



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 11:10 am GMT

PDB ID : 7NKX
EMDB ID : EMD-12449
Title : RNA polymerase II-Spt4/5-nucleosome-Chd1 structure
Authors : Farnung, L.; Ochmann, M.; Engholm, M.; Cramer, P.
Deposited on : 2021-02-19
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

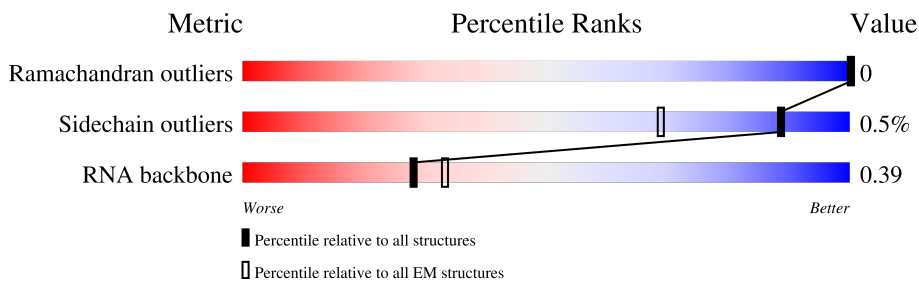
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.90 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	45% 80% 19%
2	B	1224	46% 90% 9%
3	C	318	28% 82% 17%
4	E	215	41% 98%
5	F	155	30% 55% 44%
6	H	146	36% 90% 9%
7	I	122	77% 95%
8	J	70	30% 93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	K	120	42% 93%
10	L	70	47% 63% 37%
11	a	136	31% 54% 44%
11	e	136	48% 71% 29%
12	b	103	40% 77% 22%
12	f	103	38% 76% 24%
13	c	130	36% 77% 21%
13	g	130	59% 71% 28%
14	d	123	31% 72% 25%
14	h	123	54% 73% 24%
15	T	185	37% 72% 25%
16	N	176	37% 71% 27%
17	W	1468	37% 42% 58%
18	P	69	12% 16% 7% 77%
19	Y	102	96% 96%
20	Z	1066	15% 15% 85%
21	D	221	81% 80% 19%
22	G	171	100% 98%

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 49720 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1409	11086	6984	1940	2100	62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

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

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	a	76	620	393	115	109	3	0	0
11	e	97	801	504	155	139	3	0	0

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 12 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	b	80	638	401	125	111	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 13 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	103	Total	C	N	O	0	0
			795	501	155	139		
13	g	93	Total	C	N	O	0	0
			718	450	142	126		

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 14 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
14	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 15 is a DNA chain called DNA (139-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	139	Total	C	N	O	P	0	0
			2834	1346	526	824	138		

- Molecule 16 is a DNA chain called DNA (128-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	N	128	2640	1251	486	775	128	0	0

- Molecule 17 is a protein called Chromo domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	622	5129	3254	900	953	22	0	0

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	P	16	330	148	49	117	16	0	0

- Molecule 19 is a protein called Chromatin elongation factor SPT4.

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

- Molecule 20 is a protein called Transcription elongation factor SPT5.

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-2	SER	-	expression tag	UNP P27692
Z	-1	ASN	-	expression tag	UNP P27692
Z	0	ALA	-	expression tag	UNP P27692
Z	376	LEU	LYS	conflict	UNP P27692
Z	377	GLU	SER	conflict	UNP P27692

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

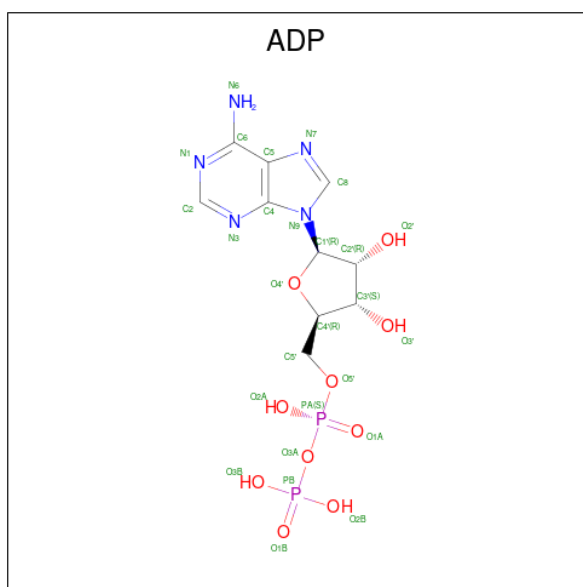
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

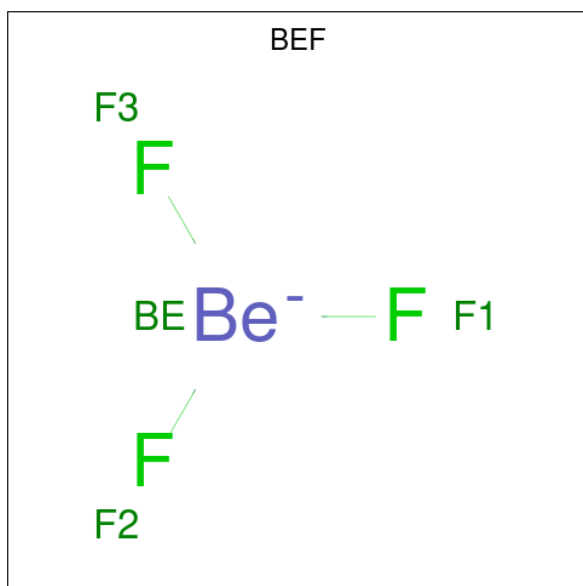
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	

- Molecule 25 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 26 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).

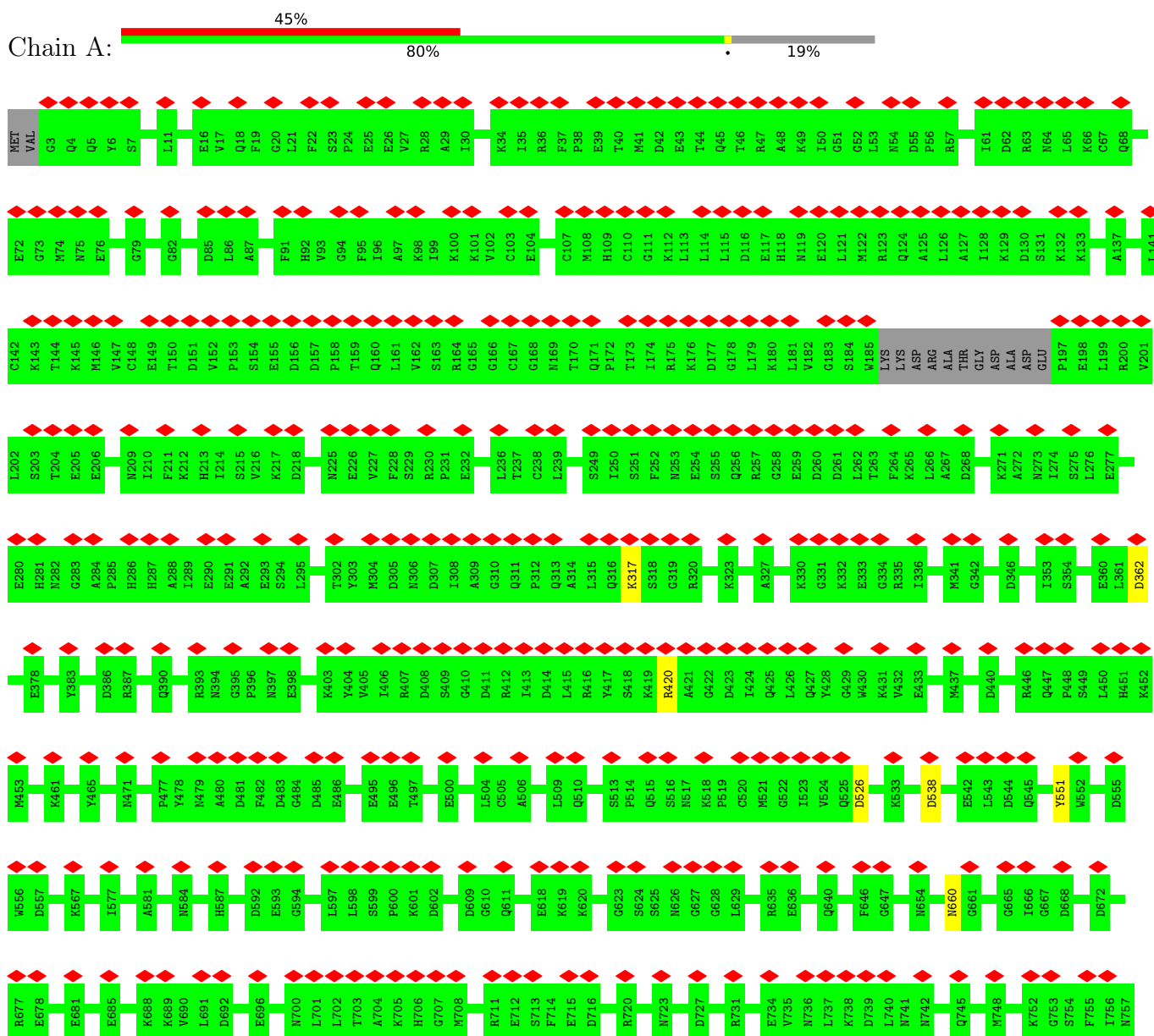


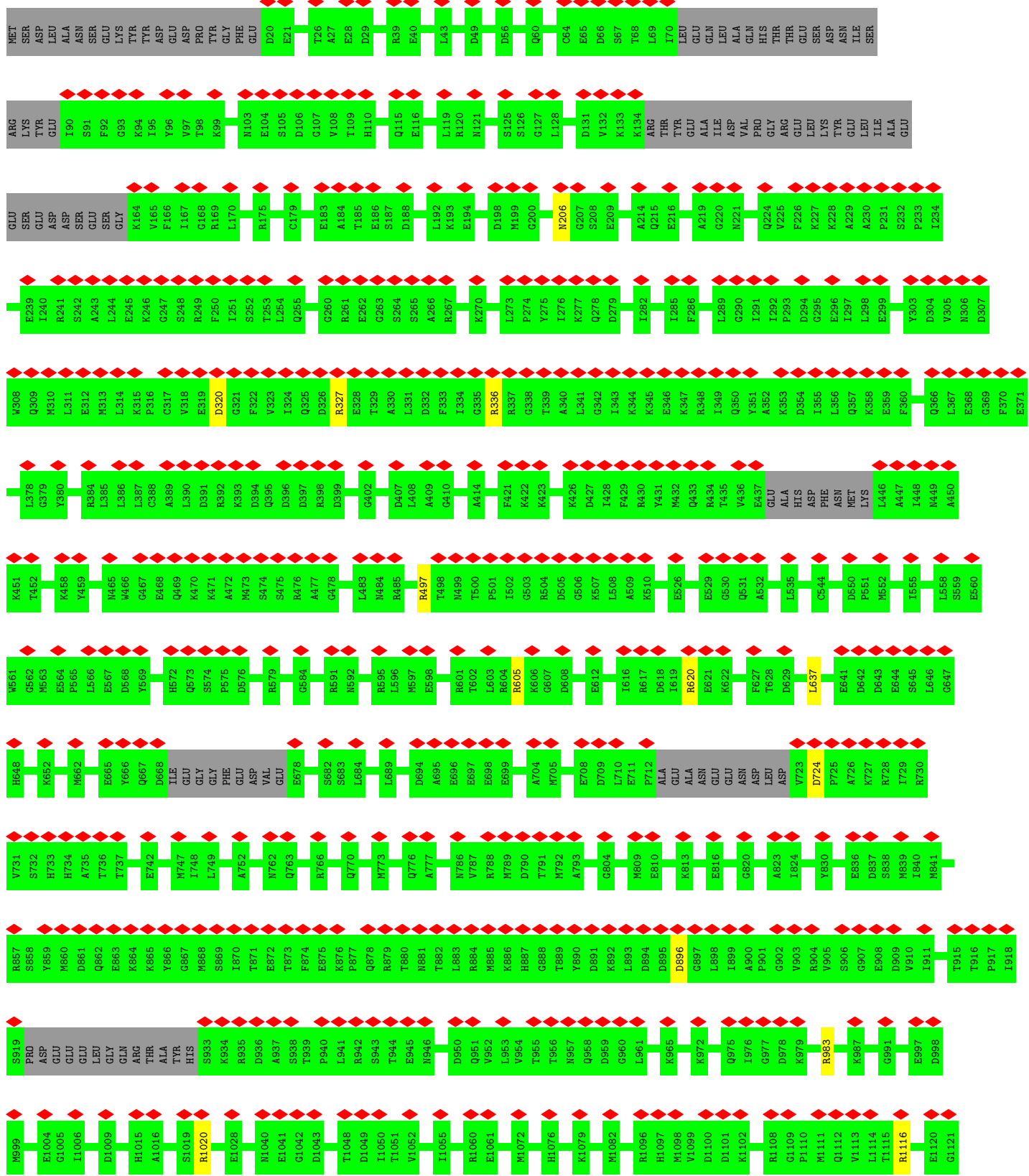
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
26	W	1	4	1	3	0

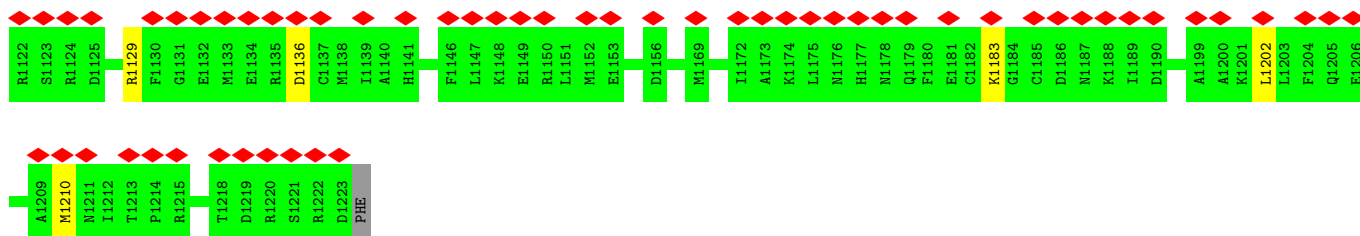
3 Residue-property plots

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.

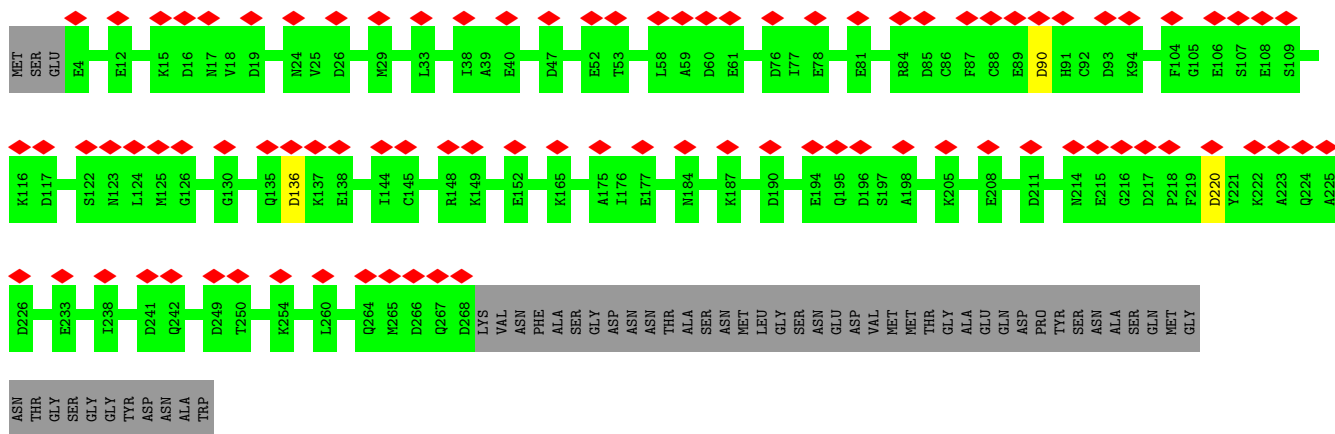
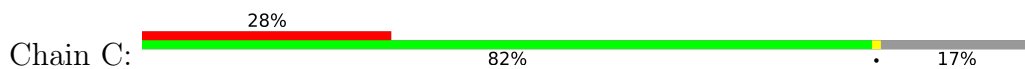
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



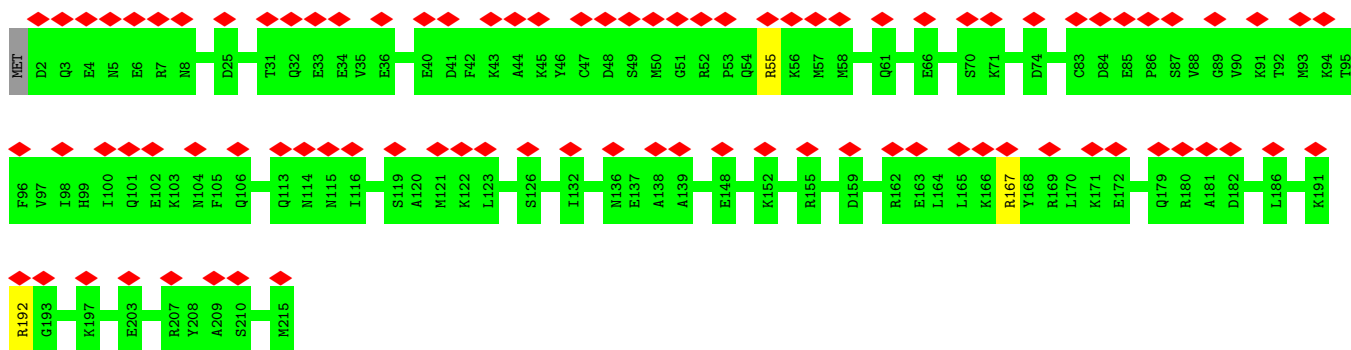
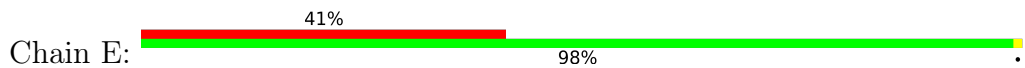




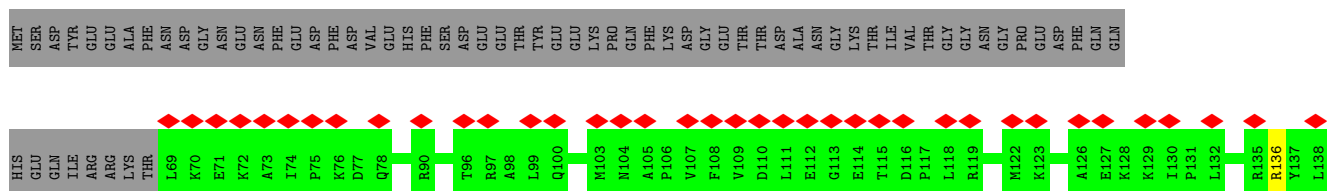
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

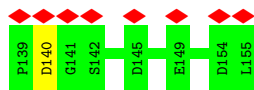


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

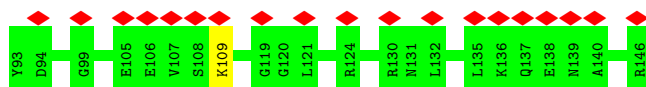
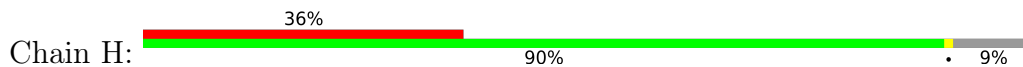


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

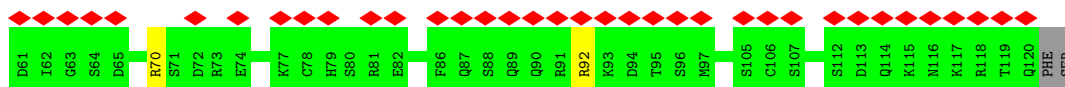
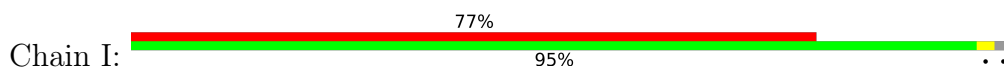




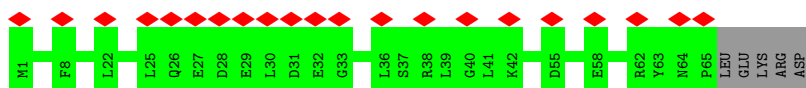
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



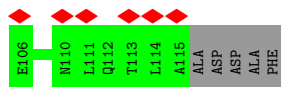
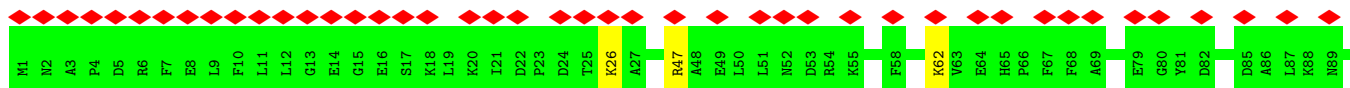
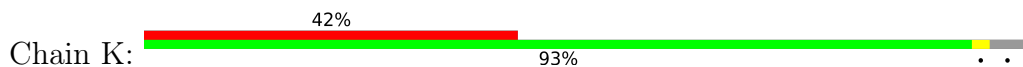
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

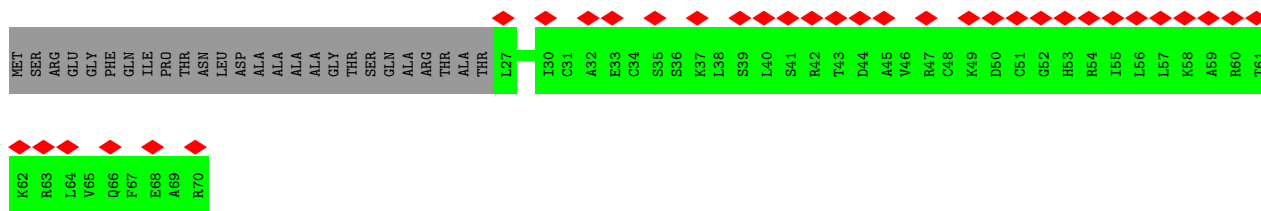


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

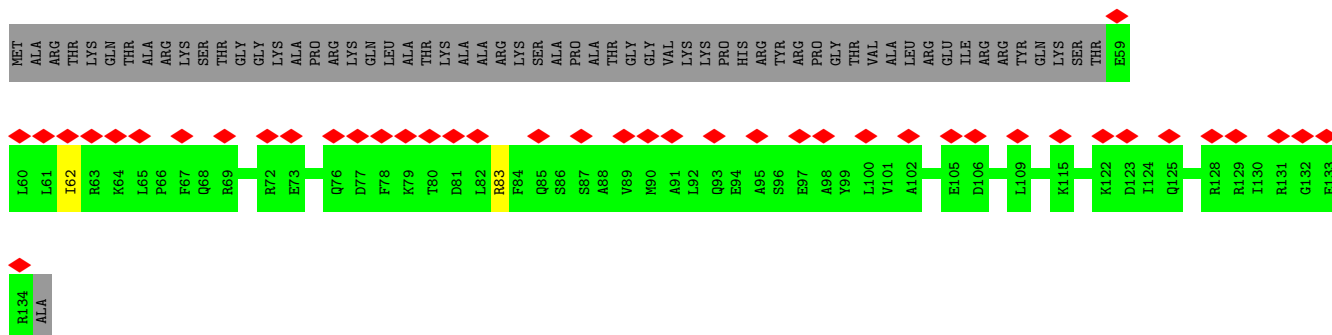


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

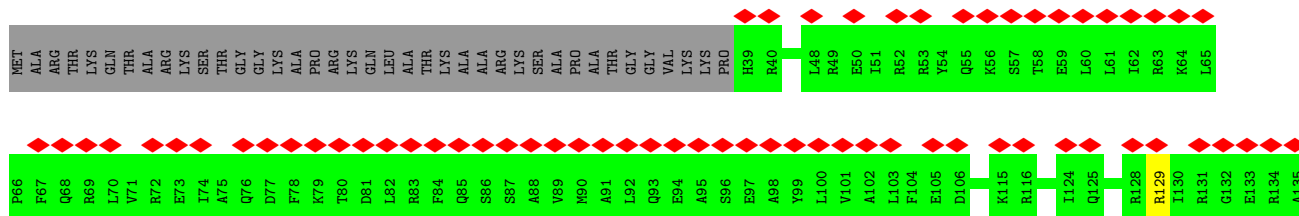




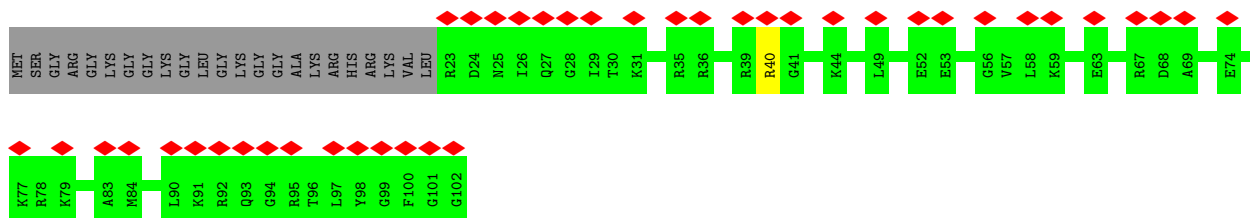
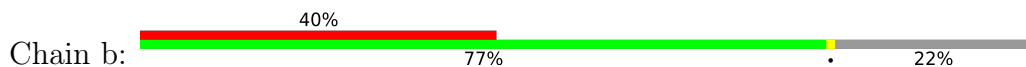
• Molecule 11: Histone H3.2



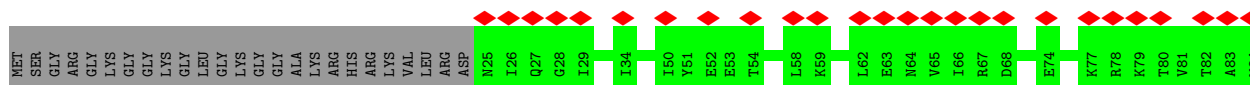
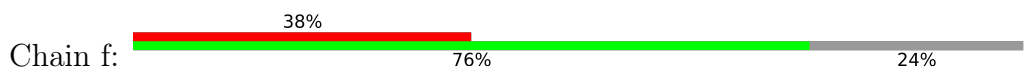
• Molecule 11: Histone H3.2

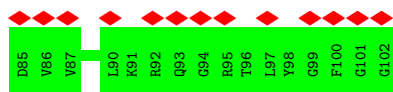


• Molecule 12: Histone H4

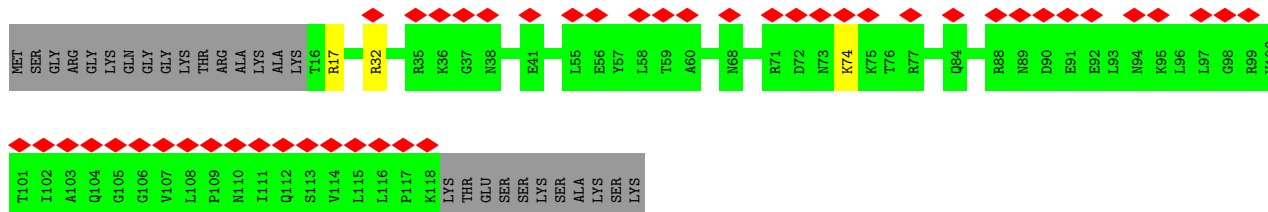
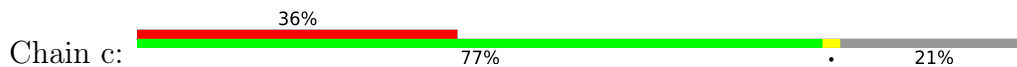


• Molecule 12: Histone H4

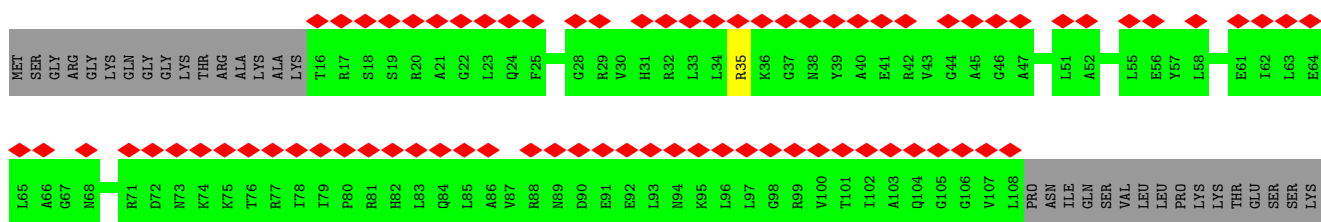




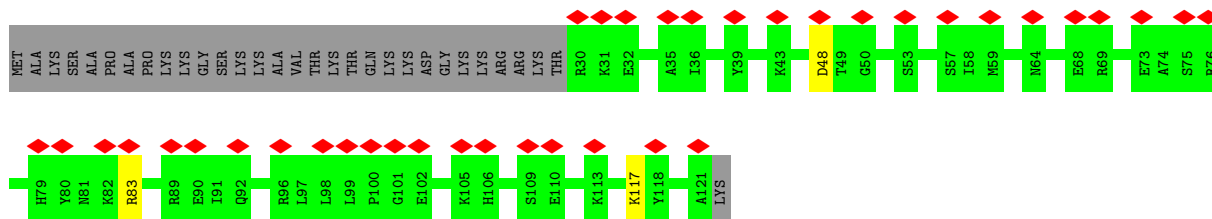
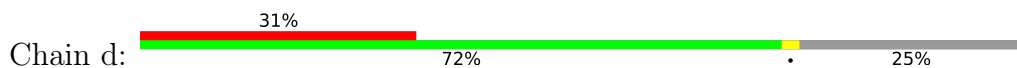
• Molecule 13: Histone H2A type 1



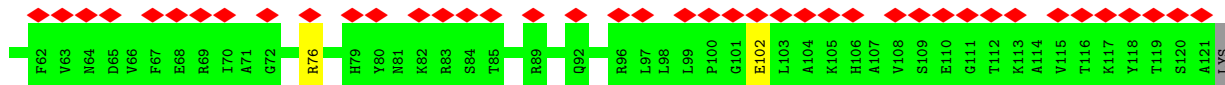
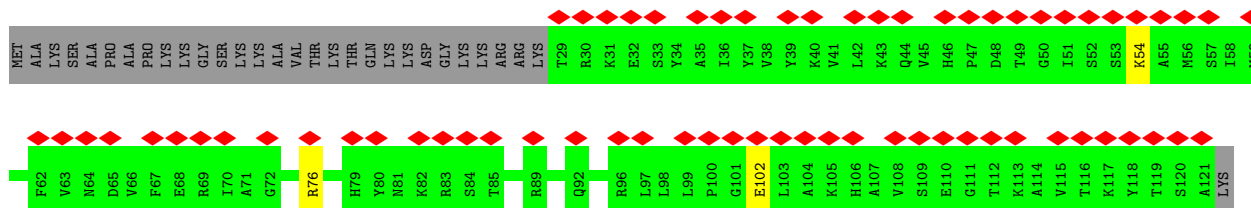
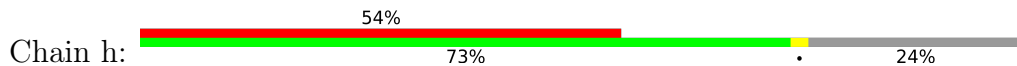
• Molecule 13: Histone H2A type 1

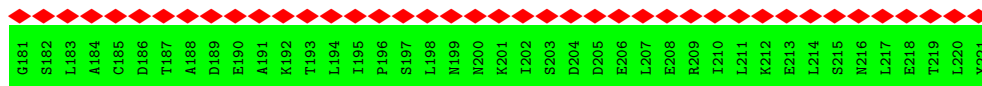


• Molecule 14: Histone H2B 1.1

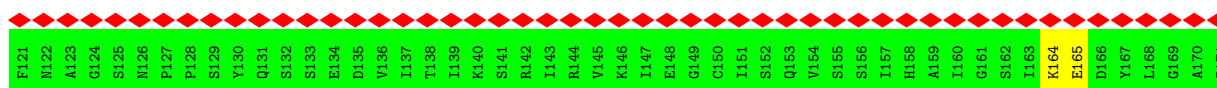
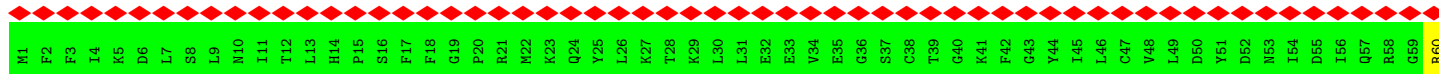


• Molecule 14: Histone H2B 1.1





- Molecule 22: DNA-directed RNA polymerase II subunit RPB7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	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	0.072	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.02	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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	1/11284 (0.0%)	0.73	11/15258 (0.1%)
2	B	0.40	0/9037	0.74	13/12184 (0.1%)
3	C	0.40	0/2124	0.70	2/2879 (0.1%)
4	E	0.40	0/1788	0.74	4/2406 (0.2%)
5	F	0.48	0/717	0.84	2/967 (0.2%)
6	H	0.44	0/1086	0.73	0/1470
7	I	0.41	0/989	0.80	2/1331 (0.2%)
8	J	0.44	0/541	0.70	0/727
9	K	0.46	0/938	0.84	3/1267 (0.2%)
10	L	0.44	0/353	0.89	0/468
11	a	0.39	0/627	0.83	2/841 (0.2%)
11	e	0.43	0/812	0.85	2/1088 (0.2%)
12	b	0.39	0/645	0.85	1/862 (0.1%)
12	f	0.40	0/626	0.76	0/837
13	c	0.44	0/805	0.82	1/1088 (0.1%)
13	g	0.42	0/726	0.78	1/979 (0.1%)
14	d	0.41	0/730	0.83	2/983 (0.2%)
14	h	0.40	0/737	0.77	1/993 (0.1%)
15	T	0.89	1/3179 (0.0%)	1.04	6/4900 (0.1%)
16	N	0.88	0/2961	1.03	5/4571 (0.1%)
17	W	0.37	0/5230	0.71	3/7057 (0.0%)
18	P	0.54	0/365	0.95	0/564
19	Y	0.33	0/755	0.64	0/1021
20	Z	0.38	0/1271	0.73	1/1702 (0.1%)
21	D	0.37	0/1454	0.76	1/1949 (0.1%)
22	G	0.44	0/1368	0.95	2/1844 (0.1%)
All	All	0.49	2/51148 (0.0%)	0.80	65/70236 (0.1%)

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
3	C	0	1
11	a	0	1
13	c	0	1
14	h	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	-24	DG	C3'-O3'	5.94	1.51	1.44
1	A	551	TYR	CD2-CE2	-5.40	1.31	1.39

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1129	ARG	NE-CZ-NH2	-8.28	116.16	120.30
16	N	27	DG	O4'-C1'-N9	7.63	113.34	108.00
14	d	83	ARG	NE-CZ-NH2	-7.44	116.58	120.30
11	a	83	ARG	NE-CZ-NH1	7.33	123.96	120.30
4	E	167	ARG	CG-CD-NE	-7.21	96.67	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	90	ASP	Peptide
11	a	62	ILE	Peptide
13	c	74	LYS	Peptide
14	h	102	GLU	Peptide

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	A	1399/1733 (81%)	1315 (94%)	84 (6%)	0	100	100
2	B	1102/1224 (90%)	1047 (95%)	55 (5%)	0	100	100
3	C	263/318 (83%)	242 (92%)	21 (8%)	0	100	100
4	E	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
5	F	85/155 (55%)	79 (93%)	6 (7%)	0	100	100
6	H	129/146 (88%)	115 (89%)	14 (11%)	0	100	100
7	I	117/122 (96%)	106 (91%)	11 (9%)	0	100	100
8	J	63/70 (90%)	59 (94%)	4 (6%)	0	100	100
9	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	40 (95%)	2 (5%)	0	100	100
11	a	74/136 (54%)	71 (96%)	3 (4%)	0	100	100
11	e	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
12	b	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
12	f	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
13	c	101/130 (78%)	93 (92%)	8 (8%)	0	100	100
13	g	91/130 (70%)	89 (98%)	2 (2%)	0	100	100
14	d	90/123 (73%)	87 (97%)	3 (3%)	0	100	100
14	h	91/123 (74%)	88 (97%)	3 (3%)	0	100	100
17	W	610/1468 (42%)	584 (96%)	26 (4%)	0	100	100
19	Y	96/102 (94%)	91 (95%)	5 (5%)	0	100	100
20	Z	152/1066 (14%)	142 (93%)	10 (7%)	0	100	100
21	D	176/221 (80%)	159 (90%)	17 (10%)	0	100	100
22	G	169/171 (99%)	159 (94%)	10 (6%)	0	100	100
All	All	5424/8185 (66%)	5125 (94%)	299 (6%)	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	
1	A	1232/1520 (81%)	1226 (100%)	6 (0%)	88	96
2	B	967/1061 (91%)	962 (100%)	5 (0%)	88	96
3	C	233/274 (85%)	233 (100%)	0	100	100
4	E	196/197 (100%)	196 (100%)	0	100	100
5	F	77/137 (56%)	77 (100%)	0	100	100
6	H	117/128 (91%)	116 (99%)	1 (1%)	78	93
7	I	113/116 (97%)	112 (99%)	1 (1%)	78	93
8	J	60/65 (92%)	60 (100%)	0	100	100
9	K	99/102 (97%)	99 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	a	66/111 (60%)	66 (100%)	0	100	100
11	e	84/111 (76%)	84 (100%)	0	100	100
12	b	65/79 (82%)	65 (100%)	0	100	100
12	f	63/79 (80%)	63 (100%)	0	100	100
13	c	82/102 (80%)	81 (99%)	1 (1%)	71	91
13	g	72/102 (71%)	72 (100%)	0	100	100
14	d	78/103 (76%)	77 (99%)	1 (1%)	69	90
14	h	79/103 (77%)	78 (99%)	1 (1%)	69	90
17	W	567/1313 (43%)	563 (99%)	4 (1%)	84	95
19	Y	82/87 (94%)	82 (100%)	0	100	100
20	Z	136/878 (16%)	136 (100%)	0	100	100
21	D	161/200 (80%)	159 (99%)	2 (1%)	71	91
22	G	152/152 (100%)	151 (99%)	1 (1%)	84	95
All	All	4820/7077 (68%)	4797 (100%)	23 (0%)	89	96

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	d	117	LYS
17	W	323	ASN
17	W	295	ARG
17	W	463	ARG
2	B	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	188	HIS
6	H	137	GLN
21	D	150	ASN
17	W	579	GLN
21	D	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	P	15/69 (21%)	4 (26%)	2 (13%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	P	35	U
18	P	36	G
18	P	37	U
18	P	39	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	P	36	G
18	P	38	C

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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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
26	BEF	W	1502	17	0,3,3	-	-	-		
25	ADP	W	1501	-	24,29,29	0.92	1 (4%)	29,45,45	1.51	5 (17%)

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
25	ADP	W	1501	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	1501	ADP	C5-C4	2.22	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	1501	ADP	N3-C2-N1	-3.79	122.76	128.68
25	W	1501	ADP	C3'-C2'-C1'	3.32	105.98	100.98
25	W	1501	ADP	PA-O3A-PB	-2.99	122.57	132.83
25	W	1501	ADP	O5'-C5'-C4'	2.62	118.01	108.99
25	W	1501	ADP	C4-C5-N7	-2.40	106.90	109.40

There are no chirality outliers.

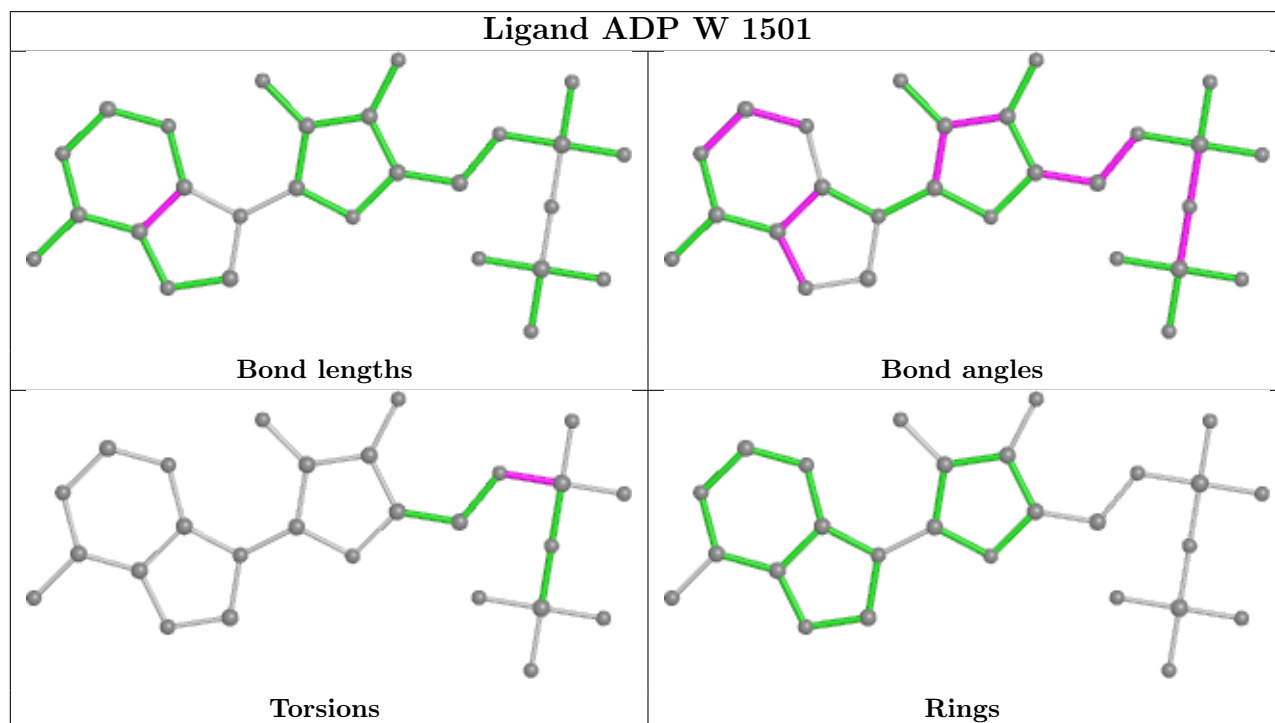
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	W	1501	ADP	C5'-O5'-PA-O1A
25	W	1501	ADP	C5'-O5'-PA-O2A
25	W	1501	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

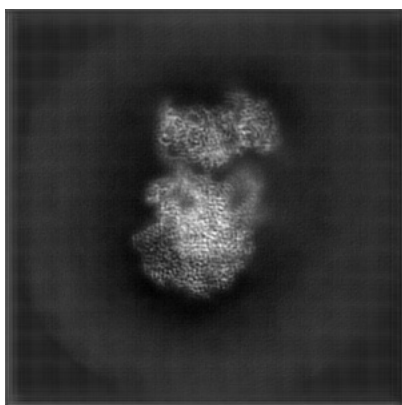
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12449. These allow visual inspection of the internal detail of the map and identification of artifacts.

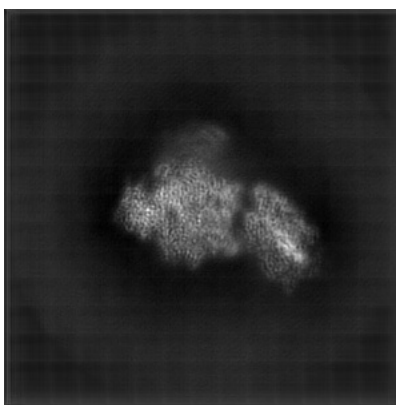
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

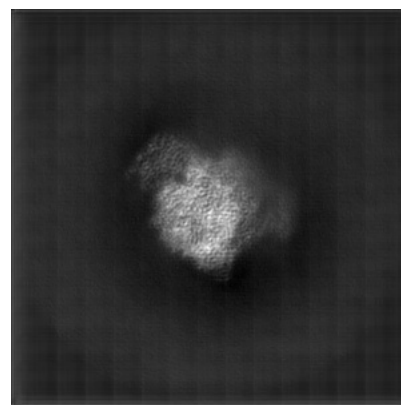
6.1.1 Primary map



X



Y

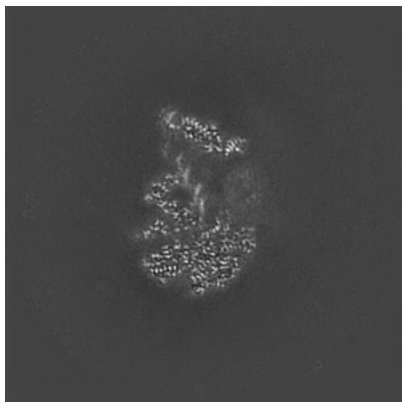


Z

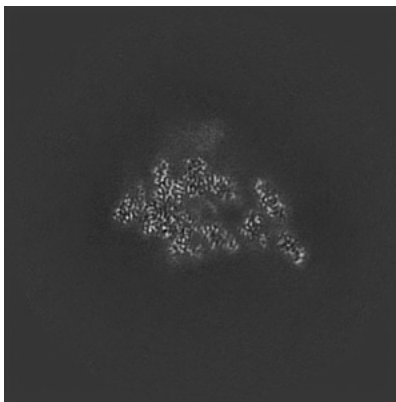
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

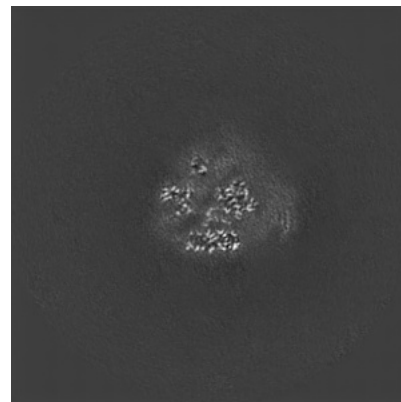
6.2.1 Primary map



X Index: 200



Y Index: 200

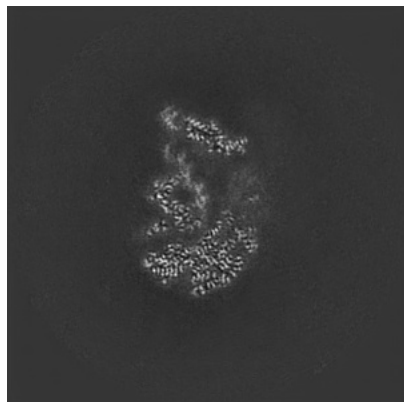


Z Index: 200

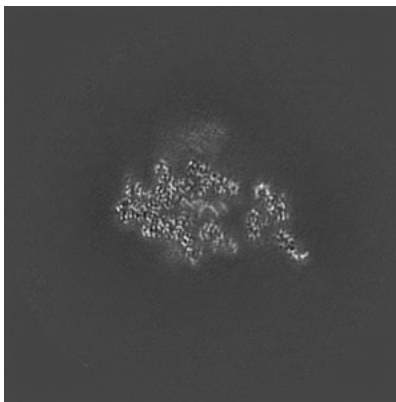
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

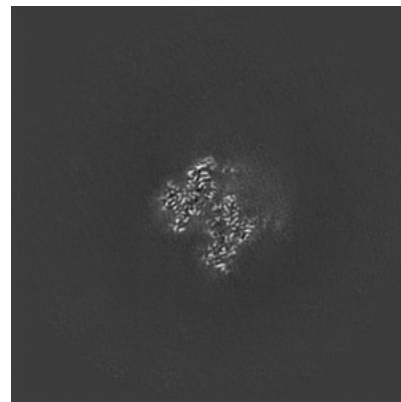
6.3.1 Primary map



X Index: 198



Y Index: 195



Z Index: 176

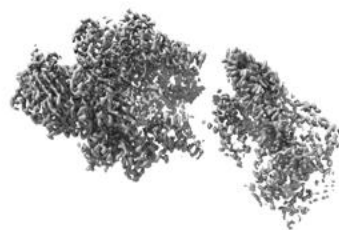
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

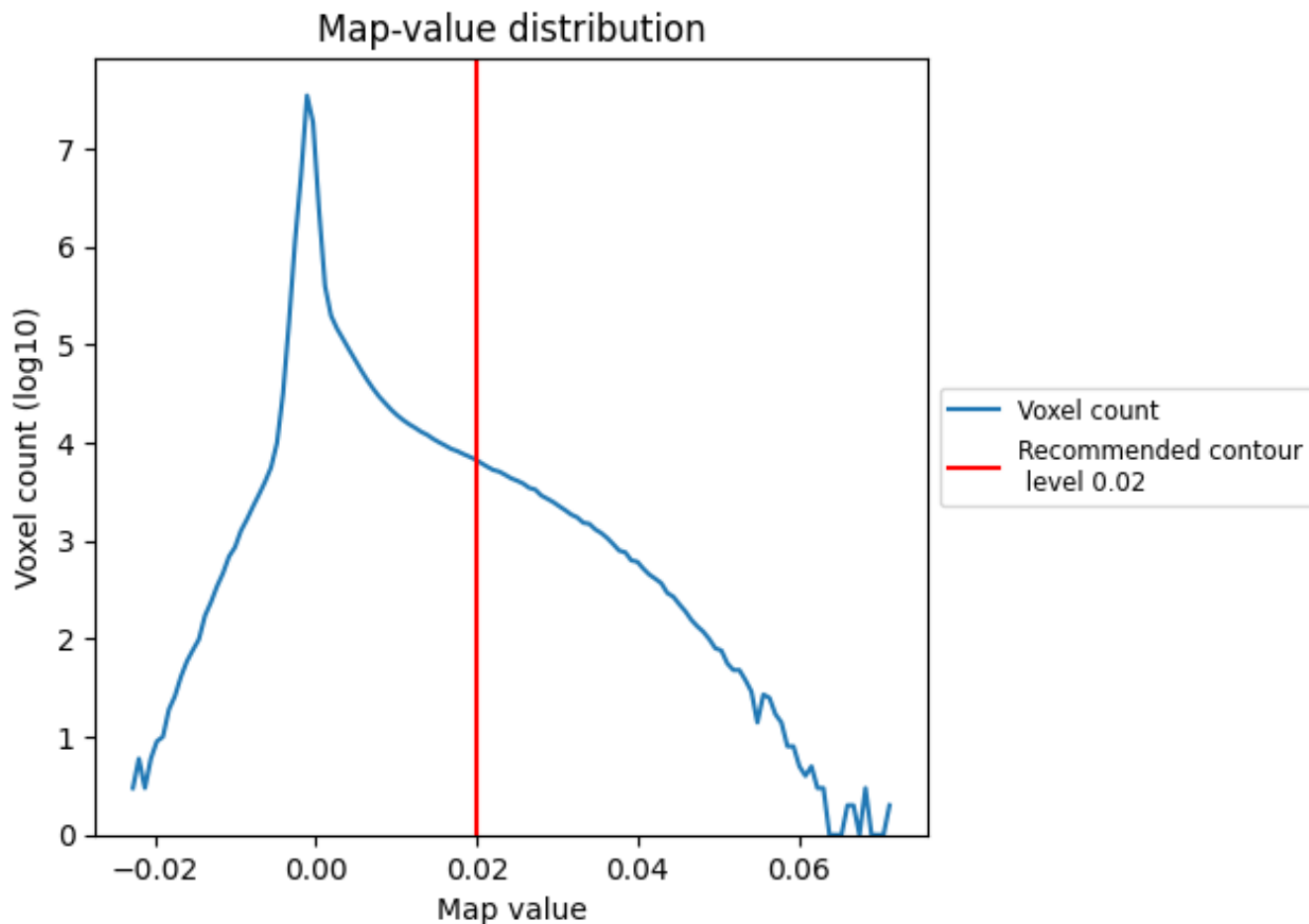
6.5 Mask visualisation

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

7 Map analysis [i](#)

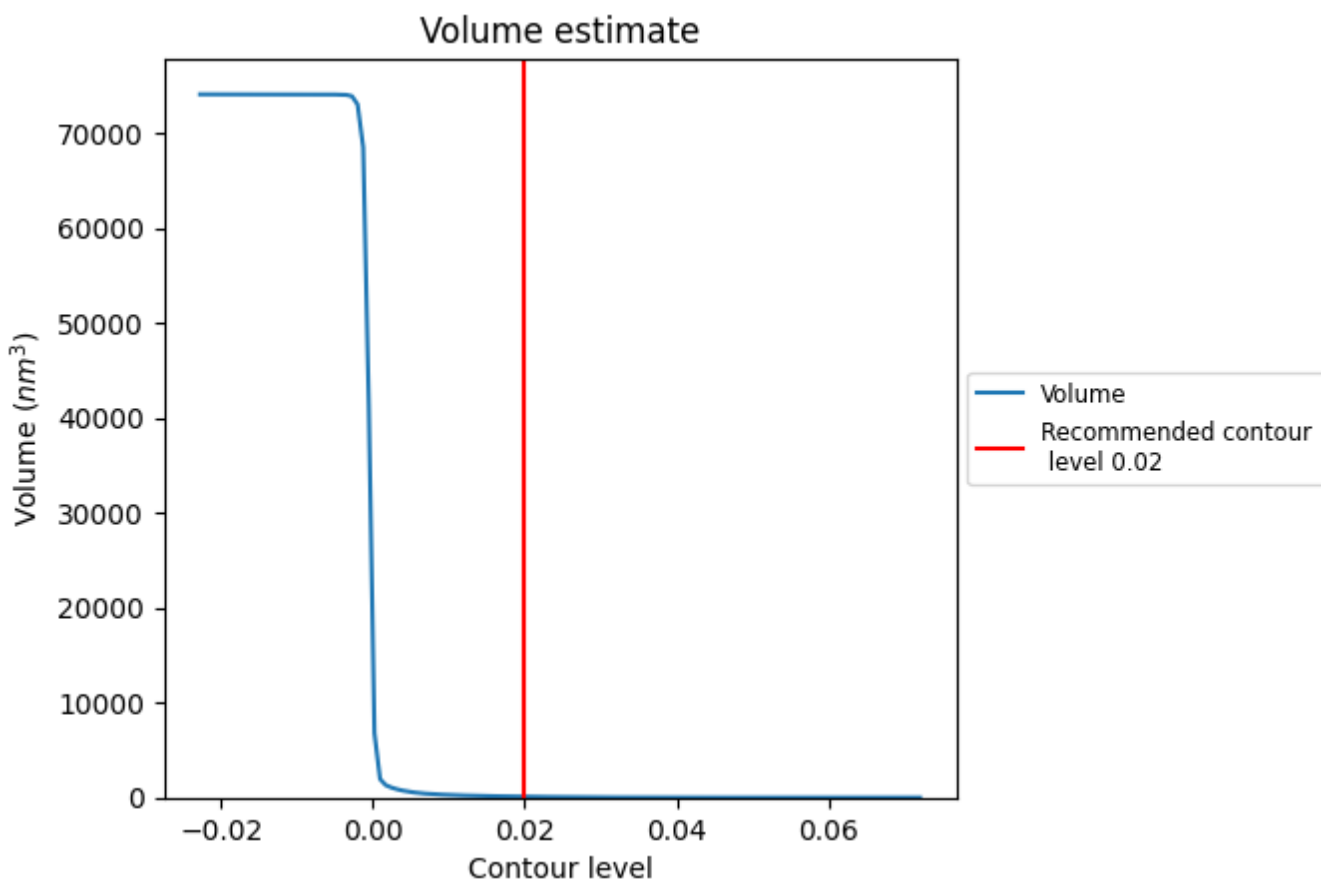
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

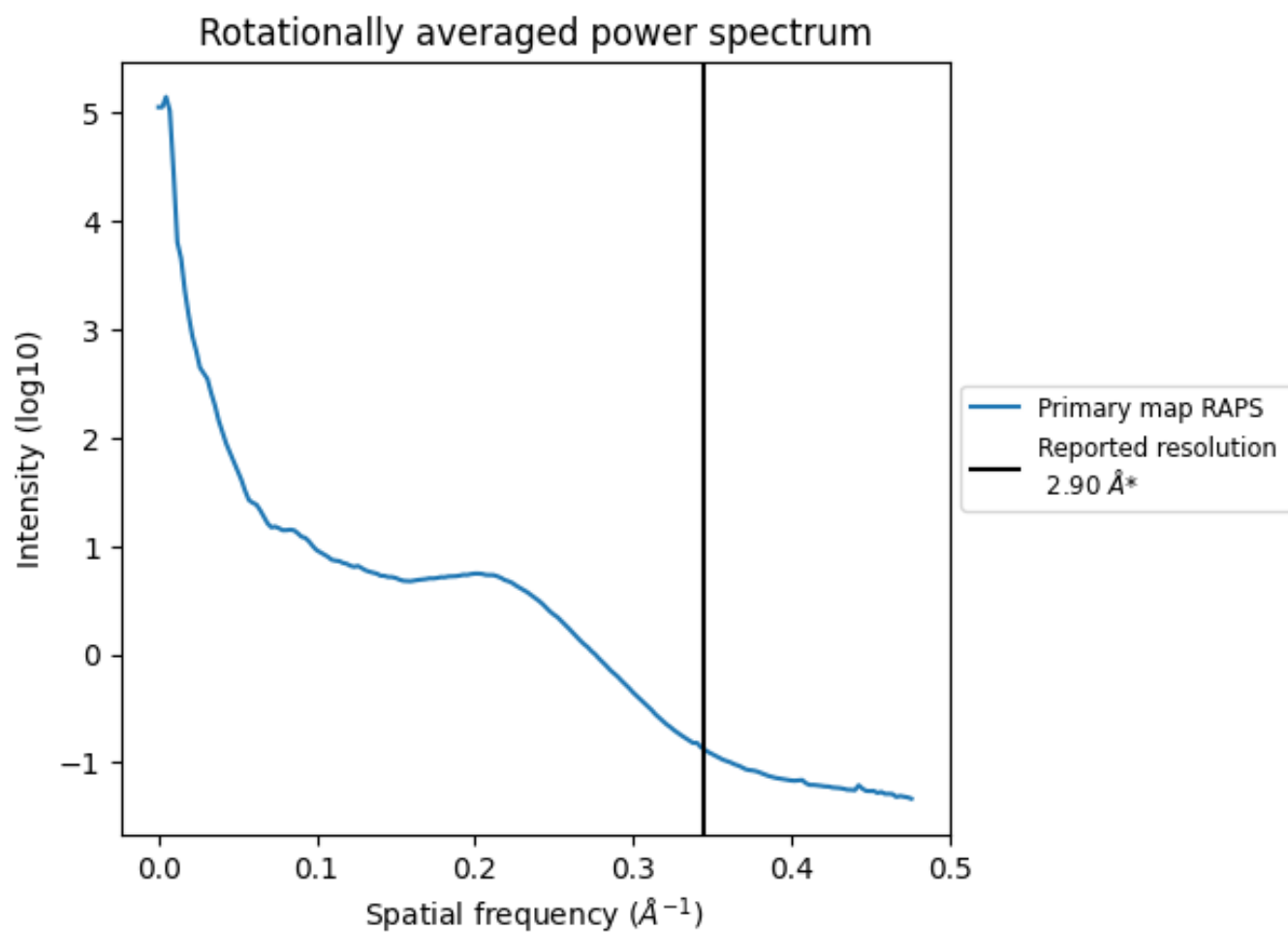
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm³; this corresponds to an approximate mass of 85 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 0.345 Å⁻¹

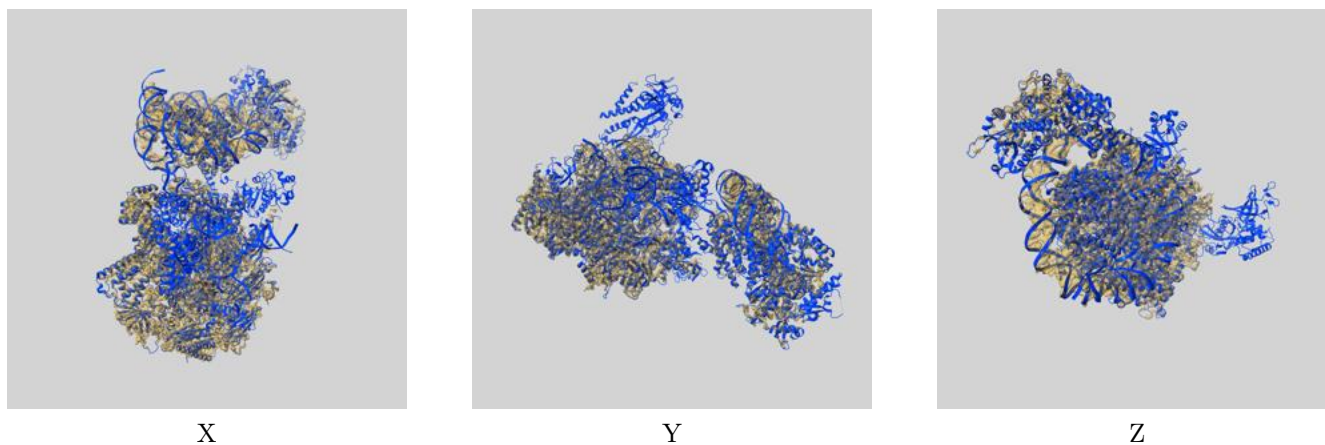
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

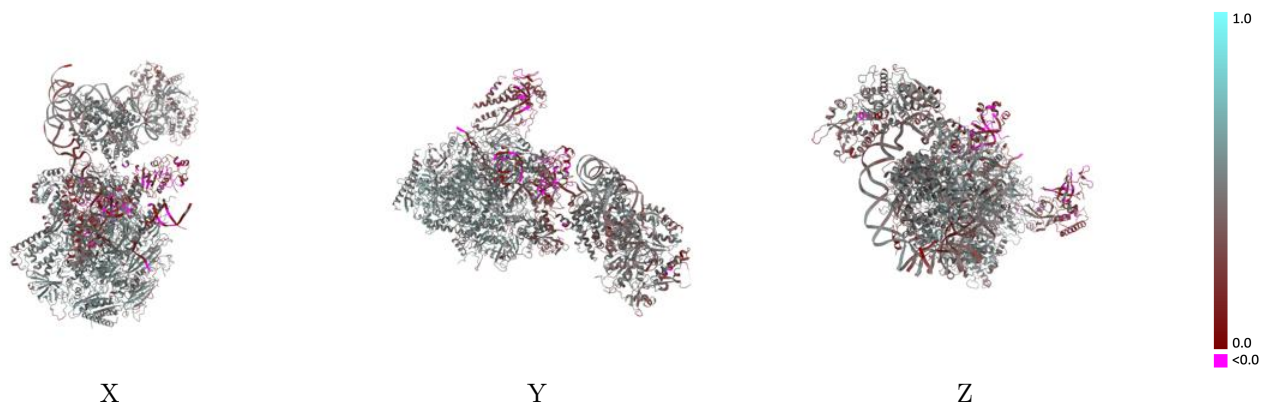
This section contains information regarding the fit between EMDB map EMD-12449 and PDB model 7NKX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



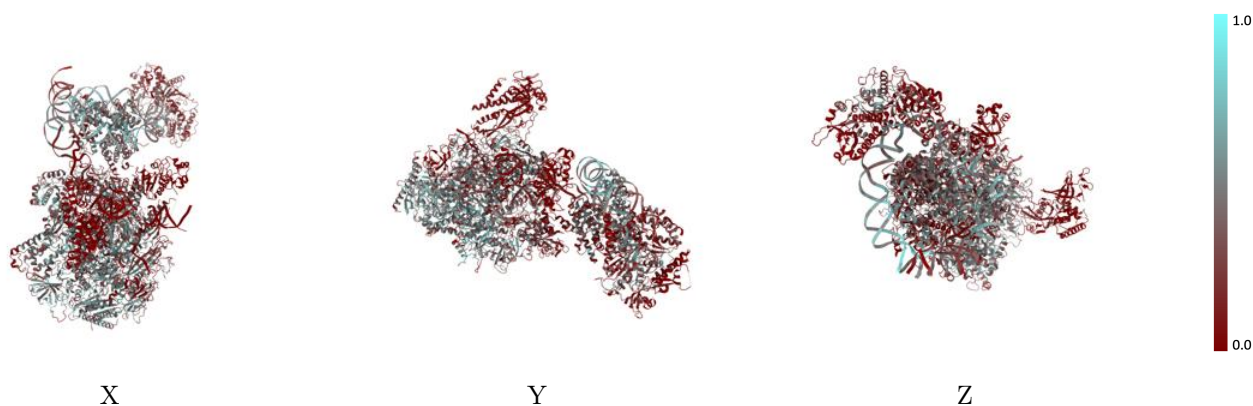
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



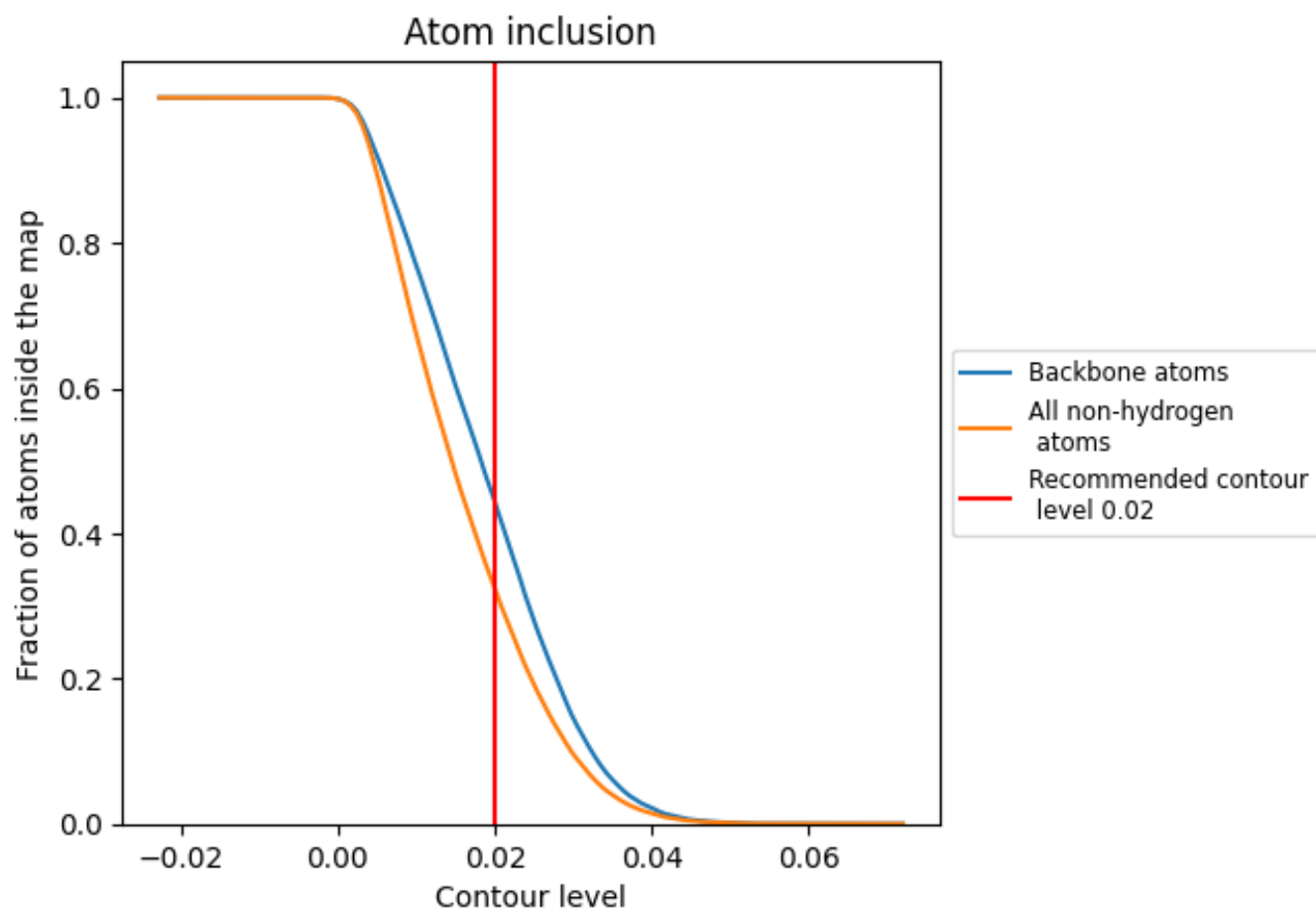
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 32% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3243	 0.4440
A	 0.3644	 0.4840
B	 0.3895	 0.5010
C	 0.4920	 0.5190
D	 0.0000	 0.2480
E	 0.4529	 0.4830
F	 0.3916	 0.4980
G	 0.0030	 0.2450
H	 0.4635	 0.4980
I	 0.1934	 0.3710
J	 0.5513	 0.5330
K	 0.4146	 0.5120
L	 0.2743	 0.4640
N	 0.3917	 0.3710
P	 0.3182	 0.3410
T	 0.3878	 0.3770
W	 0.1681	 0.4200
Y	 0.0000	 0.1590
Z	 0.0008	 0.2830
a	 0.3661	 0.4880
b	 0.3971	 0.5000
c	 0.4130	 0.4830
d	 0.4330	 0.4630
e	 0.3117	 0.4710
f	 0.4118	 0.4980
g	 0.1890	 0.4410
h	 0.2779	 0.4460

