



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:20 am GMT

PDB ID : 6GYL
EMDB ID : EMD-0091
Title : Structure of a yeast closed complex with distorted DNA (core CCdist)
Authors : Dienemann, C.; Schwalb, B.; Schilbach, S.; Cramer, P.
Deposited on : 2018-06-30
Resolution : 4.80 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
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

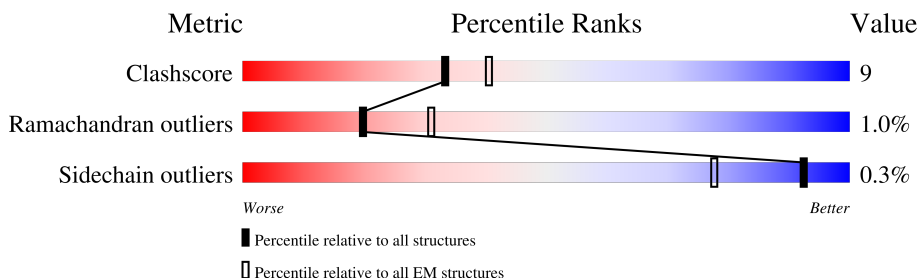
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.





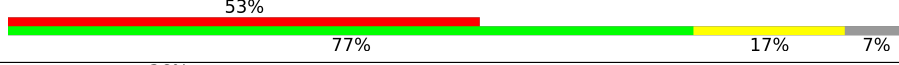
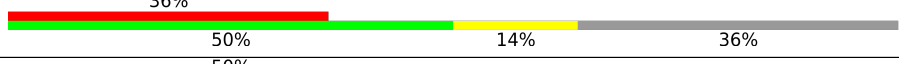
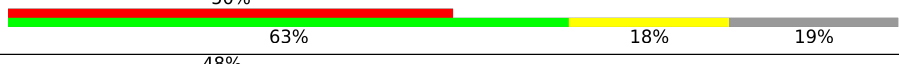
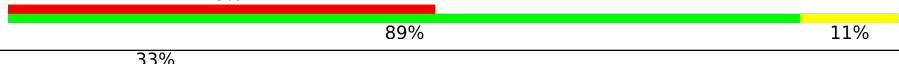
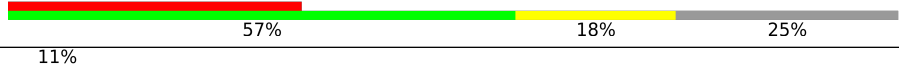



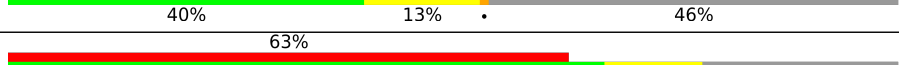


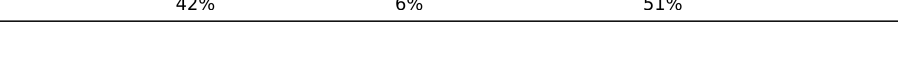
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	44% (Poor fit) 67% (0 outliers) 14% (1 outlier) 19% (2+ outliers)
2	B	1224	53% (0 outliers) 73% (1 outlier) 21% (2 outliers) 6% (2+ outliers)
3	C	318	42% (0 outliers) 68% (1 outlier) 14% (2 outliers) 18% (2+ outliers)
4	D	221	56% (0 outliers) 61% (1 outlier) 10% (2 outliers) 29% (2+ outliers)
5	E	215	57% (0 outliers) 88% (1 outlier) 11% (2 outliers)
6	F	155	26% (Poor fit) 43% (0 outliers) 10% (1 outlier) 46% (2+ outliers)
7	G	171	57% (0 outliers) 65% (1 outlier) 35% (2+ outliers)
8	H	146	50% (0 outliers) 71% (1 outlier) 23% (2 outliers) 7% (2+ outliers)

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Mol	Chain	Length	Quality of chain
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	56	
15	O	240	
16	Q	735	
17	R	400	
18	T	56	
19	U	171	
20	V	129	
21	W	586	
22	X	328	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 43409 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	1398	10997	6931	1927	2078	61	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	1152	9178	5807	1608	1708	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	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	0	0

- Molecule 5 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		
5	E	213	1744	1107	308	318	11	0	0

- Molecule 6 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		
6	F	83	670	428	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 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		
8	H	136	1089	686	184	215	4	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	944	581	172	181	10	0	0

- Molecule 10 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		
10	J	65	532	339	93	94	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	112	904	580	154	168	2	0	0

- Molecule 12 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		
12	L	45	358	221	71	62	4	0	0

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	279	2175	1382	373	403	17	0	0

- Molecule 14 is a DNA chain called GAT1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	56	1129	540	204	329	56	0	0

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	180	1416	921	242	247	6	0	0

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	148	1144	733	195	212	4	0	0

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	190	1303	812	238	246	7	0	0

- Molecule 18 is a DNA chain called GAT1 promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	T	56	1149	546	222	325	56	0	0

- Molecule 19 is a protein called Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	92	757	474	130	150	3	0	0

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	100	782	492	130	156	4	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	123	LYS	-	expression tag	UNP P32774
V	124	HIS	-	expression tag	UNP P32774
V	125	HIS	-	expression tag	UNP P32774
V	126	HIS	-	expression tag	UNP P32774
V	127	HIS	-	expression tag	UNP P32774
V	128	HIS	-	expression tag	UNP P32774
V	129	HIS	-	expression tag	UNP P32774

- Molecule 21 is a protein called Transcription initiation factor IIE subunit alpha,Tfa1,Tfa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	191	1469	932	254	277	6	0	0

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	160	1004	620	184	196	4	0	0

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

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

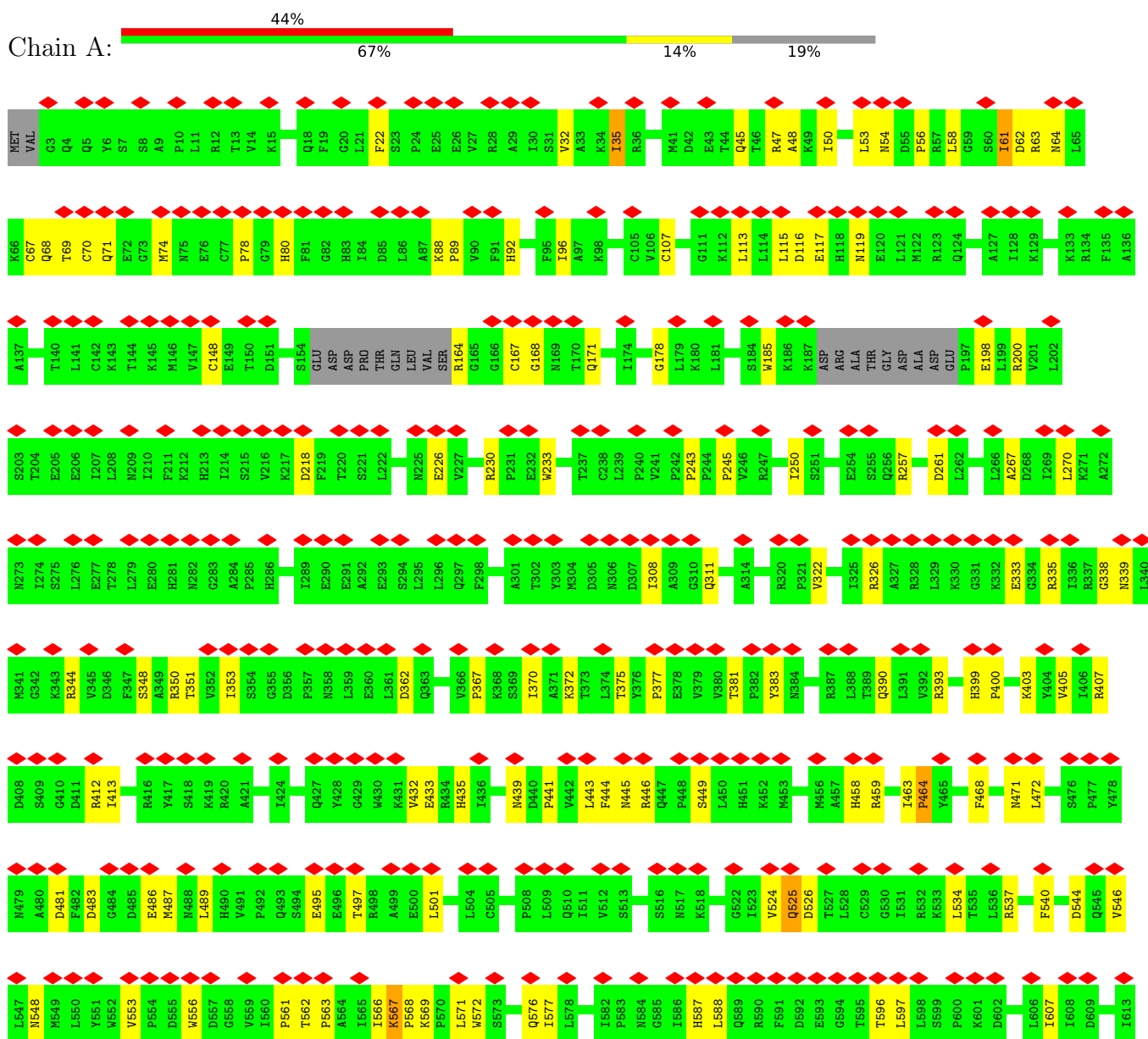
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

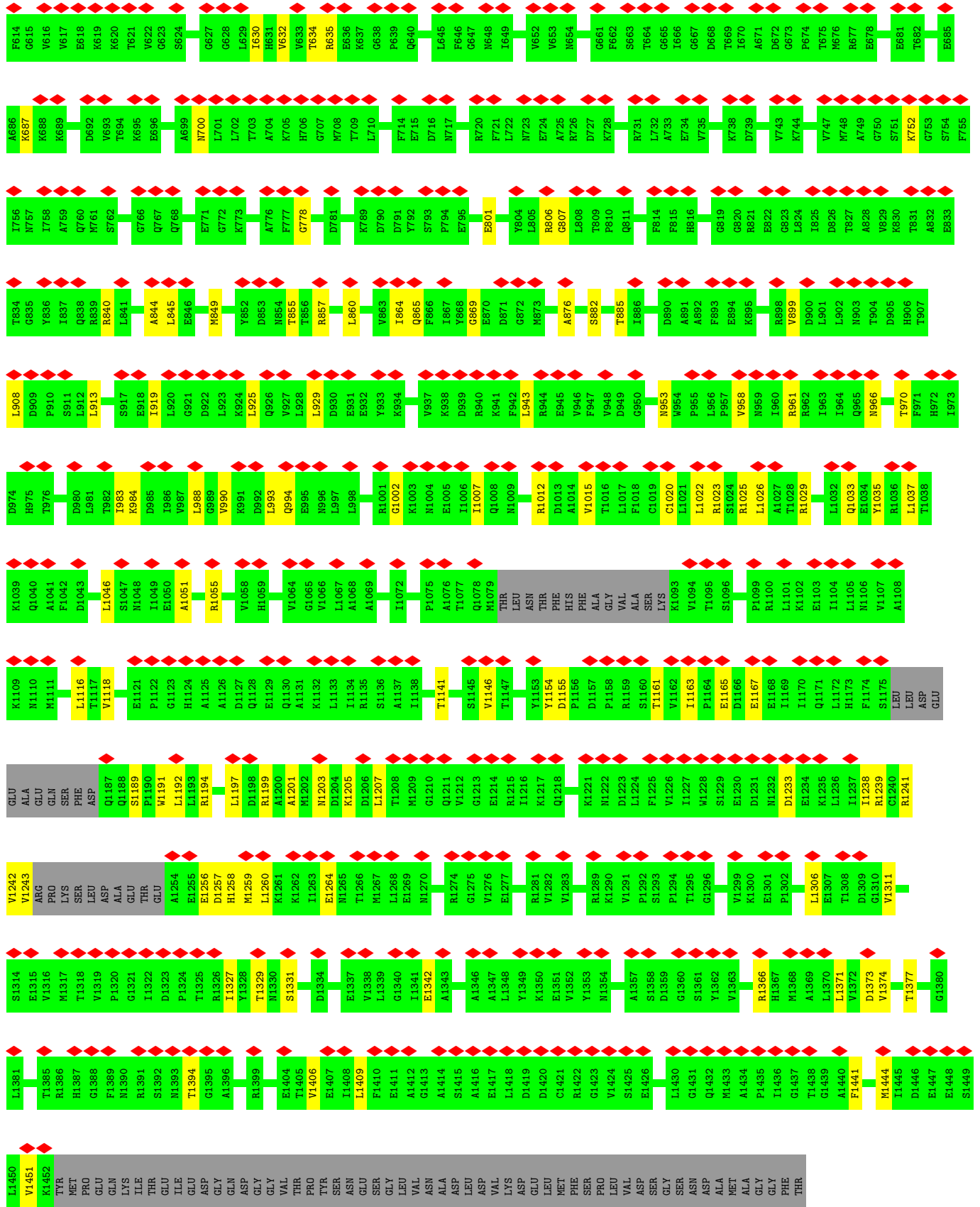
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total 1	Mg 1	0

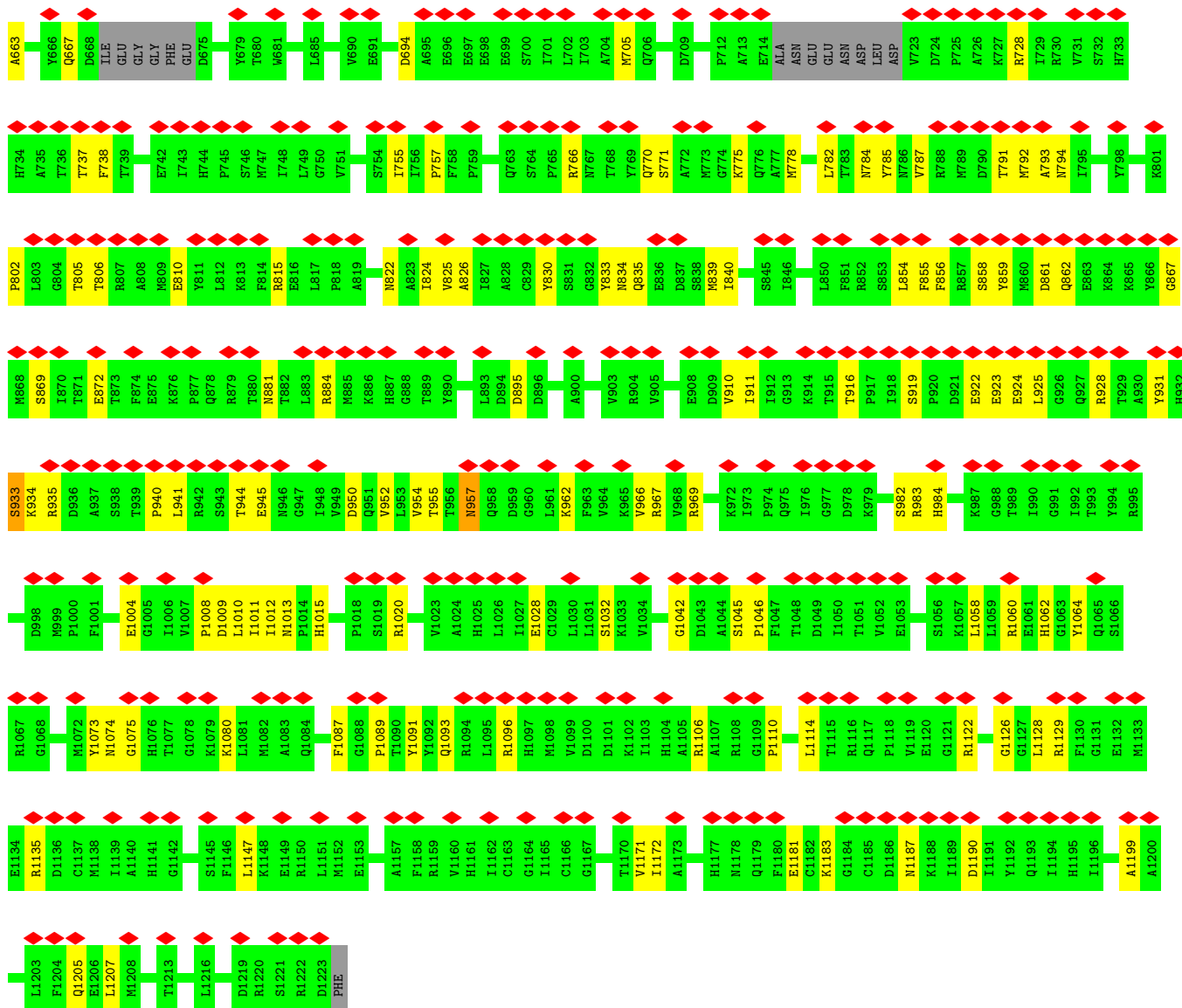
3 Residue-property plots

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

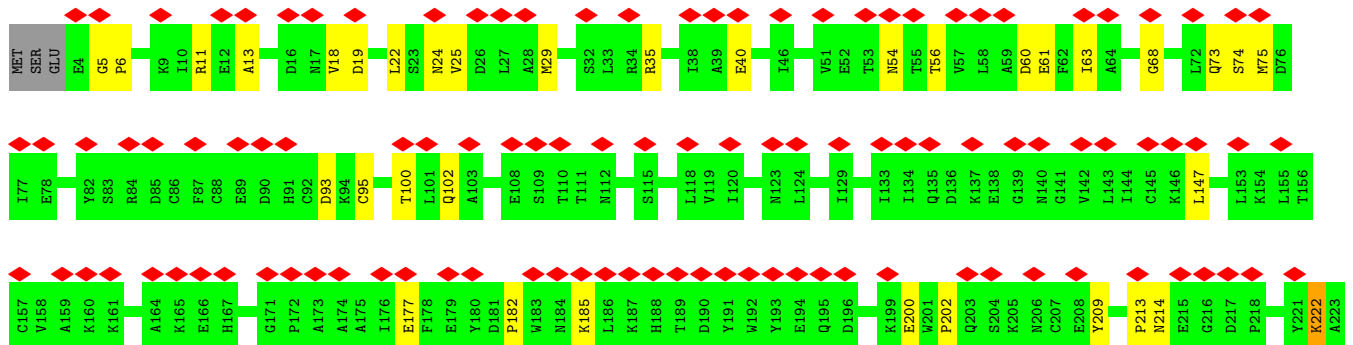
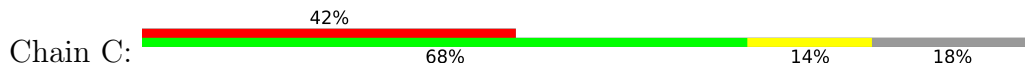
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

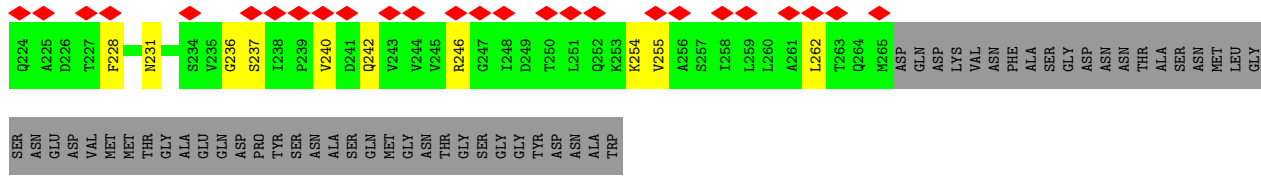




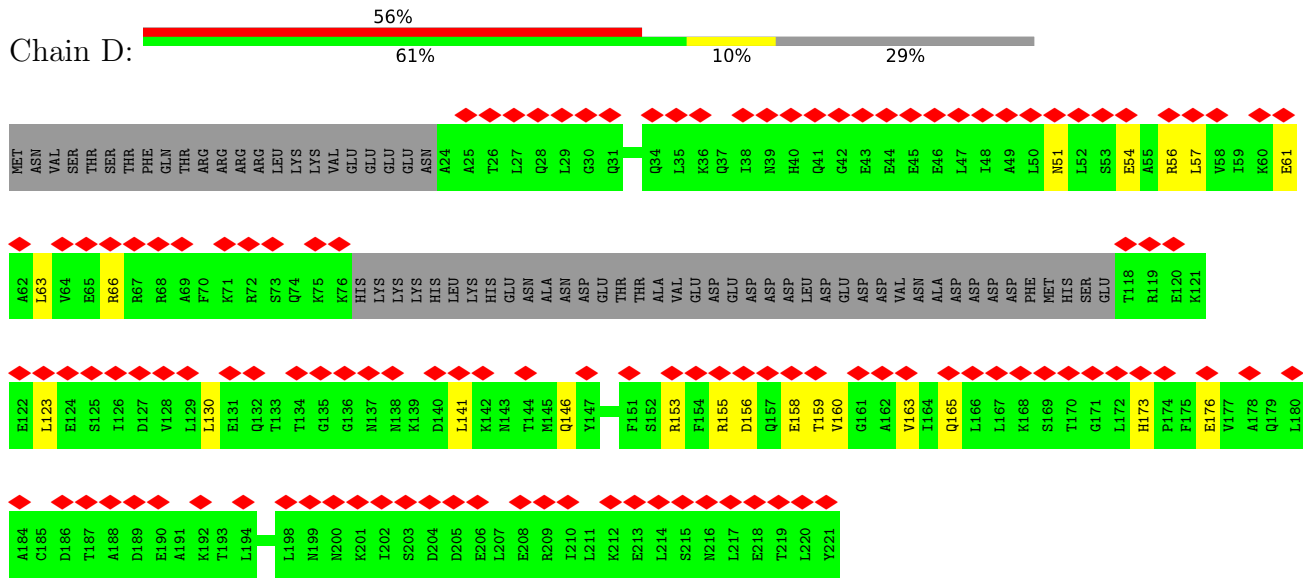


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

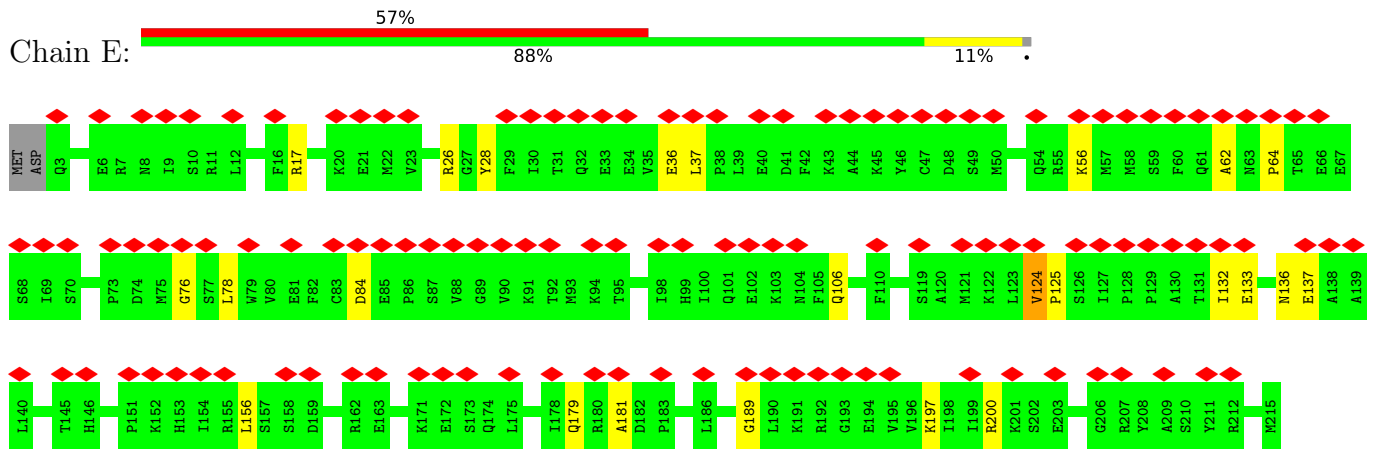




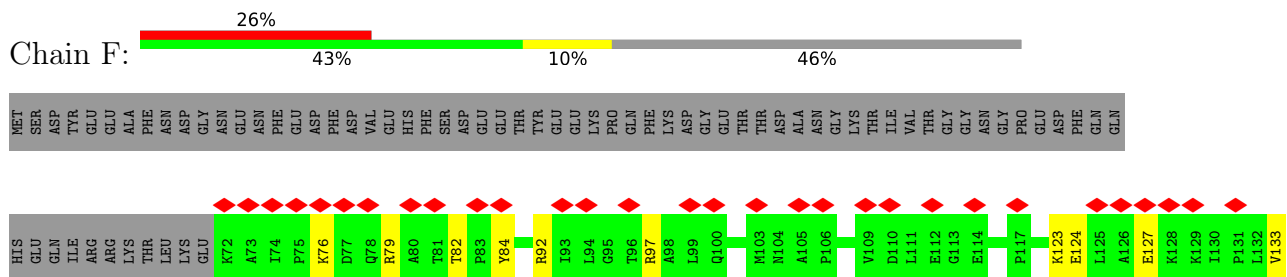
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

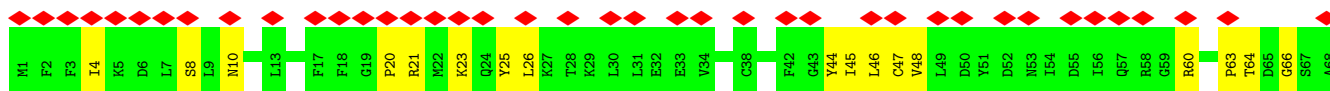


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

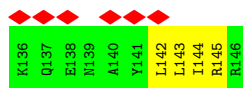
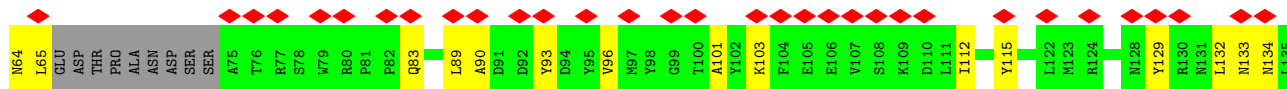
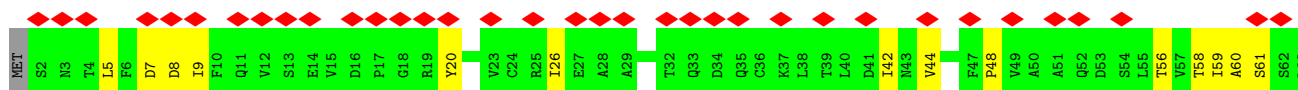




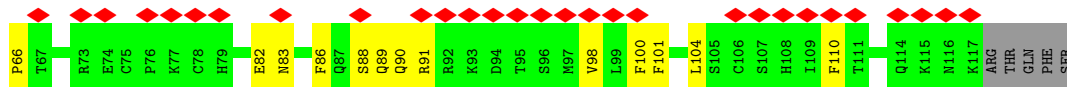
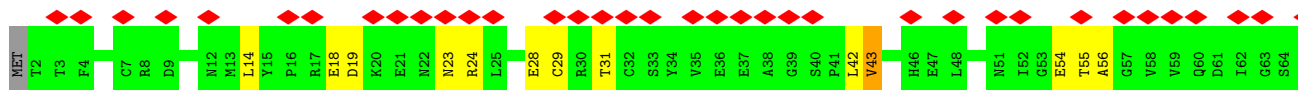
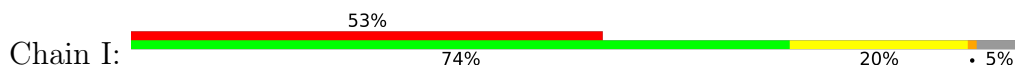
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



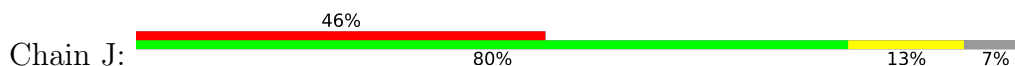
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

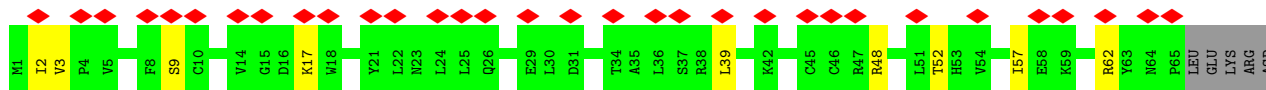


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

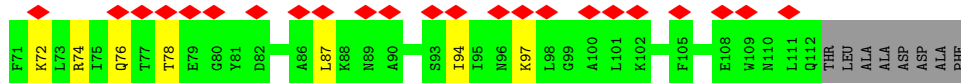
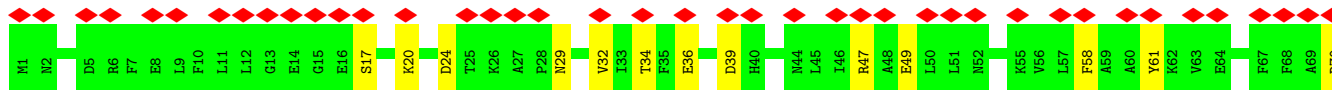
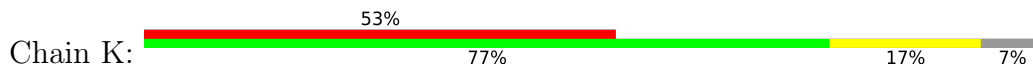


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

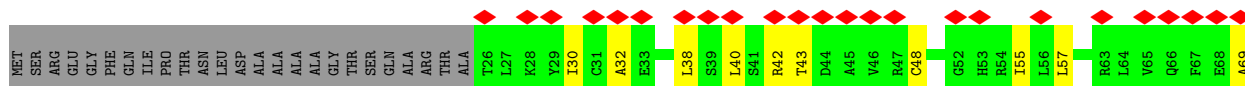




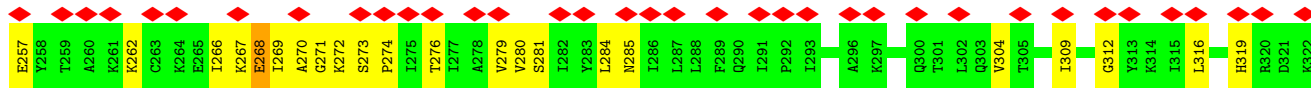
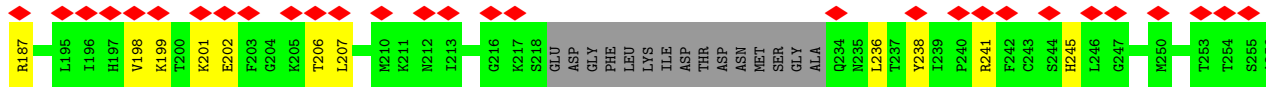
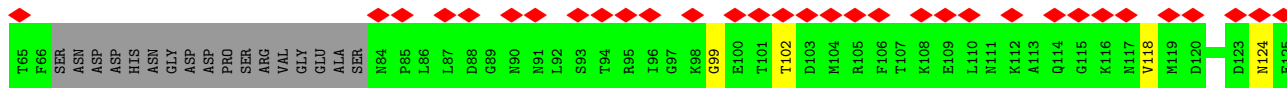
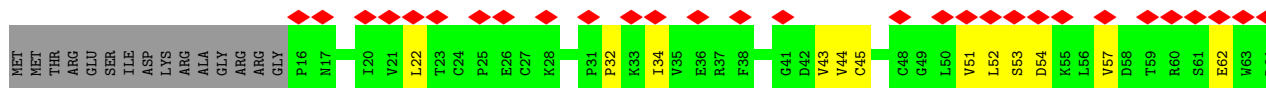
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

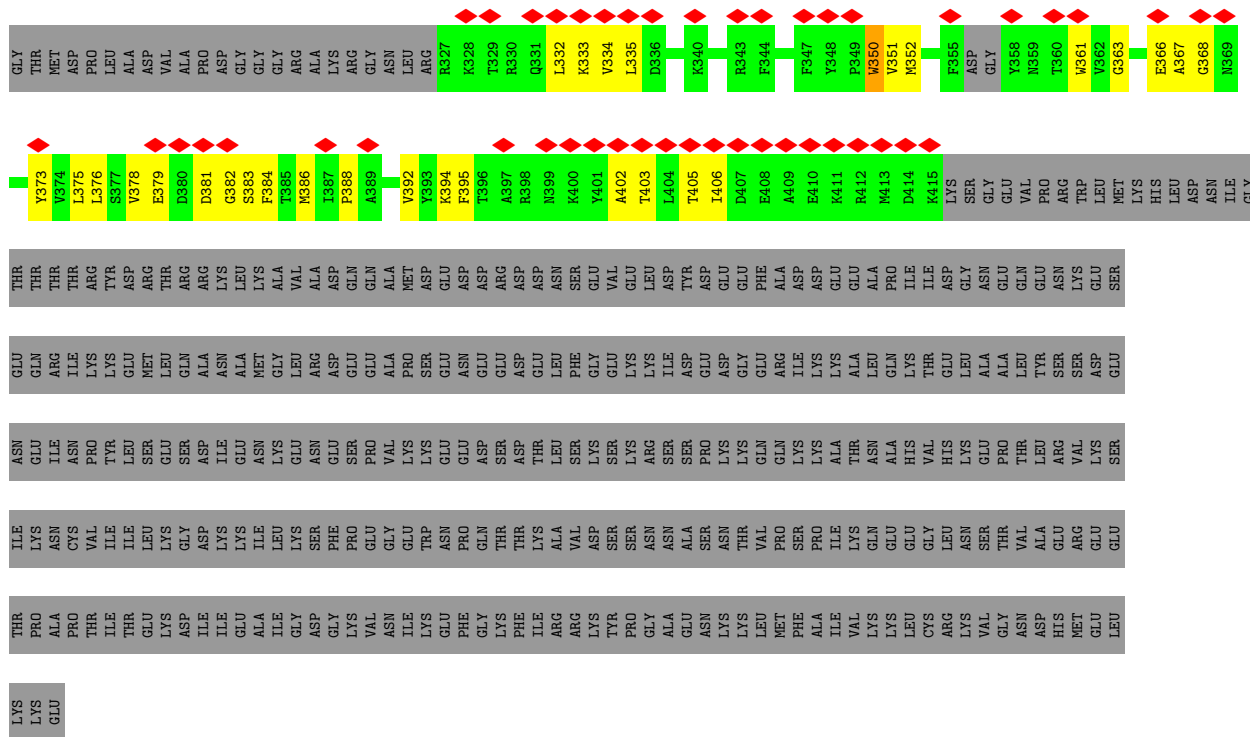


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

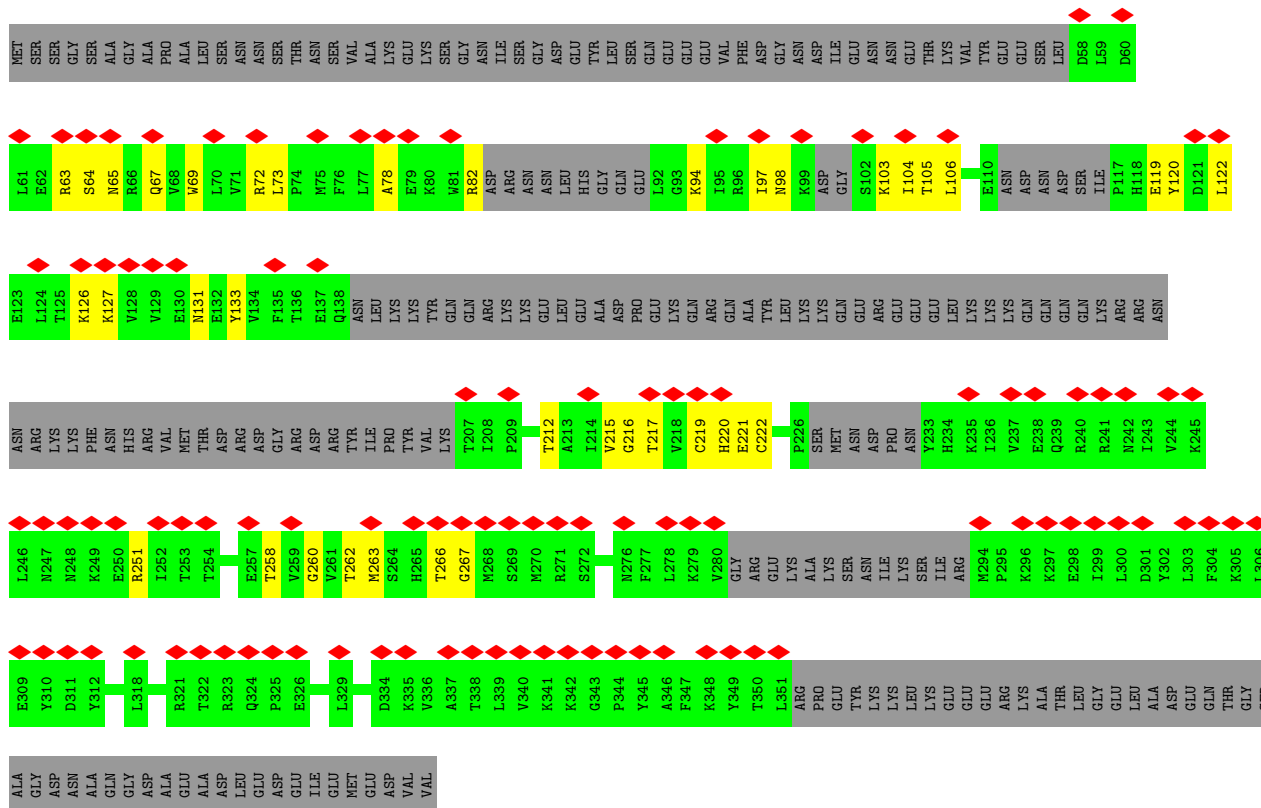
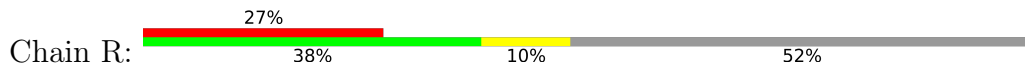


• Molecule 13: Transcription initiation factor IIB

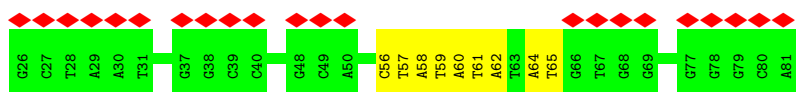
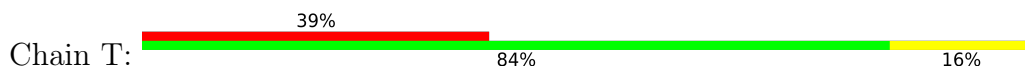




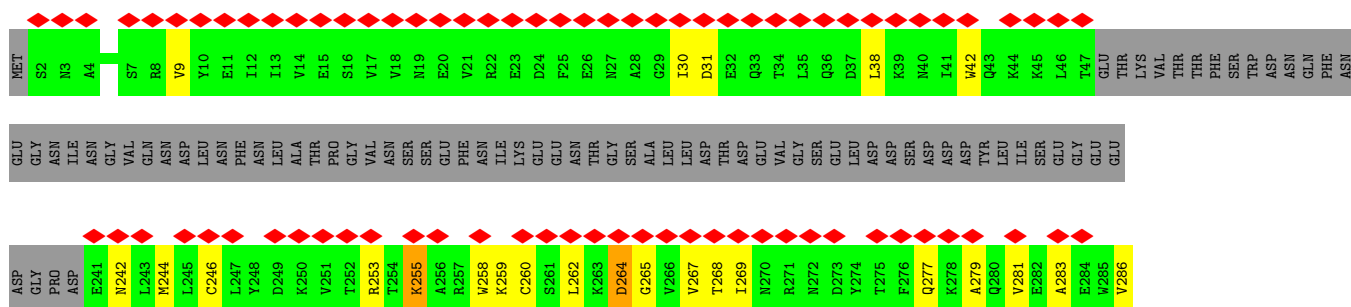
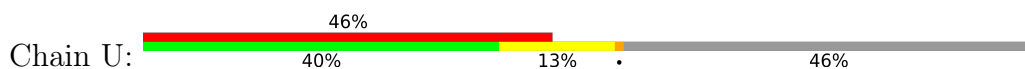
● Molecule 17: Transcription initiation factor IIF subunit beta



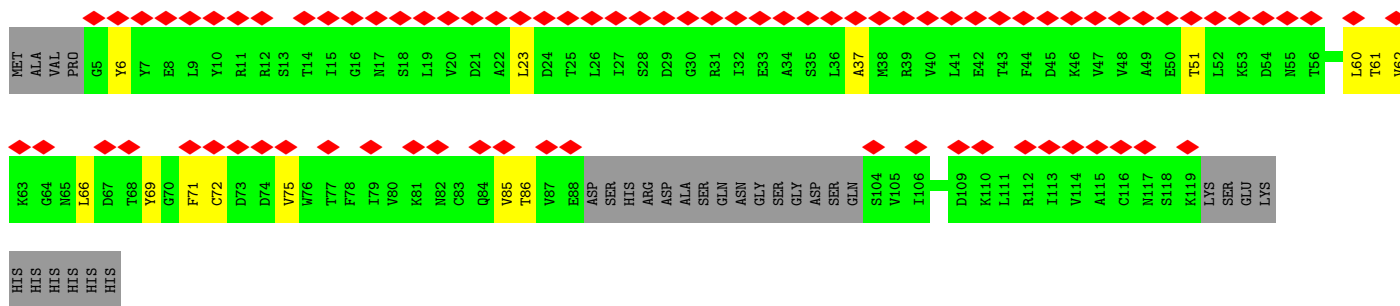
• Molecule 18: GAT1 promoter DNA



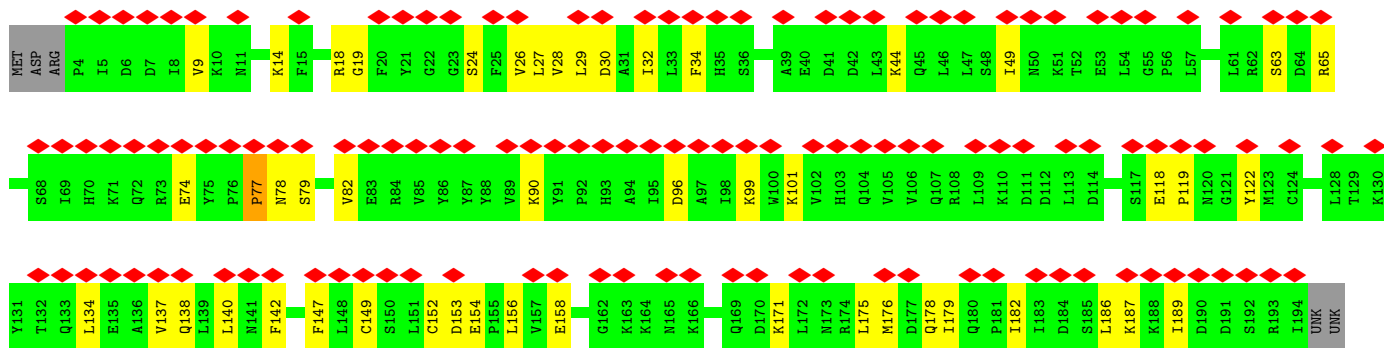
• Molecule 19: Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit



• Molecule 20: Transcription initiation factor IIA subunit 2



• Molecule 21: Transcription initiation factor IIE subunit alpha, Tfa1, Tfa1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38000	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 ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.011	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0028	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/11192	0.41	0/15128
2	B	0.24	0/9357	0.40	0/12618
3	C	0.24	0/2099	0.40	0/2845
4	D	0.23	0/1262	0.37	0/1693
5	E	0.24	0/1780	0.38	0/2395
6	F	0.24	0/682	0.38	0/922
7	G	0.25	0/1368	0.42	0/1844
8	H	0.25	0/1107	0.42	0/1499
9	I	0.24	0/962	0.43	0/1295
10	J	0.28	0/541	0.41	0/727
11	K	0.24	0/922	0.39	0/1244
12	L	0.23	0/360	0.45	0/478
13	M	0.24	0/2204	0.40	0/2963
14	N	0.50	0/1264	0.85	0/1933
15	O	0.25	0/1443	0.43	0/1942
16	Q	0.26	0/1168	0.45	0/1579
17	R	0.24	0/1312	0.42	0/1777
18	T	0.49	0/1292	0.81	0/1981
19	U	0.22	0/766	0.38	0/1032
20	V	0.23	0/789	0.39	0/1066
21	W	0.24	0/1490	0.38	0/2014
22	X	0.24	0/1013	0.40	0/1385
All	All	0.27	0/44373	0.44	0/60360

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

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	A	10997	0	11081	159	0
2	B	9178	0	9195	163	0
3	C	2061	0	2029	29	0
4	D	1253	0	1275	12	0
5	E	1744	0	1772	13	0
6	F	670	0	690	10	0
7	G	1340	0	1357	76	0
8	H	1089	0	1062	20	0
9	I	944	0	899	28	0
10	J	532	0	542	6	0
11	K	904	0	911	13	0
12	L	358	0	381	7	0
13	M	2175	0	2283	50	0
14	N	1129	0	629	8	0
15	O	1416	0	1493	77	0
16	Q	1144	0	1034	29	0
17	R	1303	0	1110	29	0
18	T	1149	0	627	51	0
19	U	757	0	747	23	0
20	V	782	0	790	14	0
21	W	1469	0	1431	97	0
22	X	1004	0	730	38	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	43409	0	42068	748	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 9.

The worst 5 of 748 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)
15:O:99:PHE:CD2	18:T:58:DA:H1'	1.23	1.65
15:O:98:ARG:HG2	18:T:58:DA:C5'	1.46	1.43
15:O:99:PHE:CG	18:T:58:DA:H1'	1.57	1.37
15:O:99:PHE:CZ	18:T:58:DA:N3	1.95	1.35
7:G:158:HIS:HB2	21:W:138:GLN:NE2	1.40	1.32

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	A	1386/1733 (80%)	1298 (94%)	77 (6%)	11 (1%)	19	59
2	B	1136/1224 (93%)	1064 (94%)	62 (6%)	10 (1%)	17	56
3	C	260/318 (82%)	236 (91%)	20 (8%)	4 (2%)	10	46
4	D	153/221 (69%)	145 (95%)	7 (5%)	1 (1%)	22	62
5	E	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	29	68
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	25	65
8	H	132/146 (90%)	117 (89%)	12 (9%)	3 (2%)	6	36
9	I	114/122 (93%)	99 (87%)	15 (13%)	0	100	100
10	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	30
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	273/345 (79%)	252 (92%)	16 (6%)	5 (2%)	8	41
15	O	178/240 (74%)	164 (92%)	13 (7%)	1 (1%)	25	65
16	Q	140/735 (19%)	119 (85%)	17 (12%)	4 (3%)	4	31
17	R	176/400 (44%)	160 (91%)	15 (8%)	1 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	88/171 (52%)	82 (93%)	4 (4%)	2 (2%)	6	36
20	V	96/129 (74%)	92 (96%)	3 (3%)	1 (1%)	15	53
21	W	189/586 (32%)	183 (97%)	4 (2%)	2 (1%)	14	51
22	X	156/328 (48%)	129 (83%)	23 (15%)	4 (3%)	5	34
All	All	5154/7499 (69%)	4781 (93%)	320 (6%)	53 (1%)	20	53

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	127	ILE
21	W	77	PRO
2	B	830	TYR
2	B	933	SER
7	G	63	PRO

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	1221/1520 (80%)	1218 (100%)	3 (0%)	93	96
2	B	1000/1061 (94%)	997 (100%)	3 (0%)	92	95
3	C	230/274 (84%)	228 (99%)	2 (1%)	78	87
4	D	139/200 (70%)	137 (99%)	2 (1%)	67	81
5	E	195/197 (99%)	194 (100%)	1 (0%)	88	93
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	108 (98%)	2 (2%)	59	77
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	245/299 (82%)	245 (100%)	0	100	100
15	O	152/205 (74%)	152 (100%)	0	100	100
16	Q	109/641 (17%)	108 (99%)	1 (1%)	78	87
17	R	107/363 (30%)	106 (99%)	1 (1%)	78	87
19	U	84/154 (54%)	84 (100%)	0	100	100
20	V	90/115 (78%)	90 (100%)	0	100	100
21	W	155/244 (64%)	155 (100%)	0	100	100
22	X	62/295 (21%)	62 (100%)	0	100	100
All	All	4440/6325 (70%)	4425 (100%)	15 (0%)	92	95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	222	LYS
16	Q	350	TRP
4	D	153	ARG
17	R	251	ARG
9	I	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	235	ASN
22	X	279	GLN
15	O	158	GLN
21	W	107	GLN
2	B	60	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

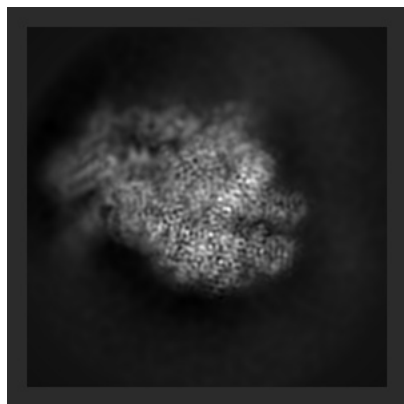
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0091. These allow visual inspection of the internal detail of the map and identification of artifacts.

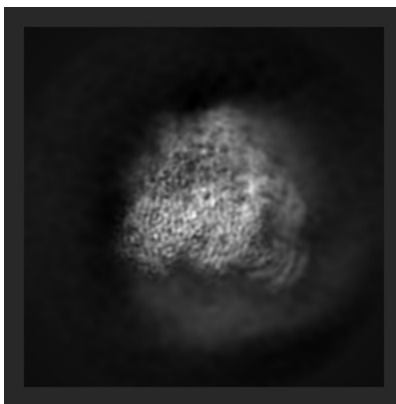
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

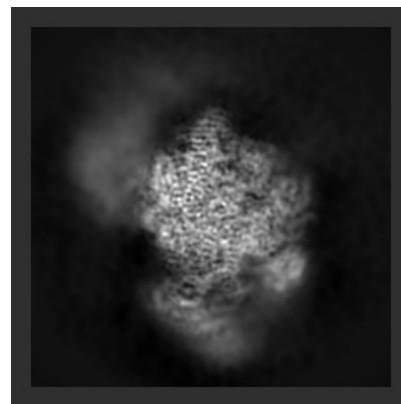
6.1.1 Primary map



X

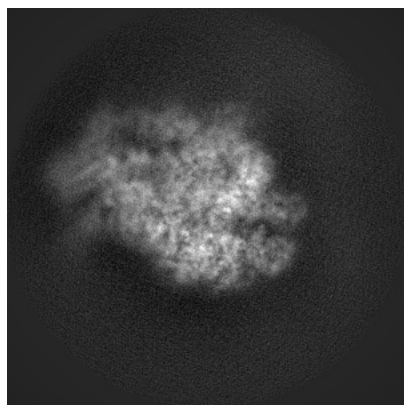


Y

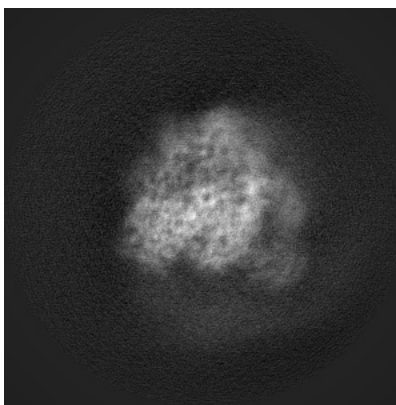


Z

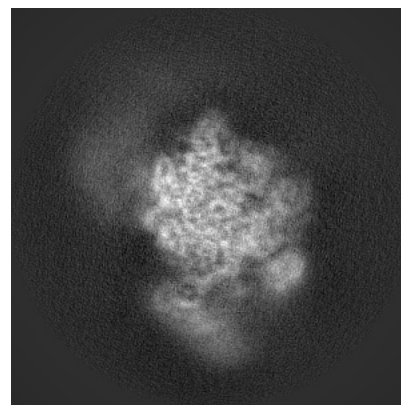
6.1.2 Raw map



X



Y

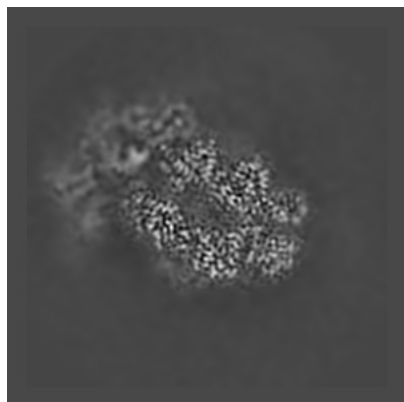


Z

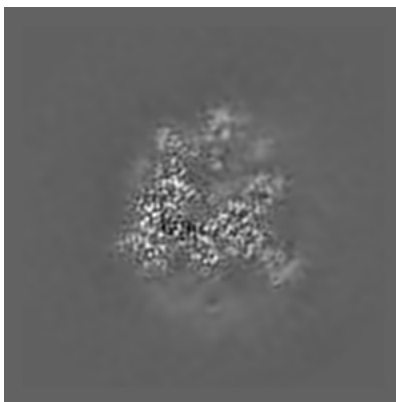
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

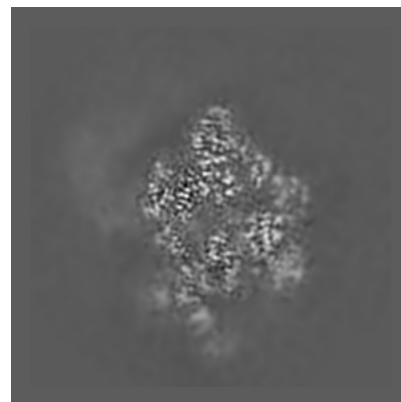
6.2.1 Primary map



X Index: 150

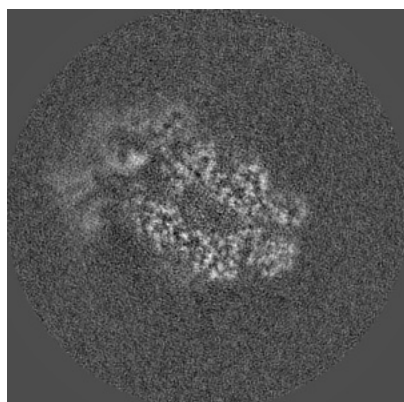


Y Index: 150

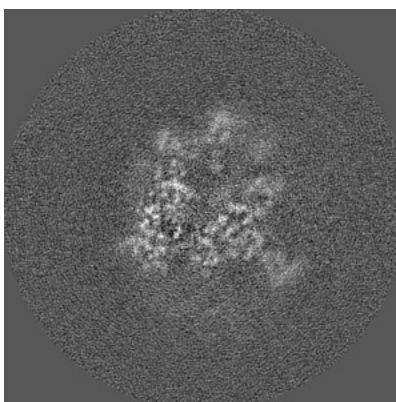


Z Index: 150

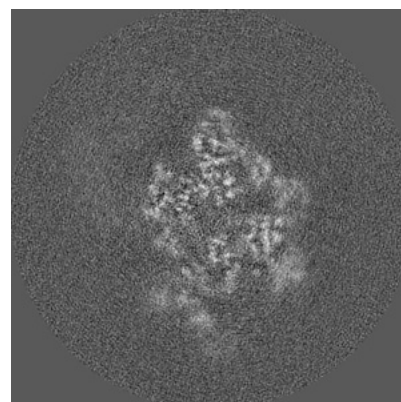
6.2.2 Raw map



X Index: 150



Y Index: 150

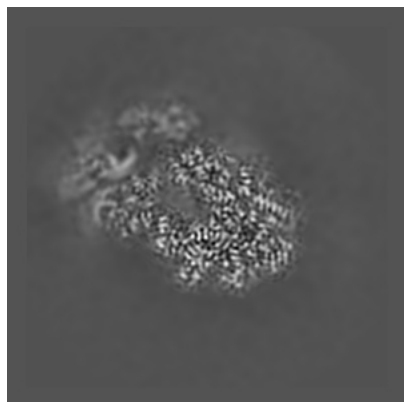


Z Index: 150

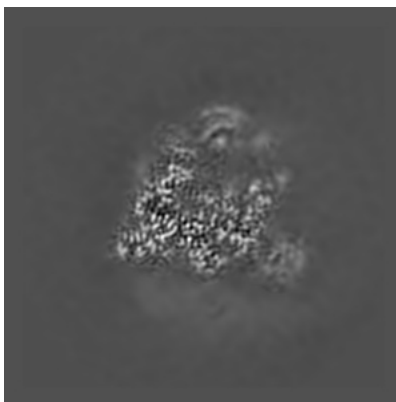
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

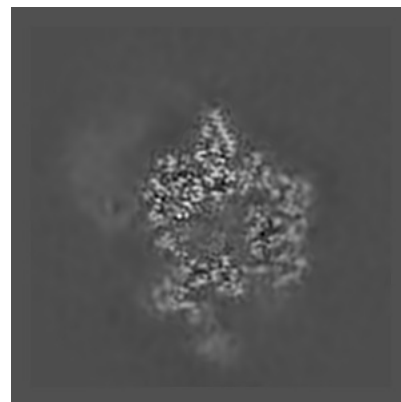
6.3.1 Primary map



X Index: 140

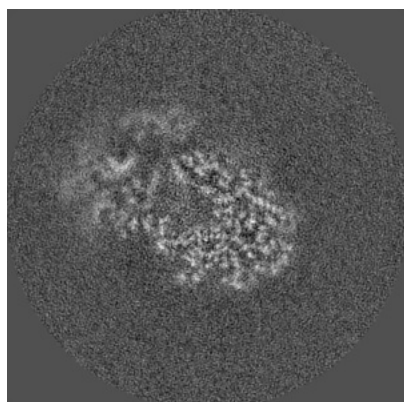


Y Index: 156

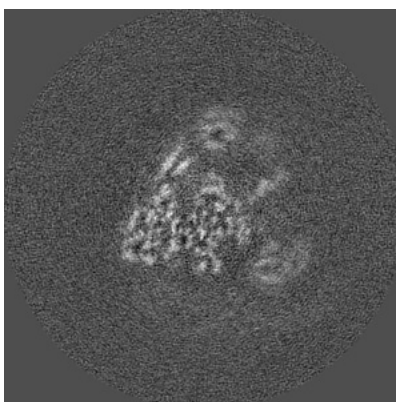


Z Index: 156

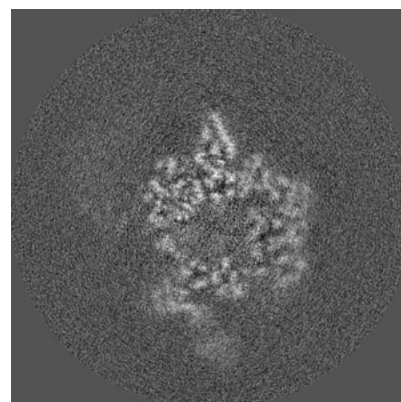
6.3.2 Raw map



X Index: 141



Y Index: 162

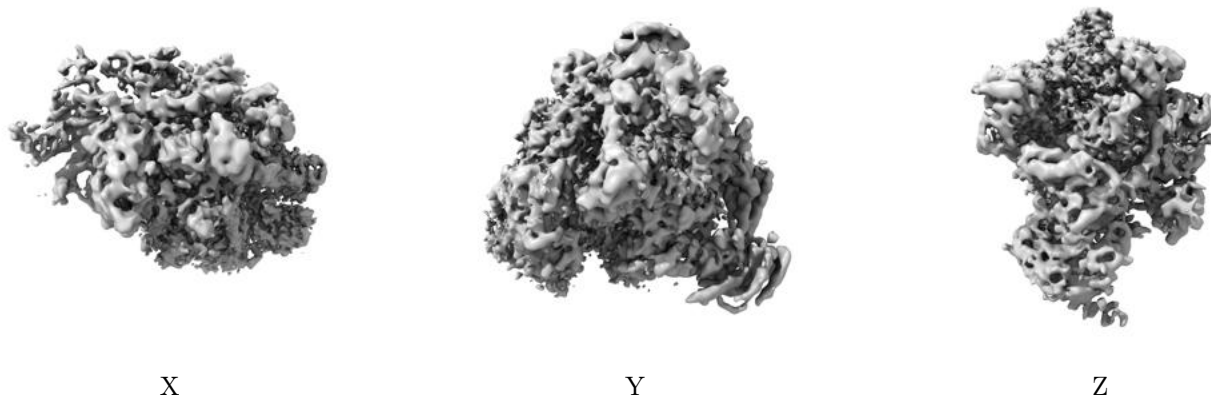


Z Index: 156

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

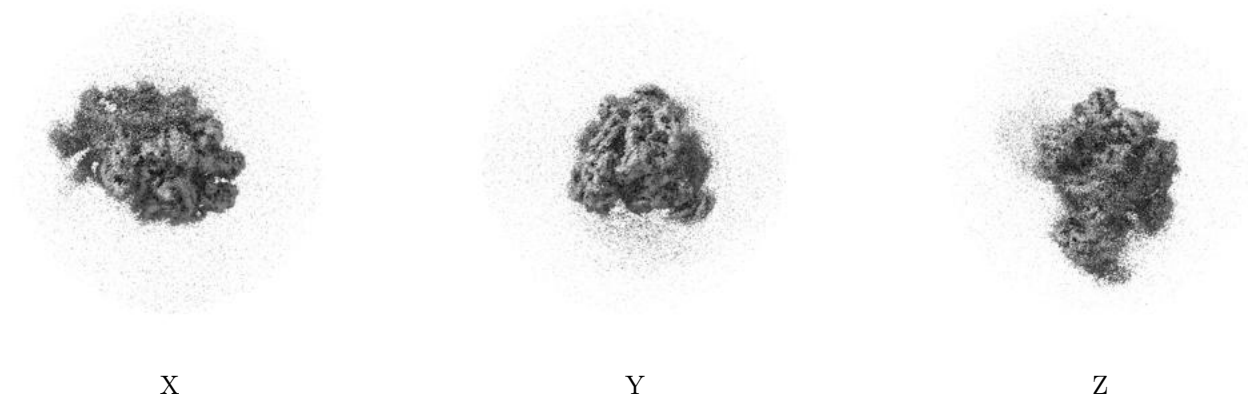
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

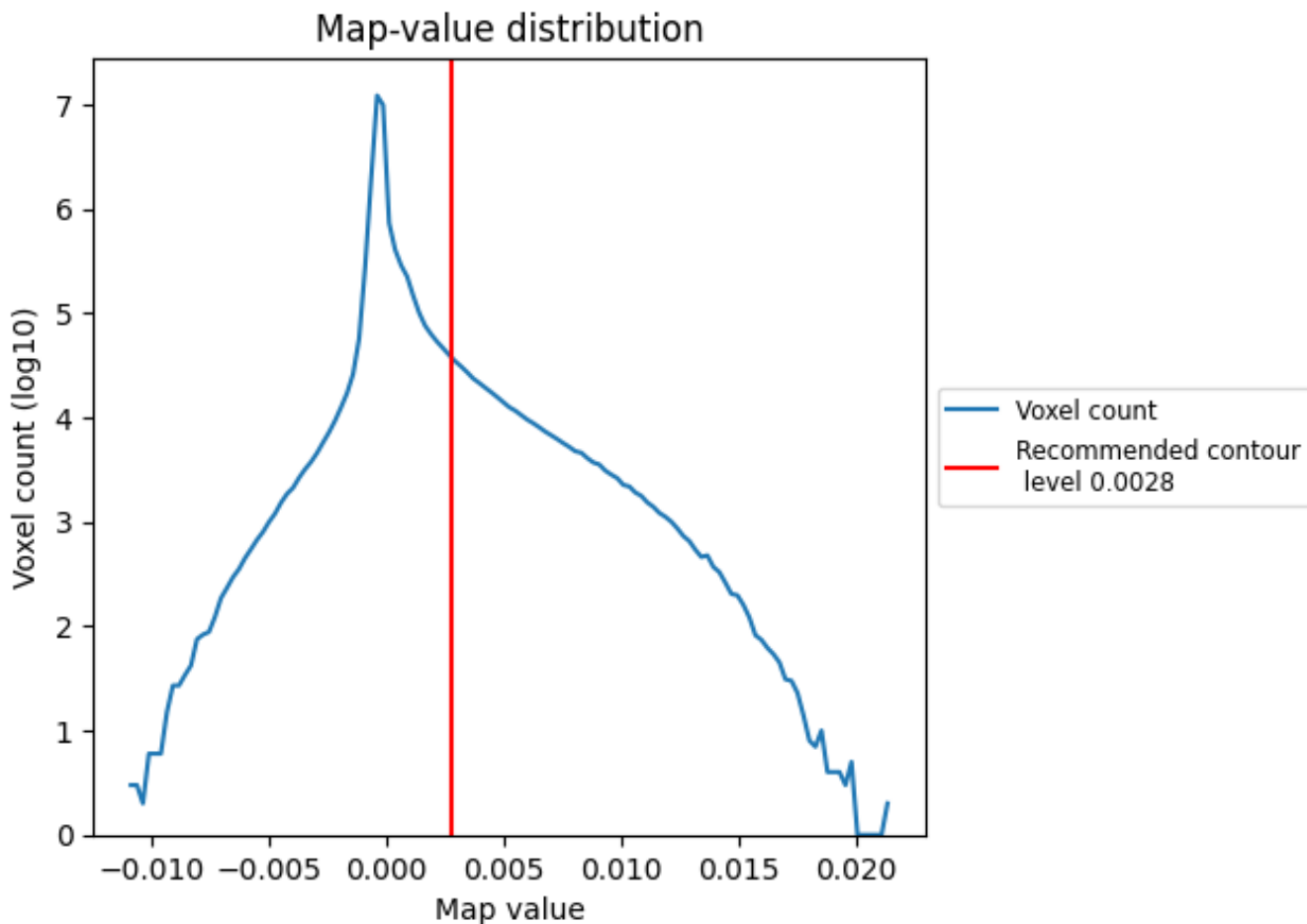
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

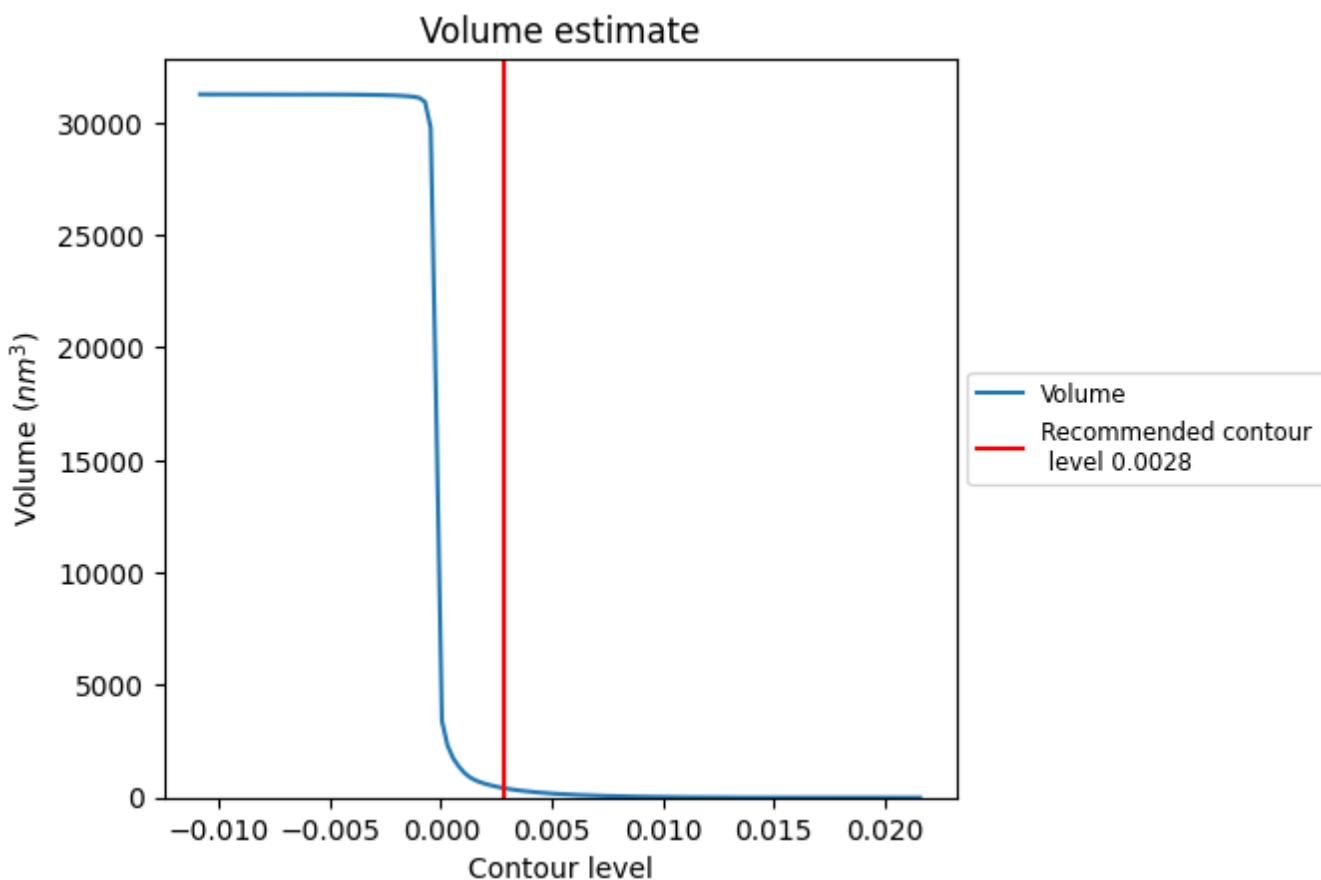
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

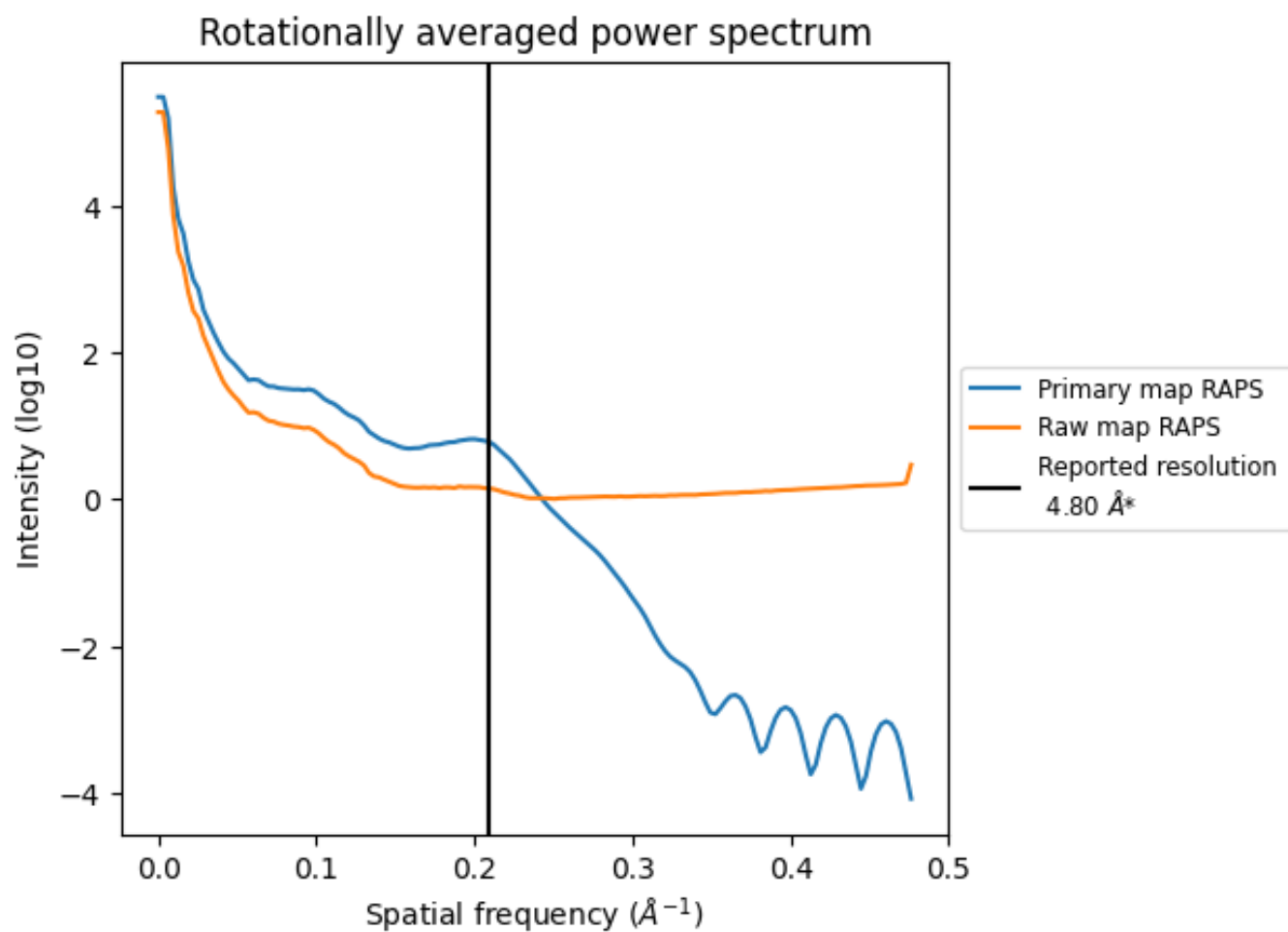
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 426 nm^3 ; this corresponds to an approximate mass of 385 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

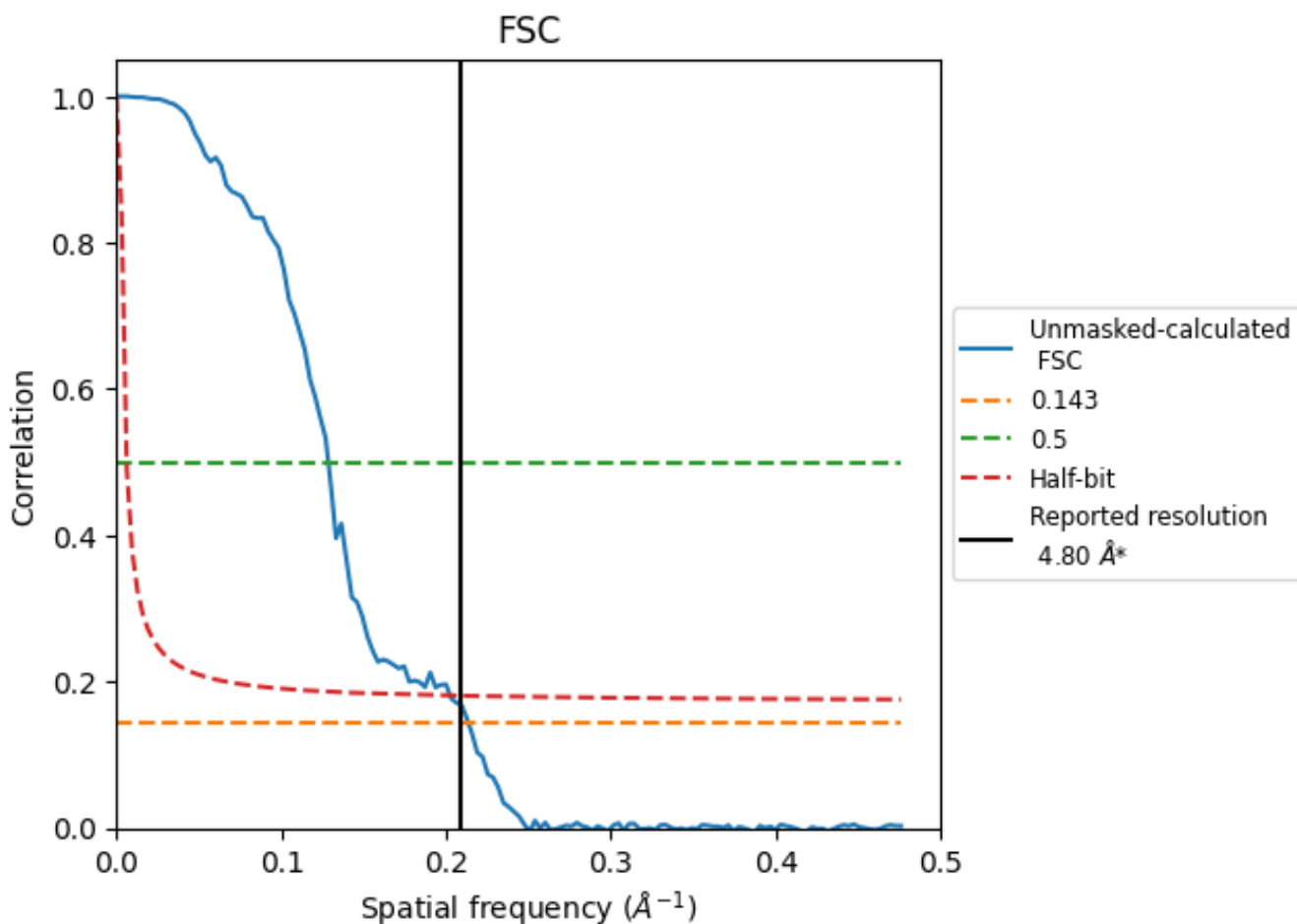


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

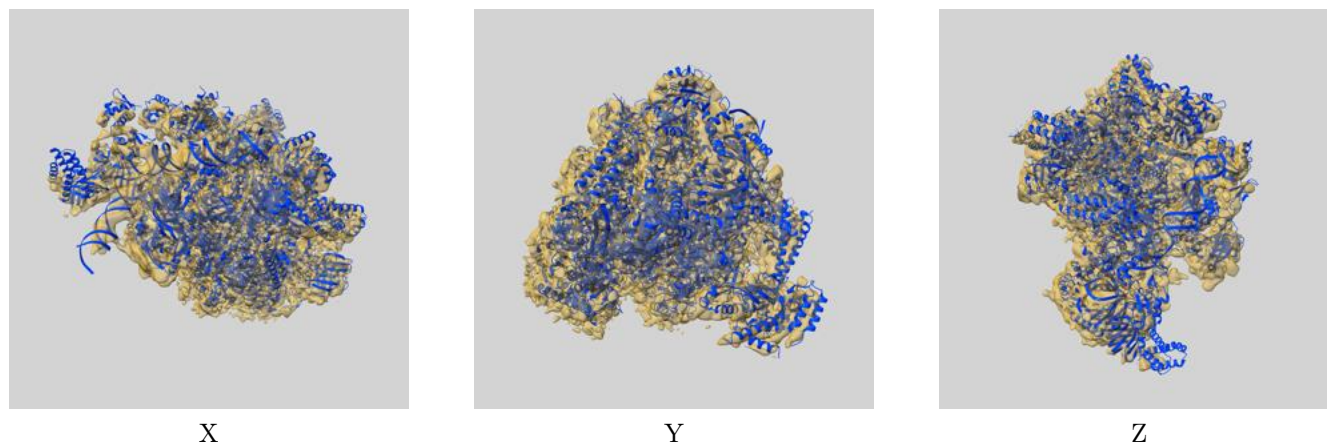
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	7.78	4.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

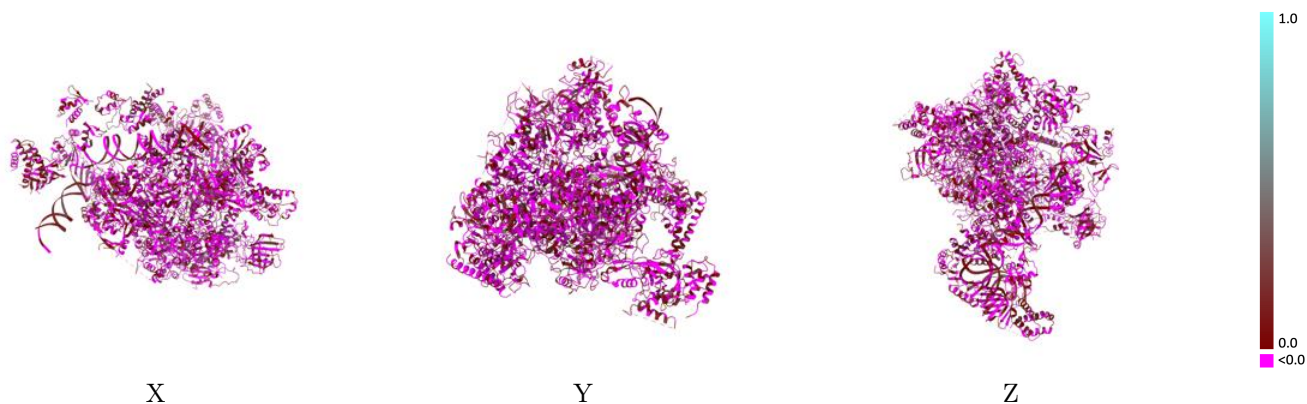
This section contains information regarding the fit between EMDB map EMD-0091 and PDB model 6GYL. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



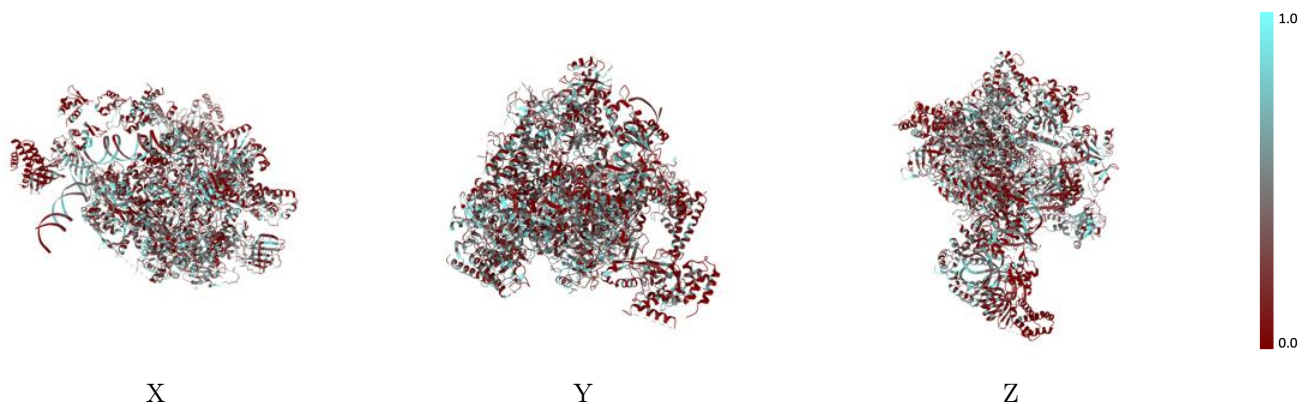
The images above show the 3D surface view of the map at the recommended contour level 0.0028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



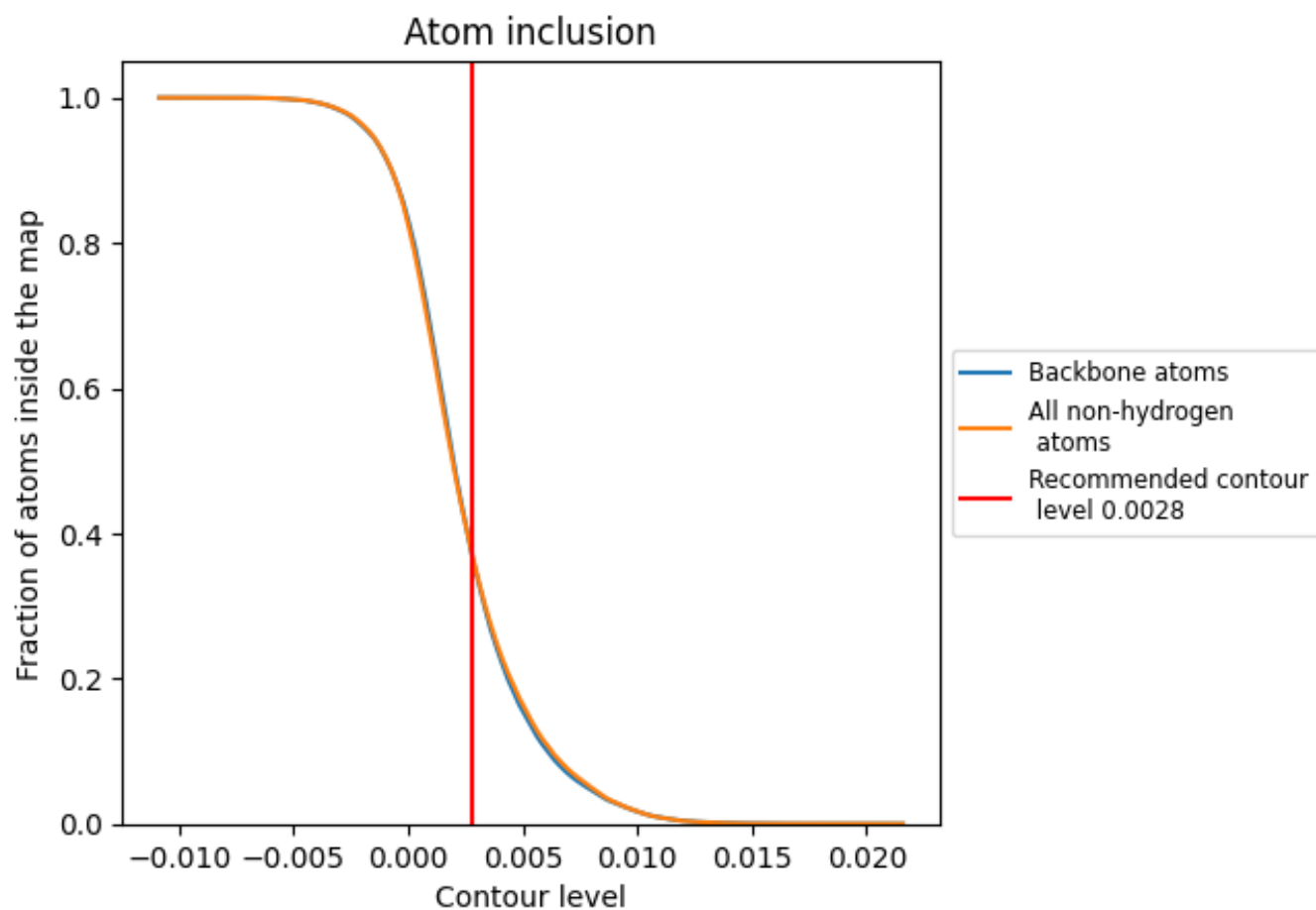
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0028).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 37% 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 (0.0028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3696	 -0.0040
A	 0.3840	 -0.0110
B	 0.3770	 -0.0240
C	 0.4248	 -0.0310
D	 0.1987	 0.0040
E	 0.3745	 0.0120
F	 0.4202	 0.0230
G	 0.3480	 -0.0030
H	 0.3779	 -0.0040
I	 0.3822	 0.0160
J	 0.4333	 -0.0570
K	 0.3850	 -0.0410
L	 0.3642	 -0.0550
M	 0.3360	 -0.0170
N	 0.4181	 0.0710
O	 0.4784	 0.0280
Q	 0.3802	 0.0040
R	 0.4093	 -0.0100
T	 0.4996	 0.0660
U	 0.1606	 0.0330
V	 0.1630	 0.0540
W	 0.3140	 0.0240
X	 0.2144	 0.0330

