



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 06:19 pm GMT

PDB ID : 5OA1
EMDB ID : EMD-3727
Title : RNA polymerase I pre-initiation complex
Authors : Sadian, Y.; Tafur, L.; Kosinski, J.; Jakobi, A.J.; Muller, C.W.
Deposited on : 2017-06-20
Resolution : 4.40 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

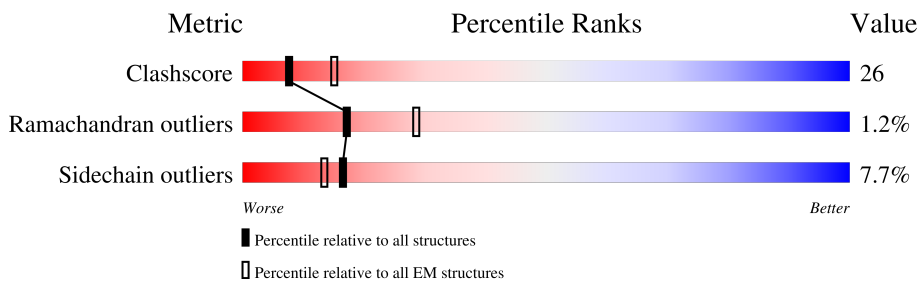
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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.



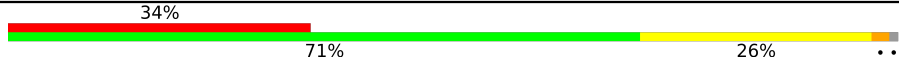






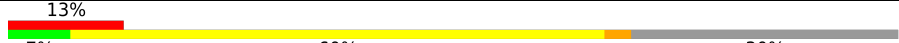
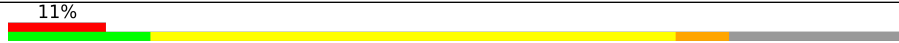

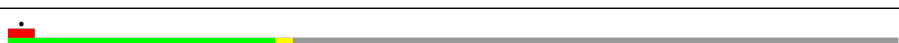


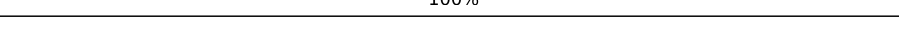
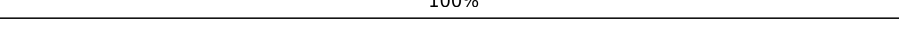
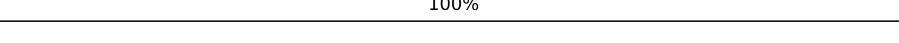
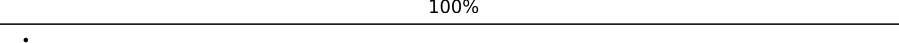
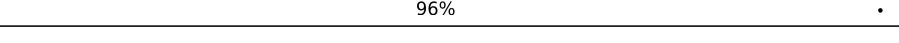
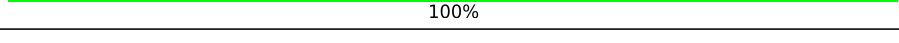
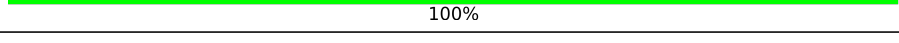
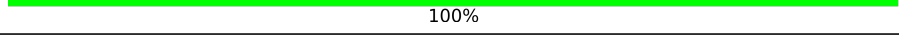
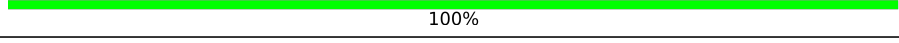
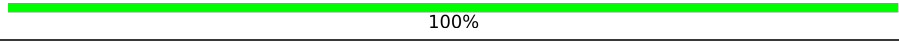
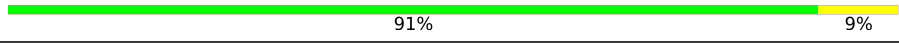

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	

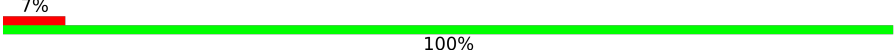
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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	S	70	
17	T	70	
18	U	514	
19	V	894	
20	W	507	
21	1	13	
22	2	19	
23	3	9	
23	9	9	
24	4	24	
25	5	16	
25	Q	16	
26	6	10	
26	8	10	
27	7	25	
28	P	22	
29	Z	15	
30	Y	12	

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Mol	Chain	Length	Quality of chain
31	R	27	 7% 100%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 43459 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
			Total	C	N	O	S		
1	A	1458	11513	7277	1997	2177	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1175	9327	5899	1635	1743	50	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	304	2418	1536	414	460	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	59	467	293	80	94	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	215	1759	1116	310	321	12	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	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	202	1600	1026	276	293	5	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	134	1072	676	181	211	4	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	124	942	584	160	189	9	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	69	569	362	101	100	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	103	810	506	132	167	5	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	359	221	71	63	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	105	831	528	137	166	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	139	Total	C	N	O	S	0	0
			1103	706	179	214	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

- Molecule 16 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	49	Total	C	N	O	P	0	0
			1028	486	210	283	49		

- Molecule 17 is a DNA chain called DNA (56-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	56	Total	C	N	O	P	0	0
			1128	543	183	346	56		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	291	Total	C	N	O	0	0
			1164	582	291	291		

- Molecule 19 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

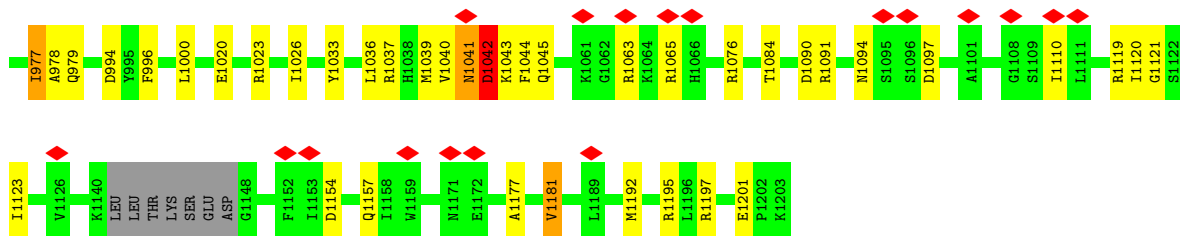
Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	288	Total	C	N	O	0	0
			1152	576	288	288		

- Molecule 20 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

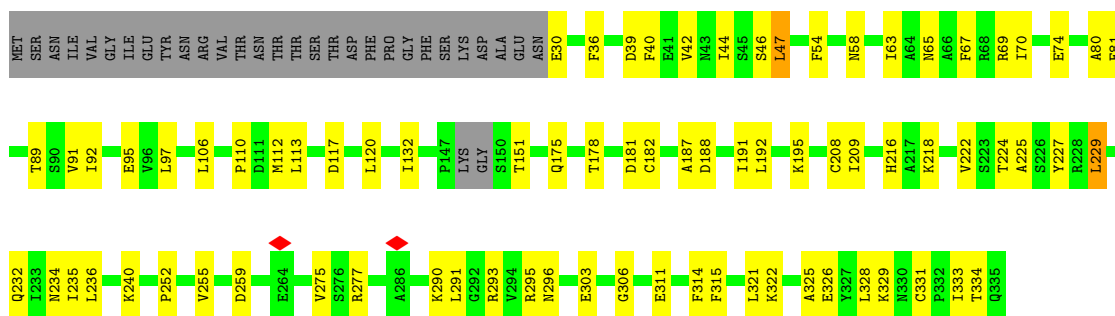
Mol	Chain	Residues	Atoms				AltConf	Trace
20	W	168	Total	C	N	O	0	0
			672	336	168	168		

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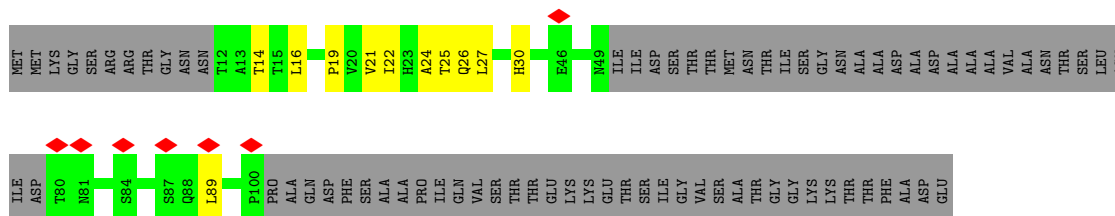
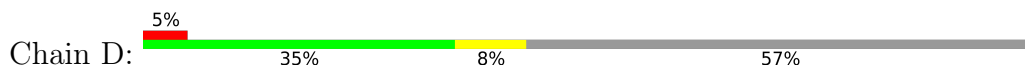
Mol	Chain	Residues	Atoms		AltConf
32	J	1	Total 1	Zn 1	0
32	L	1	Total 1	Zn 1	0



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



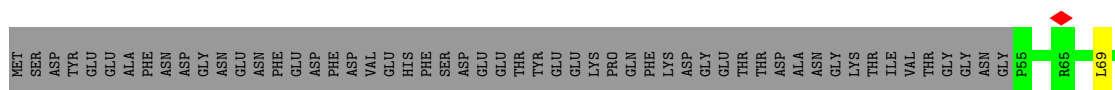
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

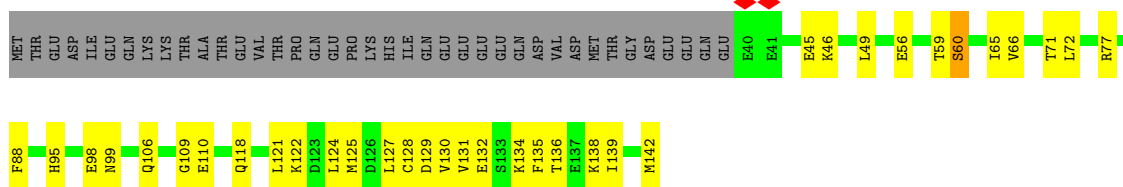


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

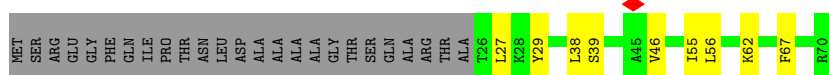


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

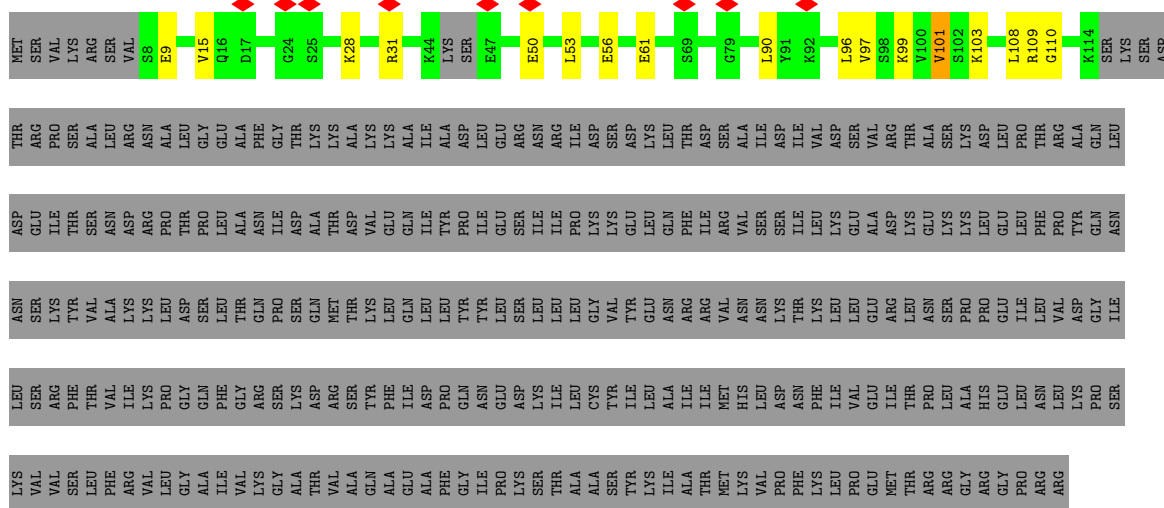




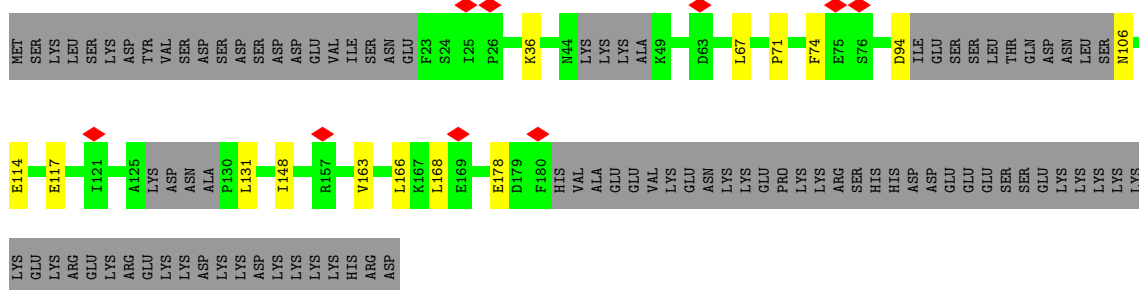
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



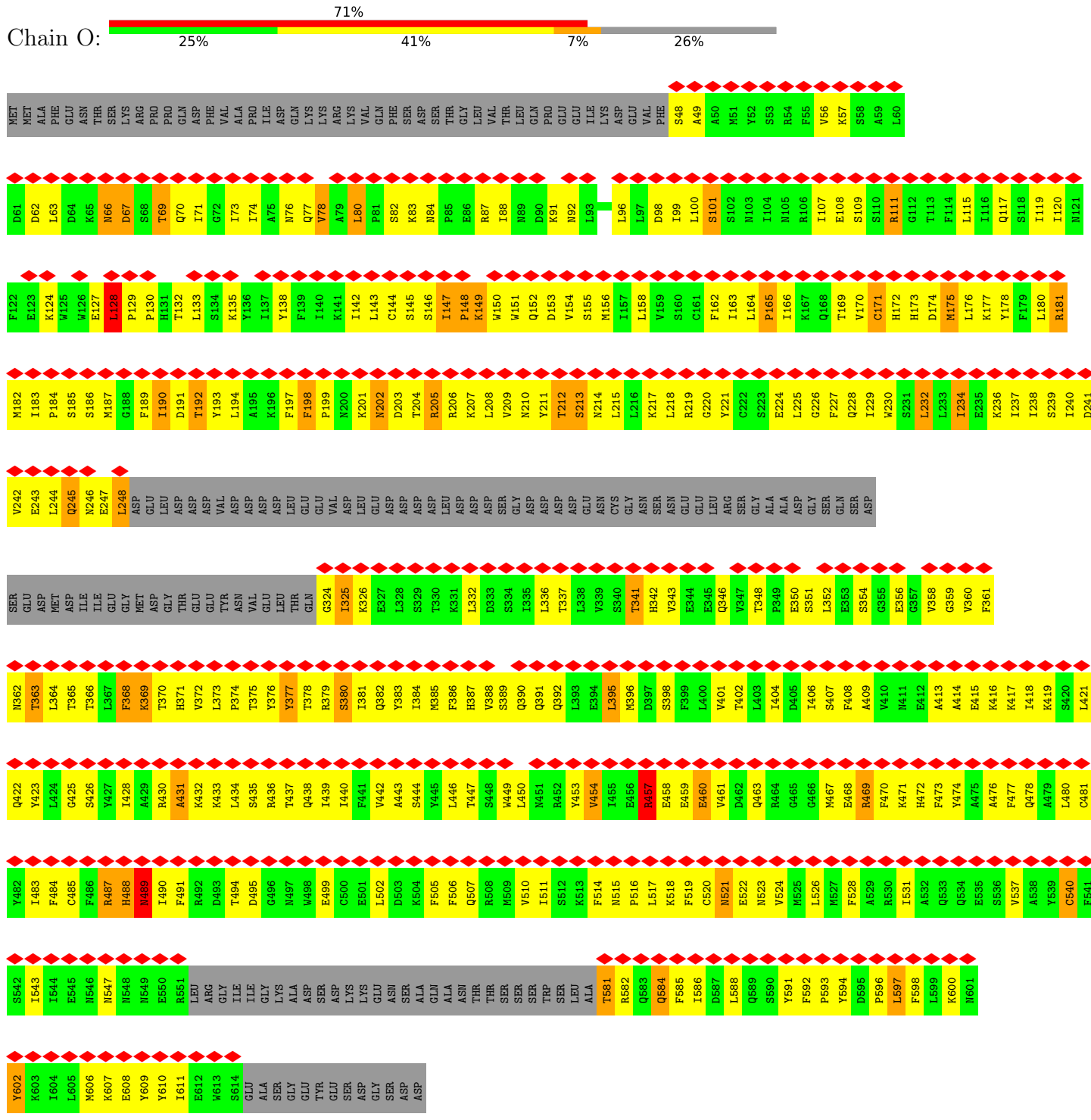
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



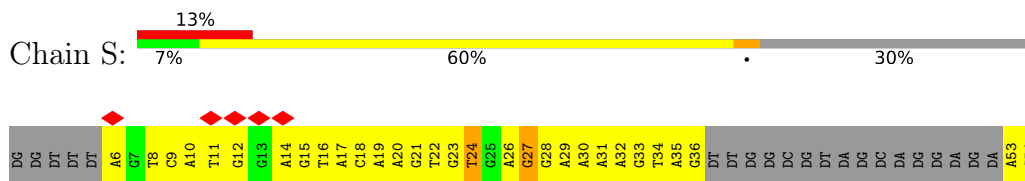
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

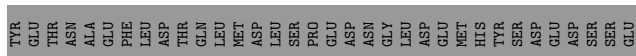
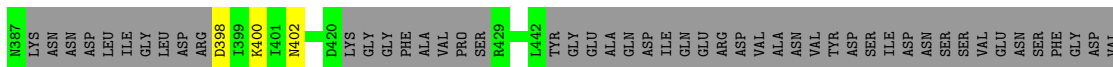


• Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3



• Molecule 16: DNA (49-MER)





- Molecule 21: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: ALA-ALA

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

Chain 9:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: ALA-ALA

Chain 4:  96%



- Molecule 25: ALA-ALA

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: ALA-ALA

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38589	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/11722	0.58	0/15832
2	B	0.38	0/9534	0.59	1/12889 (0.0%)
3	C	0.39	0/2469	0.61	0/3347
4	D	0.40	0/473	0.54	0/641
5	E	0.40	0/1795	0.55	0/2416
6	F	0.39	0/838	0.54	0/1129
7	G	0.39	0/1637	0.58	0/2226
8	H	0.39	0/1090	0.57	0/1476
9	I	0.40	0/955	0.56	0/1288
10	J	0.40	0/578	0.62	0/775
11	K	0.38	0/821	0.57	0/1108
12	L	0.38	0/361	0.61	0/478
13	M	0.38	0/846	0.53	0/1136
14	N	0.38	0/1124	0.52	0/1512
15	O	0.38	1/3897 (0.0%)	0.58	2/5268 (0.0%)
16	S	1.37	3/1160 (0.3%)	2.15	76/1790 (4.2%)
17	T	1.32	5/1256 (0.4%)	2.08	79/1930 (4.1%)
18	U	0.81	1/1155 (0.1%)	0.89	3/1428 (0.2%)
19	V	0.92	0/1136	0.91	0/1392
20	W	0.58	0/664	0.87	3/816 (0.4%)
21	1	0.53	0/51	0.92	0/62
22	2	0.54	0/75	0.97	0/92
23	3	0.15	0/35	0.27	0/42
23	9	0.55	0/35	0.95	0/42
24	4	0.39	0/91	0.69	0/112
25	5	0.54	0/63	0.97	0/77
25	Q	0.53	0/62	0.96	0/74
26	6	0.54	0/39	0.95	0/47
26	8	0.16	0/39	0.26	0/47
27	7	0.42	0/99	0.74	0/122
28	P	0.46	0/87	0.81	0/107
29	Z	0.49	0/59	0.95	0/72

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	Y	0.54	0/47	0.96	0/57
31	R	0.41	0/107	0.80	0/132
All	All	0.52	10/44400 (0.0%)	0.79	164/59962 (0.3%)

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
16	S	0	2
17	T	0	2
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	S	6	DA	O3'-P	10.54	1.73	1.61
17	T	43	DC	O3'-P	8.45	1.71	1.61
17	T	42	DT	O3'-P	8.06	1.70	1.61
15	O	198	PHE	C-N	-7.16	1.20	1.34
18	U	139	LYS	C-O	6.23	1.35	1.23

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	35	DA	N1-C6-N6	-11.19	111.89	118.60
17	T	63	DA	N1-C6-N6	-10.14	112.52	118.60
17	T	47	DA	O4'-C1'-N9	10.13	115.09	108.00
17	T	48	DC	N3-C2-O2	-9.96	114.93	121.90
17	T	63	DA	C5-C6-N1	9.24	122.32	117.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	S	24	DT	Sidechain
16	S	27	DG	Sidechain
17	T	38	DC	Sidechain
17	T	47	DA	Sidechain

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	11513	0	11582	500	0
2	B	9327	0	9191	643	0
3	C	2418	0	2401	60	0
4	D	467	0	468	4	0
5	E	1759	0	1788	7	0
6	F	823	0	841	7	0
7	G	1600	0	1594	115	0
8	H	1072	0	1042	26	0
9	I	942	0	935	50	0
10	J	569	0	585	14	0
11	K	810	0	801	49	0
12	L	359	0	381	36	0
13	M	831	0	820	11	0
14	N	1103	0	1106	5	0
15	O	3811	0	3792	805	0
16	S	1028	0	548	49	0
17	T	1128	0	637	57	0
18	U	1164	0	289	29	0
19	V	1152	0	292	5	0
20	W	672	0	166	9	0
21	1	52	0	12	0	0
22	2	76	0	18	0	0
23	3	36	0	8	0	0
23	9	36	0	8	0	0
24	4	92	0	22	0	0
25	5	64	0	15	0	0
25	Q	64	0	14	0	0
26	6	40	0	9	0	0
26	8	40	0	9	0	0
27	7	100	0	24	0	0
28	P	88	0	21	4	0
29	Z	60	0	14	4	0
30	Y	48	0	11	0	0
31	R	108	0	26	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	J	1	0	0	0	0
32	L	1	0	0	0	0
All	All	43459	0	39470	2074	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 26.

The worst 5 of 2074 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)
1:A:1261:VAL:CG2	1:A:1306:TYR:HB3	1.20	1.66
15:O:162:PHE:CB	15:O:214:ASN:CB	1.76	1.62
2:B:74:PHE:CE2	2:B:94:LYS:CG	1.77	1.62
2:B:74:PHE:CE2	2:B:94:LYS:HG2	1.27	1.61
1:A:1261:VAL:HG21	1:A:1306:TYR:CB	1.21	1.59

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	1438/1664 (86%)	1365 (95%)	67 (5%)	6 (0%)	34	72
2	B	1169/1203 (97%)	1093 (94%)	71 (6%)	5 (0%)	34	72
3	C	300/335 (90%)	285 (95%)	15 (5%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	196/326 (60%)	184 (94%)	11 (6%)	1 (0%)	29	68
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	122/125 (98%)	109 (89%)	11 (9%)	2 (2%)	9	45
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	123 (94%)	8 (6%)	0	100	100
15	O	457/627 (73%)	400 (88%)	38 (8%)	19 (4%)	3	25
18	U	273/514 (53%)	245 (90%)	14 (5%)	14 (5%)	2	22
19	V	256/894 (29%)	235 (92%)	11 (4%)	10 (4%)	3	26
20	W	152/507 (30%)	141 (93%)	4 (3%)	7 (5%)	2	24
21	1	11/13 (85%)	11 (100%)	0	0	100	100
22	2	17/19 (90%)	17 (100%)	0	0	100	100
23	3	7/9 (78%)	7 (100%)	0	0	100	100
23	9	7/9 (78%)	7 (100%)	0	0	100	100
24	4	21/24 (88%)	21 (100%)	0	0	100	100
25	5	14/16 (88%)	14 (100%)	0	0	100	100
25	Q	12/16 (75%)	12 (100%)	0	0	100	100
26	6	8/10 (80%)	8 (100%)	0	0	100	100
26	8	8/10 (80%)	8 (100%)	0	0	100	100
27	7	23/25 (92%)	23 (100%)	0	0	100	100
28	P	20/22 (91%)	20 (100%)	0	0	100	100
29	Z	13/15 (87%)	13 (100%)	0	0	100	100
30	Y	10/12 (83%)	10 (100%)	0	0	100	100
31	R	25/27 (93%)	25 (100%)	0	0	100	100
All	All	5498/8005 (69%)	5135 (93%)	298 (5%)	65 (1%)	17	50

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1441	LYS
1	A	1500	GLN
2	B	90	TYR
2	B	1042	ASP
15	O	165	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	1287/1465 (88%)	1210 (94%)	77 (6%)	19	46
2	B	1024/1053 (97%)	932 (91%)	92 (9%)	9	32
3	C	269/296 (91%)	244 (91%)	25 (9%)	9	30
4	D	56/116 (48%)	50 (89%)	6 (11%)	6	26
5	E	197/197 (100%)	192 (98%)	5 (2%)	47	68
6	F	90/137 (66%)	86 (96%)	4 (4%)	28	54
7	G	180/291 (62%)	167 (93%)	13 (7%)	14	41
8	H	116/128 (91%)	111 (96%)	5 (4%)	29	55
9	I	109/110 (99%)	98 (90%)	11 (10%)	7	28
10	J	64/65 (98%)	57 (89%)	7 (11%)	6	26
11	K	93/130 (72%)	84 (90%)	9 (10%)	8	29
12	L	40/57 (70%)	37 (92%)	3 (8%)	13	40
13	M	94/371 (25%)	89 (95%)	5 (5%)	22	50
14	N	128/220 (58%)	118 (92%)	10 (8%)	12	38
15	O	427/576 (74%)	378 (88%)	49 (12%)	5	24
All	All	4174/5212 (80%)	3853 (92%)	321 (8%)	16	39

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	50	THR
15	O	190	ILE
10	J	2	ILE
13	M	103	LYS
15	O	341	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	140	GLN
15	O	172	HIS
8	H	35	GLN
11	K	106	GLN
15	O	362	ASN

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 7 ligands modelled in this entry, 7 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	103:ALA	C	105:ALA	N	5.80

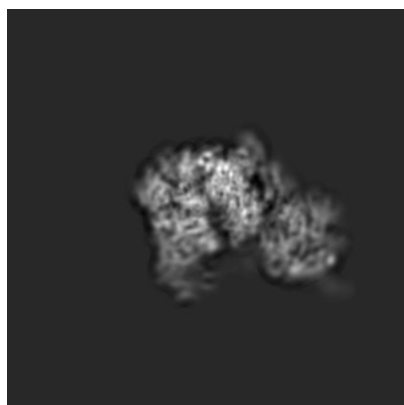
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3727. These allow visual inspection of the internal detail of the map and identification of artifacts.

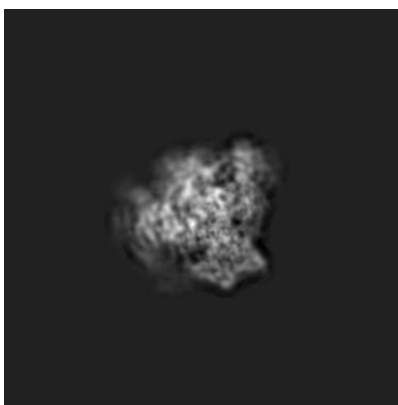
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

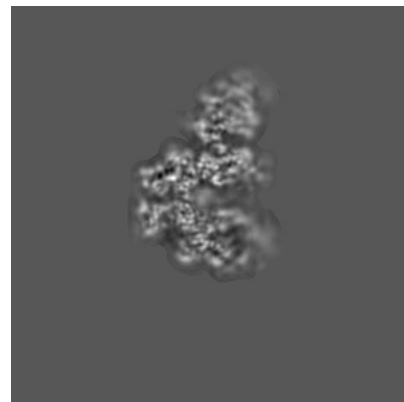
6.2.1 Primary map



X Index: 144



Y Index: 144

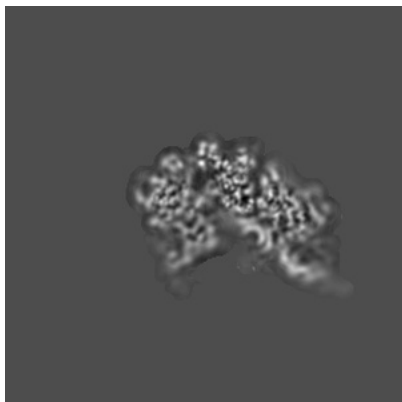


Z Index: 144

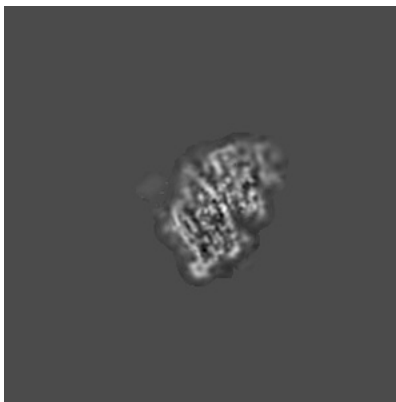
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

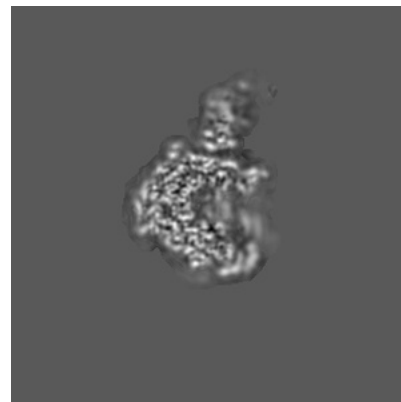
6.3.1 Primary map



X Index: 150



Y Index: 168

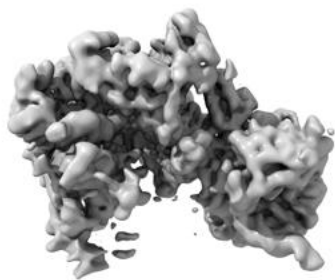


Z Index: 152

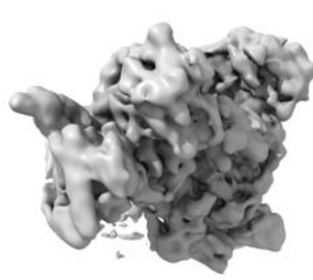
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

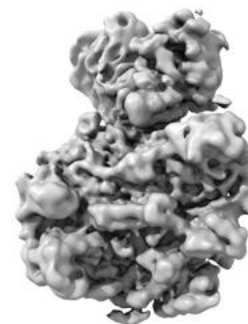
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

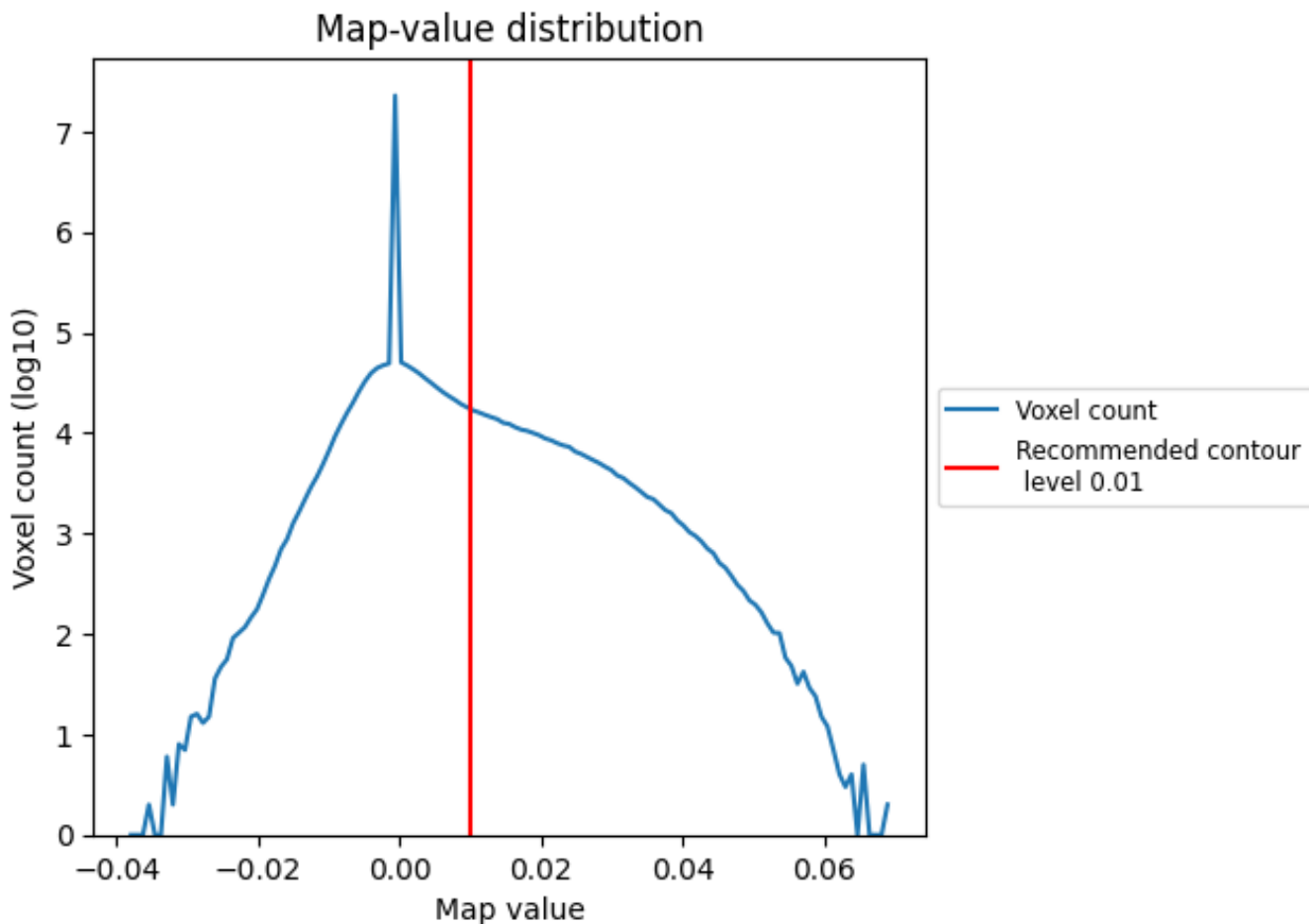
6.5 Mask visualisation

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

7 Map analysis [i](#)

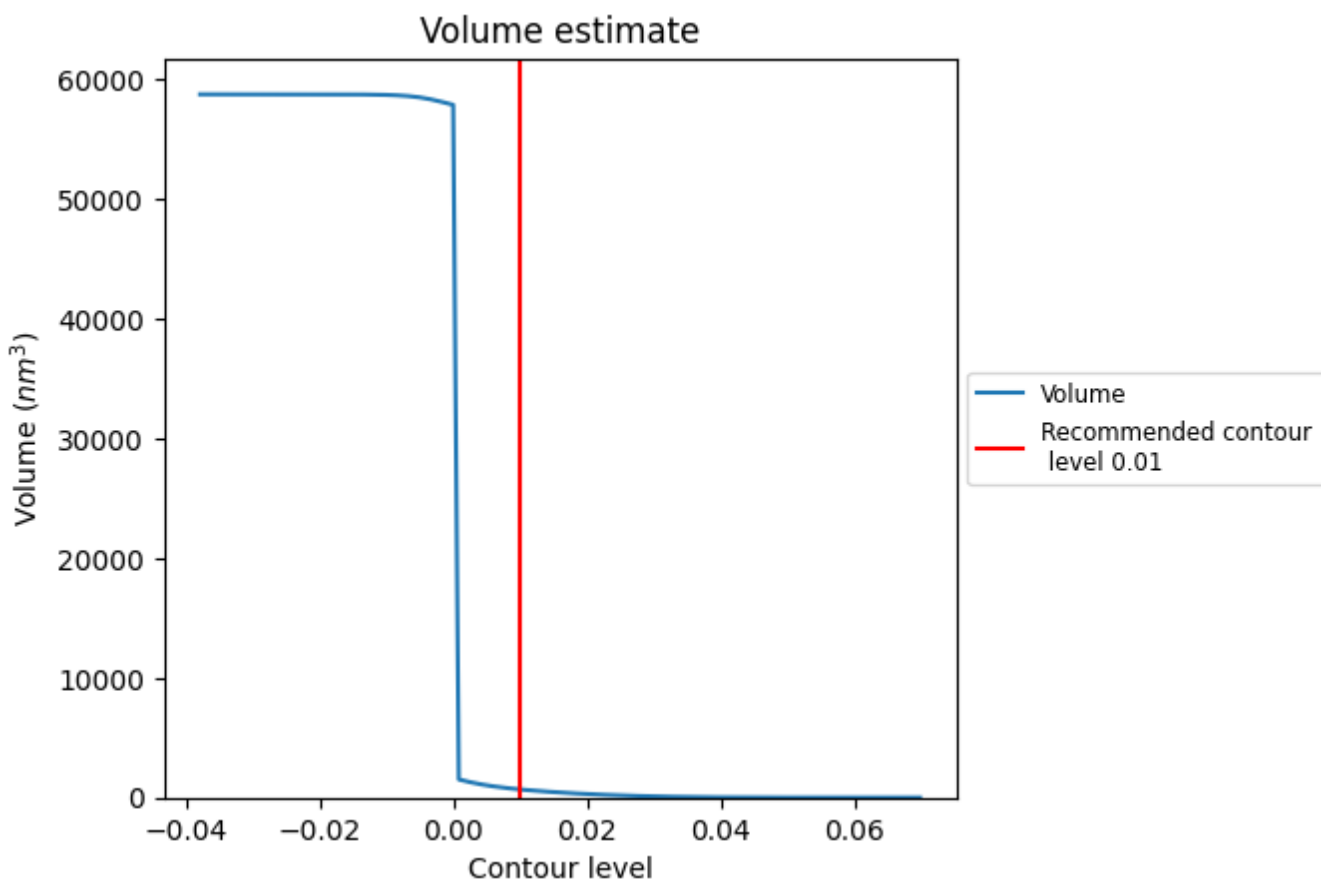
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

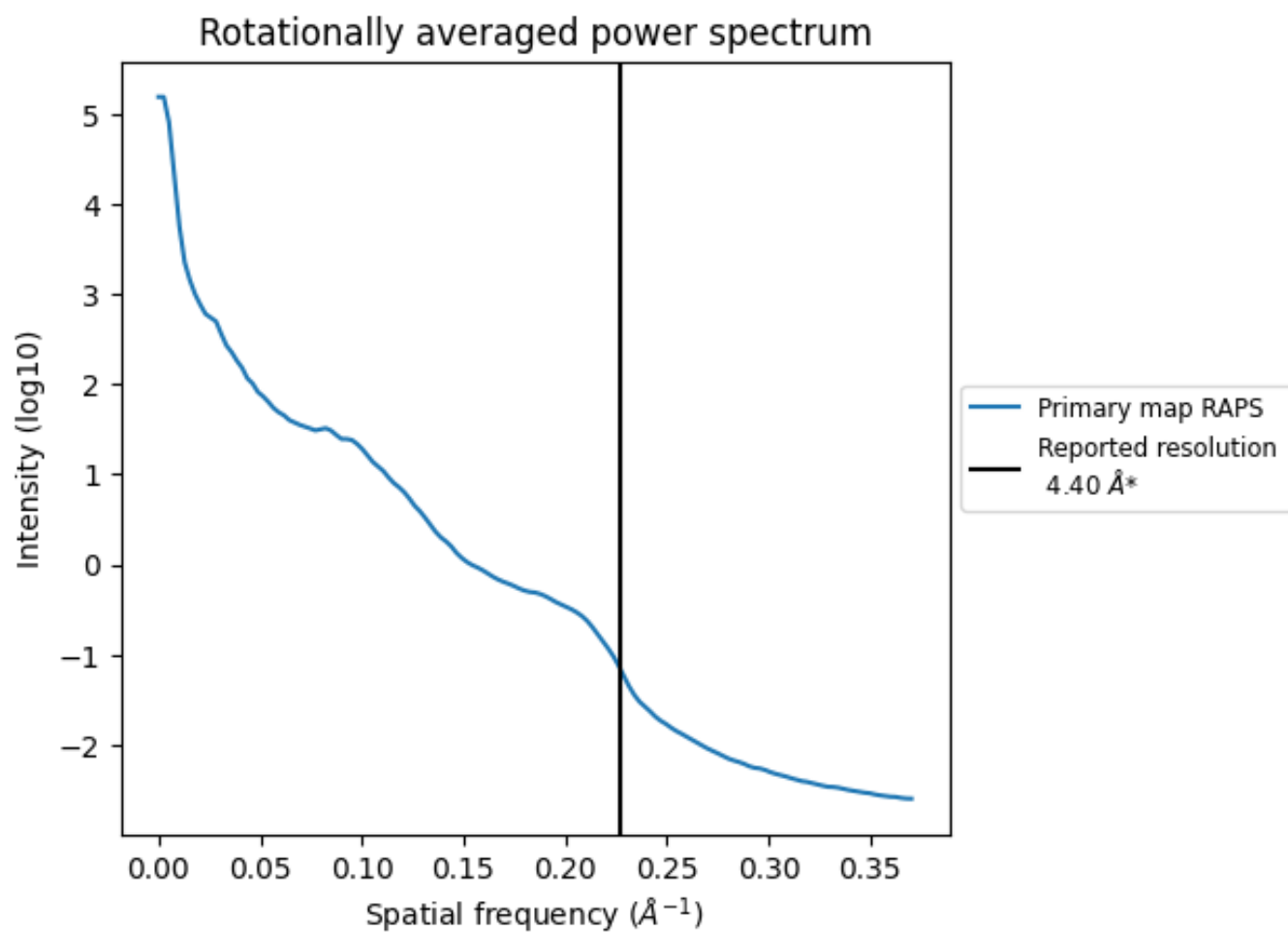
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 676 nm³; this corresponds to an approximate mass of 611 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 0.227 Å⁻¹

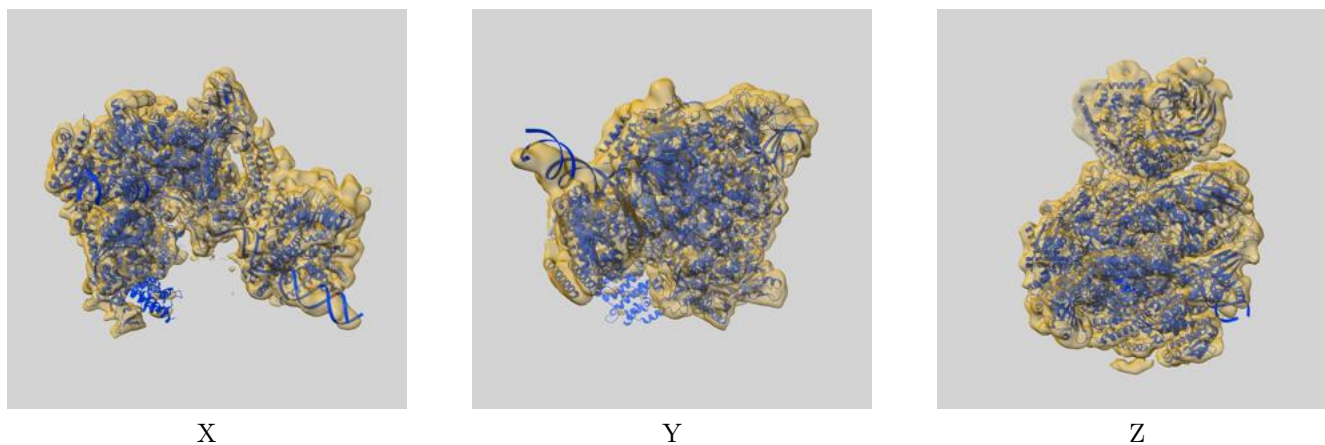
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

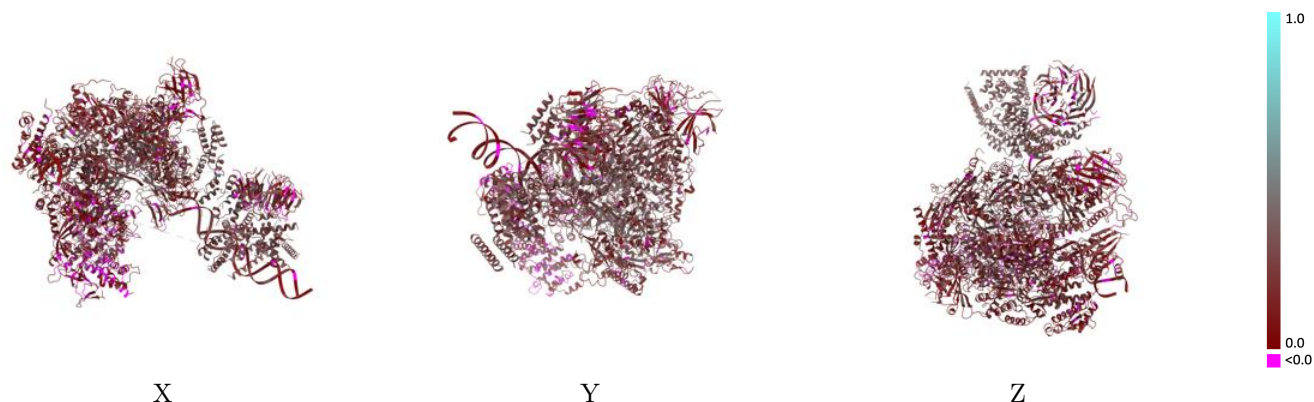
This section contains information regarding the fit between EMDB map EMD-3727 and PDB model 5OA1. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



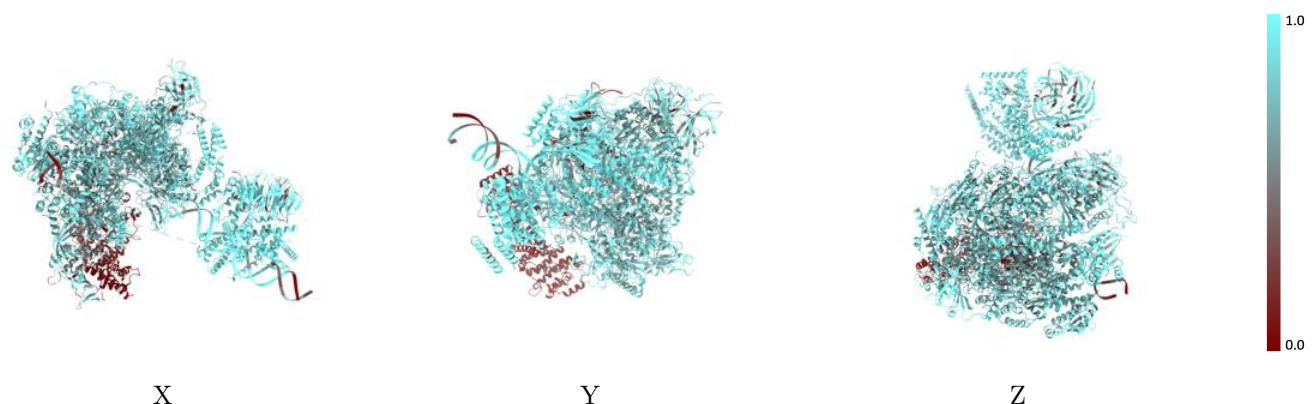
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



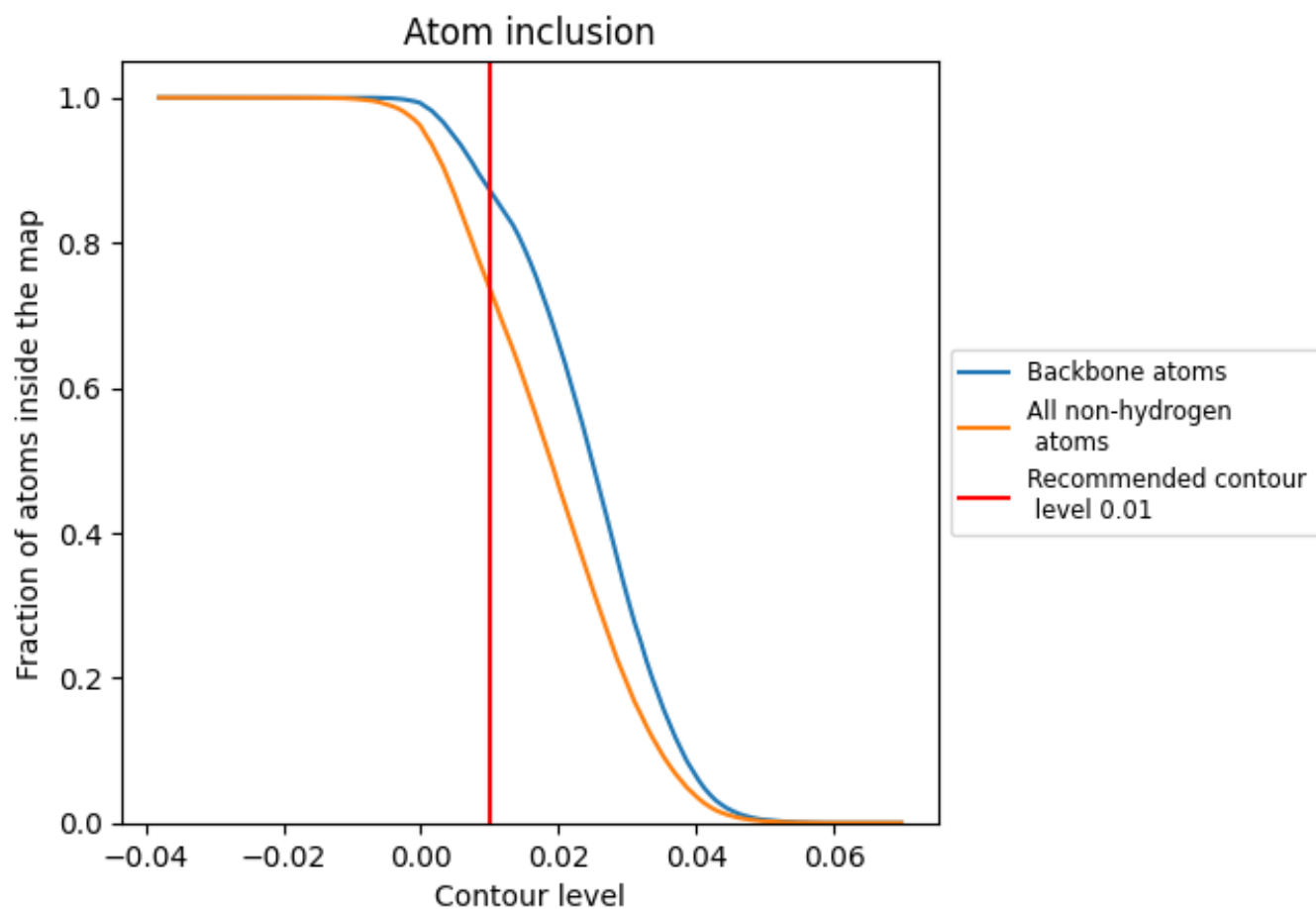
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7371	 0.1890
1	 1.0000	 0.3030
2	 1.0000	 0.2910
3	 1.0000	 0.2960
4	 0.9565	 0.3080
5	 1.0000	 0.3090
6	 1.0000	 0.3370
7	 1.0000	 0.3200
8	 1.0000	 0.2560
9	 1.0000	 0.3100
A	 0.8020	 0.1940
B	 0.7980	 0.2350
C	 0.8543	 0.2140
D	 0.7149	 0.1440
E	 0.8182	 0.1730
F	 0.8002	 0.1840
G	 0.6946	 0.0930
H	 0.8975	 0.2140
I	 0.5557	 0.1360
J	 0.8333	 0.2440
K	 0.8340	 0.1920
L	 0.7810	 0.2000
M	 0.7463	 0.1400
N	 0.7516	 0.1660
O	 0.0444	 0.0600
P	 0.9432	 0.2990
Q	 0.9688	 0.2640
R	 0.8981	 0.2740
S	 0.7529	 0.1600
T	 0.7509	 0.1720
U	 0.9132	 0.2880
V	 0.8498	 0.1500
W	 0.9777	 0.3230
Y	 1.0000	 0.3080
Z	 1.0000	 0.3170

