



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:38 pm BST

PDB ID : 6GYL / pdb_00006gyl
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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

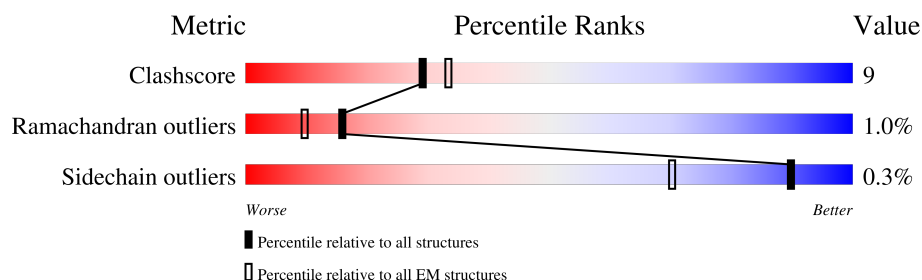
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>44%</div> <div>67%</div> <div>14%</div> <div>19%</div> </div>
2	B	1224	<div> <div>53%</div> <div>73%</div> <div>21%</div> <div>6%</div> </div>
3	C	318	<div> <div>42%</div> <div>68%</div> <div>14%</div> <div>18%</div> </div>
4	D	221	<div> <div>56%</div> <div>61%</div> <div>10%</div> <div>29%</div> </div>
5	E	215	<div> <div>57%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
6	F	155	<div> <div>26%</div> <div>43%</div> <div>10%</div> <div>46%</div> </div>
7	G	171	<div> <div>57%</div> <div>65%</div> <div>35%</div> </div>
8	H	146	<div> <div>50%</div> <div>71%</div> <div>23%</div> <div>7%</div> </div>

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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

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
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			9178	5807	1608	1708	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

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

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

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

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
21	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

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

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

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

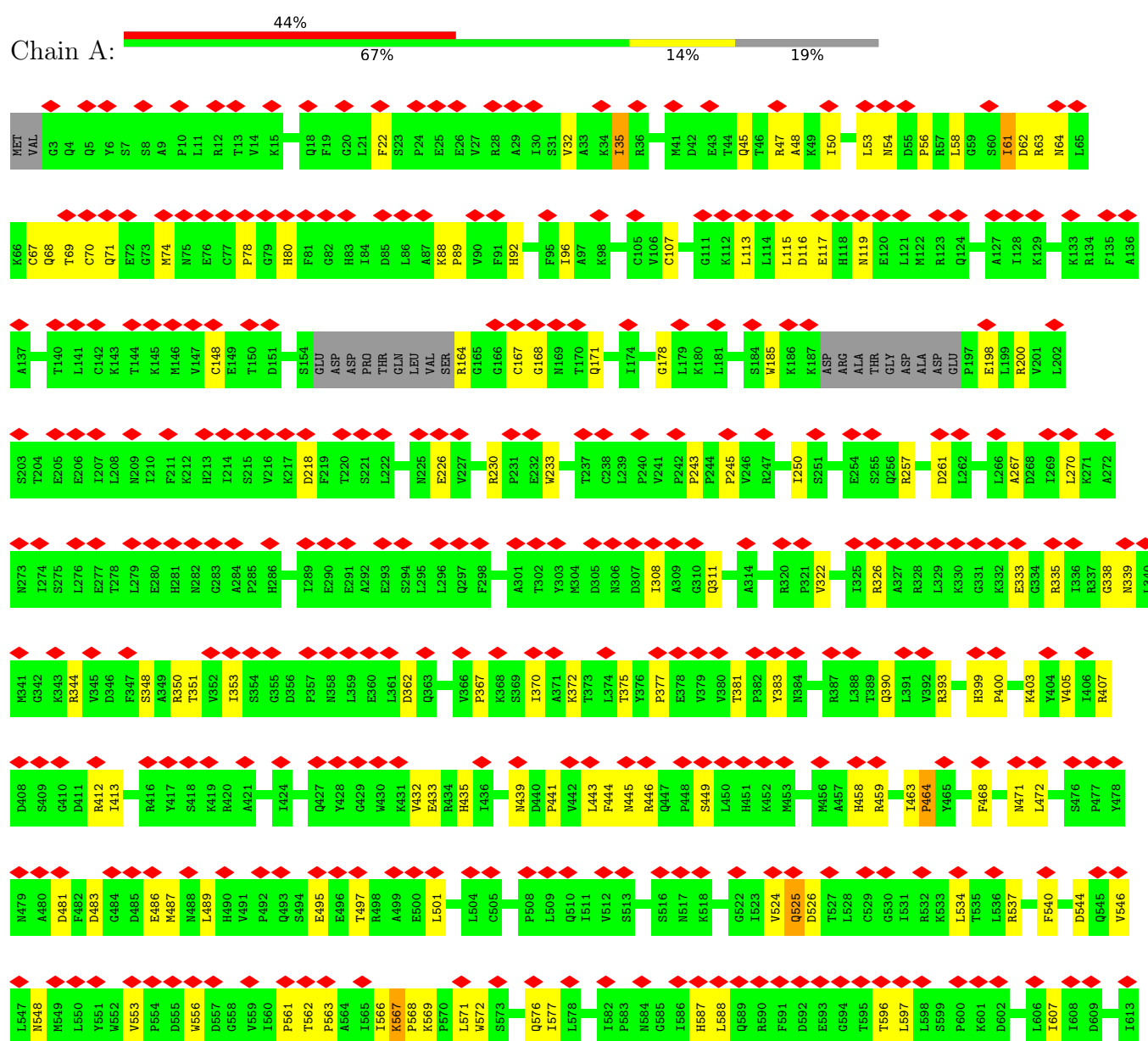
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots

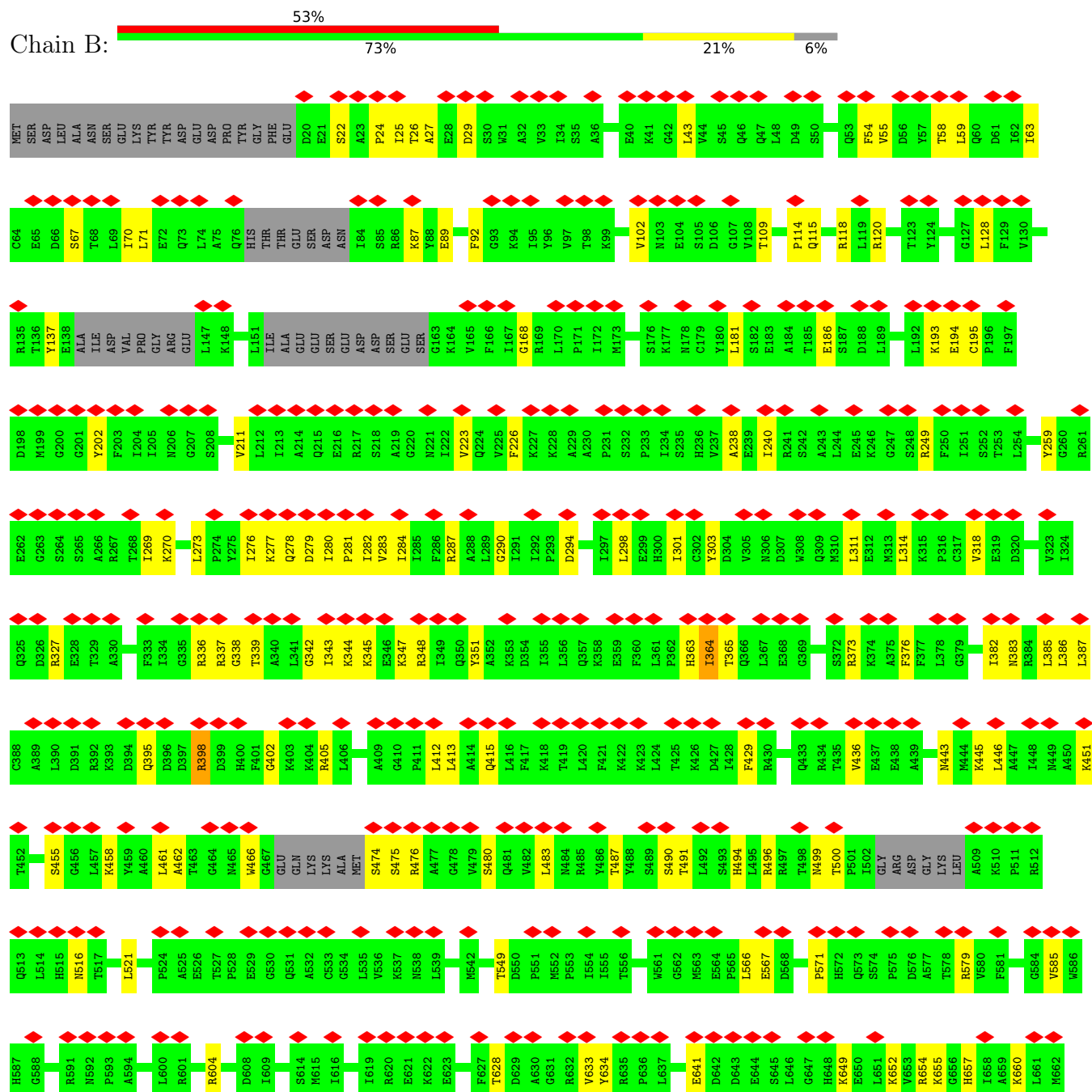
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

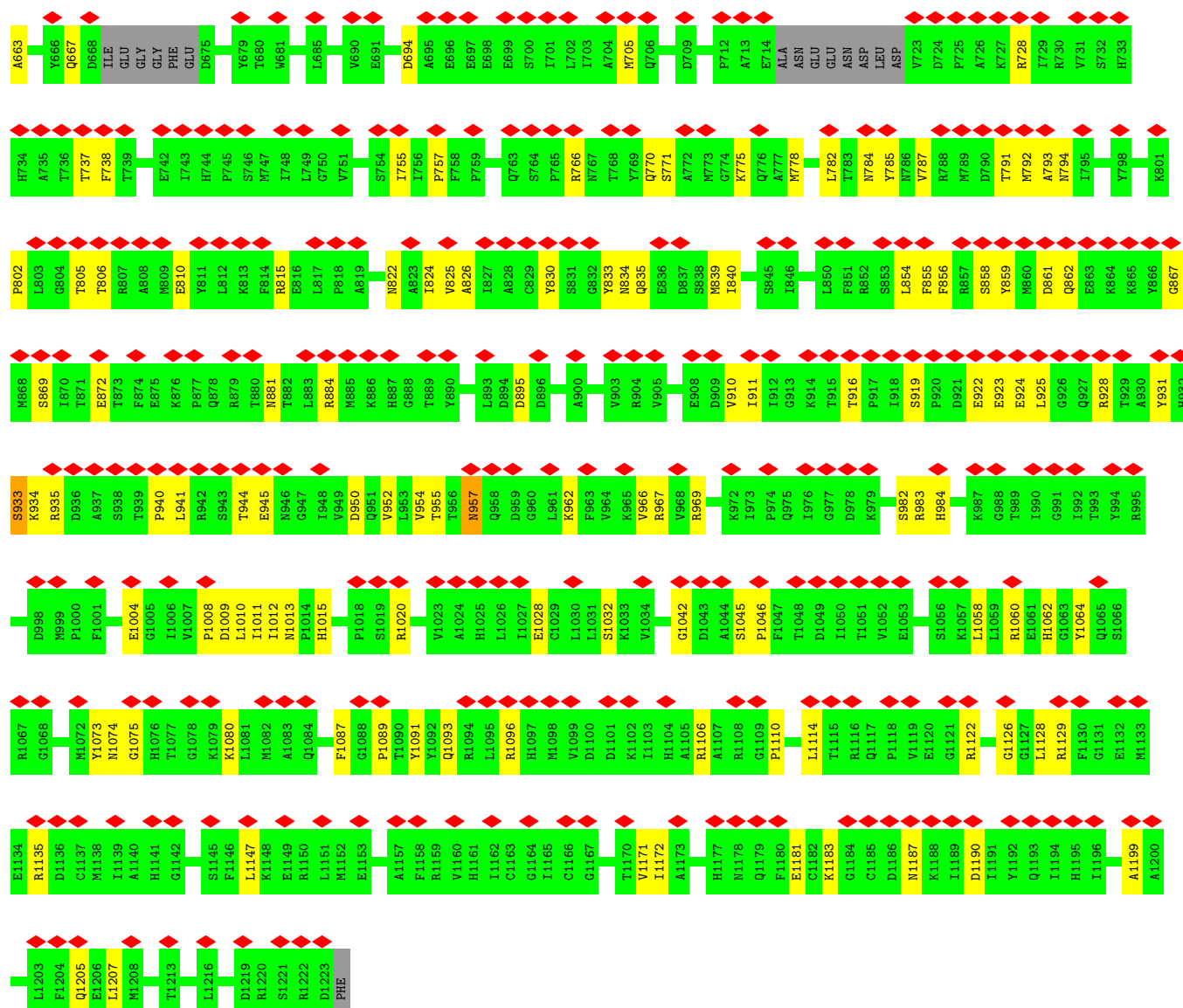
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



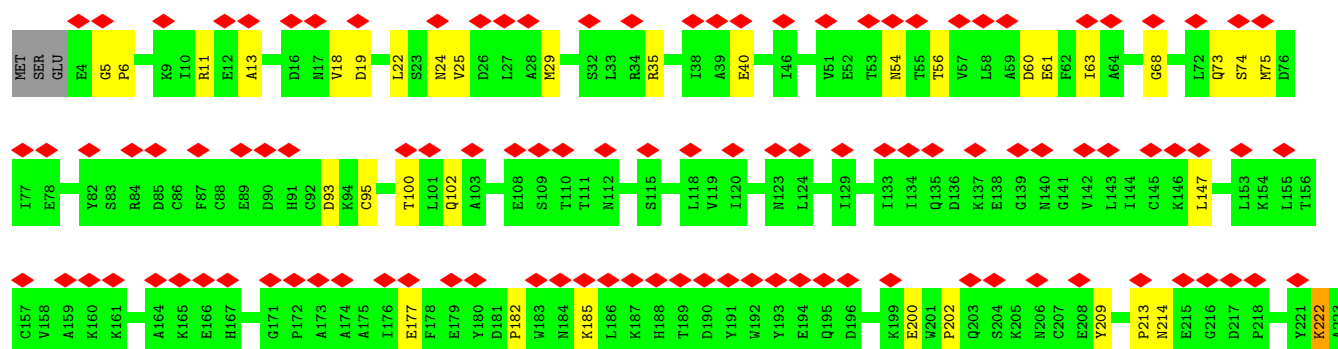
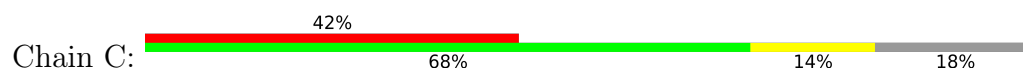


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

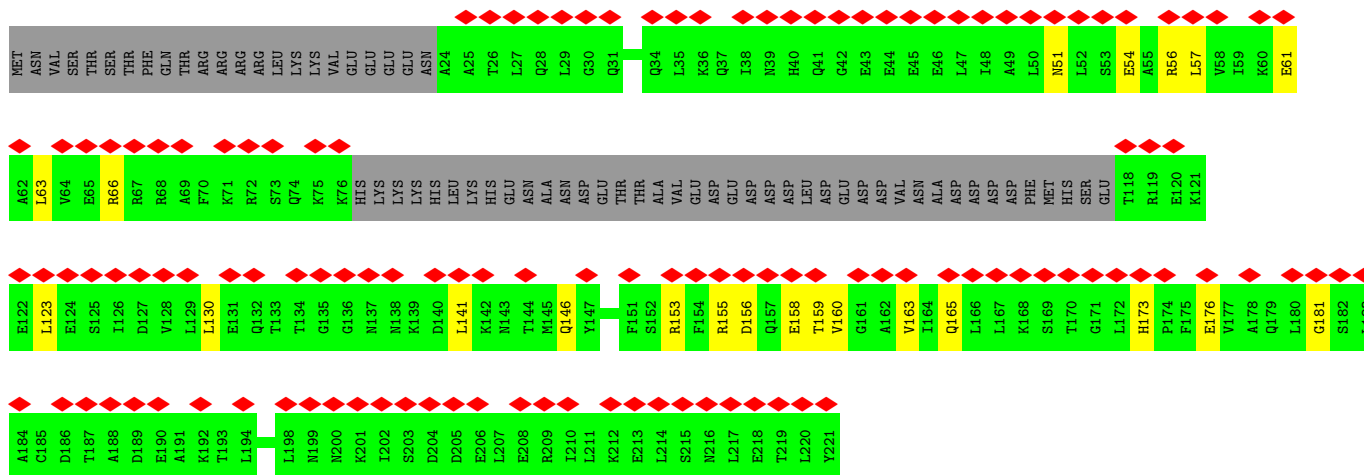




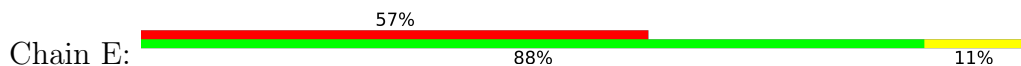
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



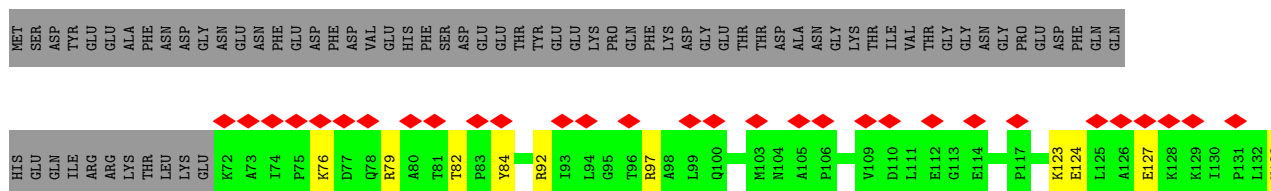
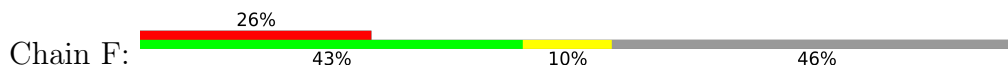
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



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

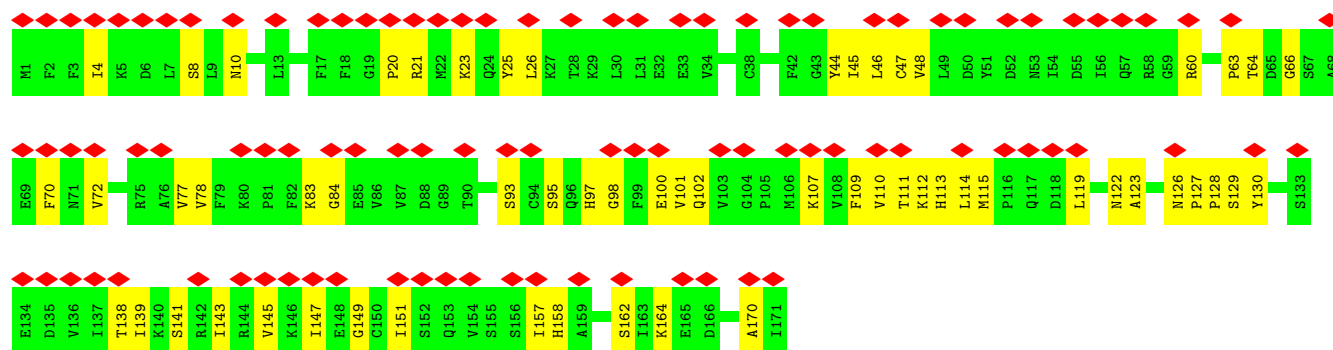


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

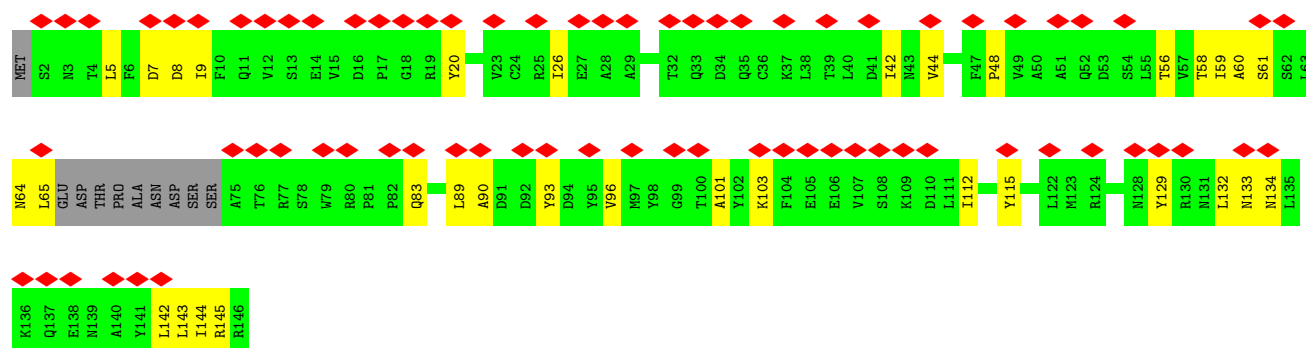




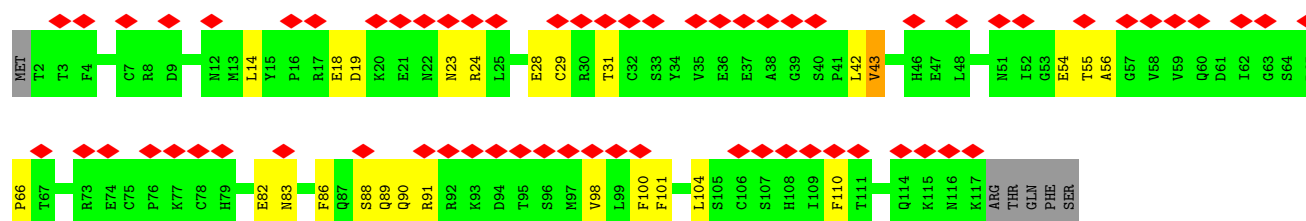
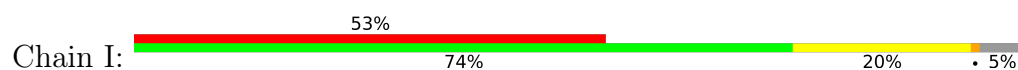
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



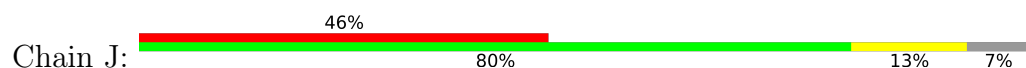
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

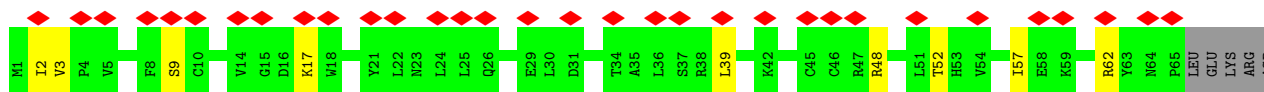


• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

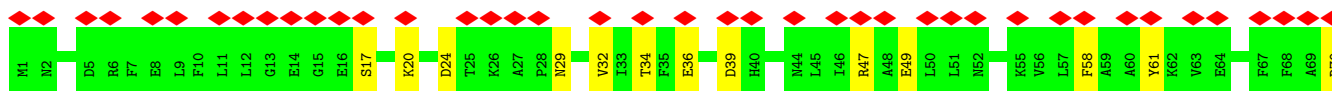
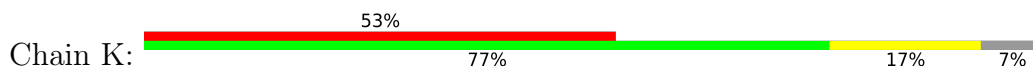


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

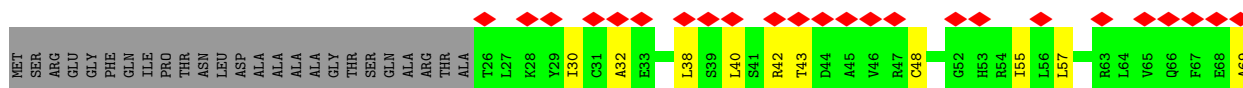




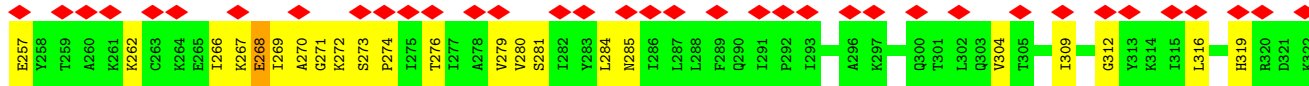
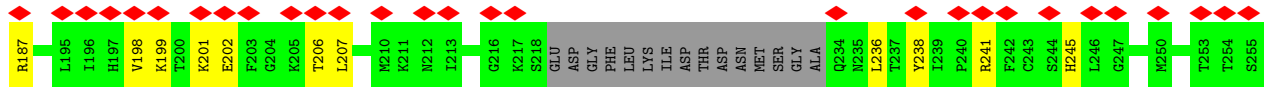
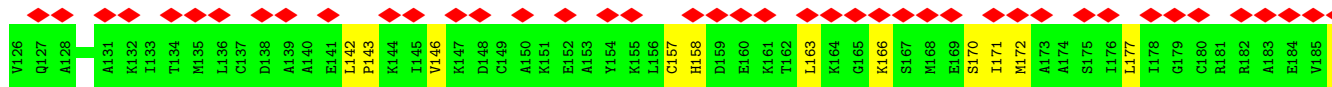
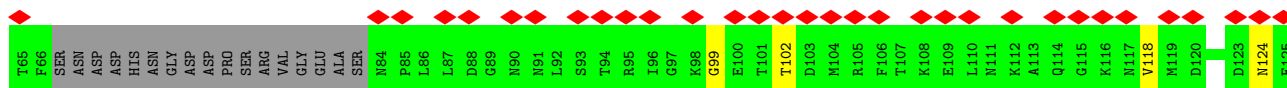
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



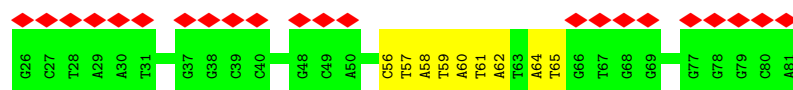
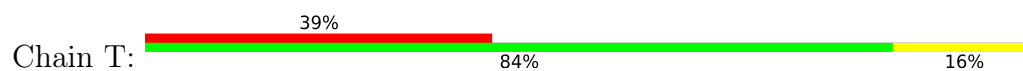
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



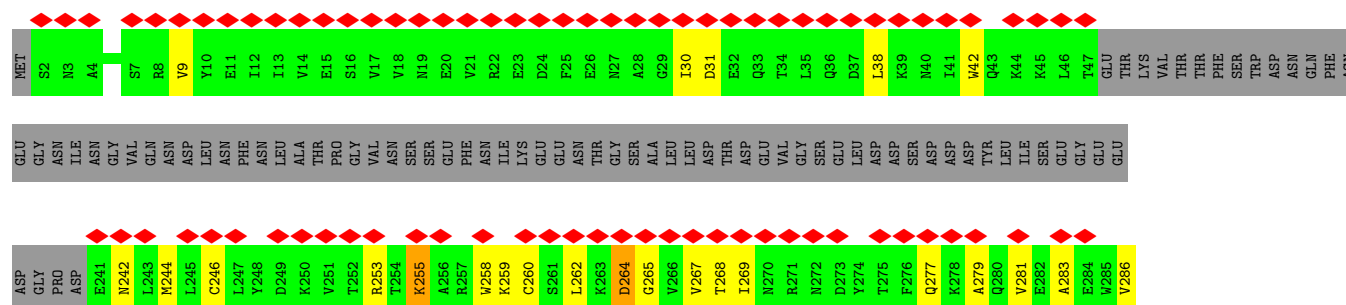
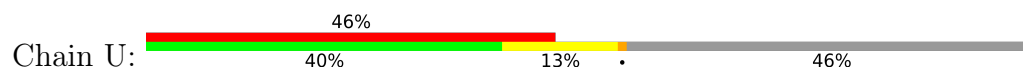
- Molecule 13: Transcription initiation factor IIB



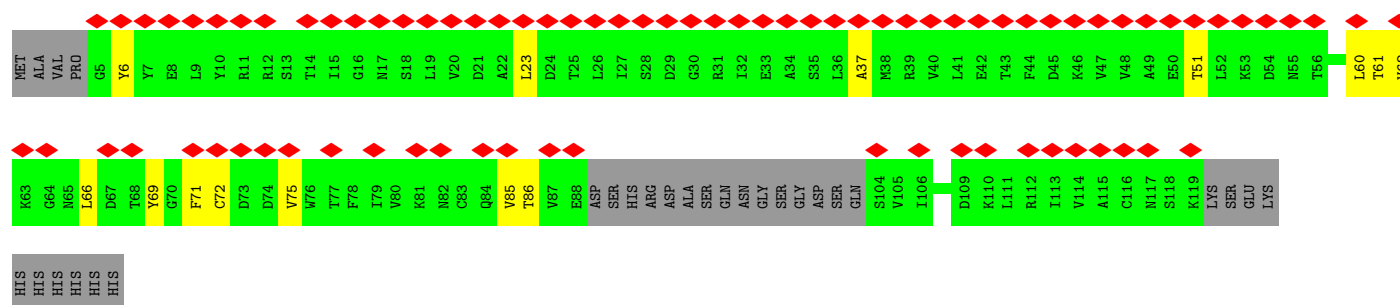
- Molecule 18: GAT1 promoter DNA



- 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



[illegible]

- Molecule 22: Transcription initiation factor IIE subunit beta

Chain X:  39% 42% 6% 51%

GLY	G249	◆	T183	LYS	◆
LYS	G250	◆	Y184	SER	◆
ILE	N251	◆	D185	ALA	◆
THR	L252	◆	Y186	LYS	◆
THR	K253	◆	H187	ASN	◆
MET	C254	◆	S188	PRO	◆
THR	T255	◆	P189	VAL	◆
GLY	D256	◆	S190	LEU	◆
THR	E257	◆	E191	VAL	◆
ILE	E258	◆	L192	ILE	◆
LEU	E259	◆	L193	ASN	◆
LYS	F260	◆	K194	LYS	◆
ASP	K261	◆	L195	GLU	◆
TYR	N262	◆	L196	ALA	◆
THR	W263	◆	R197	GLY	◆
HIS	E264	◆	S198	Y134	◆
SER	N265	◆	P199	T135	◆
HIS	W266	◆	Y200	K138	◆
ARG	Q267	◆	T201	GLN	◆
VAL	L268	◆	F202	K140	◆
		◆	K203	P141	◆
		◆	G204	V142	◆
		◆	T205	L143	◆
		◆	S206	V144	◆
		◆	C207	N145	◆
		◆	K208	E146	◆
		◆	D209	L147	◆
		◆	L210	L148	◆
		◆	K211	D149	◆
		◆	W214	Y150	◆
		◆	P215	L151	◆
		◆	Q216	S152	◆
		◆	C217	K155	◆
		◆	D218	D156	◆
		◆	E219	D157	◆
		◆	T220	K158	◆
		◆	T221	V159	◆
		◆	N222	I160	◆
		◆	Q223	E161	◆
		◆	L224	L162	◆
		◆	E225	L163	◆
		◆	E226	K164	◆
		◆	D227	K165	◆
		◆	S228	L166	◆
		◆	K229	D167	◆
		◆	W232	R168	◆
		◆	L233	I169	◆
		◆	P234	E170	◆
		◆	D238	F171	◆
		◆	K239	D172	◆
		◆	T240	P173	◆
		◆	W244	K174	◆
		◆	W245	K175	◆
		◆	Y246	G176	◆
		◆	N247	T177	◆
		◆	S248	F178	◆
		◆		K179	◆
		◆		Y180	◆
		◆		L181	◆
		◆		SER	◆

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1386/1733 (80%)	1298 (94%)	77 (6%)	11 (1%)	16	53
2	B	1136/1224 (93%)	1064 (94%)	62 (6%)	10 (1%)	14	50
3	C	260/318 (82%)	236 (91%)	20 (8%)	4 (2%)	8	39
4	D	153/221 (69%)	145 (95%)	7 (5%)	1 (1%)	19	56
5	E	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	25	64
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	22	59
8	H	132/146 (90%)	117 (89%)	12 (9%)	3 (2%)	5	28
9	I	114/122 (93%)	99 (87%)	15 (13%)	0	100	100
10	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	21
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%)	7	34
15	O	178/240 (74%)	164 (92%)	13 (7%)	1 (1%)	22	59
16	Q	140/735 (19%)	119 (85%)	17 (12%)	4 (3%)	3	23
17	R	176/400 (44%)	160 (91%)	15 (8%)	1 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	88/171 (52%)	82 (93%)	4 (4%)	2 (2%)	5	28
20	V	96/129 (74%)	92 (96%)	3 (3%)	1 (1%)	13	48
21	W	189/586 (32%)	183 (97%)	4 (2%)	2 (1%)	12	46
22	X	156/328 (48%)	129 (83%)	23 (15%)	4 (3%)	4	25
All	All	5154/7499 (69%)	4781 (93%)	320 (6%)	53 (1%)	16	48

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 ⓘ

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%)	92	94
2	B	1000/1061 (94%)	997 (100%)	3 (0%)	91	92
3	C	230/274 (84%)	228 (99%)	2 (1%)	75	83
4	D	139/200 (70%)	137 (99%)	2 (1%)	62	76
5	E	195/197 (99%)	194 (100%)	1 (0%)	86	90
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%)	54	71
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%)	75	83
17	R	107/363 (30%)	106 (99%)	1 (1%)	75	83
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%)	90	92

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 ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

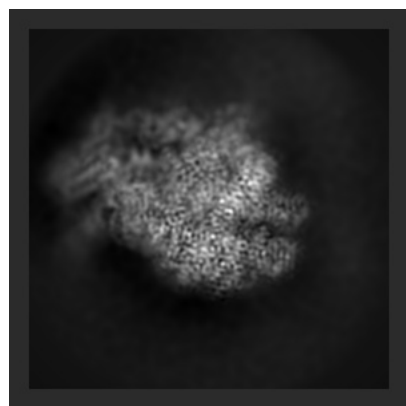
6 Map visualisation [i](#)

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.

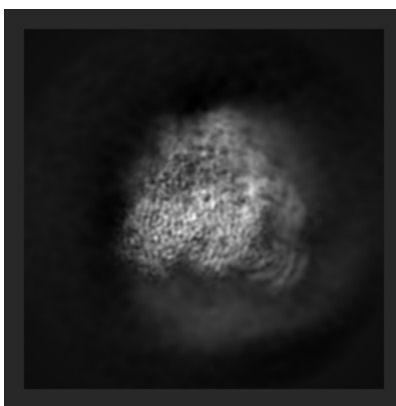
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

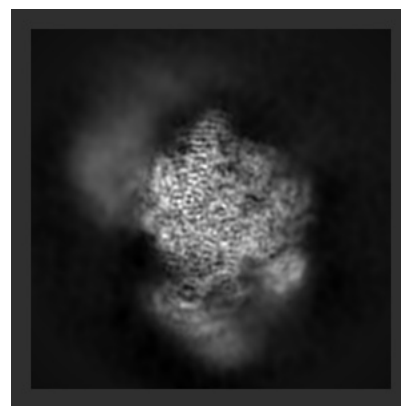
6.1.1 Primary map



X

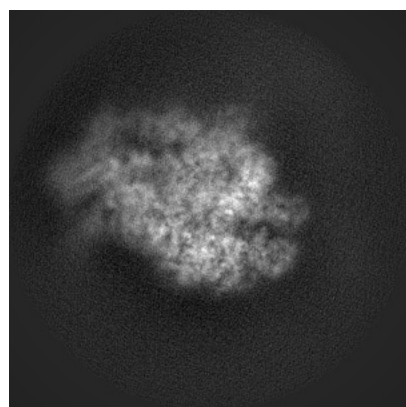


Y

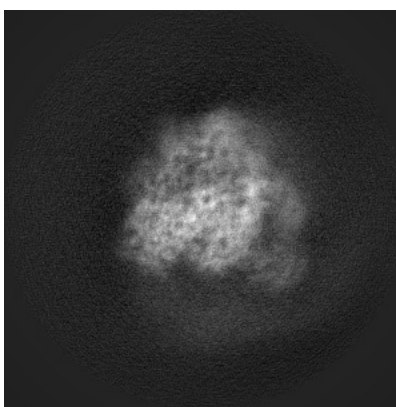


Z

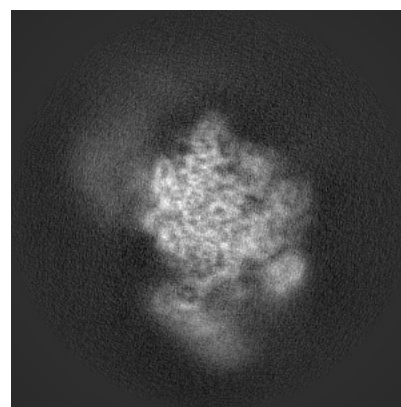
6.1.2 Raw map



X



Y

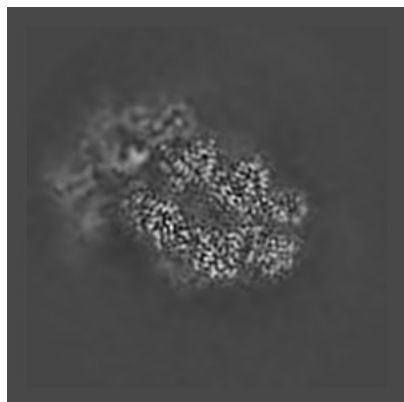


Z

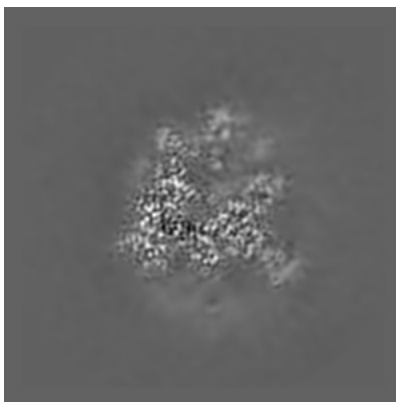
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

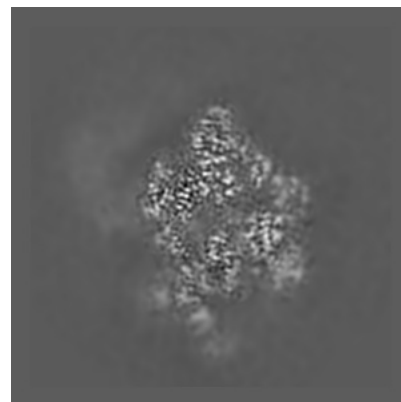
6.2.1 Primary map



X Index: 150

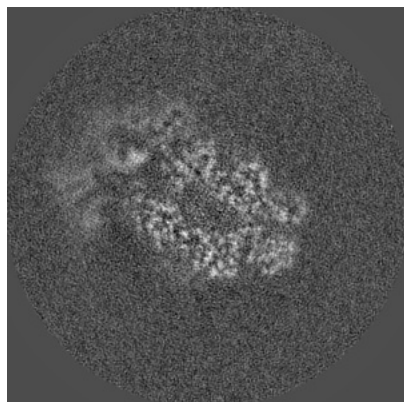


Y Index: 150

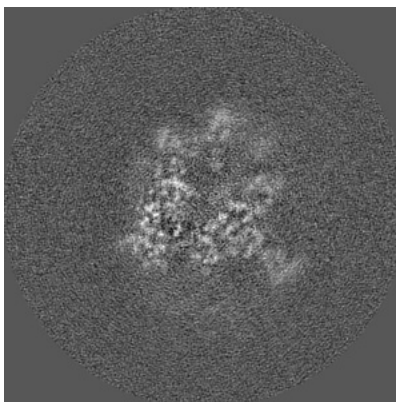


Z Index: 150

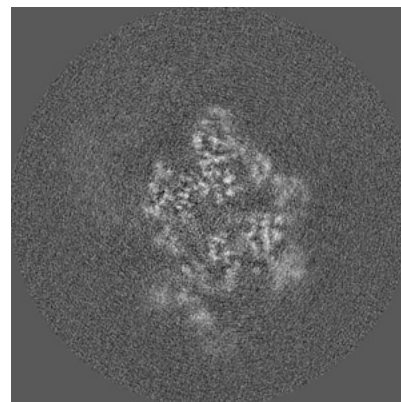
6.2.2 Raw map



X Index: 150



Y Index: 150

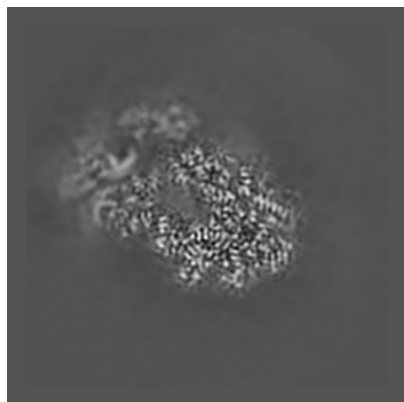


Z Index: 150

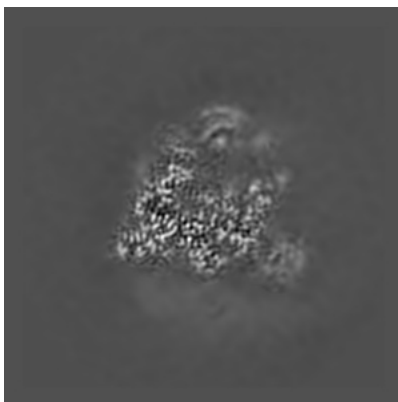
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

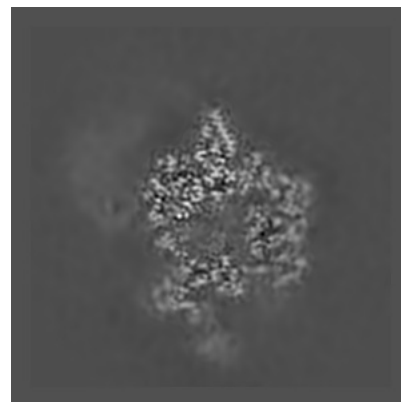
6.3.1 Primary map



X Index: 140

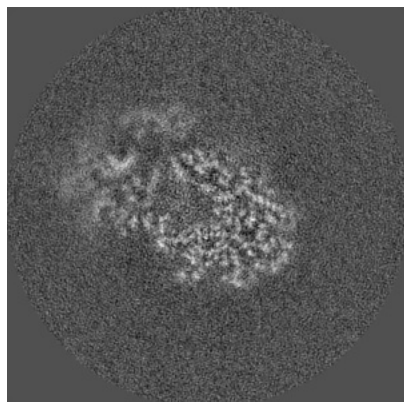


Y Index: 156

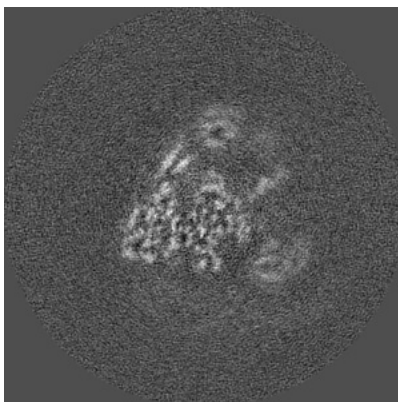


Z Index: 156

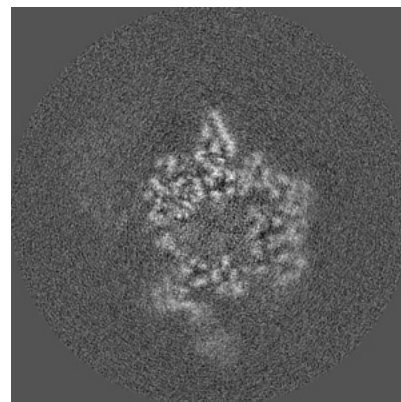
6.3.2 Raw map



X Index: 141



Y Index: 162

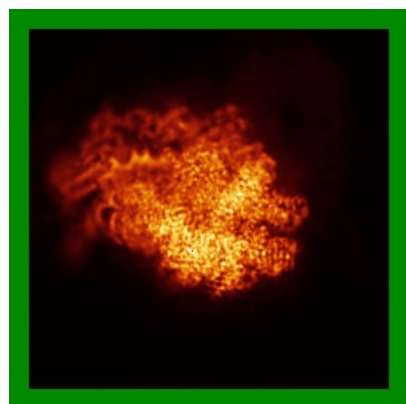


Z Index: 156

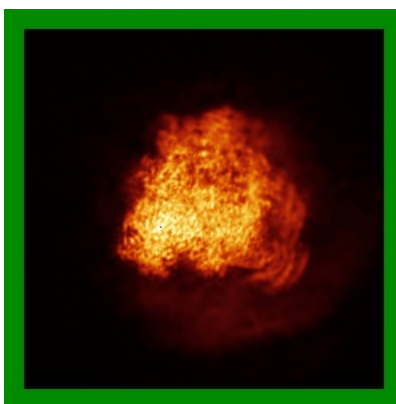
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

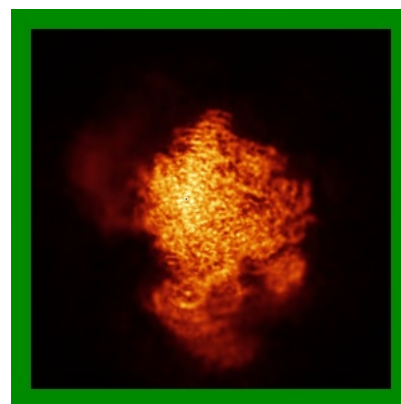
6.4.1 Primary map



X

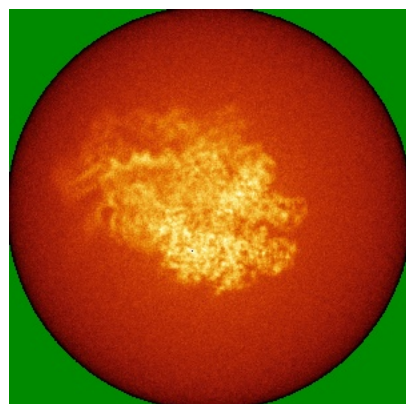


Y

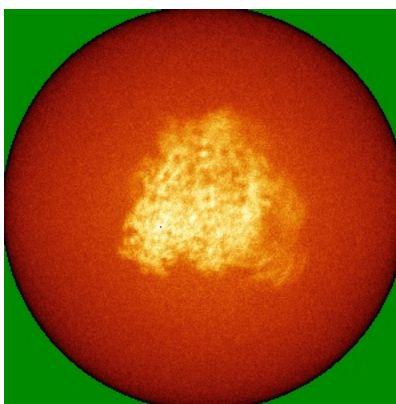


Z

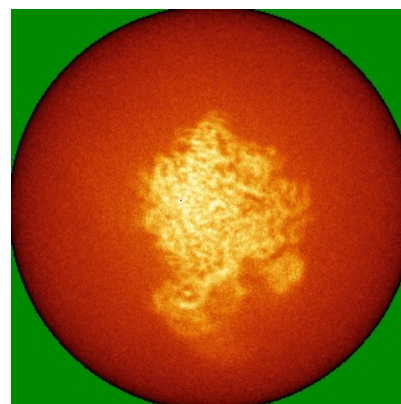
6.4.2 Raw map



X



Y

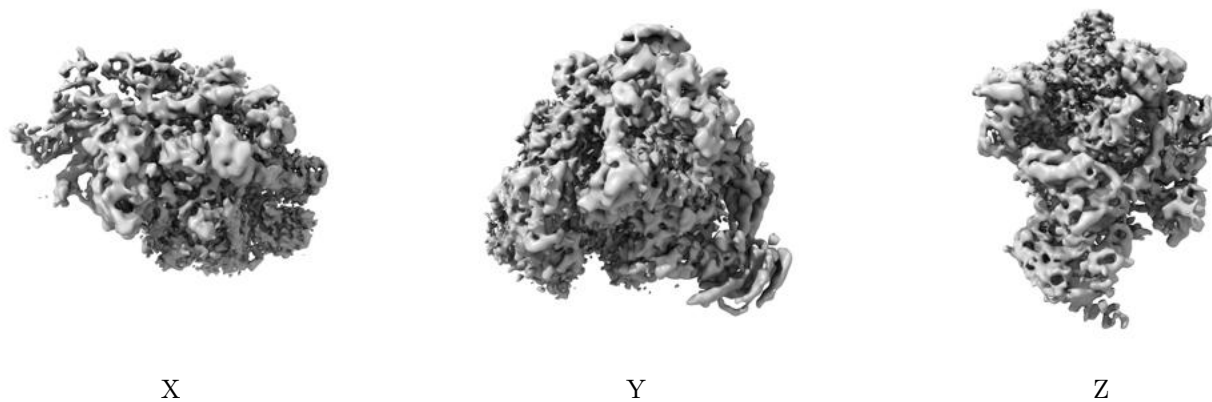


Z

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.

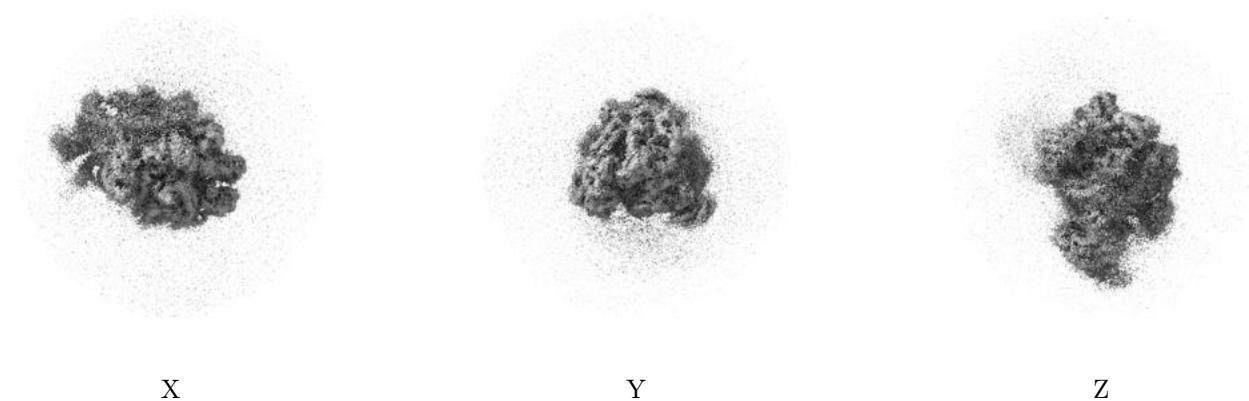
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 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.

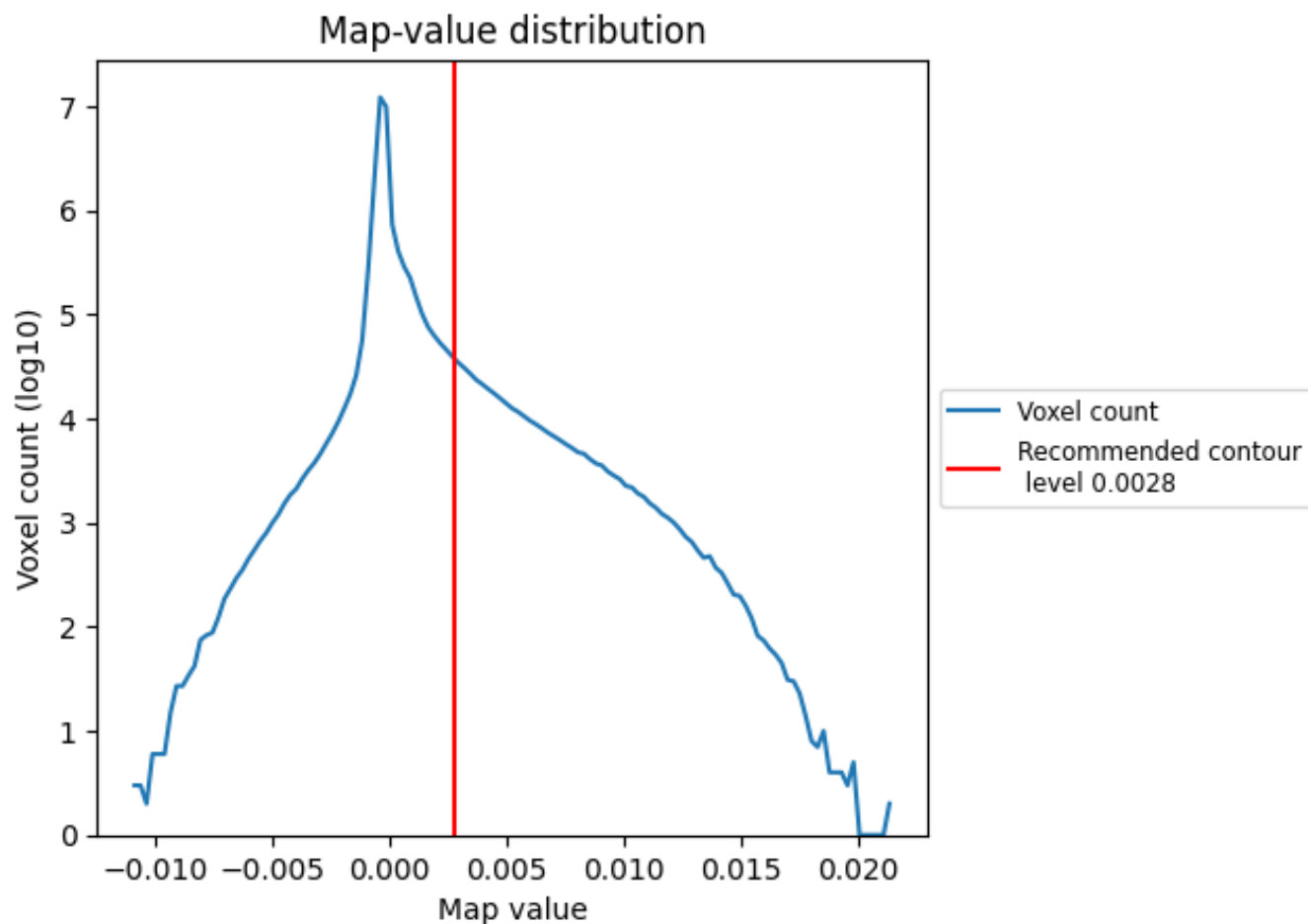
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

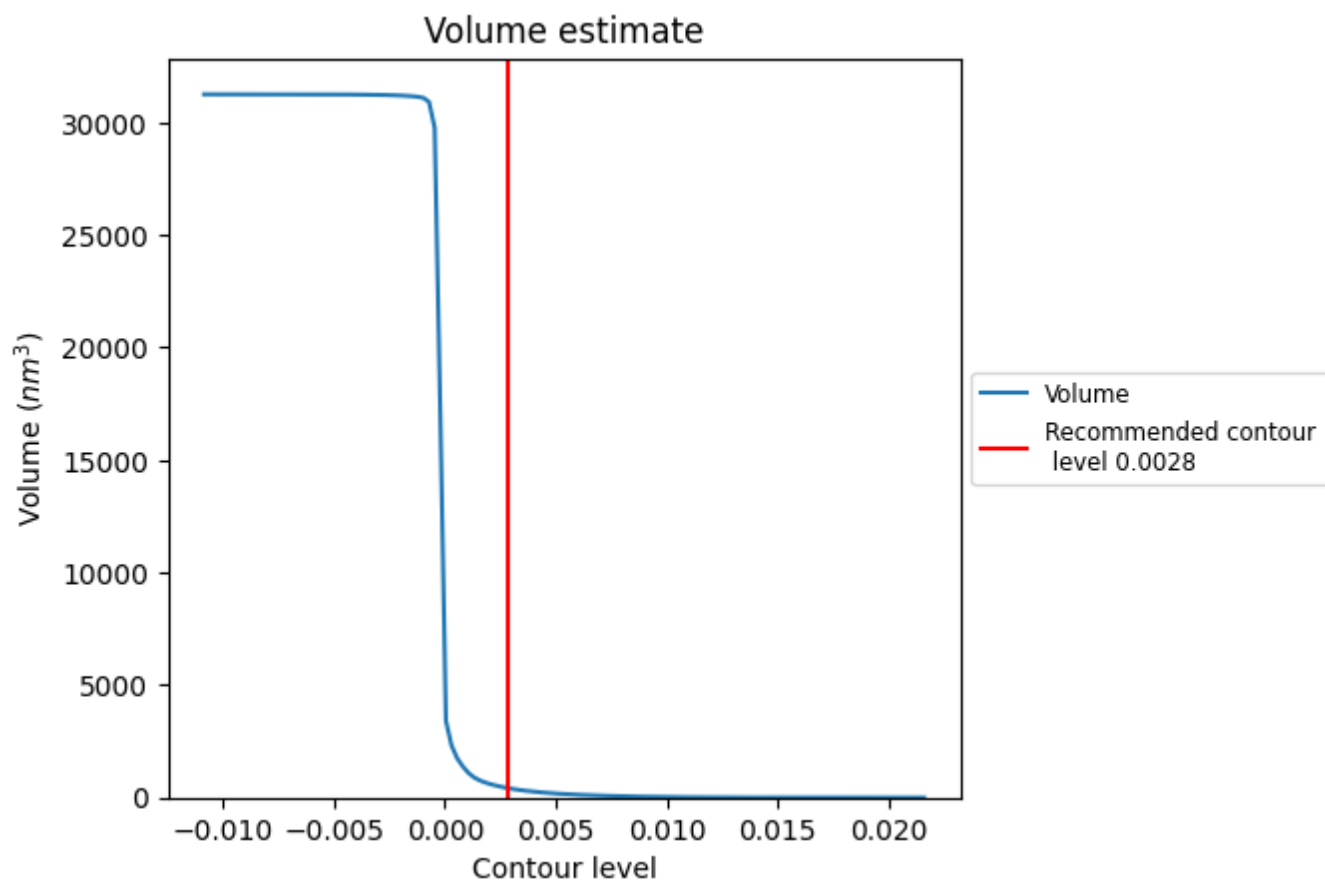
This section contains the results of statistical analysis of the map.

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.

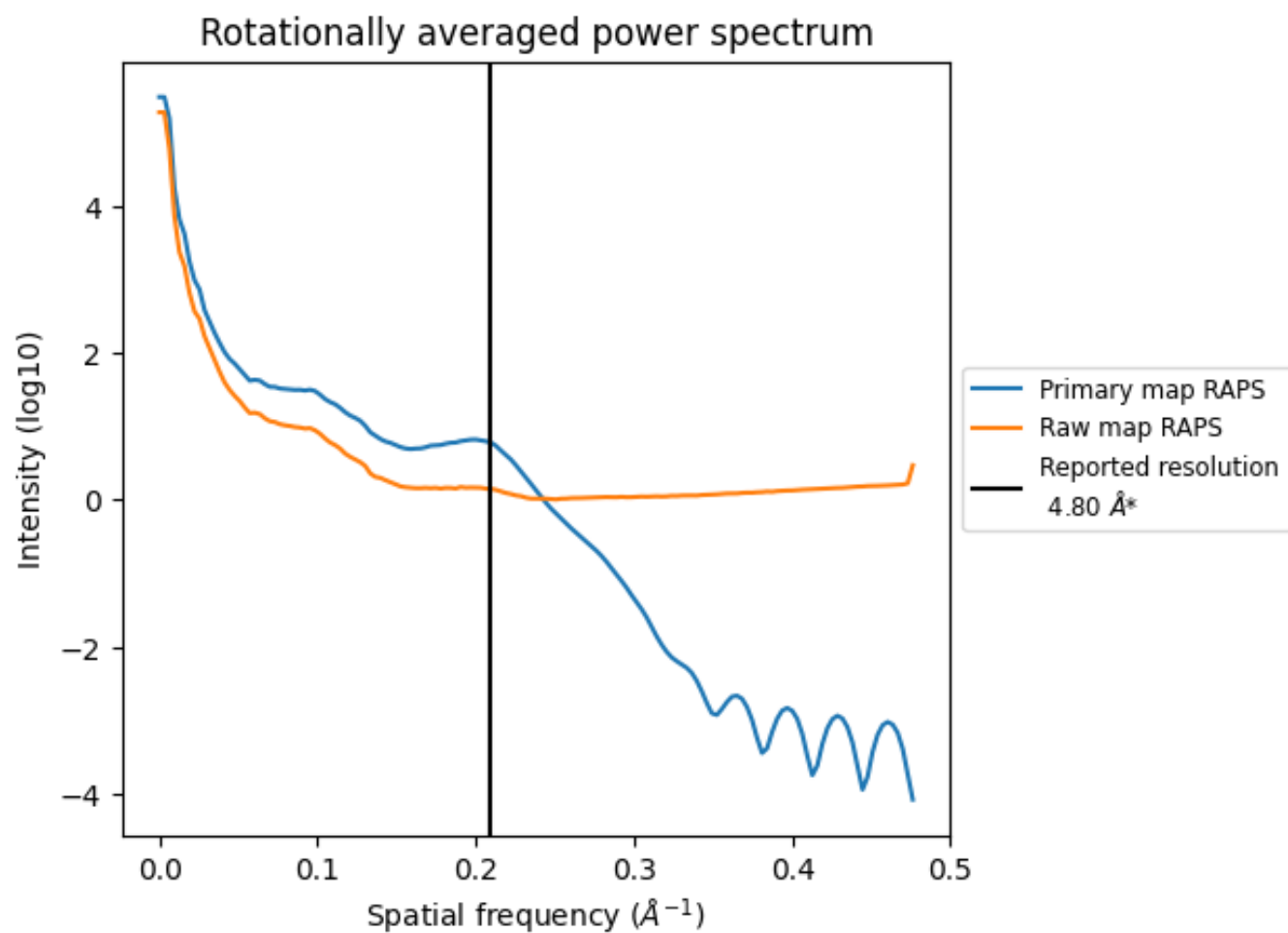
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 426 nm³; 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 ⓘ

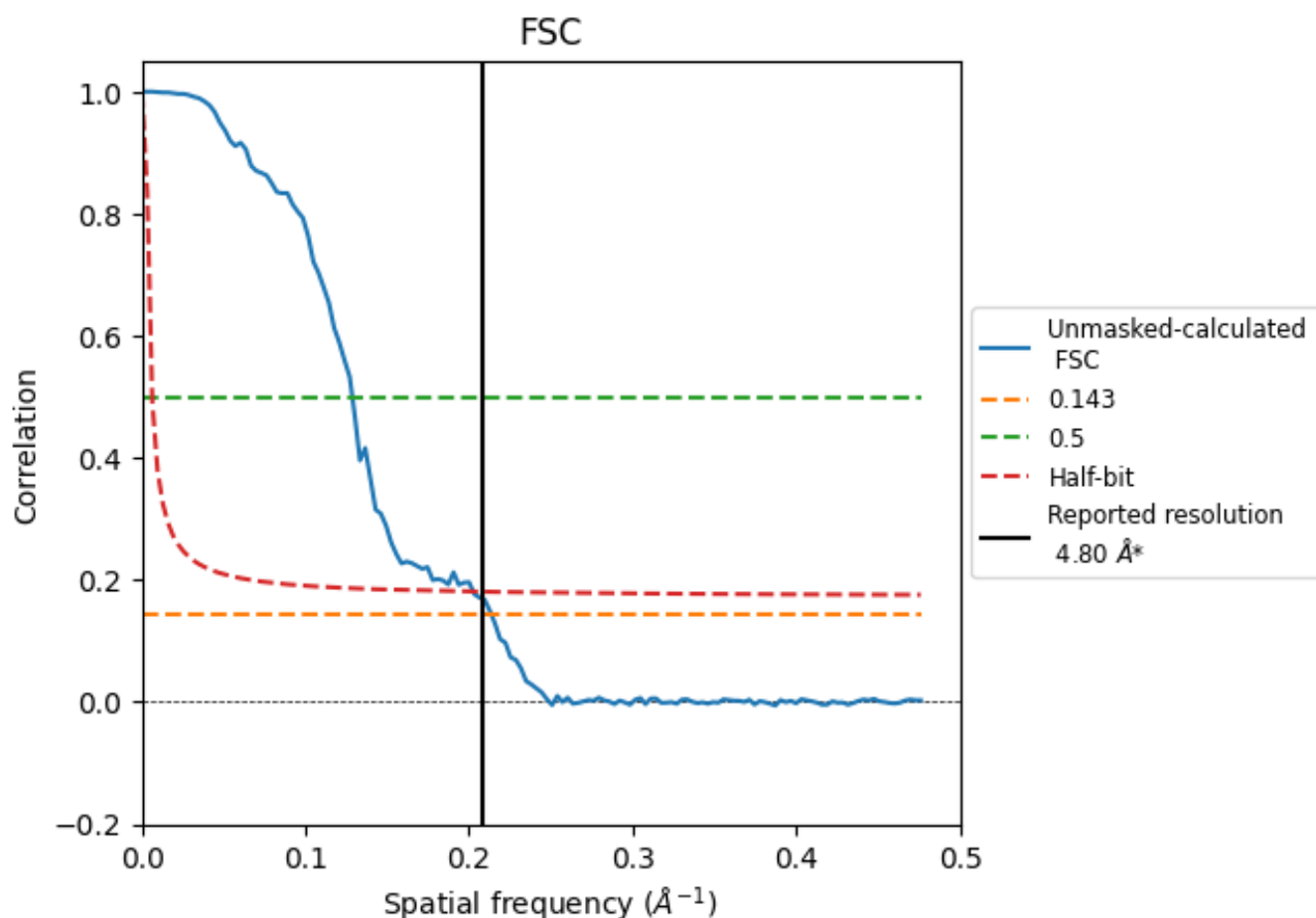


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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](#)

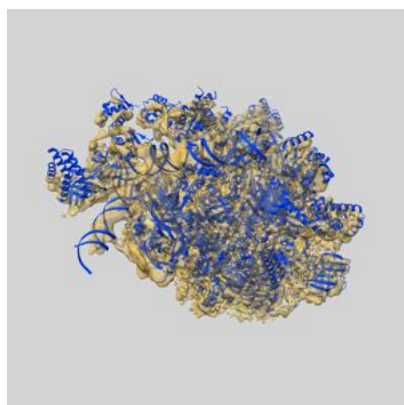
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	7.78	4.94

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

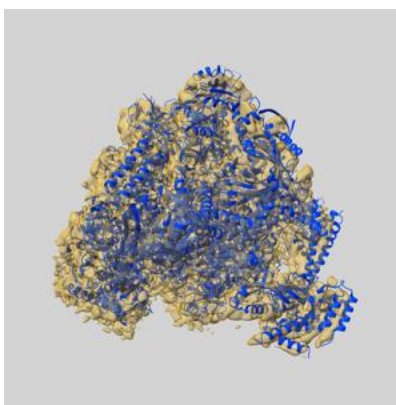
9 Map-model fit [i](#)

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](#).

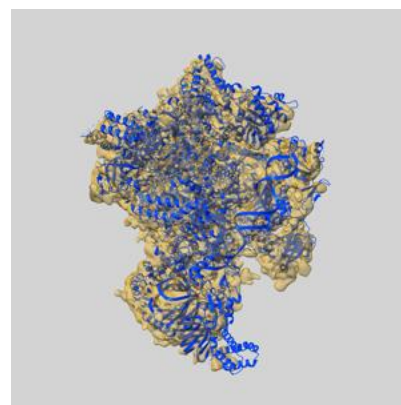
9.1 Map-model overlay [i](#)



X



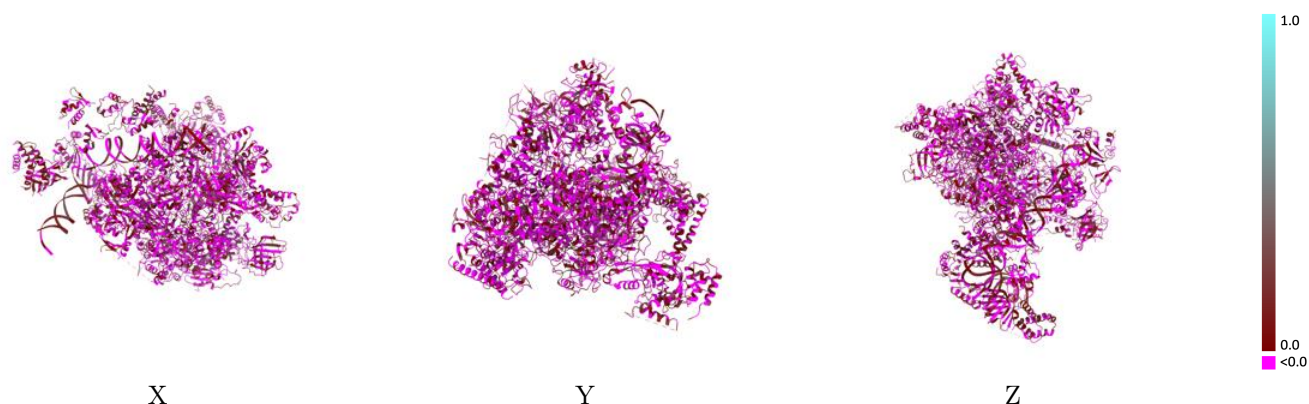
Y



Z

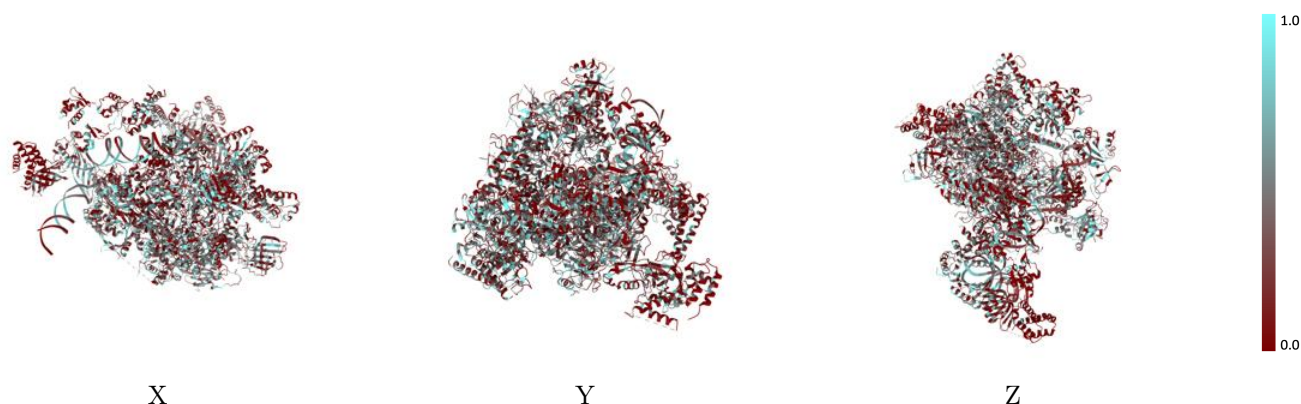
The images above show the 3D surface view of the map at the recommended contour level 0.0028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



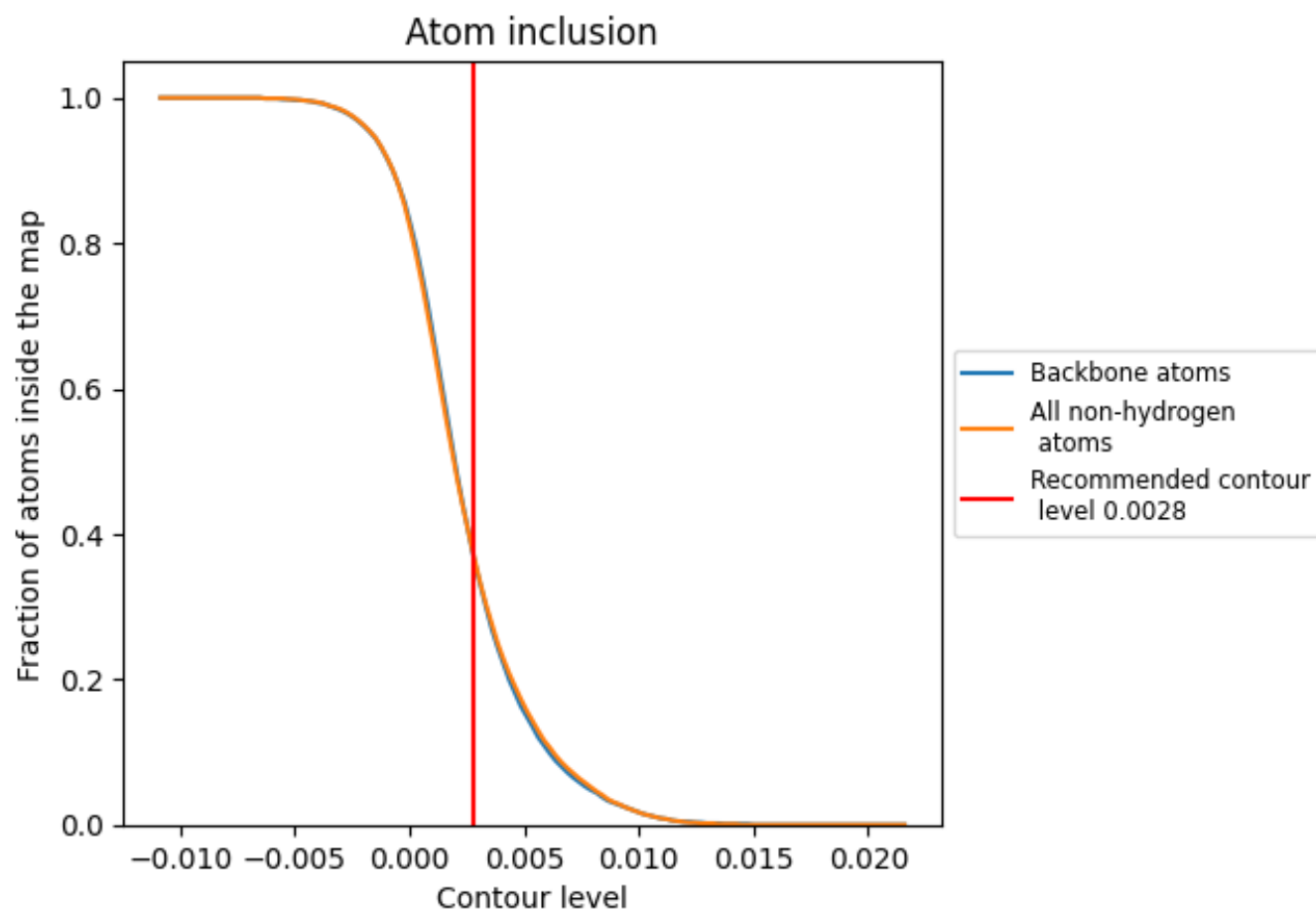
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.3700	 -0.0040
A	 0.3840	 -0.0110
B	 0.3770	 -0.0240
C	 0.4250	 -0.0310
D	 0.1990	 0.0040
E	 0.3740	 0.0120
F	 0.4200	 0.0230
G	 0.3480	 -0.0030
H	 0.3780	 -0.0040
I	 0.3820	 0.0160
J	 0.4330	 -0.0570
K	 0.3850	 -0.0410
L	 0.3640	 -0.0550
M	 0.3360	 -0.0170
N	 0.4180	 0.0710
O	 0.4780	 0.0280
Q	 0.3800	 0.0050
R	 0.4090	 -0.0100
T	 0.5000	 0.0660
U	 0.1610	 0.0330
V	 0.1630	 0.0540
W	 0.3140	 0.0240
X	 0.2140	 0.0330

