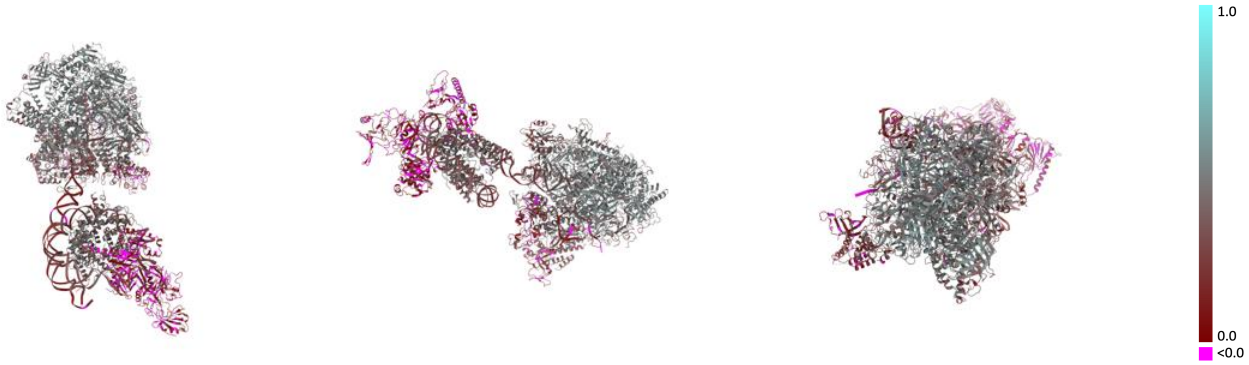
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0023 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.

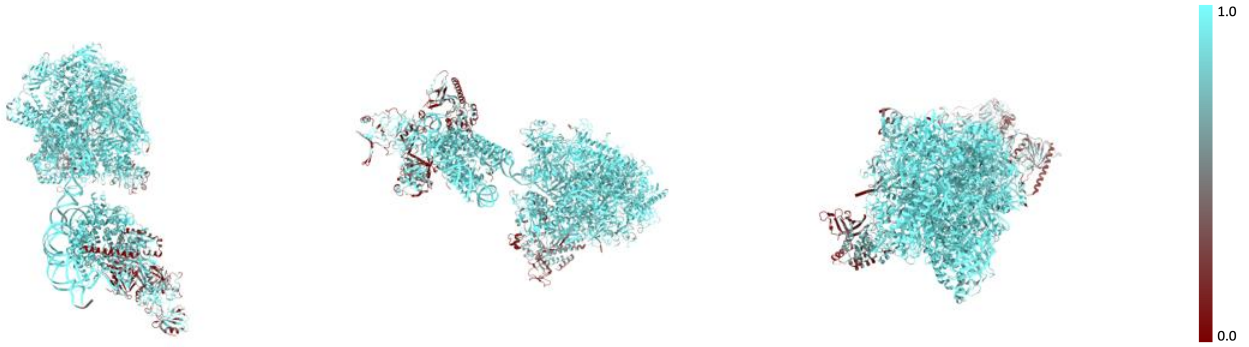
9.2 Q-score mapped to coordinate model



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.

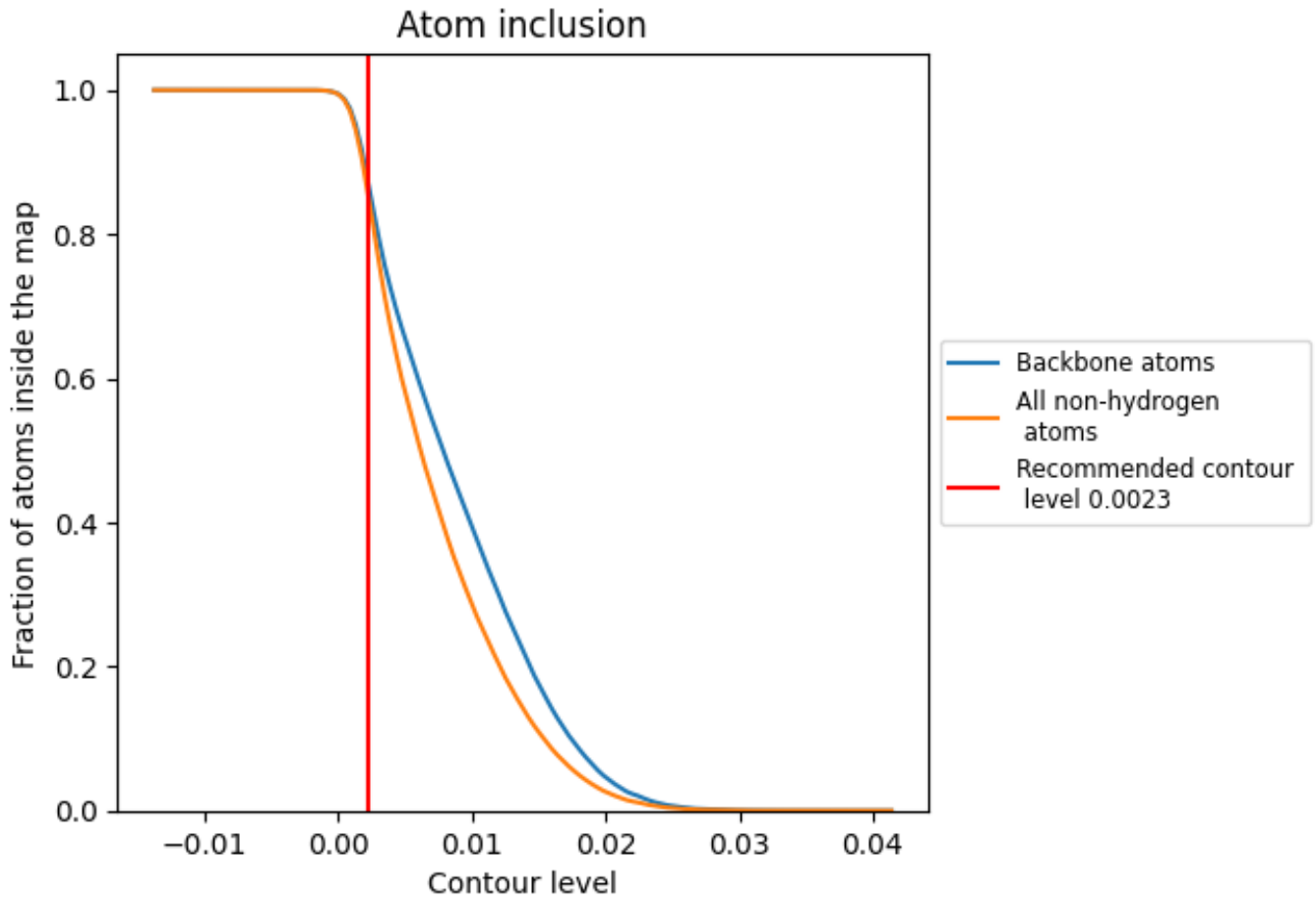
9.3 Atom inclusion mapped to coordinate model



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 (0.0023).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.0023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8459	0.3580
A	0.9506	0.4510
B	0.9661	0.4630
C	0.9495	0.4760
D	0.4676	0.2060
E	0.9555	0.4440
F	0.9389	0.4840
G	0.5121	0.2440
H	0.8913	0.4460
I	0.8256	0.3360
J	0.9807	0.4940
K	0.9261	0.4840
L	0.8997	0.3860
N	0.9121	0.2540
O	0.4988	0.1010
P	0.8062	0.2940
Q	0.4502	0.0840
T	0.9216	0.2670
Y	0.6442	0.1750
Z	0.7365	0.2450
a	0.9296	0.3960
b	0.9151	0.4240
c	0.9382	0.4350
d	0.9093	0.4130
e	0.9558	0.4050
f	0.9748	0.4390
g	0.9141	0.3900
h	0.9041	0.3910