



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 10:46 pm BST

PDB ID : 5M3F
EMDB ID : EMD-4147
Title : Yeast RNA polymerase I elongation complex at 3.8Å
Authors : Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.;
Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on : 2016-10-14
Resolution : 3.80 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.39

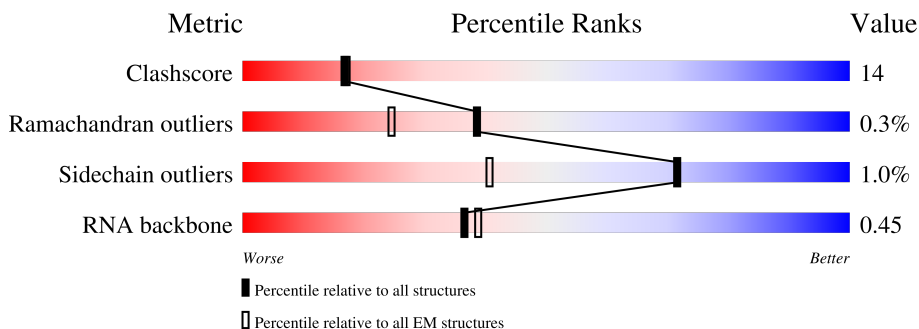
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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
RNA backbone	6643	2191

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	1664	<div> <div>38%</div> <div>65%</div> <div>22%</div> <div>12%</div> </div>
2	B	1203	<div> <div>32%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>
3	C	335	<div> <div>35%</div> <div>72%</div> <div>19%</div> <div>9%</div> </div>
4	E	215	<div> <div>67%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
5	F	155	<div> <div>30%</div> <div>49%</div> <div>15%</div> <div>35%</div> </div>
6	H	146	<div> <div>36%</div> <div>71%</div> <div>19%</div> <div>10%</div> </div>
7	I	125	<div> <div>50%</div> <div>30%</div> <div>20%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
8	J	70	
9	K	142	
10	L	70	
11	T	39	
12	U	39	
13	R	20	
14	M	415	
15	N	233	
16	D	137	
17	G	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	SO4	B	1301	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 34032 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1459	Total	C	N	O	S	0	0
			11526	7281	2004	2180	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1177	Total	C	N	O	S	0	0
			9350	5913	1639	1747	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	63	Total	C	N	O	S	0	0
			466	292	77	93	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	25	Total	C	N	O	P	0	0
			509	244	95	146	24		

- Molecule 12 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	14	Total	C	N	O	P	0	0
			285	138	51	83	13		

- Molecule 13 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	8	Total	C	N	O	P	0	0
			173	77	34	54	8		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	108	Total	C	N	O	0	0
			856	543	142	171		

- Molecule 15 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 16 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	D	54	Total	C	N	O	0	0
			431	270	73	88		

- Molecule 17 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	5		

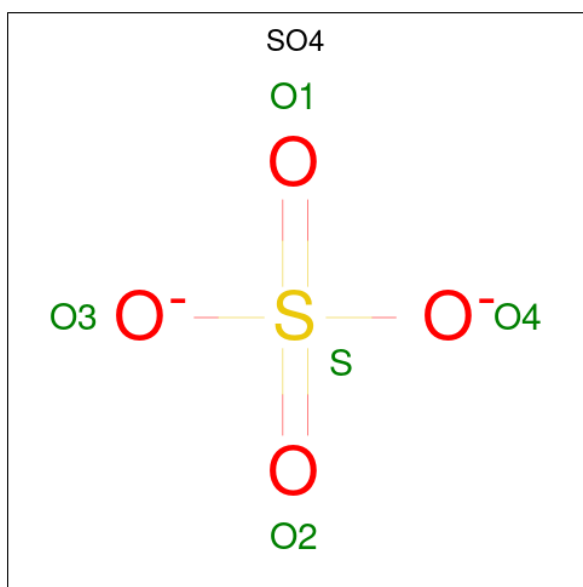
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

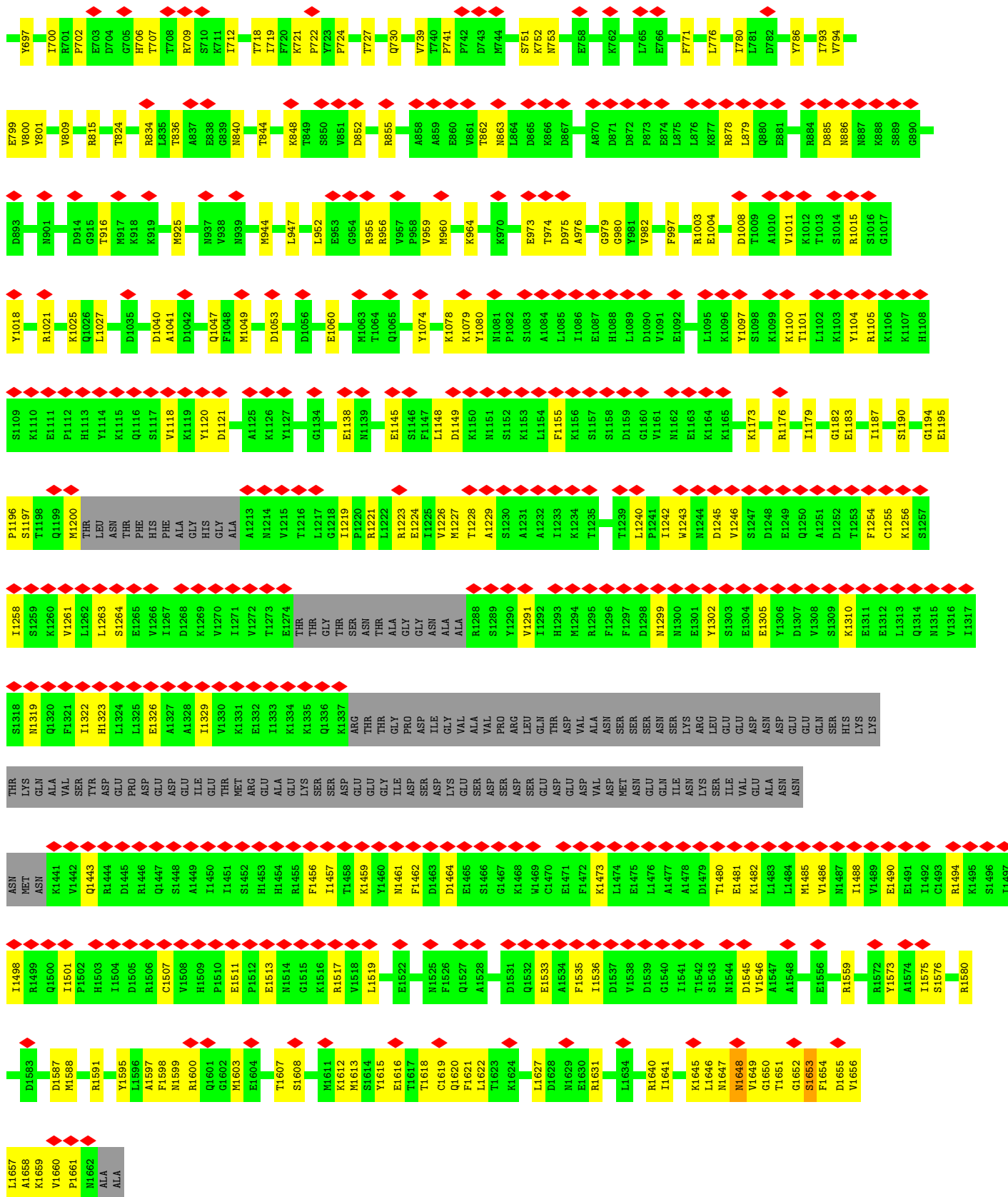
- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

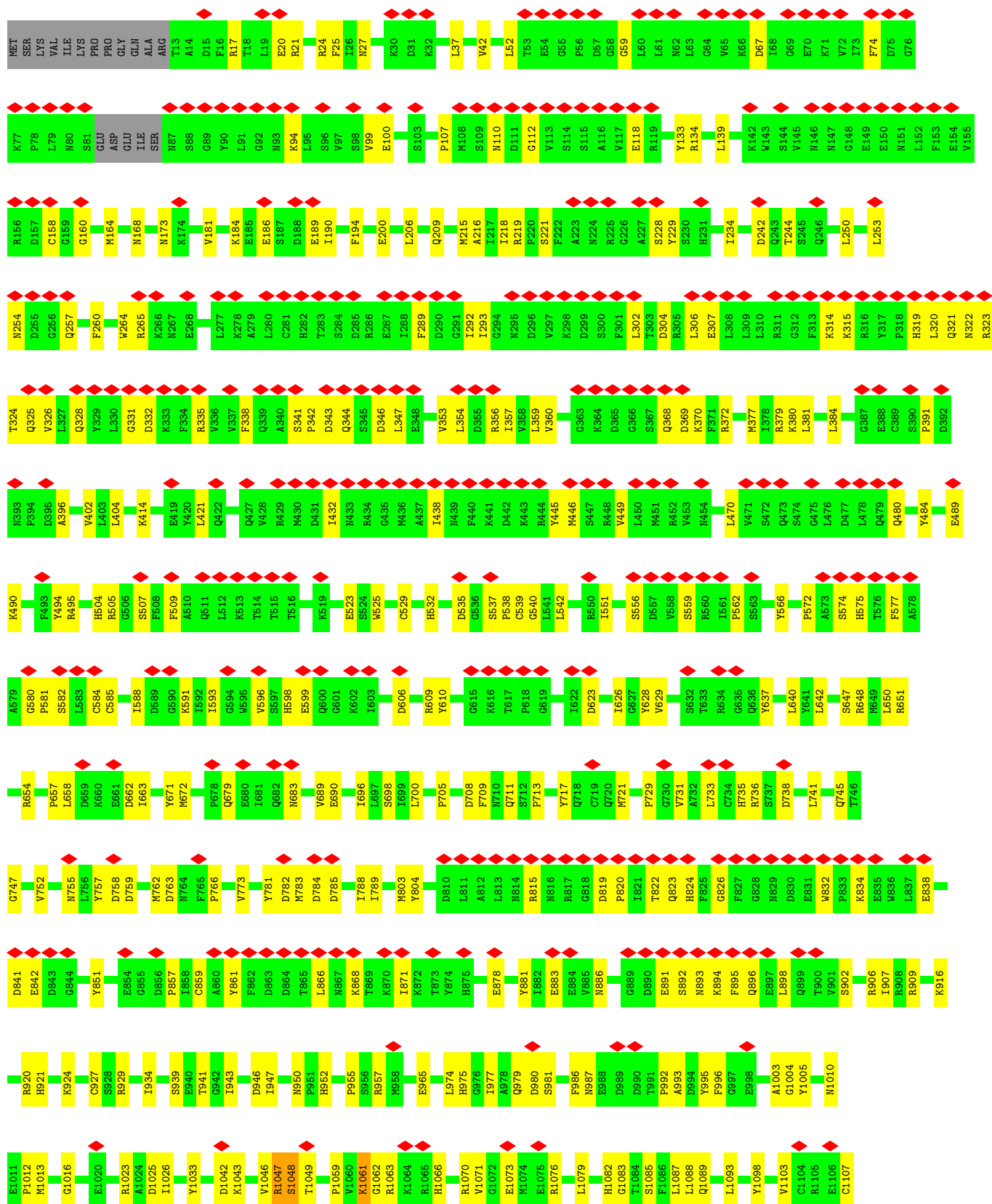
- Molecule 20 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

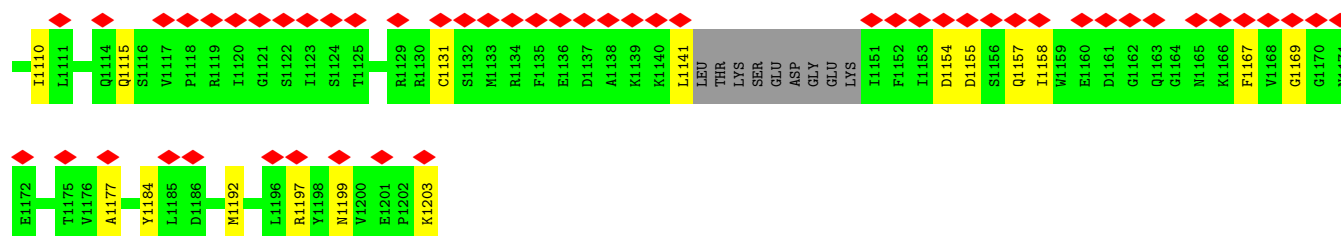


Mol	Chain	Residues	Atoms			AltConf
			Total	O	S	
20	B	1	5	4	1	0

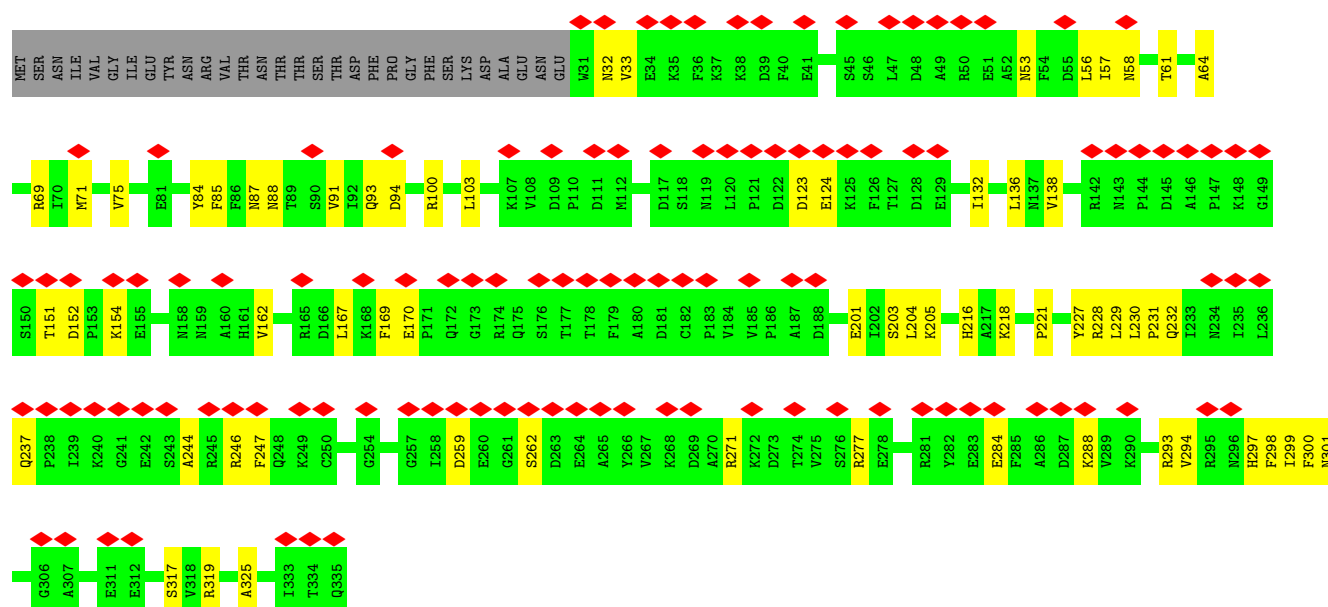
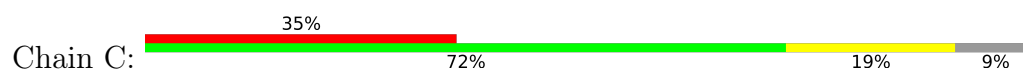


Chain B: 

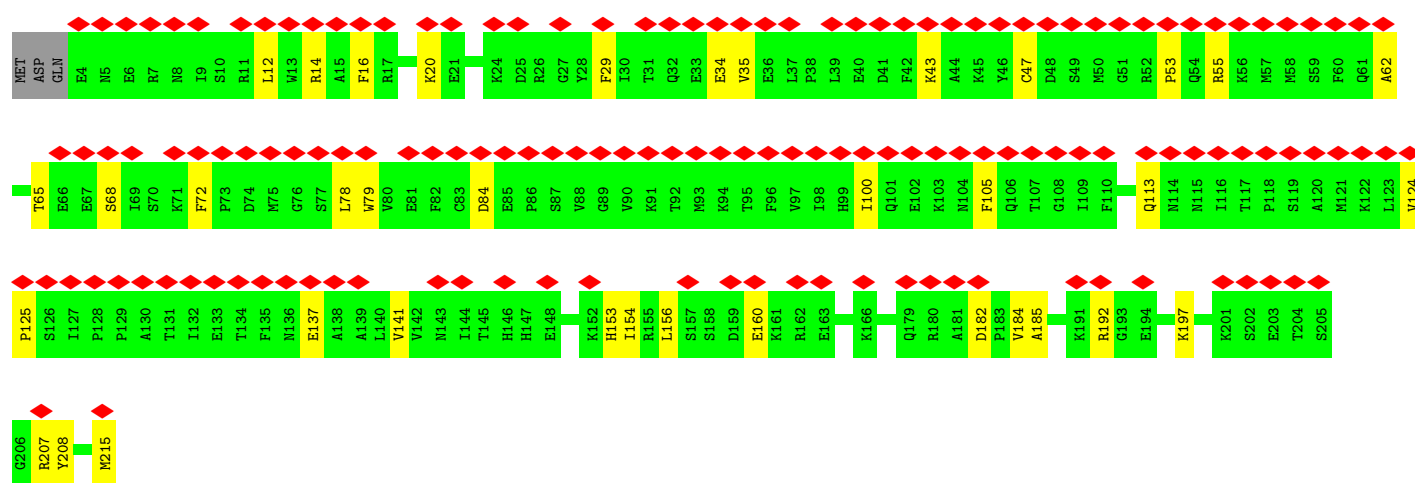
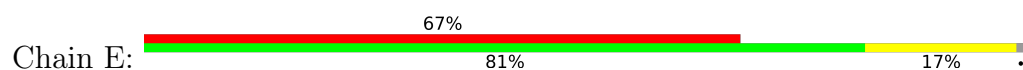




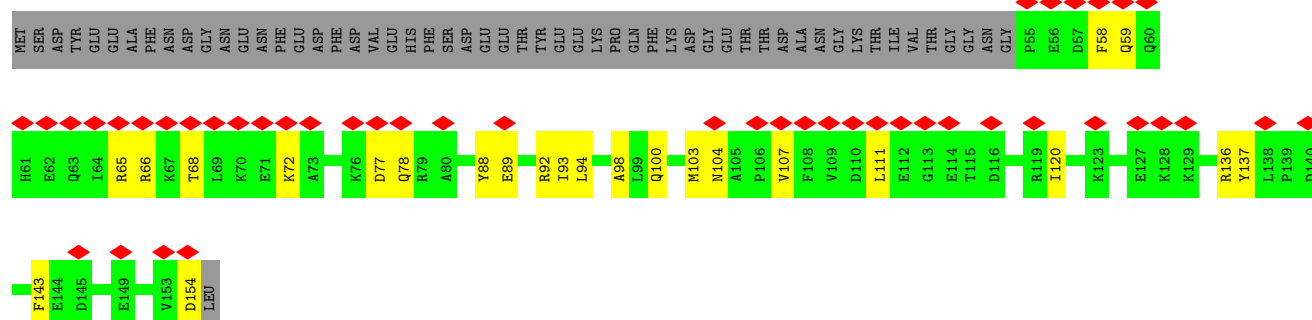
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



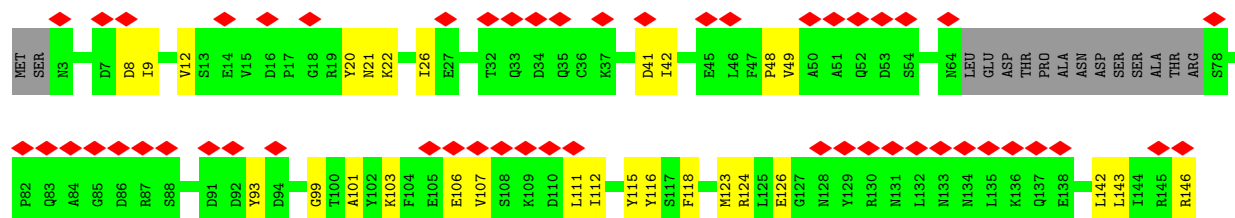
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



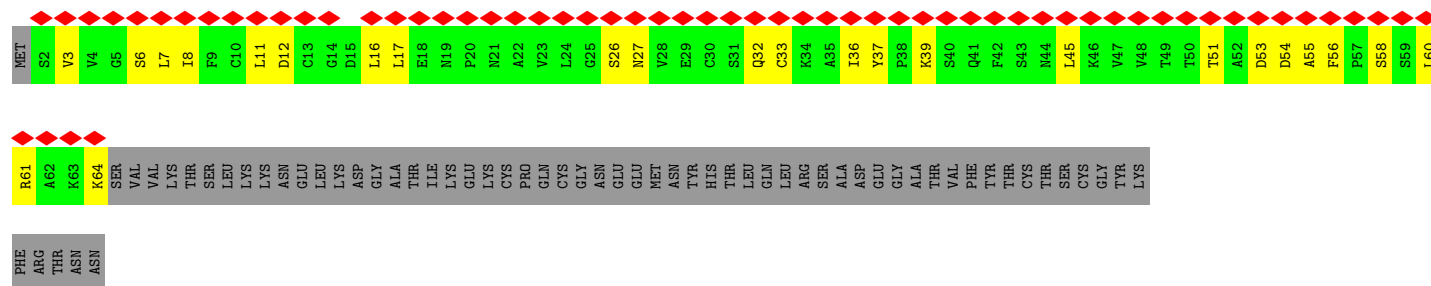
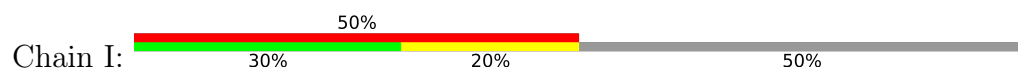
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



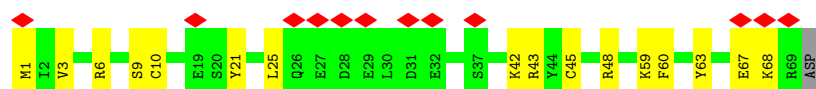
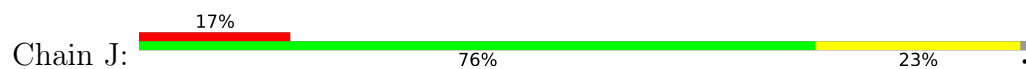
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 7: DNA-directed RNA polymerase I subunit RPA12



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

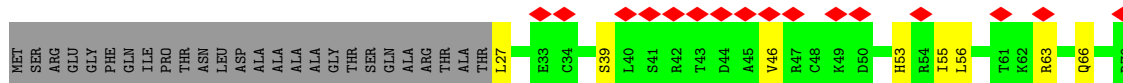


- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

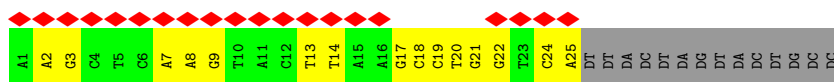
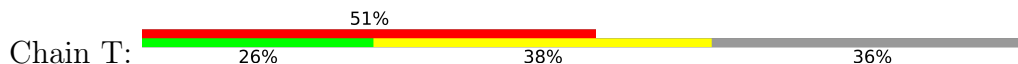




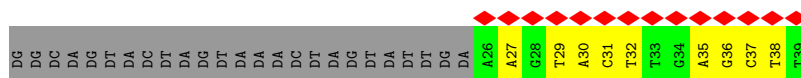
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



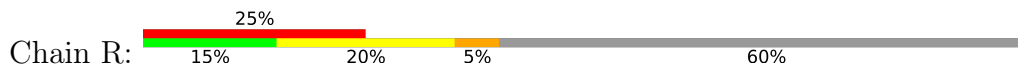
- Molecule 11: template DNA



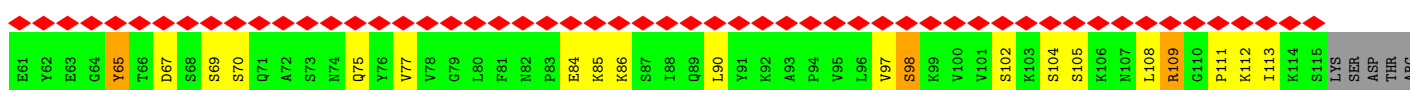
- Molecule 12: non-template DNA



- Molecule 13: RNA

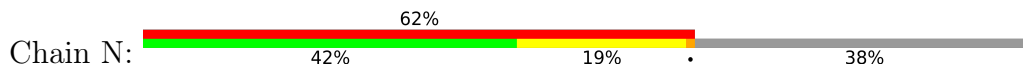


- Molecule 14: DNA-directed RNA polymerase I subunit RPA49



[illegible]

- Molecule 15: DNA-directed RNA polymerase I subunit RPA34



HIS	VAL	I121	N61	NET	
	ALA	A122	V62		SER
	GLU	S123	D63		LYS
	GLU	T124	I64		LEU
	VAL	A125	S65		SER
	LYS	K126	K66		ASP
	GLY	D127	L67		TYR
	ASN	N128	K68		VAL
	LYS	A129	S69		SER
	GLY	P130	L70		ASP
PRO	LYS	L131	P71	ASP	
LYS	LYS	Q132	V72	SER	
ARG	ARG	F133	ASP	ASP	
SER	SER	F133	ASP	GLU	
HIS	HIS	D134	PHE	VAL	
HIS	ASP	K135	SER	ILE	
ASP	ASP	V136	SER	SER	
ASP	GLU	F137	SER	ASN	
GLU	GLU	S138	T78	GLU	
GLY	GLY	V139	T79	PHE	
SER	SER	S140	T81	S24	
GLU	GLU	E141	I82	I25	
LYS	LYS	T142	D83	P26	
LYS	LYS	A143	K84	D27	
LYS	LYS	K144	H85	G28	
LYS	LYS	I145	D86	F29	
LYS	LYS	P146	E87	K30	
GLU	GLU	A147	K88	K31	
ARG	ARG	I148	I89	K33	
GLY	GLY	D149	M90	H34	
LYS	LYS	V150	D91	L35	
ARG	GLU	S151	D92	K36	
LYS	LYS	K152	T93	N37	
LYS	LYS	V153	D94	F38	
ASP	ASP	R154	I95	P39	
LYS	LYS	V155	E96	L40	
ASP	ASP	P156	S97	N41	
LYS	LYS	R157	S98	GLY	
LYS	LYS	K158	L99	ASP	
LYS	LYS	D159	T100	ASN	
HIS	HIS	V160	Q101	LYS	
ARG	ARG	P161	D102	LYS	
ASP	ASP	K162	M103	ALA	
		V163	L104	K49	
		G165	S105	O50	
		L166	M106	Q51	
		K167	M107	V53	
		L168	T108	W54	
		E169	L109	L55	
		H170	L110	I56	
		F171	V111	K57	
		A172	P112	F58	
		T173	S113	P59	
		G174	E114	S60	
		V175	K116		
		A177	E117		
		E178	S118		
		D179	L119		
		F180	K120		

- Molecule 16: DNA-directed RNA polymerase I subunit RPA14

[illegible]

- Molecule 17: DNA-directed RNA polymerase I subunit RPA43



V61	V62	K63	Q64	H65	L66	P67	N68	L69	V70	M71	K72	Y73	N74	N75	K76	V77	G78	G79	V80	V81	L82	G83	Y84	E85	G86	L87	K88	L89	L90	D91	A92	D93	P94	L95	K96	K97	E98	D99	T100	S101	E102	K103	L104	I105	K106	I107	T108	P109	D110	T111	P112	F113	G114	F115	T116	W117	C118	H119	W120
MT	SER	GLN	VAL	LYS	ARG	ALA	ASN	GLU	ASN	ARG	GLU	THR	A14	R15	F16	I17	K18	K19	H20	K21	K22	Q23	V24	T25	N26	P27	L28	D29	E30	K31	N32	G33	T34	S35	N36	C37	L38	V39	R40	V41	P42	I43	A44	L45	Y46	Y47	S48	I49	A50	P51	M52	Y53	L54	E55	N56	P57	L58	Q59	G60

LYS	R241	ASN	N121
	GLU	THR	L122
	ASP	ASP	Y123
	ASN	GLU	V124
	GLY	ASN	W125
	SER	ASN	Q126
	GLU	GLY	P127
	ILE	ASN	Q128
	VAL	ASN	V129
	TYR	ASN	GLI30
GLU	T248	ASN	D131
	GLU	GLI31	V132
	L249	ASP	L133
	T250	GLY	E134
	SER	GLY	G135
	THR	SER	Y136
	ASP	ASN	I137
	GLU	ASN	F138
	GLY	LEU	I139
	ILE	GLY	Q140
SER	ARG	PHE	S141
	GLN	PHE	A142
	ALA	GLY	S143
	GLU	ASN	H144
	SER	ARG	I145
	LEU	SER	G146
	PRO	LEU	L147
	ILE	G215	L148
	VAL	H216	I149
	SER	W217	H150
LYS	ASN	V218	D151
	LYS	V219	A152
	ILE	S220	F153
	VAL	N221	N154
	PHE	G222	A155
	ASP	E223	S156
	ASP	P224	I157
	GLI31	I225	K158
	GLU	D226	K159
	ASN	G227	N160
LYS	LYS	K228	N161
	GLI31	L229	I162
	SER	R230	P163
	HIS	F231	V164
	LYS	T232	D165
	GLU	V233	W166
	LEU	R234	T167
	ASP	N235	F168
	PRO	V236	V169
	GLU	H237	H170
VAL	VAL	T238	ASN
		T239	ASP
		G240	ASP
			VAL
			GLU
			GLU
			GLU
			ASP
			ALA
			ASP
		VAL	
		ILE	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	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 ($e^-/\text{\AA}^2$)	56	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	0.218	Depositor
Minimum map value	-0.142	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	241.49998, 241.49998, 241.49998	wwPDB
Map dimensions	230, 230, 230	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: MG, SO4, ZN

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	0.35	0/11738	0.50	0/15851
2	B	0.37	0/9557	0.52	0/12918
3	C	0.35	0/2475	0.49	0/3354
4	E	0.31	0/1771	0.46	0/2383
5	F	0.32	0/838	0.46	0/1129
6	H	0.34	0/1070	0.49	0/1449
7	I	0.26	0/472	0.48	0/639
8	J	0.37	0/578	0.47	0/775
9	K	0.35	0/804	0.51	0/1083
10	L	0.33	0/354	0.50	0/468
11	T	0.60	0/571	0.87	0/879
12	U	0.58	0/319	0.97	0/491
13	R	0.48	0/193	1.08	0/299
14	M	0.41	0/872	0.55	0/1170
15	N	0.42	0/1172	0.57	1/1580 (0.1%)
16	D	0.38	0/436	0.51	0/591
17	G	0.37	0/1564	0.66	3/2127 (0.1%)
All	All	0.37	0/34784	0.54	4/47186 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	241	ARG	NE-CZ-NH1	11.89	126.25	120.30
17	G	241	ARG	NE-CZ-NH2	-11.70	114.45	120.30
17	G	241	ARG	CD-NE-CZ	6.04	132.05	123.60
15	N	145	ILE	C-N-CD	5.04	138.99	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1048	SER	Peptide
2	B	1061	LYS	Peptide
2	B	319	HIS	Peptide

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	A	11526	0	11614	326	0
2	B	9350	0	9240	362	0
3	C	2423	0	2412	68	0
4	E	1735	0	1764	25	0
5	F	823	0	840	46	0
6	H	1052	0	1021	20	0
7	I	466	0	466	29	0
8	J	569	0	585	21	0
9	K	793	0	790	17	0
10	L	352	0	376	7	0
11	T	509	0	283	16	0
12	U	285	0	161	9	0
13	R	173	0	89	6	0
14	M	856	0	852	97	0
15	N	1151	0	1169	99	0
16	D	431	0	428	11	0
17	G	1526	0	1540	90	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1	0	0	0	0
19	A	1	0	0	0	0
20	B	5	0	0	2	0
All	All	34032	0	33630	918	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 14.

The worst 5 of 918 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)
2:B:328:GLN:NE2	14:M:112:LYS:HA	1.22	1.49
1:A:1661:PRO:CD	17:G:55:GLU:CA	1.86	1.44
2:B:987:ASN:ND2	15:N:157:ARG:CD	1.85	1.39
2:B:328:GLN:CD	14:M:112:LYS:HA	1.39	1.39
3:C:301:ASN:ND2	15:N:173:THR:HB	1.37	1.37

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	1447/1664 (87%)	1325 (92%)	119 (8%)	3 (0%)	44	74
2	B	1171/1203 (97%)	1109 (95%)	60 (5%)	2 (0%)	44	74
3	C	303/335 (90%)	286 (94%)	17 (6%)	0	100	100
4	E	210/215 (98%)	200 (95%)	10 (5%)	0	100	100
5	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	61/125 (49%)	53 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
9	K	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
10	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
14	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	6	33
15	N	139/233 (60%)	122 (88%)	14 (10%)	3 (2%)	5	30
16	D	50/137 (36%)	48 (96%)	2 (4%)	0	100	100
17	G	189/326 (58%)	174 (92%)	13 (7%)	2 (1%)	12	42
All	All	4109/5236 (78%)	3826 (93%)	271 (7%)	12 (0%)	38	69

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	A	1653	SER
1	A	91	PHE
2	B	1047	ARG
14	M	85	LYS

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	1289/1465 (88%)	1284 (100%)	5 (0%)	89	91
2	B	1030/1053 (98%)	1030 (100%)	0	100	100
3	C	269/296 (91%)	269 (100%)	0	100	100
4	E	194/197 (98%)	194 (100%)	0	100	100
5	F	90/137 (66%)	90 (100%)	0	100	100
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	55/110 (50%)	55 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	39/57 (68%)	39 (100%)	0	100	100
14	M	98/371 (26%)	88 (90%)	10 (10%)	6	24
15	N	135/220 (61%)	129 (96%)	6 (4%)	24	48
16	D	52/116 (45%)	47 (90%)	5 (10%)	7	26
17	G	171/291 (59%)	159 (93%)	12 (7%)	12	37
All	All	3692/4636 (80%)	3654 (99%)	38 (1%)	71	80

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	G	35	SER
17	G	230	ARG
17	G	39	VAL
17	G	167	THR
17	G	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	59	GLN
17	G	235	ASN
5	F	100	GLN
9	K	106	GLN
2	B	27	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/20 (35%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	15	C
13	R	17	A

There are no RNA pucker outliers to report.

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 8 ligands modelled in this entry, 7 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	$\# Z > 2$
20	SO4	B	1301	-	4,4,4	0.16	0	6,6,6	0.09	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1301	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

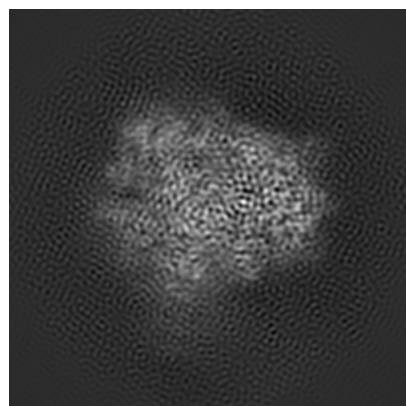
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4147. These allow visual inspection of the internal detail of the map and identification of artifacts.

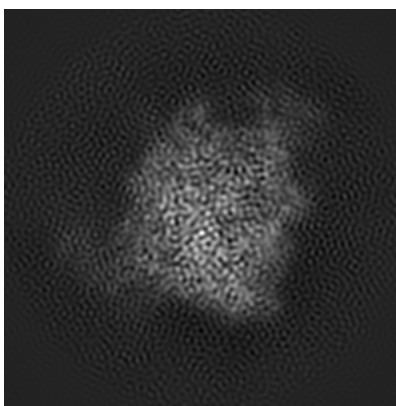
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

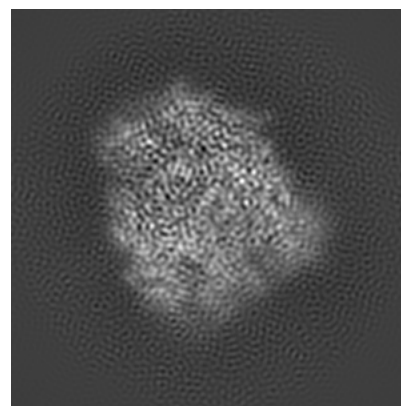
6.1.1 Primary map



X

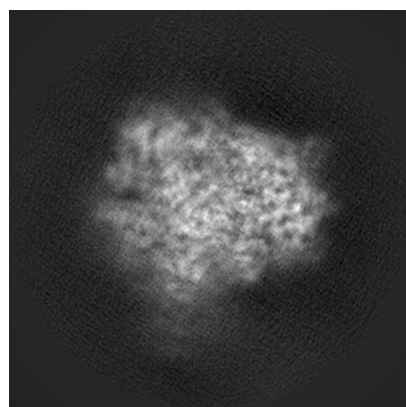


Y

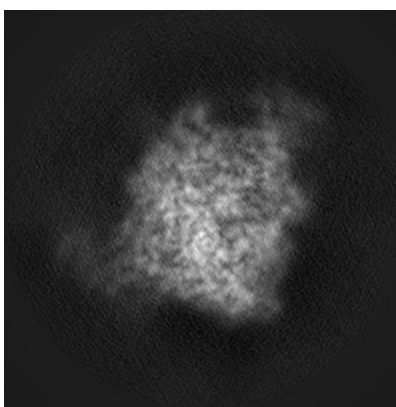


Z

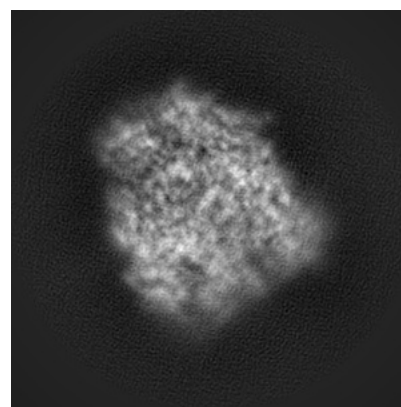
6.1.2 Raw map



X



Y

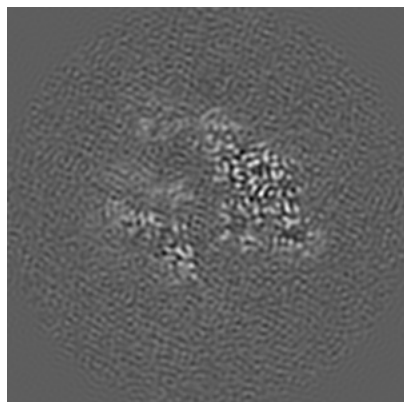


Z

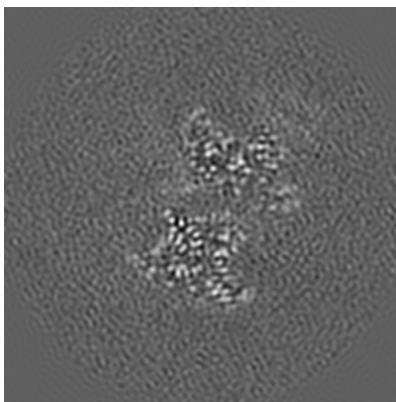
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

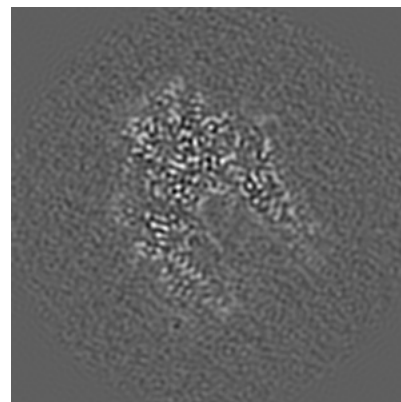
6.2.1 Primary map



X Index: 115

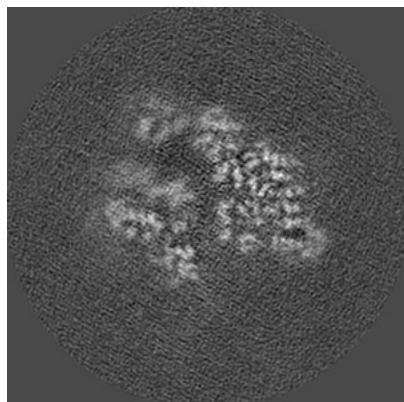


Y Index: 115

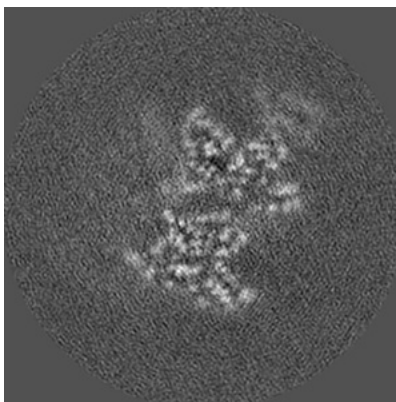


Z Index: 115

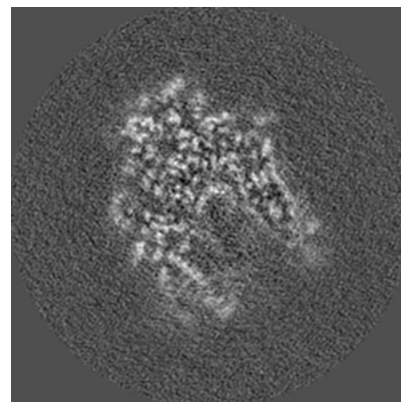
6.2.2 Raw map



X Index: 115



Y Index: 115

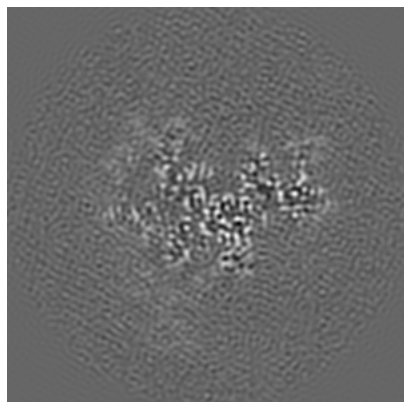


Z Index: 115

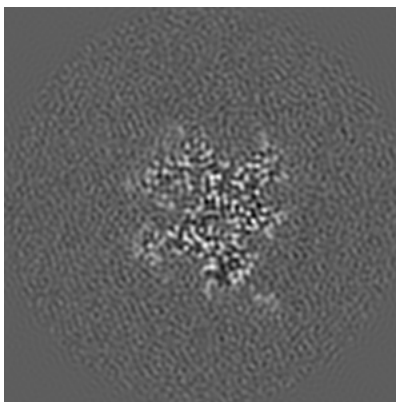
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

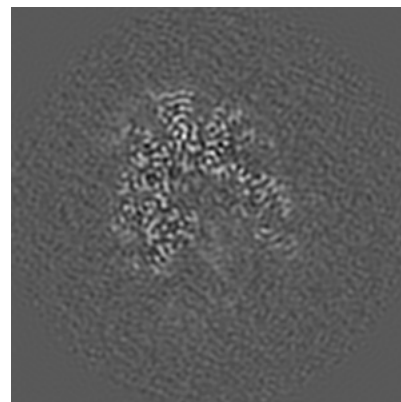
6.3.1 Primary map



X Index: 94

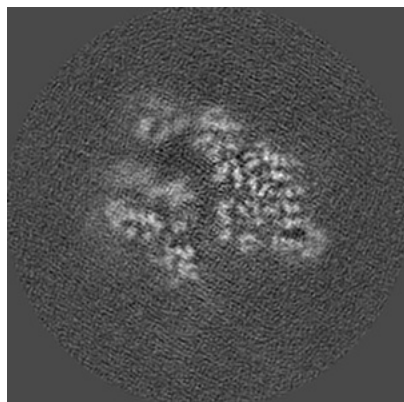


Y Index: 135

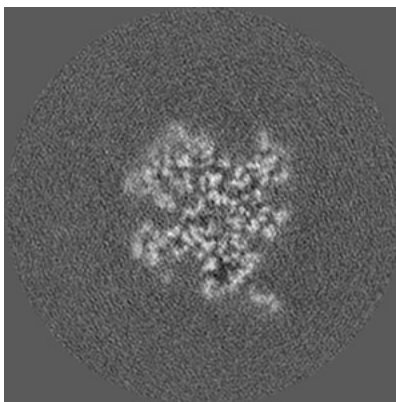


Z Index: 122

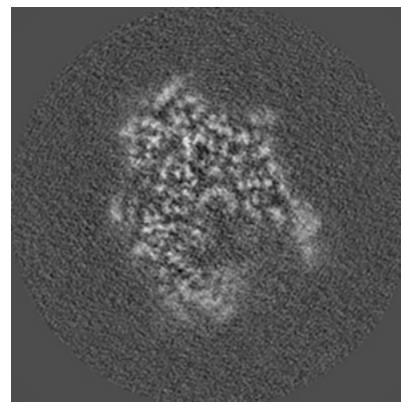
6.3.2 Raw map



X Index: 115



Y Index: 135

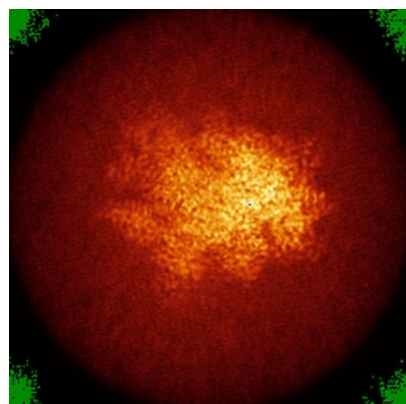


Z Index: 113

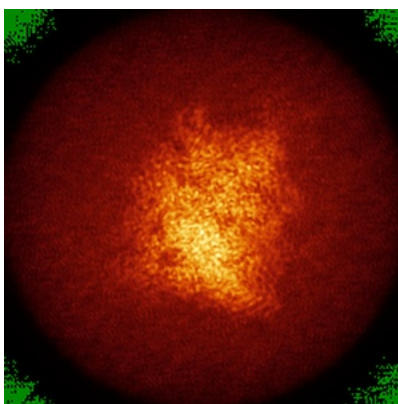
The images above show the largest variance slices of the map in three orthogonal directions.

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

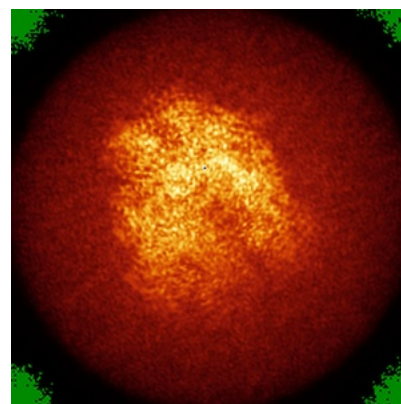
6.4.1 Primary map



X

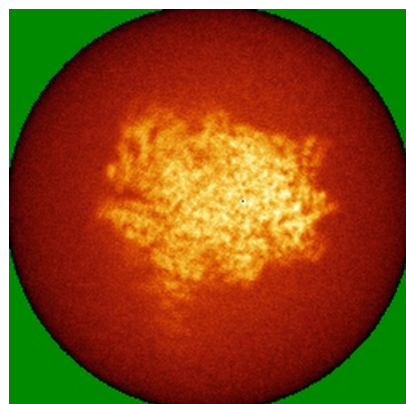


Y

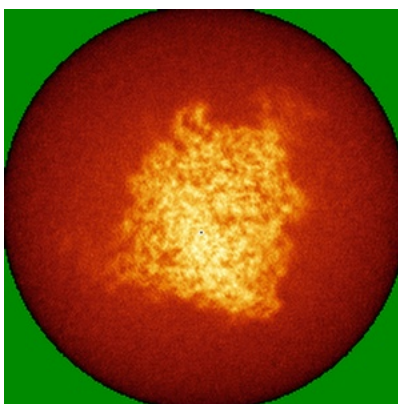


Z

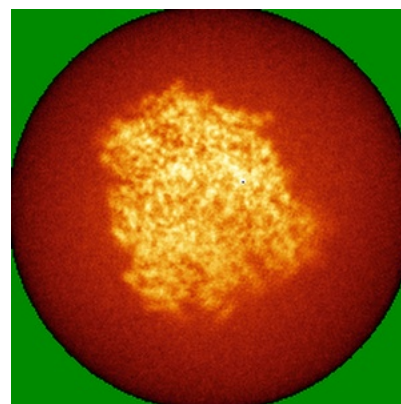
6.4.2 Raw map



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 0.045. 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.

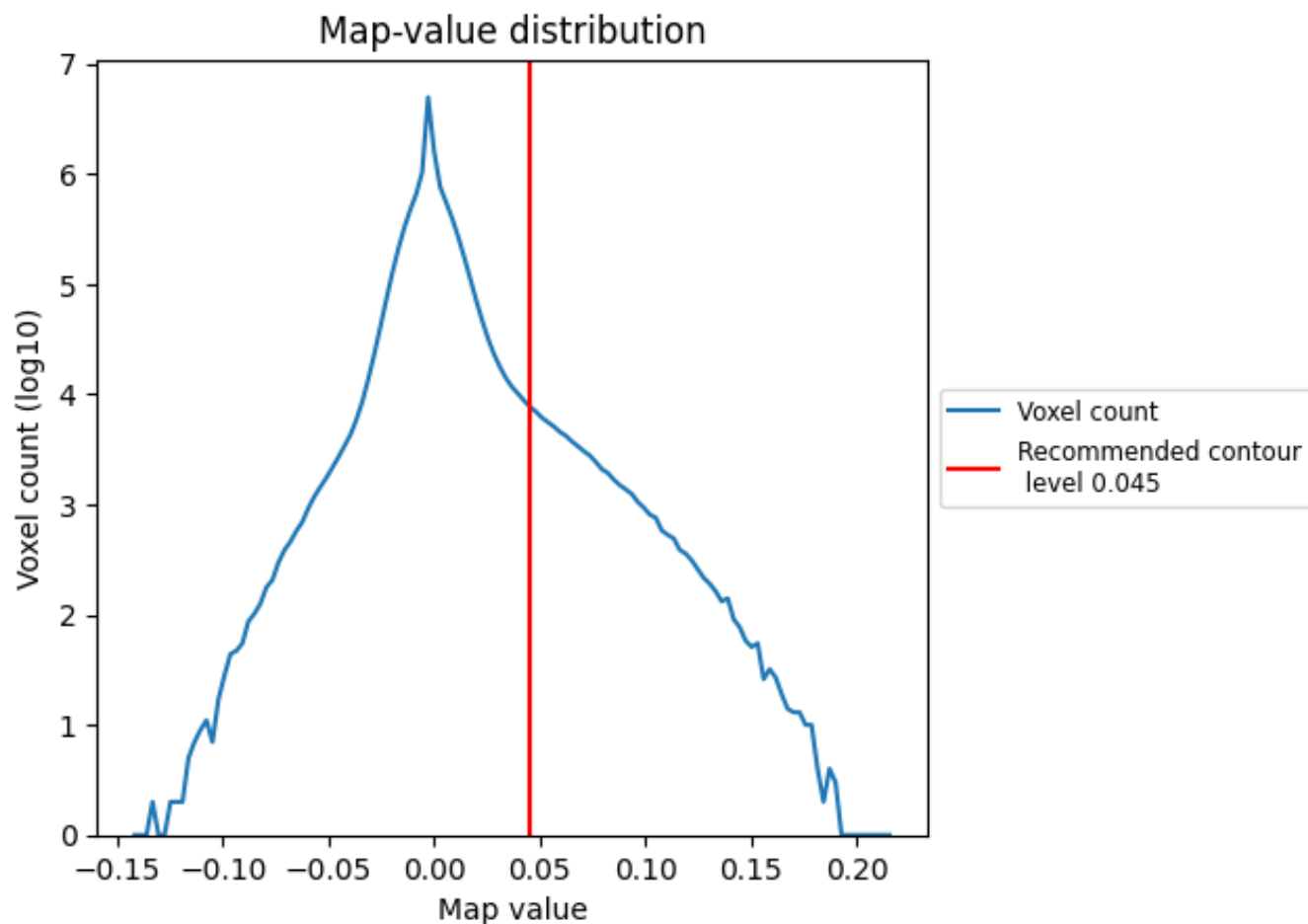
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

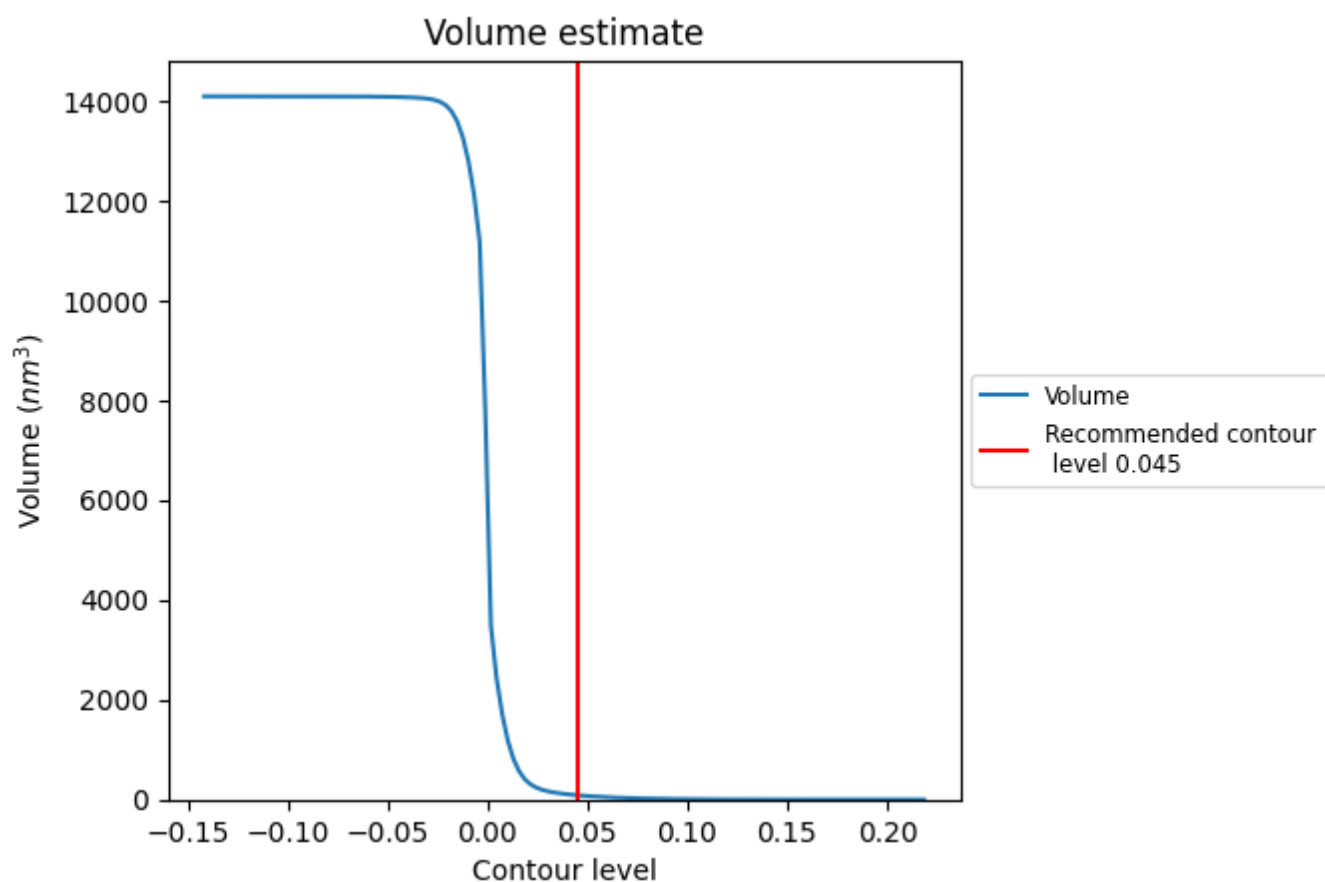
This section contains the results of statistical analysis of the map.

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.

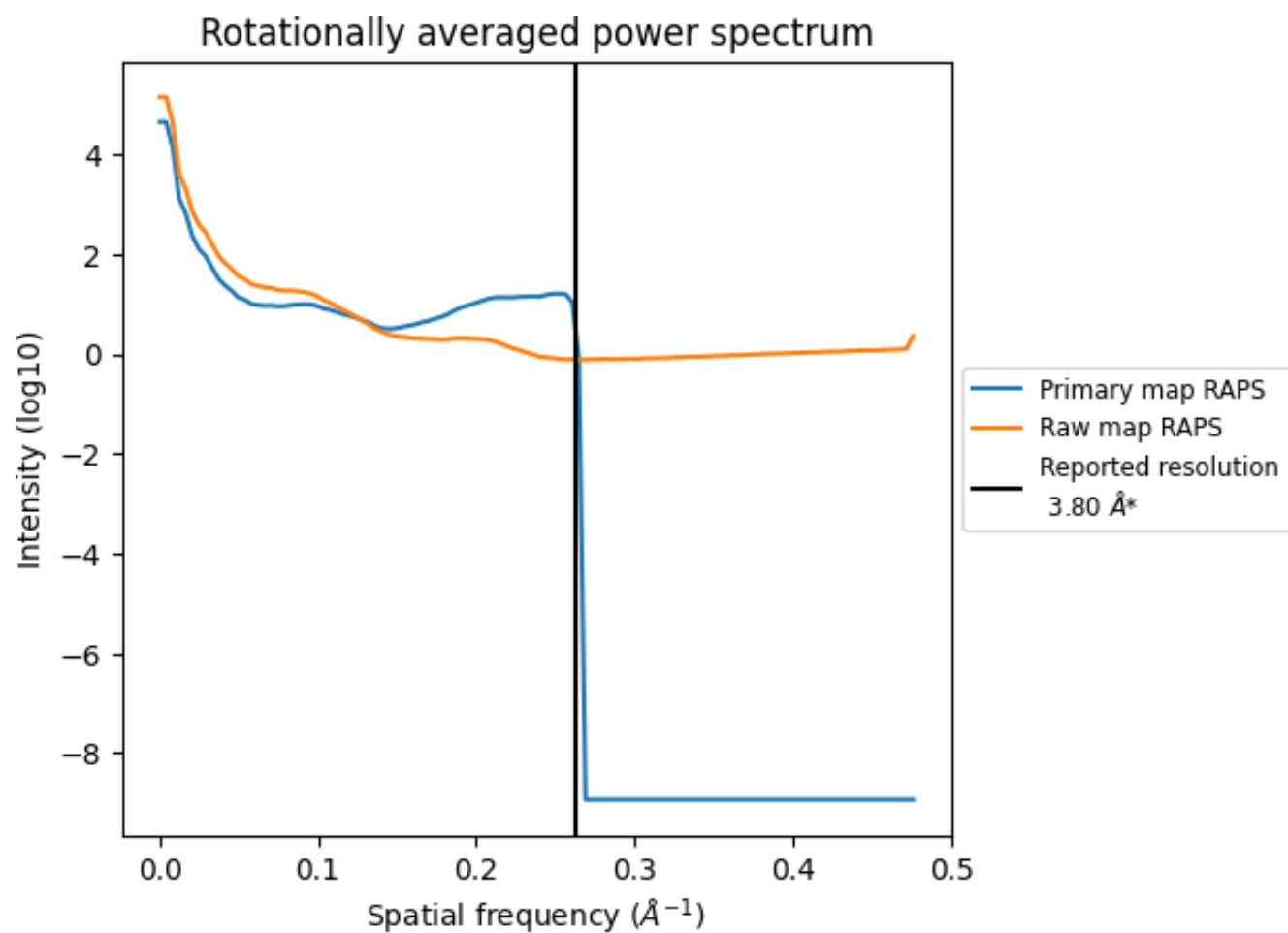
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 78 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 ⓘ

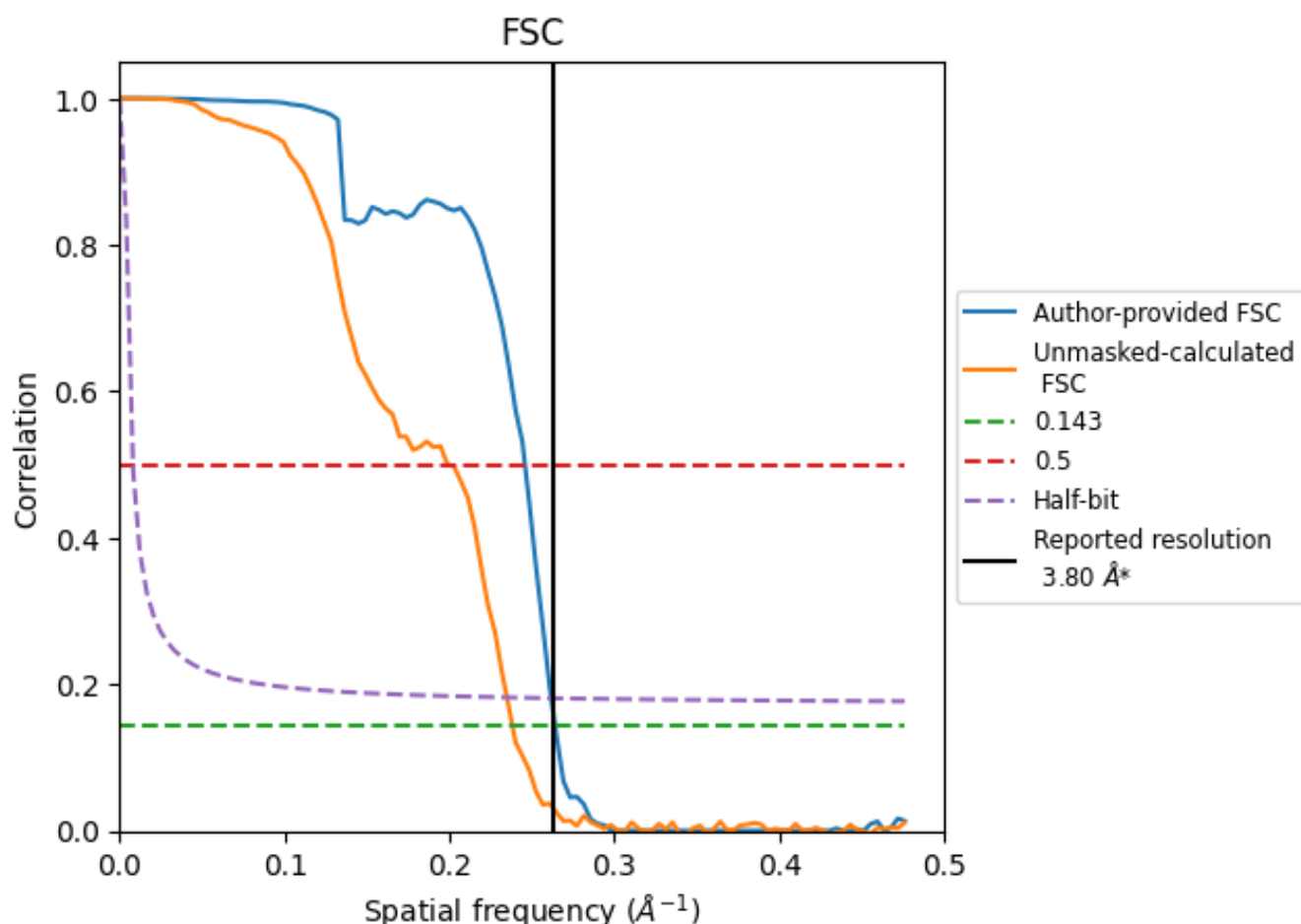


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

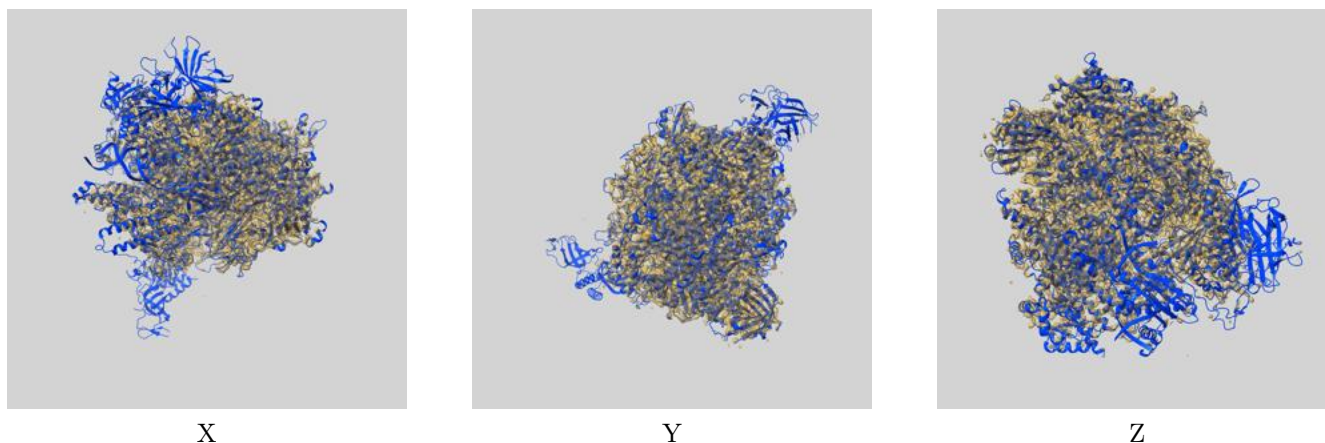
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.07	3.82
Unmasked-calculated*	4.20	5.01	4.26

*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 4.20 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

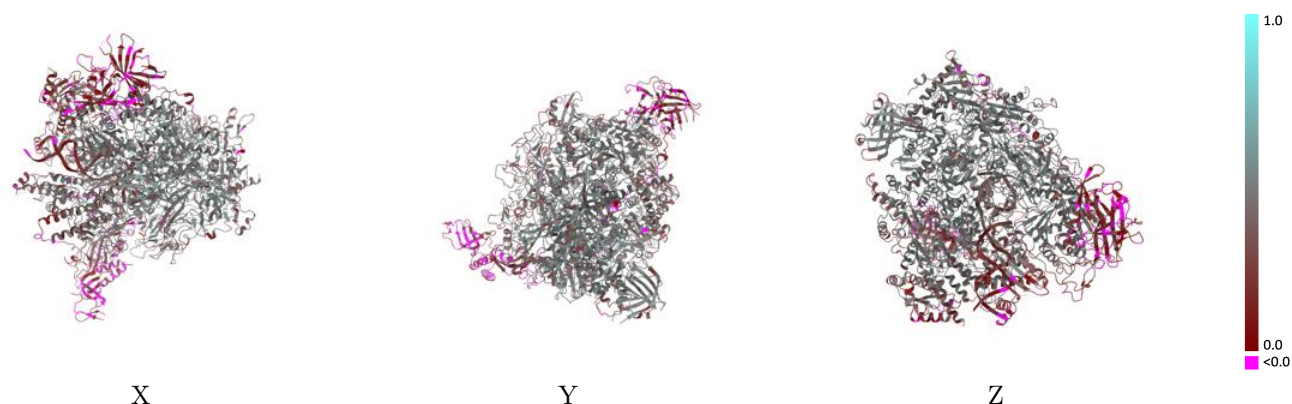
This section contains information regarding the fit between EMDB map EMD-4147 and PDB model 5M3F. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



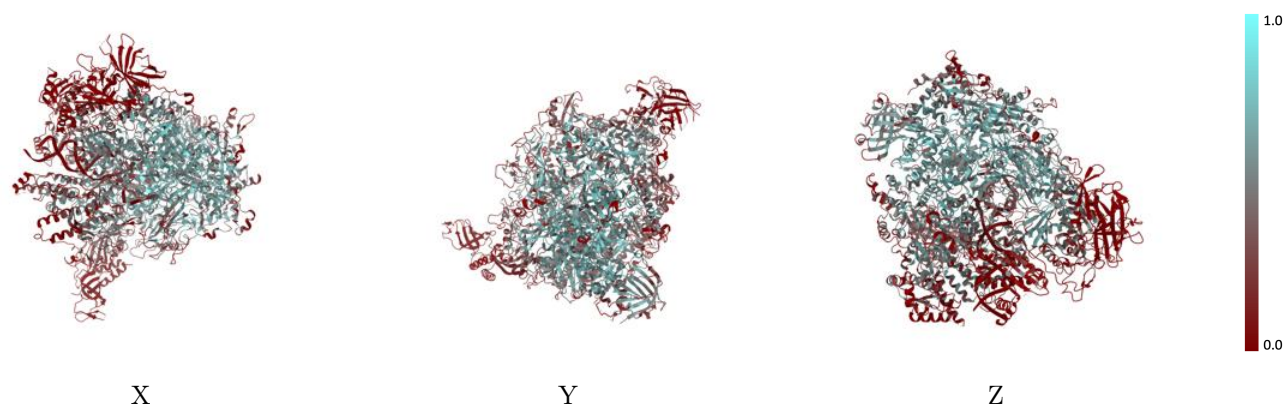
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



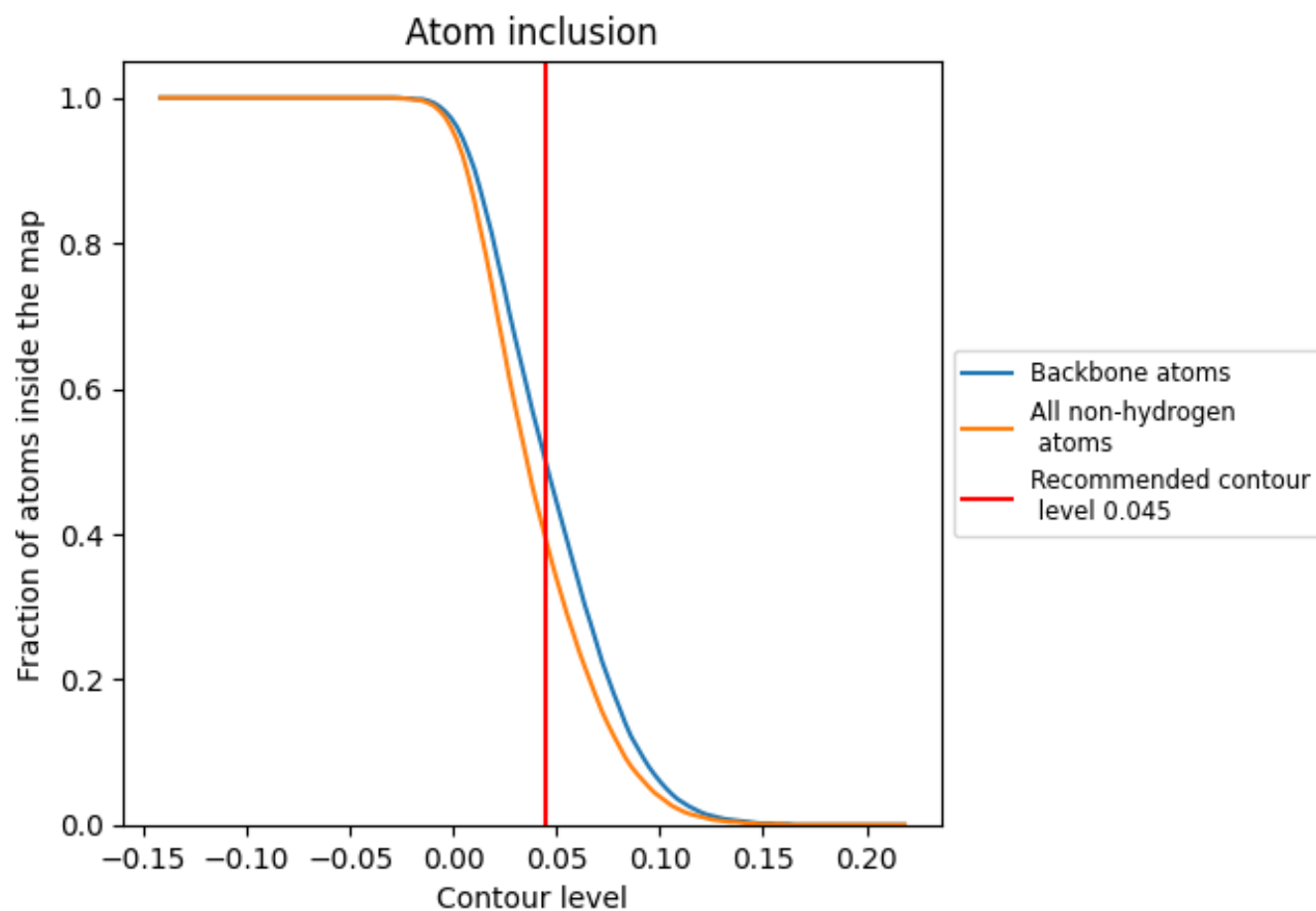
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 39% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3900	 0.3830
A	 0.4300	 0.4240
B	 0.5100	 0.4500
C	 0.4640	 0.4480
D	 0.0210	 0.0430
E	 0.2910	 0.3670
F	 0.4210	 0.4200
G	 0.0330	 0.0420
H	 0.4330	 0.4430
I	 0.0410	 0.2560
J	 0.6030	 0.4880
K	 0.4990	 0.4600
L	 0.4710	 0.4510
M	 0.0020	 0.0870
N	 0.0030	 0.0760
R	 0.2950	 0.3370
T	 0.1710	 0.2880
U	 0.0250	 0.1580

