wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 06:01 am BST

PDB ID	:	8BYQ / pdb_00008byq
EMDB ID	:	EMD-16331
Title	:	RNA polymerase II pre-initiation complex with the proximal +1 nucleosome (PIC-Nuc10W)
Authors	:	Abril-Garrido, J.; Dienemann, C.; Grabbe, F.; Velychko, T.; Lidschreiber, M.; Wang, H.; Cramer, P.
Deposited on	:	2022-12-14
Resolution	:	4.10 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:

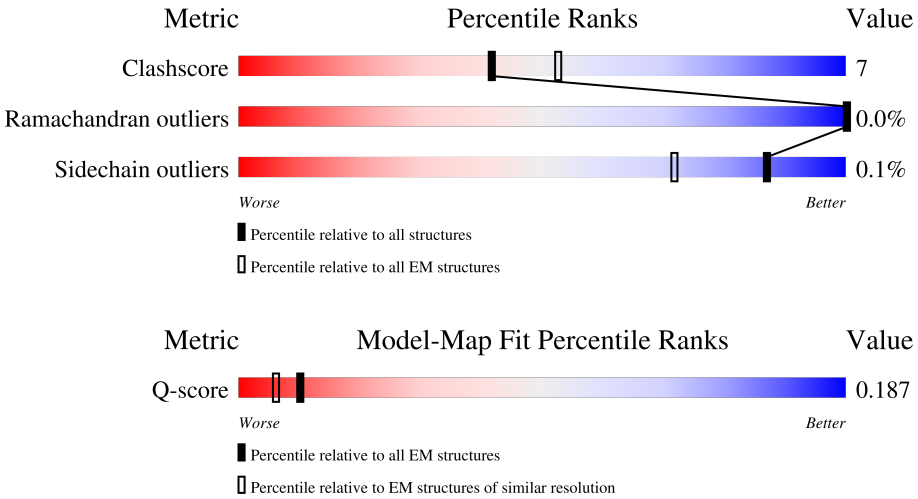
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	782	66% 17% 16%
2	1	760	75% 25%
3	2	548	67% 7% 26%
4	3	462	80% 18% ·

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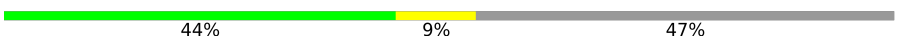
Mol	Chain	Length	Quality of chain
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	8	346	
10	9	323	
11	A	1970	
12	B	1174	
13	C	275	
14	D	142	
15	E	210	
16	F	127	
17	G	172	
18	H	150	
19	I	125	
20	J	67	
21	K	117	
22	L	58	
23	M	316	
24	N	210	
25	O	339	
26	Q	517	
27	R	249	
28	T	210	
29	U	376	

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Mol	Chain	Length	Quality of chain
30	V	109	
31	W	196	
32	X	291	
33	a	136	
33	e	136	
34	b	103	
34	f	103	
35	c	130	
35	g	130	
36	d	126	
36	h	126	

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 85971 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 XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	653	Total	C	N	O	S	0	0
			5189	3303	899	957	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	760	Total	C	N	O	S	0	0
			6034	3853	1053	1099	29		

- Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	408	Total	C	N	O	S	0	0
			2643	1646	486	503	8		

- Molecule 4 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	452	Total	C	N	O	S	0	0
			3589	2307	631	637	14		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	366	Total	C	N	O	S	0	0
			2710	1702	476	506	26		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	263	Total	C	N	O	S	0	0
			2064	1322	344	379	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	273	Total	C	N	O	S	0	0
			2233	1397	391	432	13		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	298	Total	C	N	O	S	0	0
			2370	1531	404	424	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 14 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- 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
			1351	875	219	249	8		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 22 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 24 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	198	Total	C	N	O	P	0	0
			4051	1921	746	1187	197		

- Molecule 25 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 26 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 27 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 28 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	198	Total	C	N	O	P	0	0
			4061	1924	755	1185	197		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 30 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 31 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 32 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 33 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	97	Total	C	N	O	S	0	0
			802	506	155	138	3		
33	e	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	103	ALA	GLY	engineered mutation	UNP P84233
e	103	ALA	GLY	engineered mutation	UNP P84233

- Molecule 34 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
34	f	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

- Molecule 35 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	109	Total	C	N	O	0	0
			843	531	167	145		
35	g	106	Total	C	N	O	0	0
			818	516	160	142		

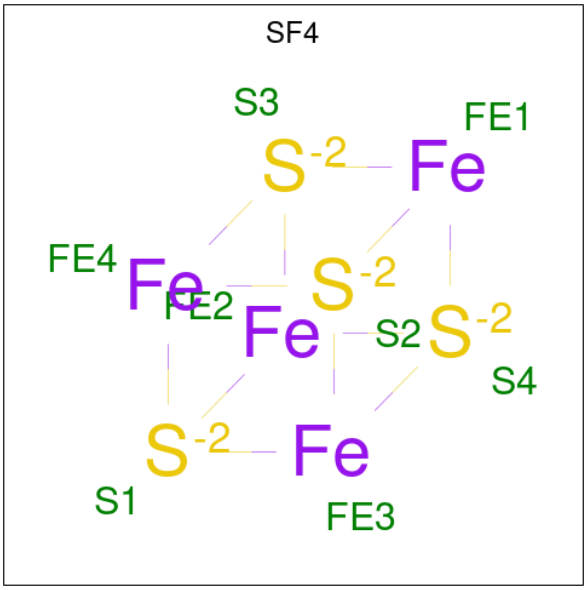
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	conflict	UNP P06897
g	100	ARG	GLY	conflict	UNP P06897

- Molecule 36 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
36	h	95	Total	C	N	O	S	0	0
			744	468	134	140	2		

- Molecule 37 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	4	3	Total	Zn	0
			3	3	
38	5	1	Total	Zn	0
			1	1	
38	7	2	Total	Zn	0
			2	2	
38	A	2	Total	Zn	0
			2	2	
38	B	1	Total	Zn	0
			1	1	
38	C	1	Total	Zn	0
			1	1	
38	I	2	Total	Zn	0
			2	2	

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

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

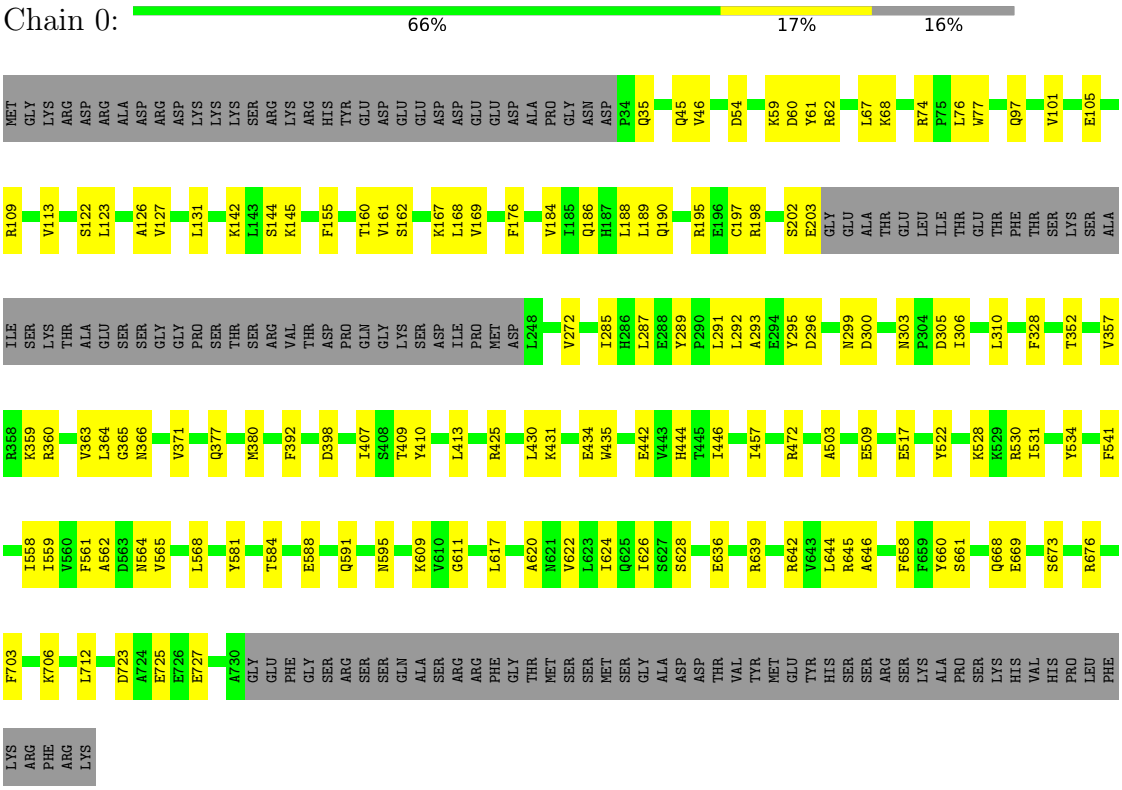
Mol	Chain	Residues	Atoms	AltConf
39	A	1	Total Mg 1 1	0

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.

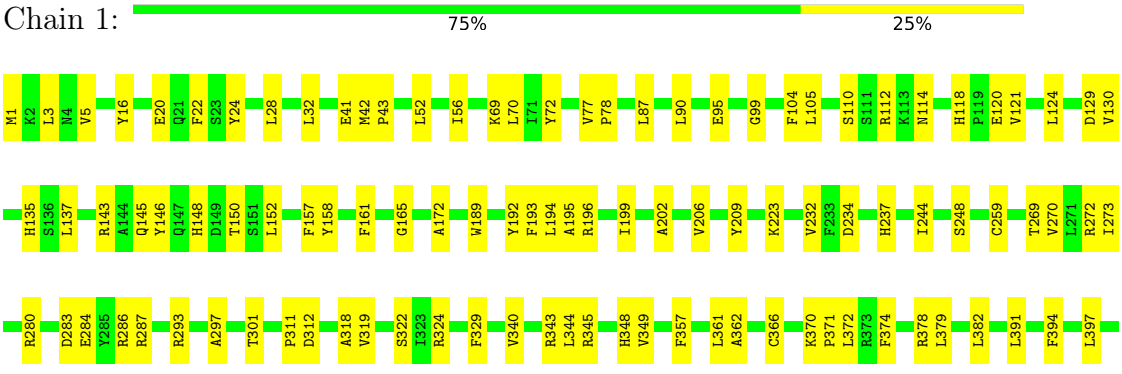
• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPB

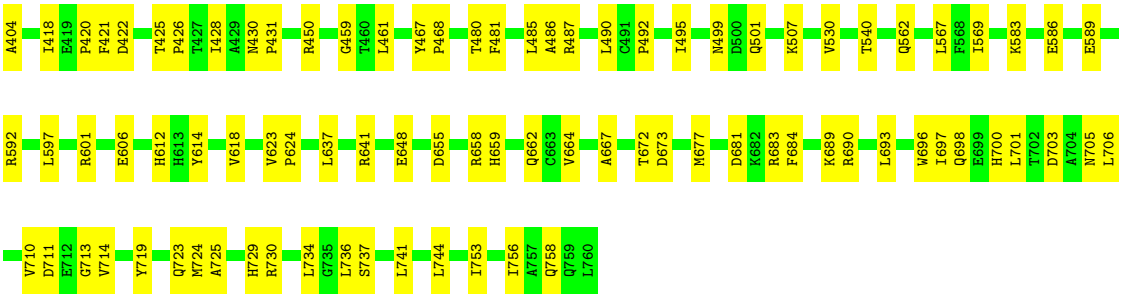
Chain 0:



• Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

Chain 1:

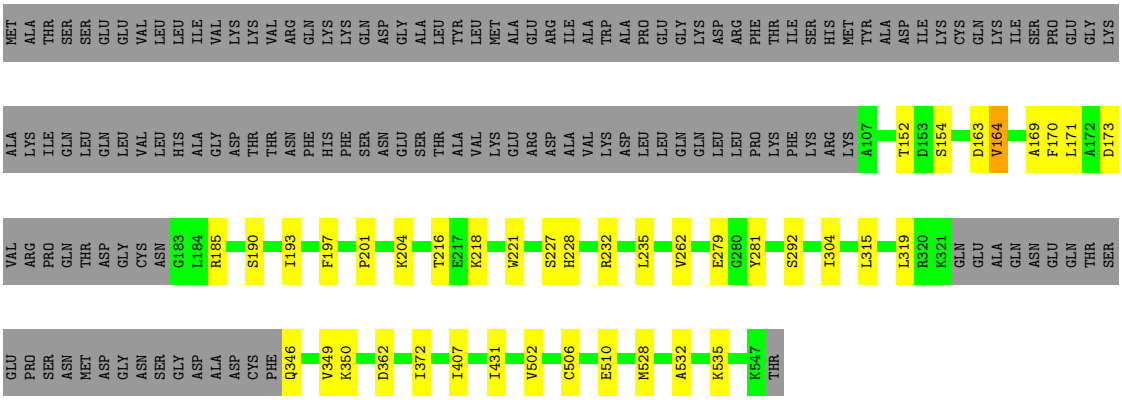




• Molecule 3: General transcription factor IIH subunit 1

Chain 2:

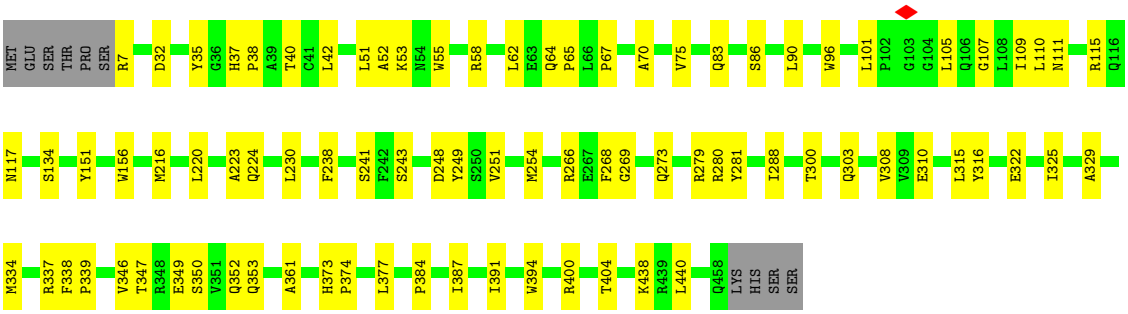




• Molecule 4: General transcription factor IIH subunit 4

Chain 3:

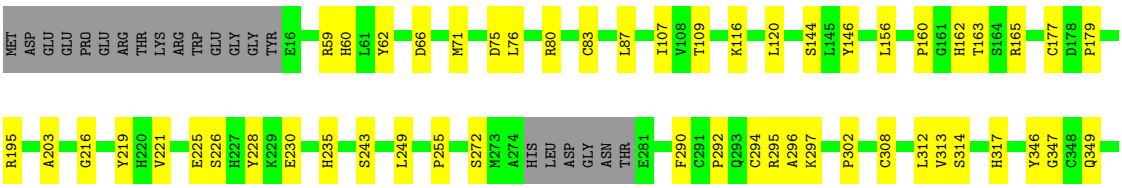


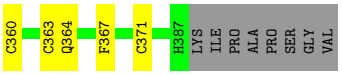


• Molecule 5: General transcription factor IIH subunit 2

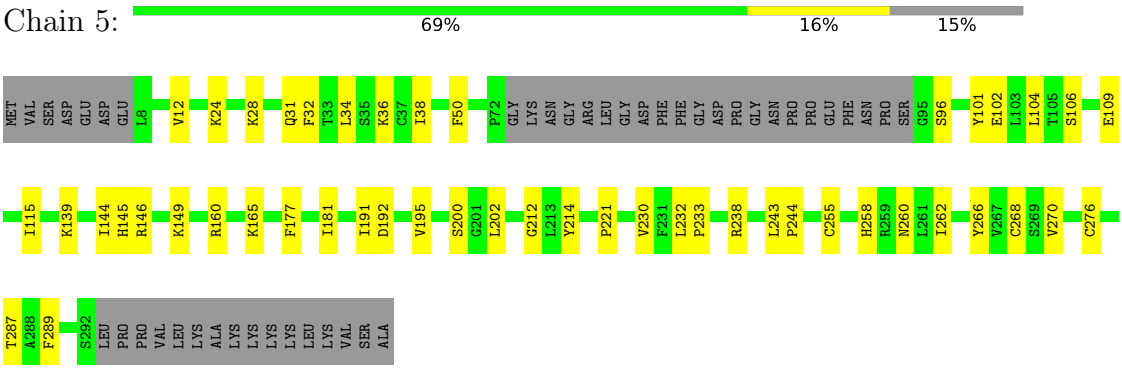
Chain 4:



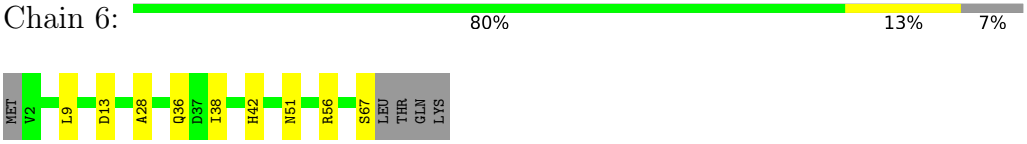




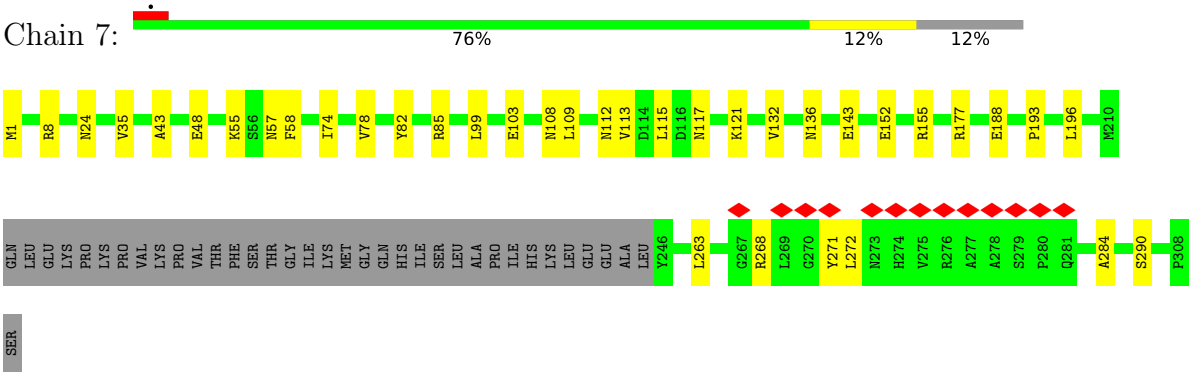
• Molecule 6: General transcription factor IIH subunit 3



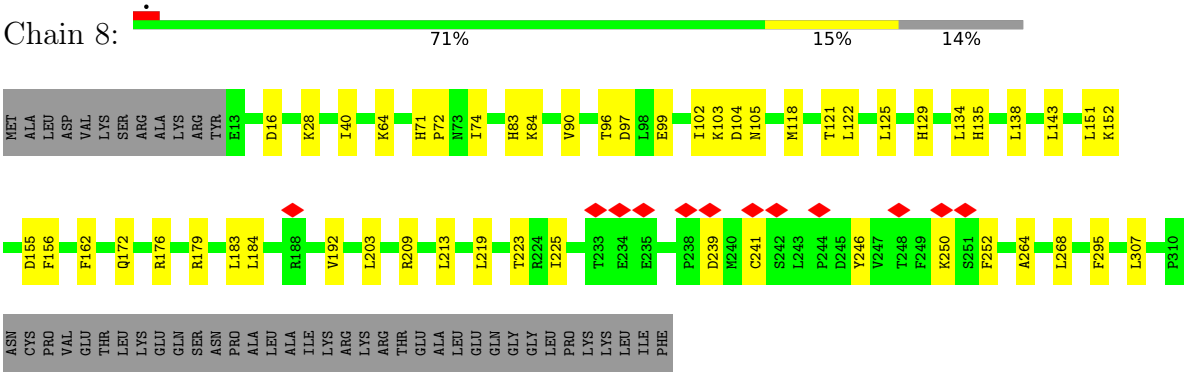
• Molecule 7: General transcription factor IIH subunit 5



• Molecule 8: CDK-activating kinase assembly factor MAT1

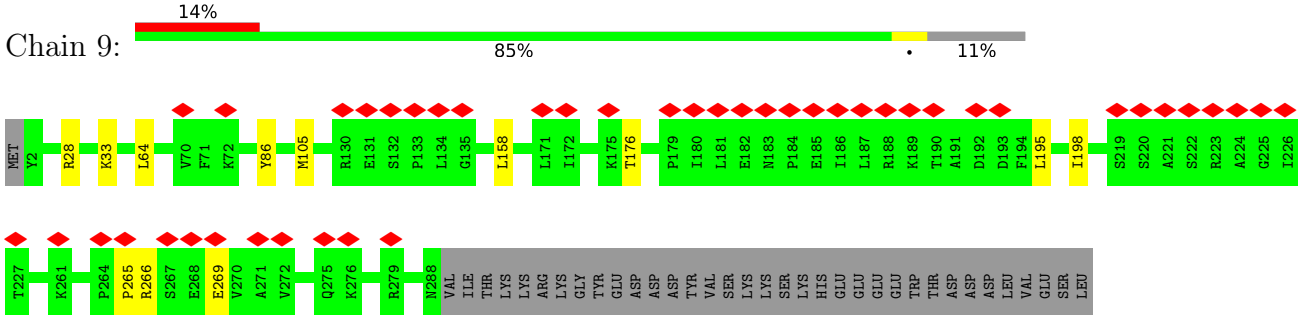


• Molecule 9: Cyclin-dependent kinase 7



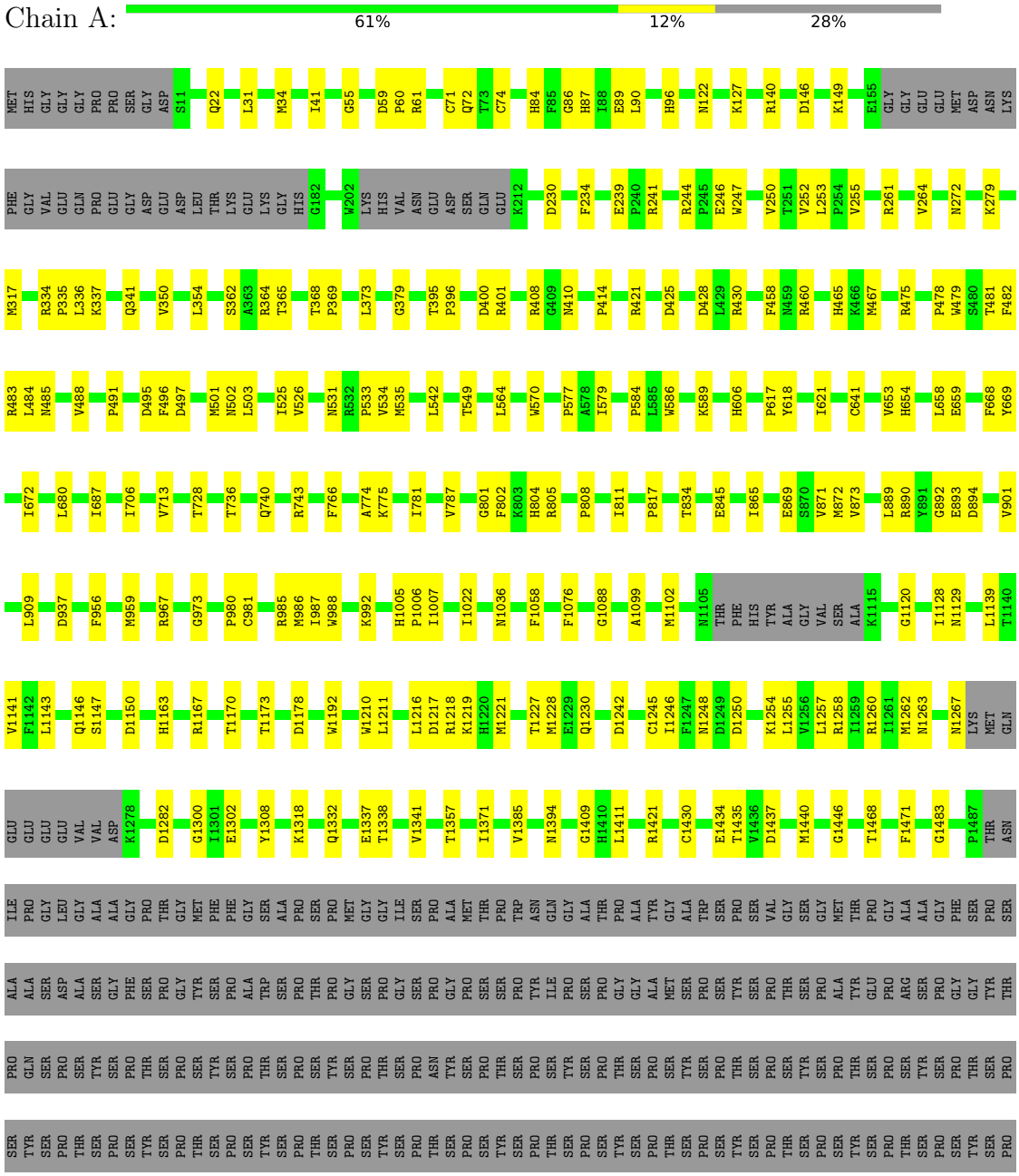
• Molecule 10: Cyclin-H

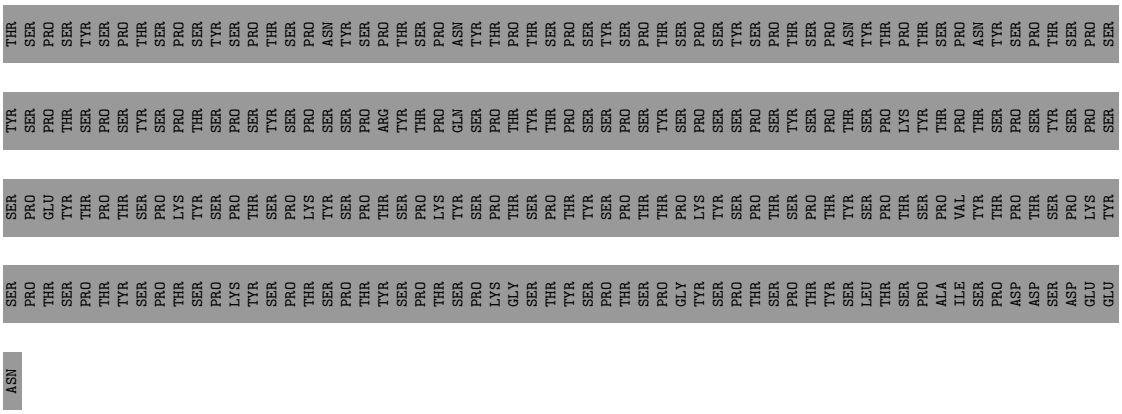
Chain 9:



• Molecule 11: DNA-directed RNA polymerase subunit

Chain A:

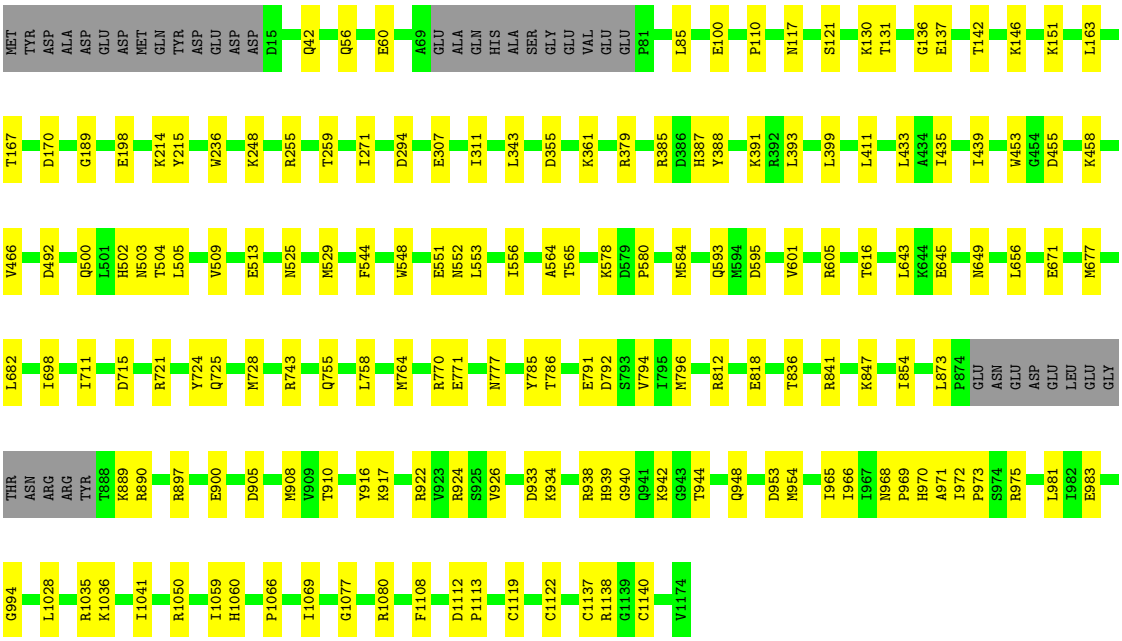




• Molecule 12: DNA-directed RNA polymerase subunit beta

Chain B:

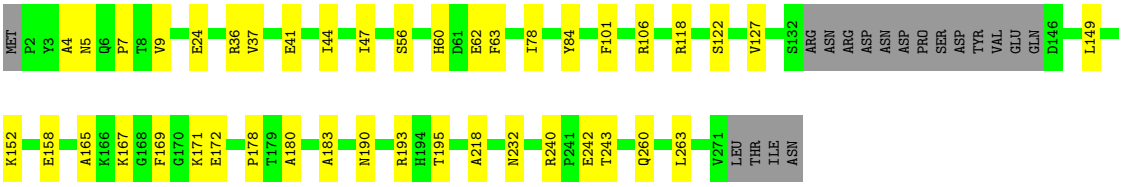




• Molecule 13: DNA-directed RNA polymerase II subunit RPB3

Chain C:

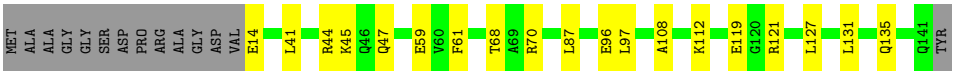




• Molecule 14: RNA polymerase II subunit D

Chain D:





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

Chain E:

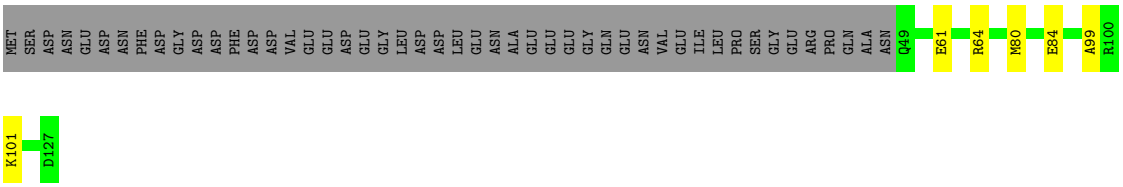




• Molecule 16: DNA-directed RNA polymerase II subunit F

Chain F:

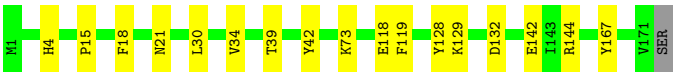




• Molecule 17: DNA-directed RNA polymerase II subunit RPB7

Chain G:

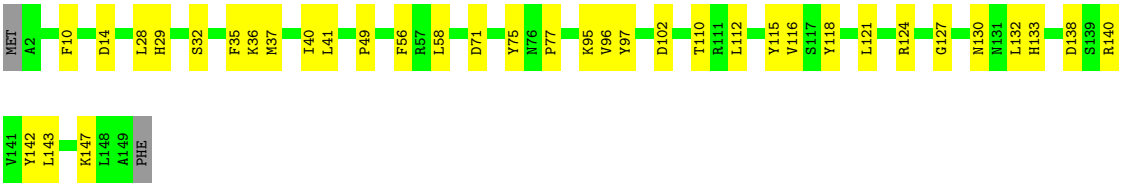




• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

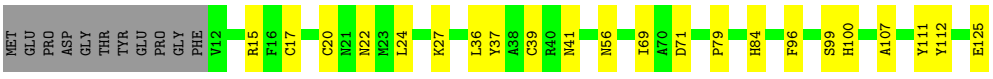




• Molecule 19: DNA-directed RNA polymerase II subunit RPB9

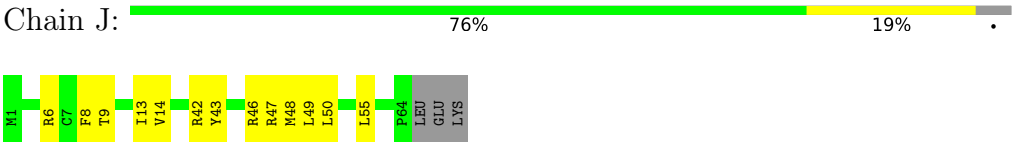
Chain I:





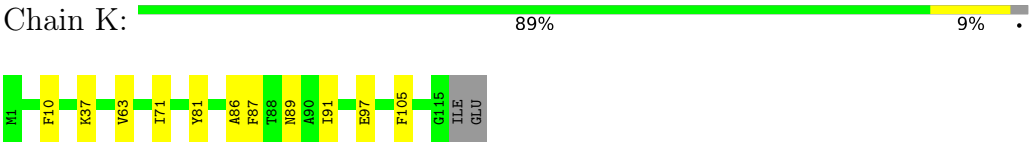
• Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



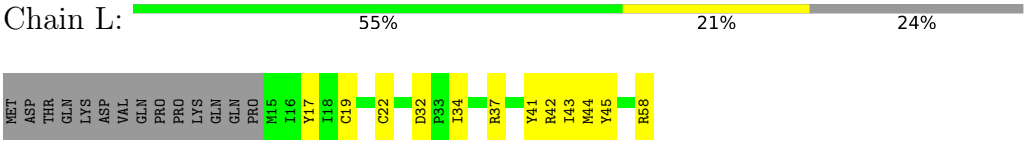
• Molecule 21: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



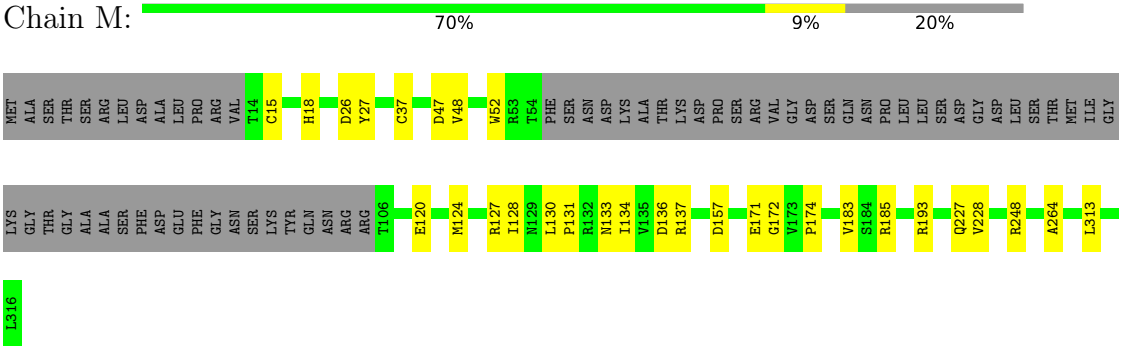
• Molecule 22: RNA polymerase II subunit K

Chain L:



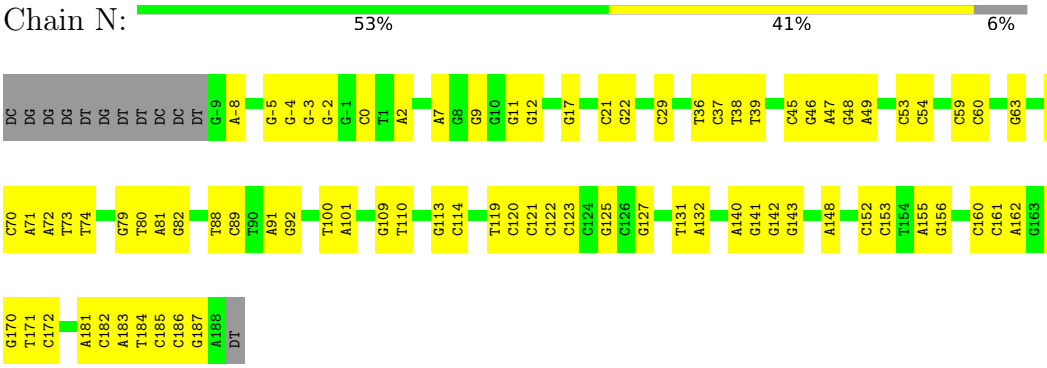
• Molecule 23: Transcription initiation factor IIB

Chain M:



• Molecule 24: Non-template DNA

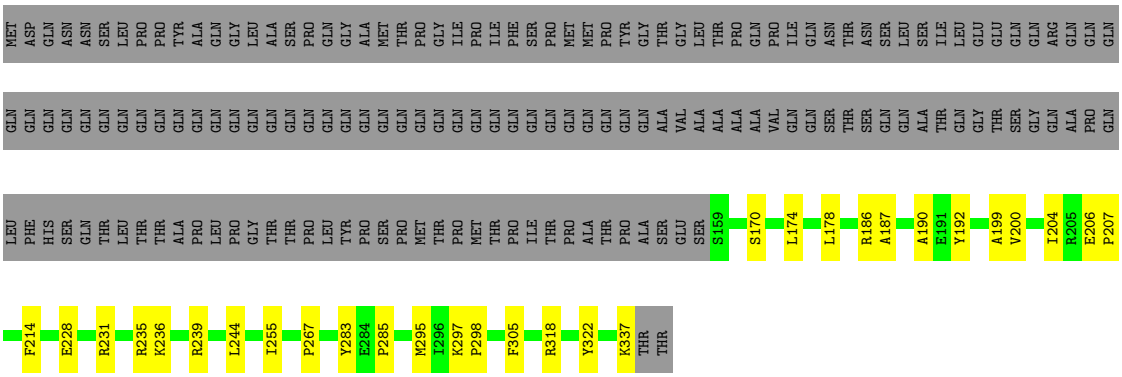
Chain N:

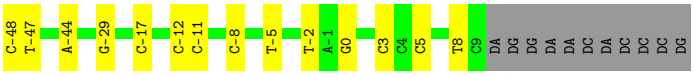


• Molecule 25: TATA-box-binding protein

Chain O:



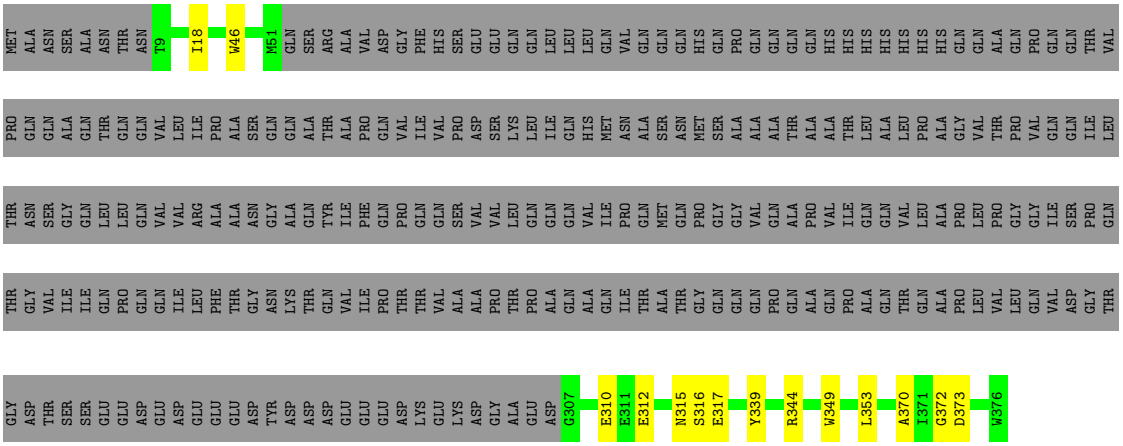

MET ASP GLN ASN SER LEU PRO PRO TYR ALA GLN GLY LEU ALA SER PRO GLN GLY ALA MET THR PRO GLY ILE PRO ILE PHE SER PRO MET MET PRO TYR GLY THR GLY LEU THR PRO GLN PRO ILE GLN ASN THR ASN SER LEU SER ILE LEU GLU GLN GLN ARG GLN GLN
GLN GLN GLN



• Molecule 29: Transcription initiation factor IIA subunit 1

Chain U:

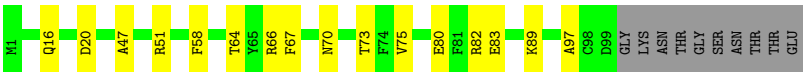




• Molecule 30: Transcription initiation factor IIA subunit 2

Chain V:

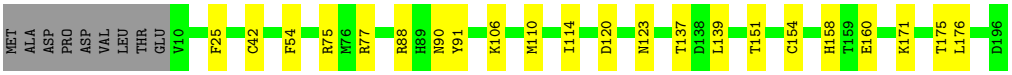




• Molecule 31: General transcription factor IIE subunit 1

Chain W:

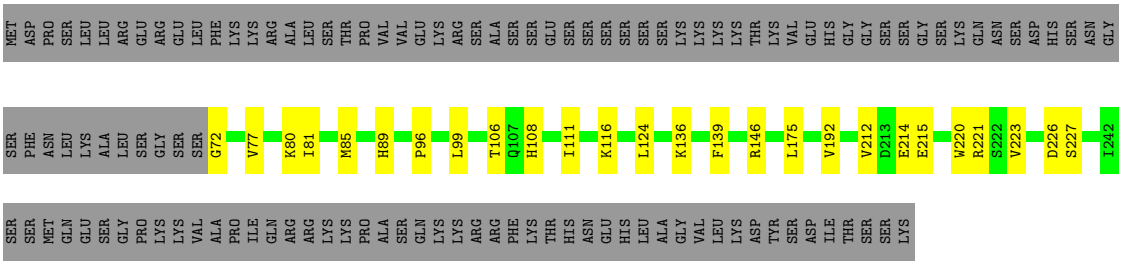




• Molecule 32: Transcription initiation factor IIE subunit beta

Chain X:





• Molecule 33: Histone H3.2

Chain a:

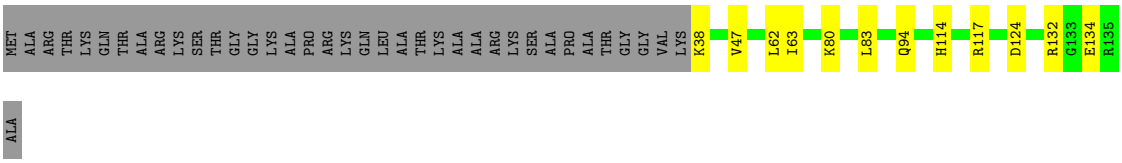




• Molecule 33: Histone H3.2

Chain e:

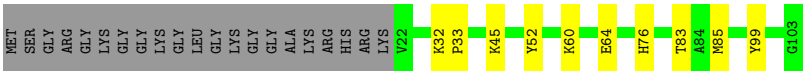




• Molecule 34: Histone H4

Chain b:

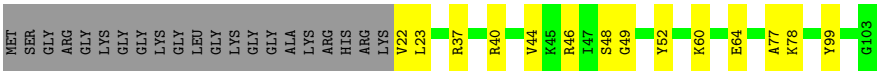




• Molecule 34: Histone H4

Chain f:

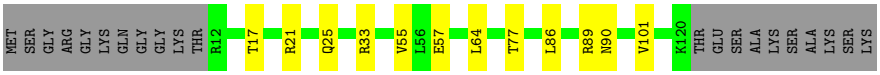




• Molecule 35: Histone H2A type 1

Chain c:





• Molecule 35: Histone H2A type 1

Chain g:





• Molecule 36: Histone H2B 1.1

Chain d:





• Molecule 36: Histone H2B 1.1

Chain h:




MET
PRO
GLU
PRO
ALA
LYS
SER
ALA
PRO
ALA
PRO
LYS
LYS
GLY
SER
LYS
LYS
ALA
VAL
THR
LYS
THR
GLN
LYS
LYS
ASP
GLY
LYS
LYS
ARG
ARG
K32
E36
V42
M60
D69
N85
K86
R87
R93
K126

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101994	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 ($e^-/Å^2$)	50.45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	21.074	Depositor
Minimum map value	-5.711	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.4	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, 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	0.15	0/5294	0.52	0/7158
2	1	0.21	0/6158	0.59	0/8342
3	2	0.32	0/2683	0.59	0/3672
4	3	0.13	0/3672	0.51	0/4979
5	4	0.15	0/2764	0.54	0/3754
6	5	0.16	0/2101	0.59	0/2843
7	6	0.13	0/528	0.43	0/713
8	7	0.17	0/2269	0.54	0/3053
9	8	0.17	0/2429	0.59	0/3295
10	9	0.16	0/2384	0.51	0/3220
11	A	0.31	0/11479	0.55	0/15496
12	B	0.38	0/9257	0.58	0/12493
13	C	0.36	0/2102	0.58	0/2857
14	D	0.13	0/1064	0.41	0/1428
15	E	0.24	0/1752	0.47	0/2366
16	F	0.31	0/646	0.55	0/871
17	G	0.18	0/1382	0.48	0/1874
18	H	0.29	0/1207	0.53	0/1628
19	I	0.20	0/949	0.48	0/1284
20	J	0.41	0/516	0.66	0/696
21	K	0.34	0/939	0.52	0/1271
22	L	0.35	0/378	0.74	0/500
23	M	0.26	0/1983	0.49	0/2679
24	N	0.32	0/4543	0.67	0/7009
25	O	0.18	0/1448	0.47	0/1948
26	Q	0.13	0/1167	0.40	0/1576
27	R	0.17	0/1817	0.41	0/2445
28	T	0.30	0/4557	0.63	0/7033
29	U	0.14	0/945	0.41	0/1274
30	V	0.14	0/816	0.41	0/1105
31	W	0.15	0/1560	0.47	0/2097
32	X	0.13	0/1427	0.42	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	a	0.11	0/814	0.45	0/1092
33	e	0.12	0/823	0.41	0/1104
34	b	0.10	0/660	0.40	0/883
34	f	0.13	0/660	0.44	0/883
35	c	0.10	0/853	0.37	0/1149
35	g	0.11	0/828	0.41	0/1117
36	d	0.16	0/777	0.46	0/1041
36	h	0.18	0/755	0.43	0/1013
All	All	0.25	0/88386	0.54	0/121157

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5189	0	5164	93	0
2	1	6034	0	6002	135	0
3	2	2643	0	2044	32	0
4	3	3589	0	3621	61	0
5	4	2710	0	2538	36	0
6	5	2064	0	2099	39	0
7	6	522	0	528	8	0
8	7	2233	0	2210	30	0
9	8	2370	0	2391	28	0
10	9	2334	0	2357	8	0
11	A	11274	0	11406	149	0
12	B	9076	0	9116	105	0
13	C	2059	0	2008	31	0
14	D	1050	0	1033	11	0
15	E	1721	0	1737	24	0
16	F	636	0	665	6	0
17	G	1351	0	1358	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	1186	0	1147	22	0
19	I	928	0	859	15	0
20	J	507	0	523	11	0
21	K	920	0	942	9	0
22	L	373	0	379	11	0
23	M	1953	0	1990	23	0
24	N	4051	0	2222	69	0
25	O	1422	0	1514	23	0
26	Q	1138	0	1103	14	0
27	R	1788	0	1819	29	0
28	T	4061	0	2221	49	0
29	U	930	0	888	12	0
30	V	806	0	818	9	0
31	W	1535	0	1539	17	0
32	X	1403	0	1428	19	0
33	a	802	0	841	4	0
33	e	811	0	853	8	0
34	b	653	0	696	7	0
34	f	653	0	696	11	0
35	c	843	0	908	10	0
35	g	818	0	877	5	0
36	d	766	0	797	4	0
36	h	744	0	771	8	0
37	1	8	0	0	0	0
38	4	3	0	0	0	0
38	5	1	0	0	0	0
38	7	2	0	0	0	0
38	A	2	0	0	0	0
38	B	1	0	0	0	0
38	C	1	0	0	0	0
38	I	2	0	0	0	0
38	J	1	0	0	0	0
38	L	1	0	0	0	0
38	M	1	0	0	0	0
38	W	1	0	0	0	0
39	A	1	0	0	0	0
All	All	85971	0	82108	1044	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1044 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:74:CYS:SG	11:A:84:HIS:CE1	2.49	1.04
12:B:905:ASP:OD1	12:B:924:ARG:NH1	2.11	0.84
12:B:953:ASP:OD1	13:C:36:ARG:NH2	2.13	0.82
15:E:46:ASP:O	15:E:52:ARG:NH1	2.14	0.81
5:4:349:GLN:O	6:5:146:ARG:NH2	2.13	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	649/782 (83%)	629 (97%)	20 (3%)	0	100	100
2	1	758/760 (100%)	736 (97%)	22 (3%)	0	100	100
3	2	402/548 (73%)	352 (88%)	47 (12%)	3 (1%)	18	55
4	3	450/462 (97%)	437 (97%)	13 (3%)	0	100	100
5	4	362/395 (92%)	340 (94%)	22 (6%)	0	100	100
6	5	259/308 (84%)	244 (94%)	15 (6%)	0	100	100
7	6	64/71 (90%)	64 (100%)	0	0	100	100
8	7	269/309 (87%)	264 (98%)	5 (2%)	0	100	100
9	8	296/346 (86%)	281 (95%)	15 (5%)	0	100	100
10	9	285/323 (88%)	279 (98%)	6 (2%)	0	100	100
11	A	1413/1970 (72%)	1376 (97%)	37 (3%)	0	100	100
12	B	1130/1174 (96%)	1099 (97%)	31 (3%)	0	100	100
13	C	253/275 (92%)	248 (98%)	5 (2%)	0	100	100
14	D	126/142 (89%)	125 (99%)	1 (1%)	0	100	100
15	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
18	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
19	I	112/125 (90%)	107 (96%)	5 (4%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
22	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
23	M	248/316 (78%)	242 (98%)	6 (2%)	0	100	100
25	O	177/339 (52%)	176 (99%)	1 (1%)	0	100	100
26	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
27	R	218/249 (88%)	215 (99%)	3 (1%)	0	100	100
29	U	109/376 (29%)	108 (99%)	1 (1%)	0	100	100
30	V	97/109 (89%)	94 (97%)	3 (3%)	0	100	100
31	W	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
32	X	169/291 (58%)	162 (96%)	7 (4%)	0	100	100
33	a	95/136 (70%)	95 (100%)	0	0	100	100
33	e	96/136 (71%)	96 (100%)	0	0	100	100
34	b	80/103 (78%)	80 (100%)	0	0	100	100
34	f	80/103 (78%)	80 (100%)	0	0	100	100
35	c	107/130 (82%)	107 (100%)	0	0	100	100
35	g	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
36	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
36	h	93/126 (74%)	93 (100%)	0	0	100	100
All	All	9731/12274 (79%)	9439 (97%)	289 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	164	VAL
3	2	170	PHE
3	2	169	ALA

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	0	558/688 (81%)	558 (100%)	0	100	100
2	1	639/664 (96%)	639 (100%)	0	100	100
3	2	176/484 (36%)	176 (100%)	0	100	100
4	3	384/399 (96%)	384 (100%)	0	100	100
5	4	280/352 (80%)	280 (100%)	0	100	100
6	5	234/272 (86%)	234 (100%)	0	100	100
7	6	59/64 (92%)	59 (100%)	0	100	100
8	7	250/283 (88%)	250 (100%)	0	100	100
9	8	258/299 (86%)	253 (98%)	5 (2%)	50	67
10	9	259/296 (88%)	259 (100%)	0	100	100
11	A	1254/1749 (72%)	1254 (100%)	0	100	100
12	B	994/1027 (97%)	994 (100%)	0	100	100
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/126 (94%)	118 (100%)	0	100	100
15	E	191/192 (100%)	191 (100%)	0	100	100
16	F	69/111 (62%)	69 (100%)	0	100	100
17	G	152/153 (99%)	152 (100%)	0	100	100
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	53 (100%)	0	100	100
21	K	104/106 (98%)	104 (100%)	0	100	100
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	121 (100%)	0	100	100
27	R	196/218 (90%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	U	105/324 (32%)	105 (100%)	0	100	100
30	V	90/98 (92%)	90 (100%)	0	100	100
31	W	169/177 (96%)	169 (100%)	0	100	100
32	X	154/261 (59%)	154 (100%)	0	100	100
33	a	85/111 (77%)	85 (100%)	0	100	100
33	e	86/111 (78%)	86 (100%)	0	100	100
34	b	67/79 (85%)	67 (100%)	0	100	100
34	f	67/79 (85%)	67 (100%)	0	100	100
35	c	86/101 (85%)	86 (100%)	0	100	100
35	g	84/101 (83%)	84 (100%)	0	100	100
36	d	83/106 (78%)	83 (100%)	0	100	100
36	h	81/106 (76%)	81 (100%)	0	100	100
All	All	8382/10752 (78%)	8377 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	8	64	LYS
9	8	96	THR
9	8	97	ASP
9	8	203	LEU
9	8	307	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
19	I	87	GLN
36	d	48	GLN
19	I	100	HIS
27	R	152	ASN
8	7	200	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 17 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	$\#\|Z\| > 2$
37	SF4	1	1000	2	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
37	SF4	1	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

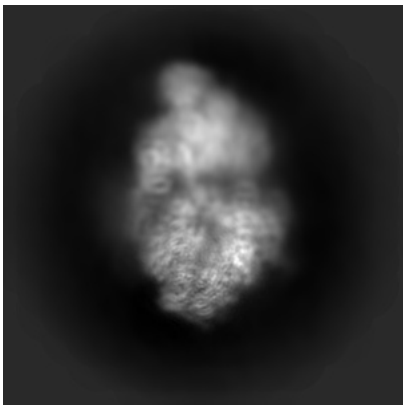
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16331. These allow visual inspection of the internal detail of the map and identification of artifacts.

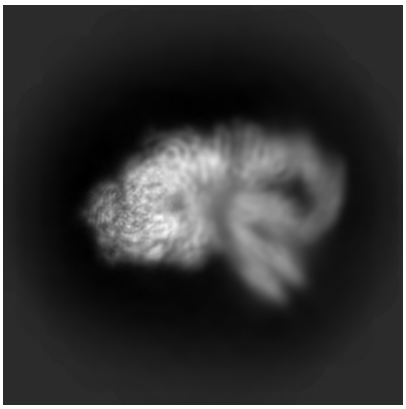
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

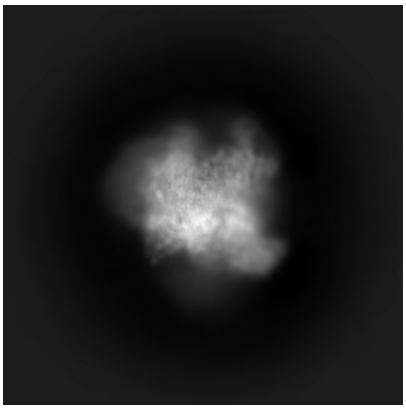
6.1.1 Primary map



X

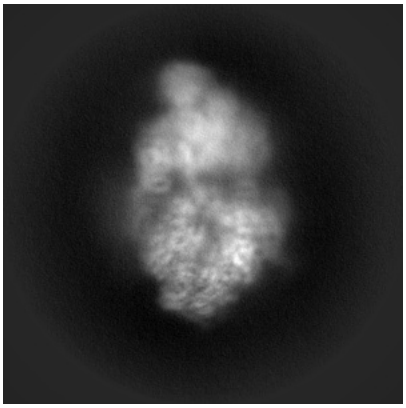


Y

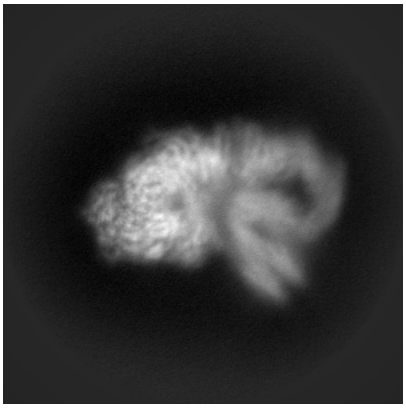


Z

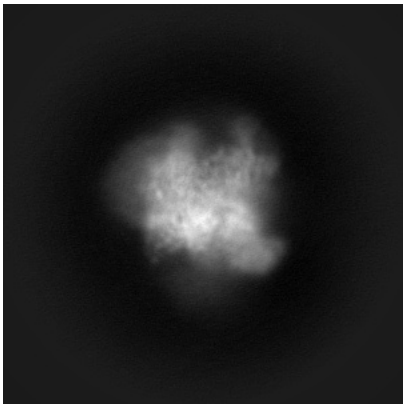
6.1.2 Raw map



X



Y

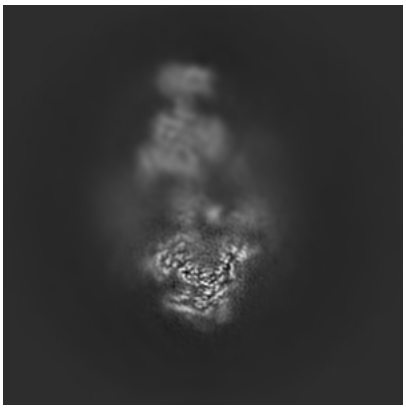


Z

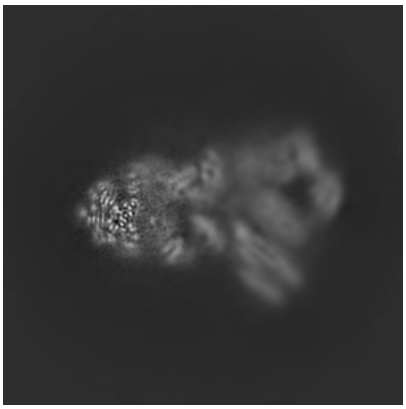
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

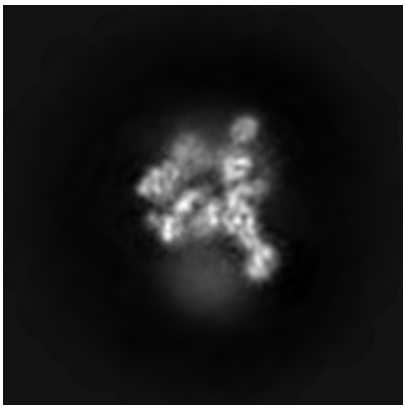
6.2.1 Primary map



X Index: 200

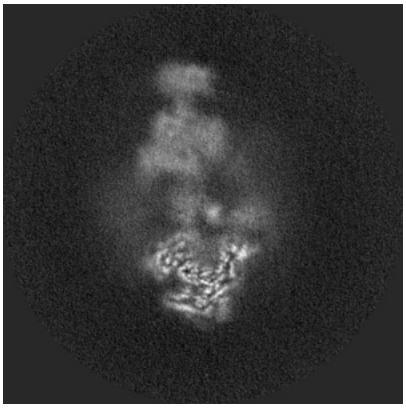


Y Index: 200

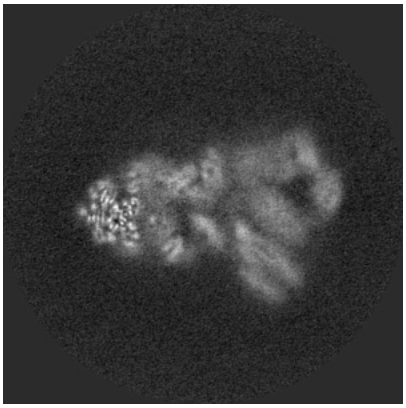


Z Index: 200

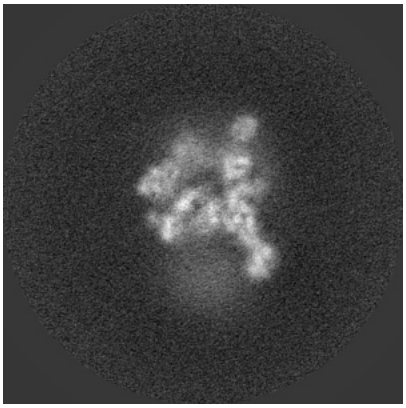
6.2.2 Raw map



X Index: 200



Y Index: 200

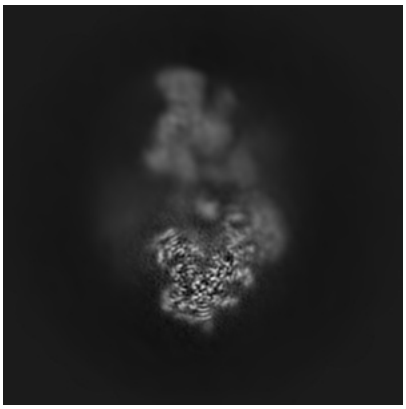


Z Index: 200

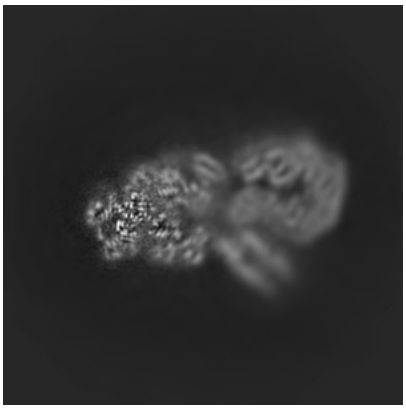
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

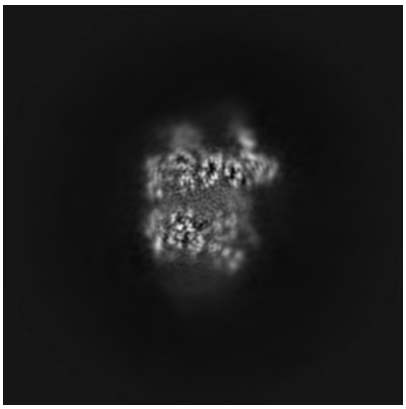
6.3.1 Primary map



X Index: 186

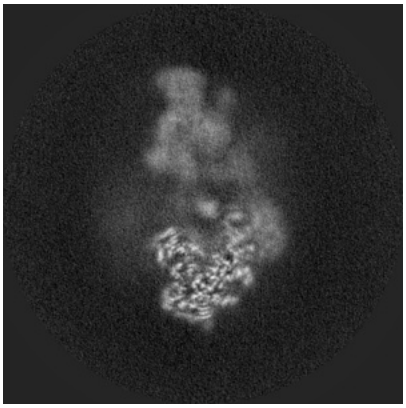


Y Index: 185

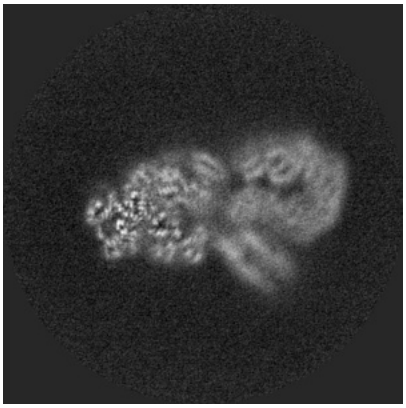


Z Index: 154

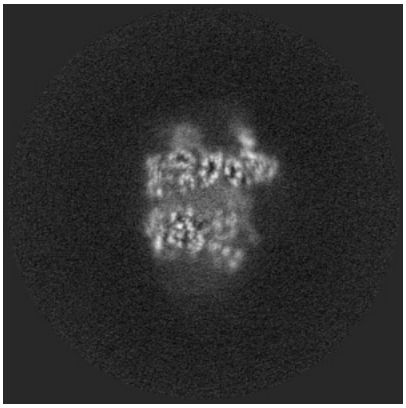
6.3.2 Raw map



X Index: 186



Y Index: 185

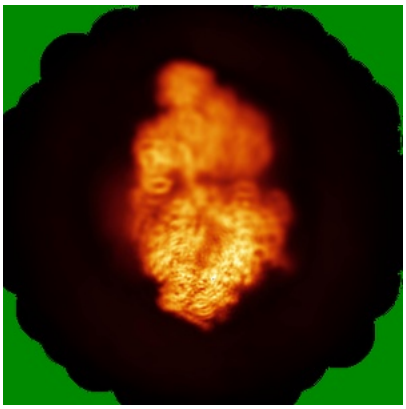


Z Index: 154

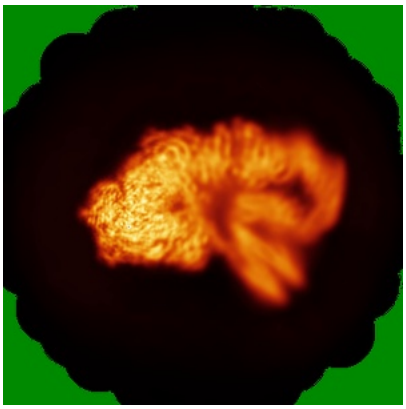
The images above show the largest variance slices of the map in three orthogonal directions.

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

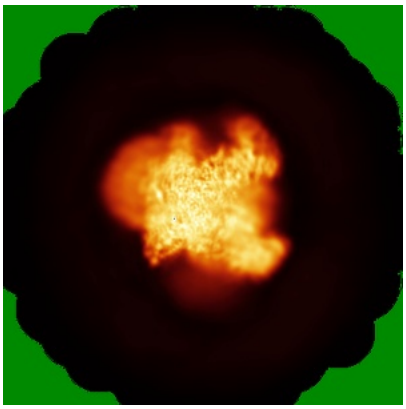
6.4.1 Primary map



X

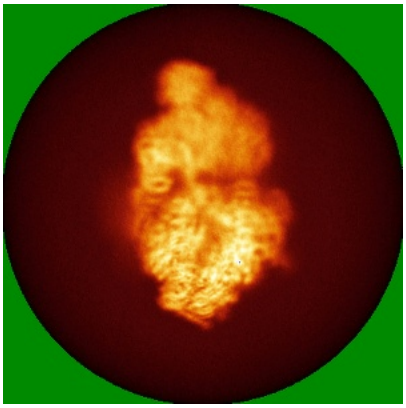


Y

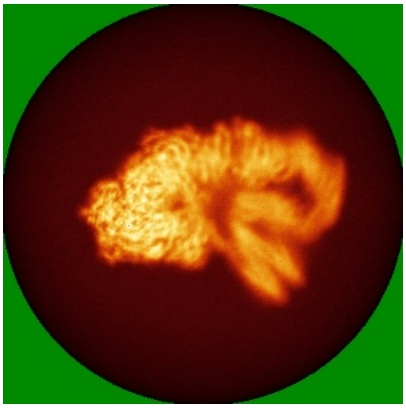


Z

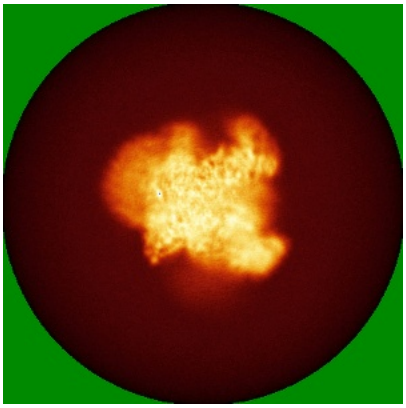
6.4.2 Raw map



X



Y

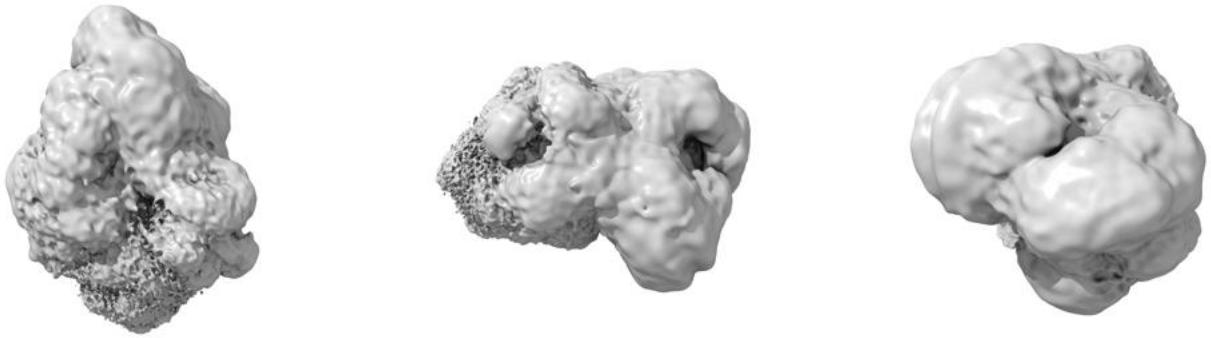


Z

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

6.5 Orthogonal surface views (i)

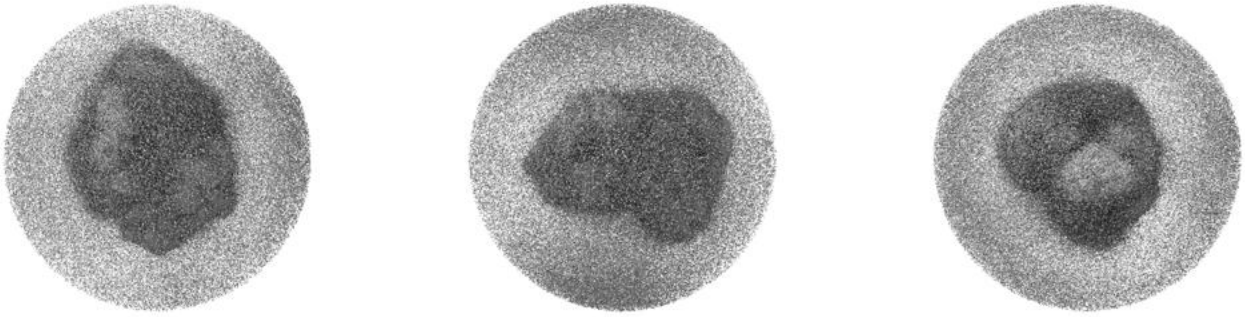
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

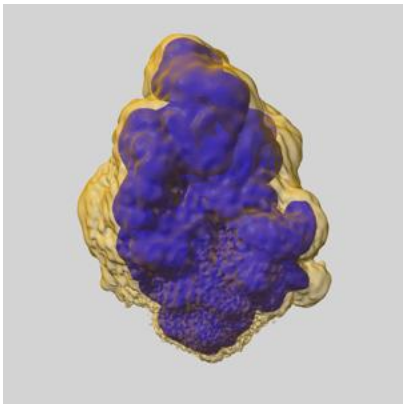
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

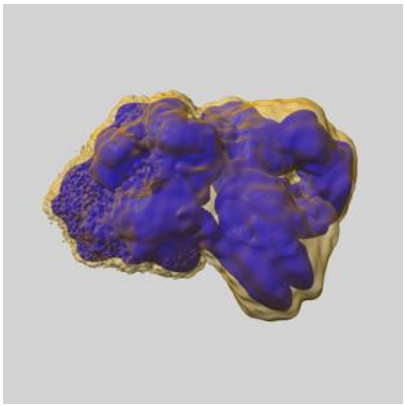
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

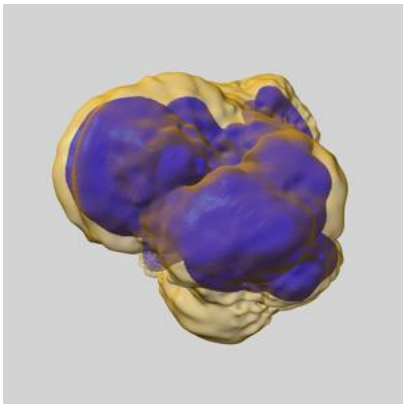
6.6.1 emd_16331_msk_1.map (i)



X



Y

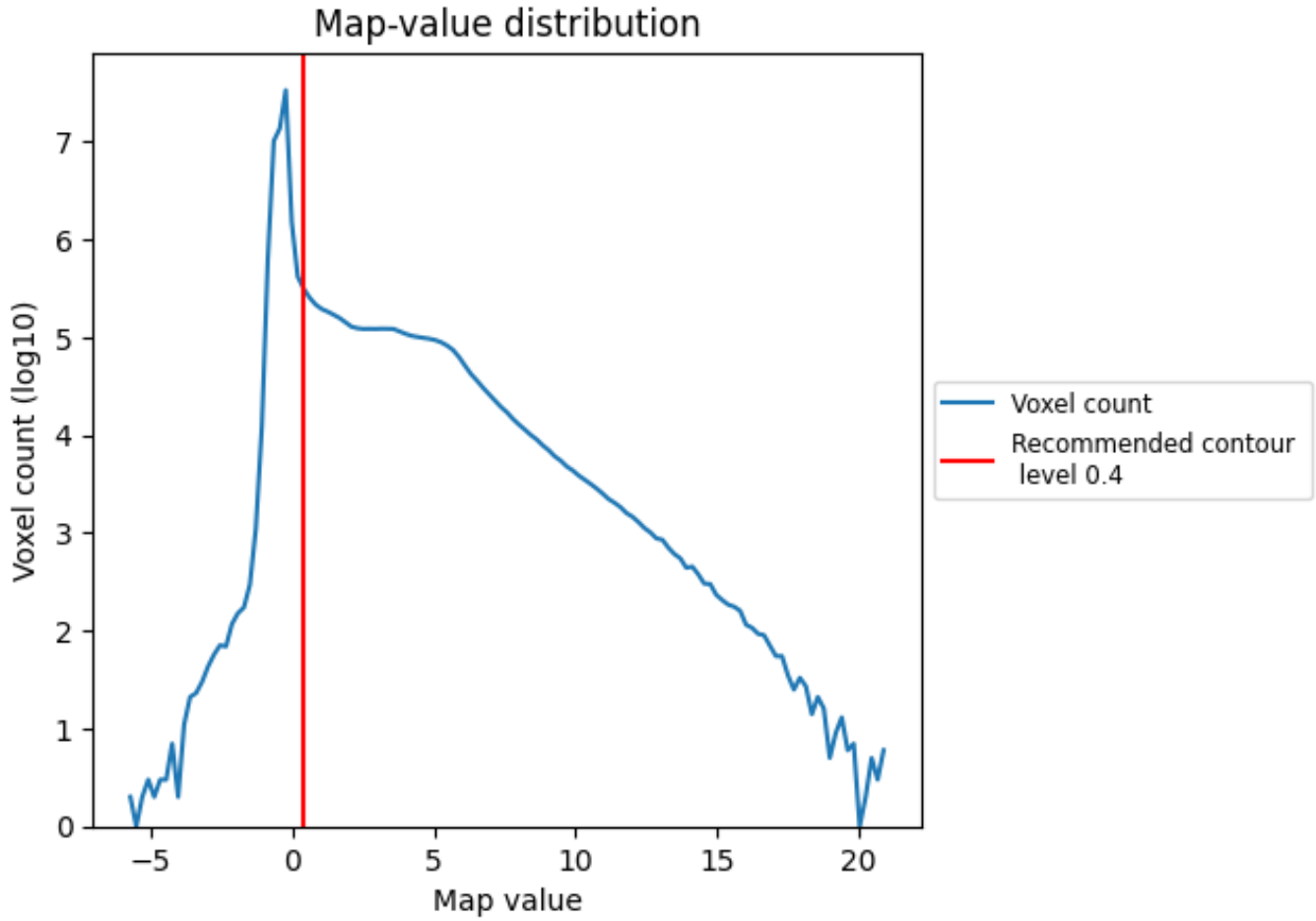


Z

7 Map analysis

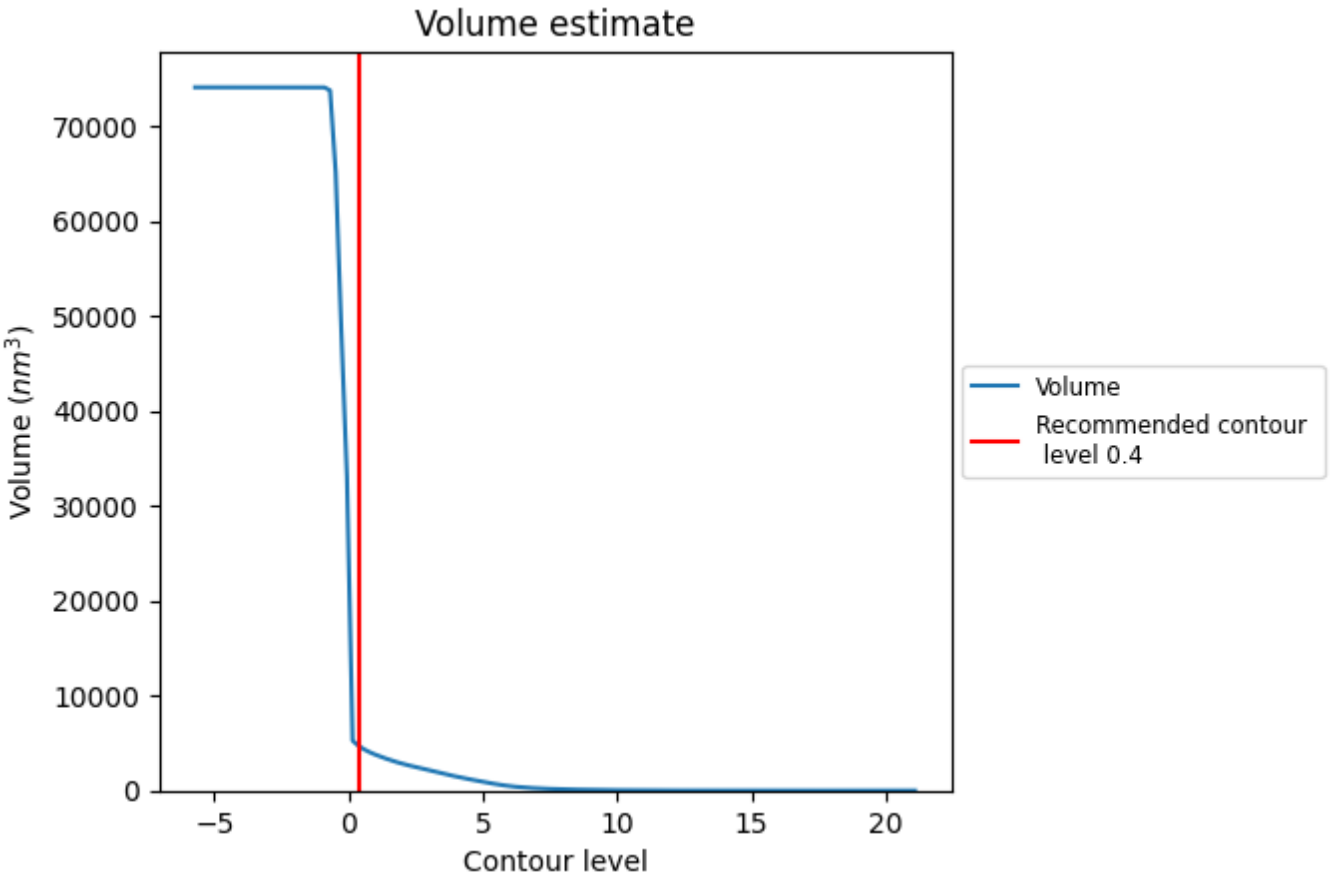
This section contains the results of statistical analysis of the map.

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.

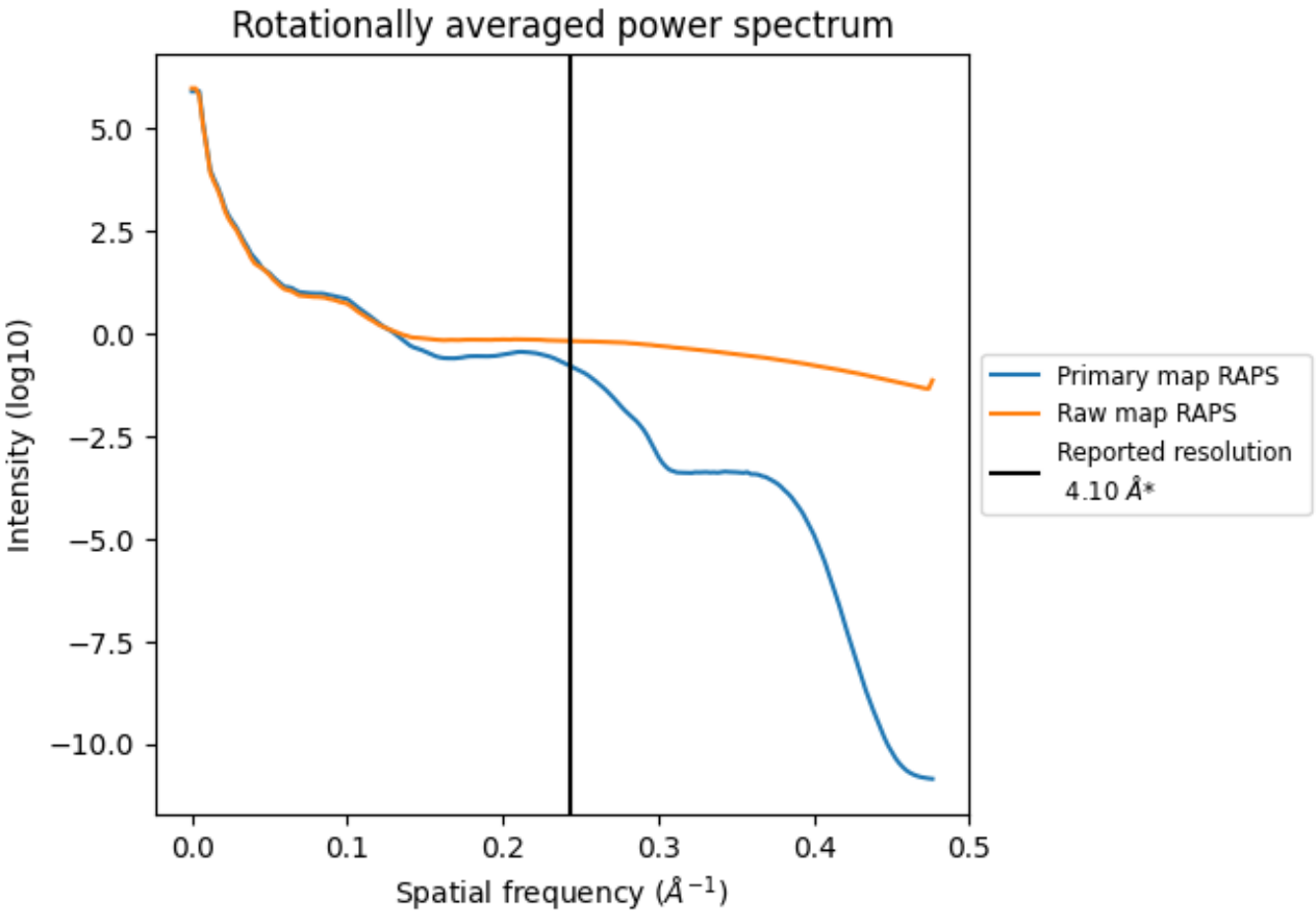
7.2 Volume estimate (i)



The volume at the recommended contour level is 4663 nm^3; this corresponds to an approximate mass of 4212 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)

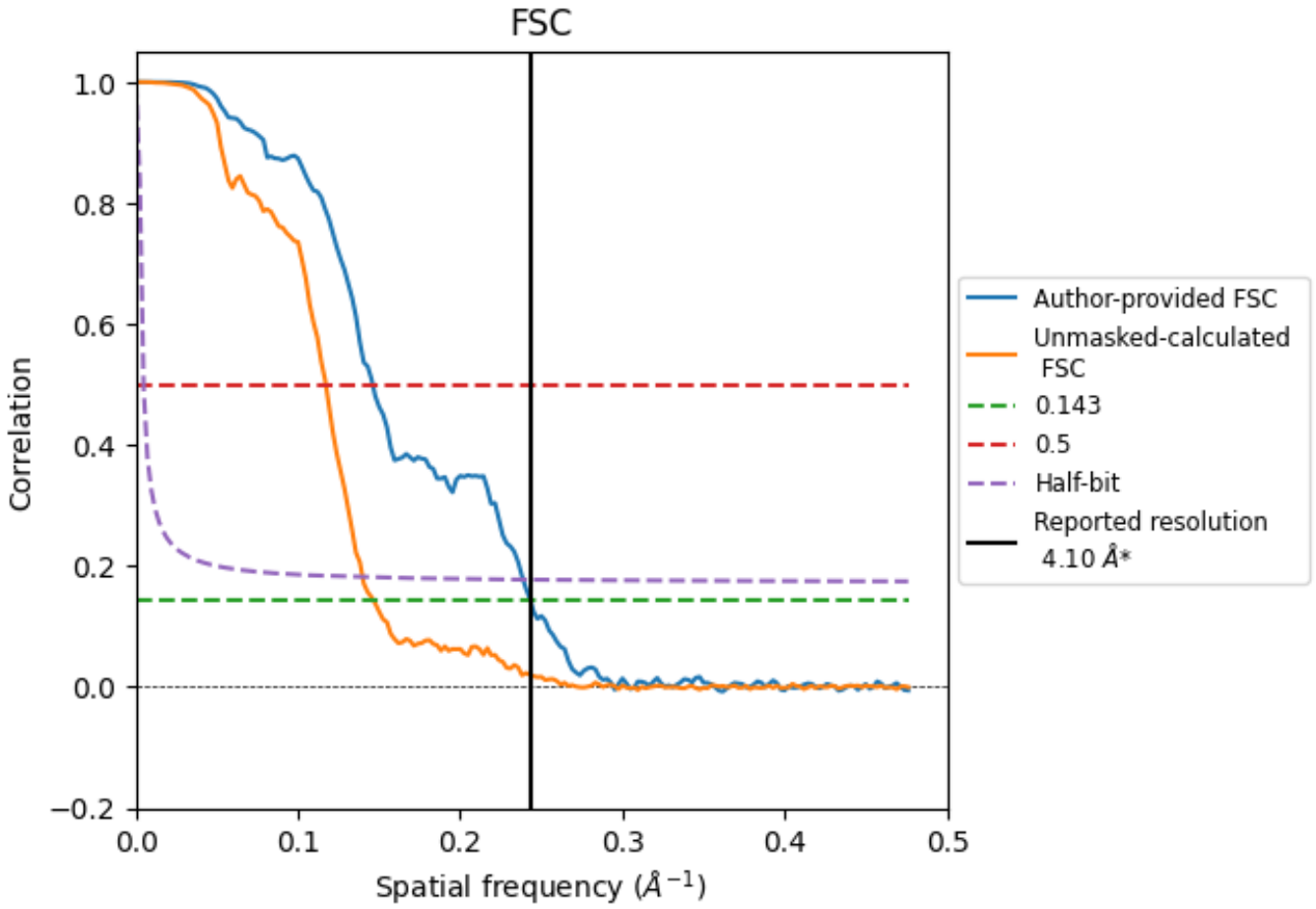


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

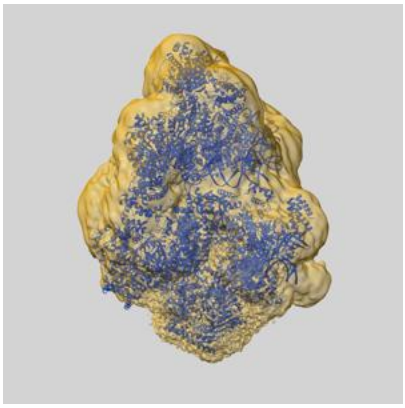
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.11	6.85	4.19
Unmasked-calculated*	6.83	8.54	7.15

*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 6.83 differs from the reported value 4.1 by more than 10 %

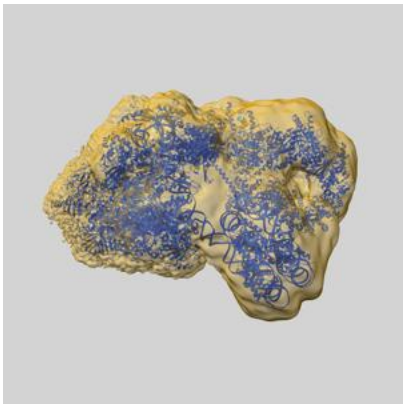
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16331 and PDB model 8BYQ. Per-residue inclusion information can be found in section 3 on page 13.

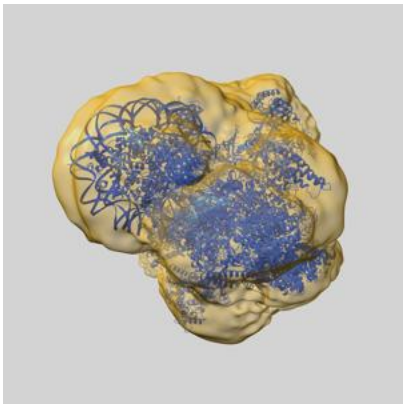
9.1 Map-model overlay



X



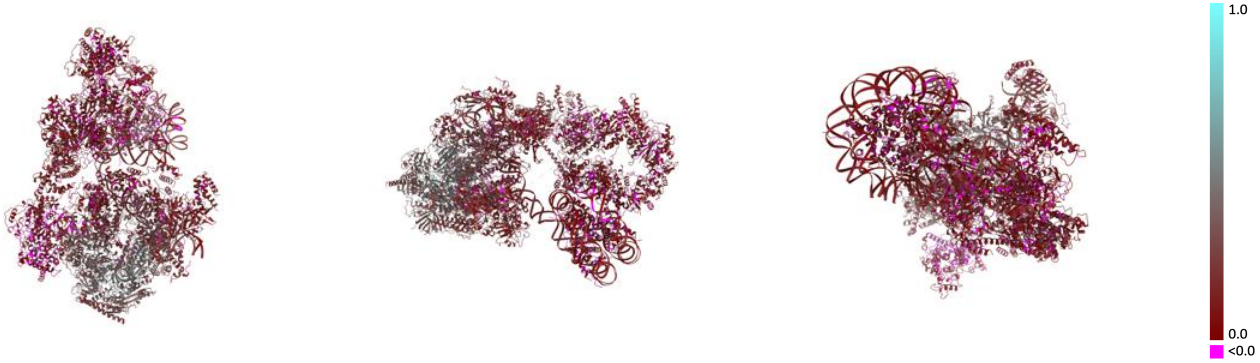
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

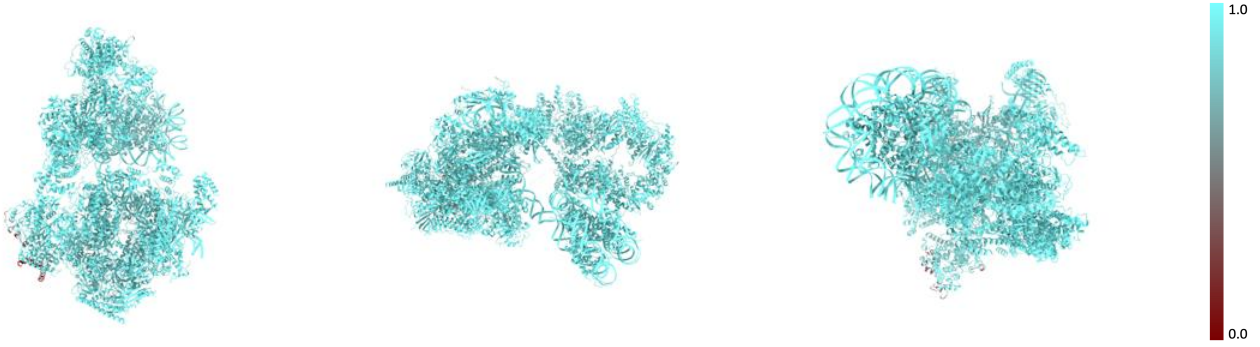
9.2 Q-score mapped to coordinate model



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.

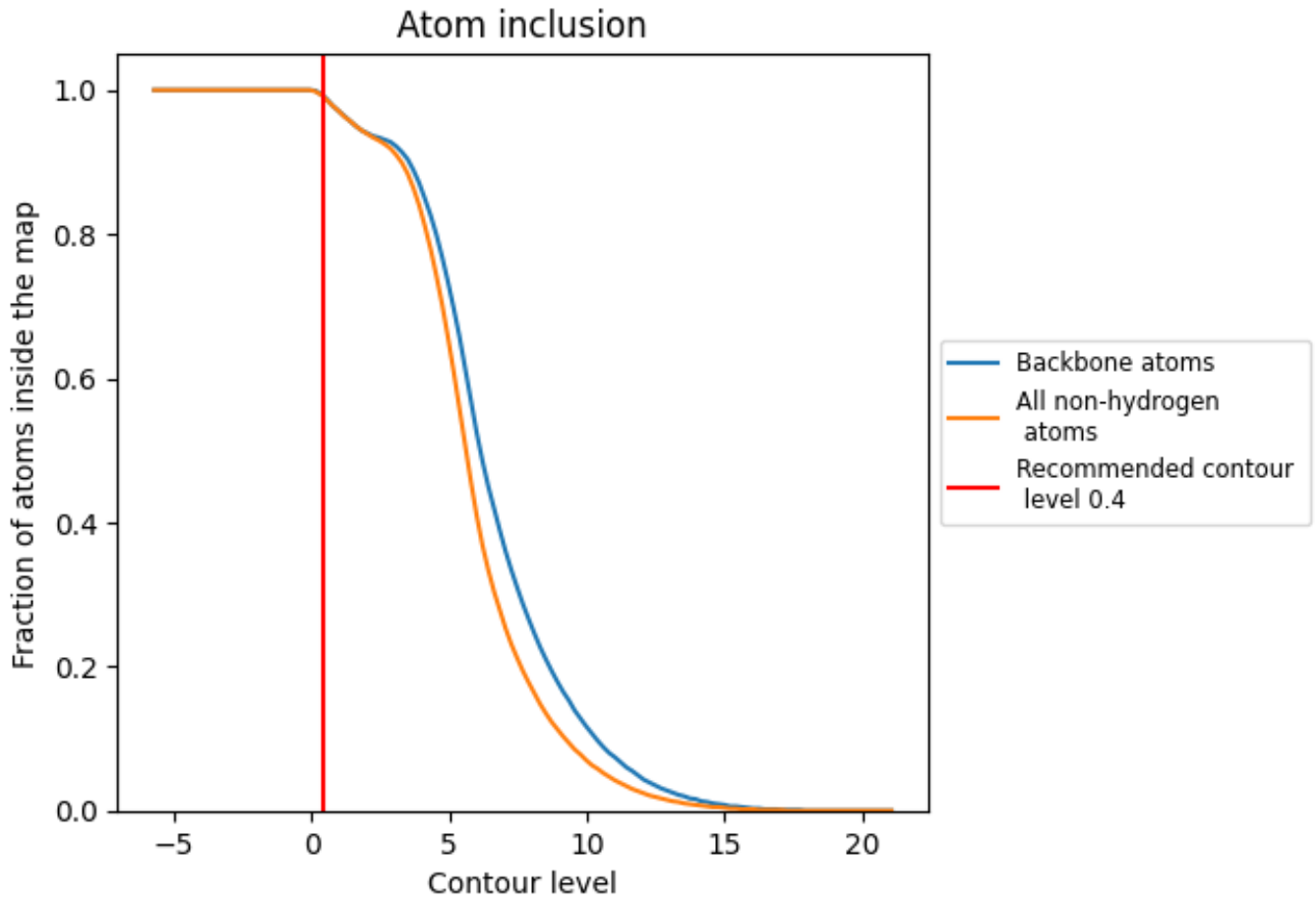
9.3 Atom inclusion mapped to coordinate model



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9920	0.1870
0	1.0000	0.1050
1	1.0000	0.1460
2	1.0000	0.0750
3	0.9990	0.1110
4	1.0000	0.1230
5	1.0000	0.1010
6	1.0000	0.0890
7	0.9570	0.1170
8	0.9540	0.0540
9	0.8120	0.0410
A	1.0000	0.2890
B	1.0000	0.3560
C	1.0000	0.3560
D	1.0000	0.1380
E	1.0000	0.2410
F	1.0000	0.3430
G	1.0000	0.1690
H	1.0000	0.3070
I	1.0000	0.2160
J	1.0000	0.3860
K	1.0000	0.3430
L	1.0000	0.3410
M	1.0000	0.2650
N	1.0000	0.1450
O	1.0000	0.1900
Q	1.0000	0.1400
R	0.9990	0.1590
T	1.0000	0.1470
U	0.9950	0.1500
V	1.0000	0.1430
W	1.0000	0.1230
X	1.0000	0.1340
a	1.0000	0.0880
b	1.0000	0.0830



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	1.0000	0.0740
d	1.0000	0.0770
e	1.0000	0.1130
f	1.0000	0.1010
g	1.0000	0.0760
h	1.0000	0.0900