wwPDB EM Validation Summary Report (i)

Nov 5, 2022 – 04:43 PM EDT

PDB ID	:	5W5Y
EMDB ID	:	EMD-8771
Title	:	RNA polymerase I Initial Transcribing Complex
Authors	:	Han, Y.; He, Y.
Deposited on	:	2017-06-16
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

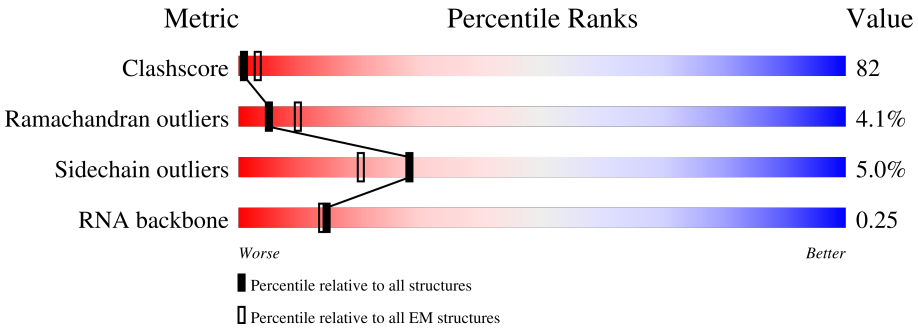
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1664	46% 40% 12%
2	B	1203	45% 50%
3	C	335	44% 45% 9%
4	D	137	21% 22% 57%
5	E	215	45% 54%
6	F	155	32% 21% 46%
7	G	326	6% 16% 44% 38%

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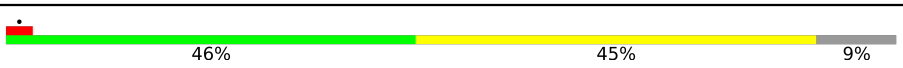
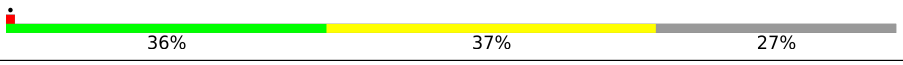
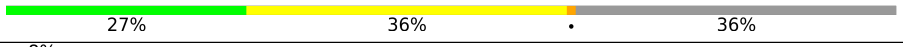
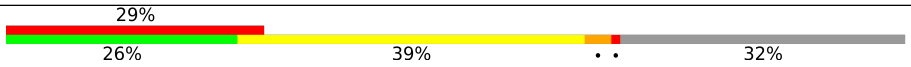
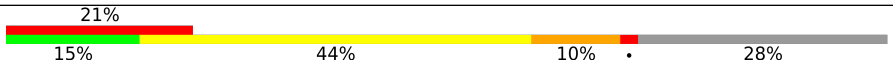
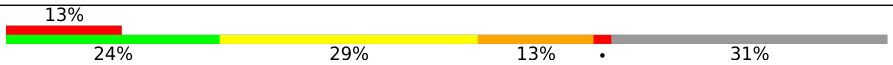
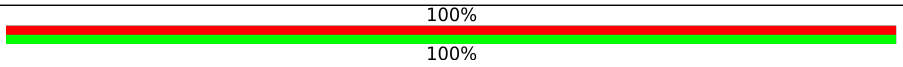
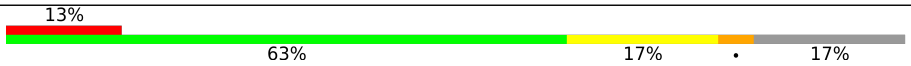
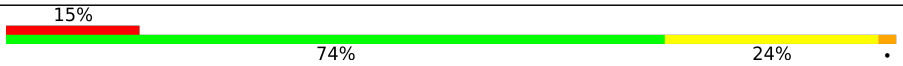
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	894	
16	P	514	
17	Q	507	
18	R	6	
19	S	54	
20	T	54	

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
21	ZN	A	1701	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 46572 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	1461	11542	7292	2004	2184	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	1178	9351	5911	1639	1750	51	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	306	2432	1544	417	463	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	1760	1116	310	322	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	83	670	428	114	125	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	201	Total	C	N	O	S	0	0
			1592	1022	275	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1071	676	181	210	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			479	300	79	96	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	103	Total	C	N	O	S	0	0
			811	506	132	168	5		

- 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
			359	221	71	63	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	106	Total	C	N	O	0	0
			841	534	139	168		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	158	Total	C	N	O	S	0	0
			1254	799	205	246	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	640	Total	C	N	O	S	0	0
			5063	3218	872	964	9		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	4	UNK	GLU	SEE REMARK 999	UNP P32786
O	5	UNK	ASP	SEE REMARK 999	UNP P32786
O	6	UNK	ALA	SEE REMARK 999	UNP P32786
O	7	UNK	LEU	SEE REMARK 999	UNP P32786
O	8	UNK	ASP	SEE REMARK 999	UNP P32786
O	9	UNK	LEU	SEE REMARK 999	UNP P32786
O	10	UNK	HIS	SEE REMARK 999	UNP P32786
O	11	UNK	ILE	SEE REMARK 999	UNP P32786
O	12	UNK	VAL	SEE REMARK 999	UNP P32786
O	13	UNK	VAL	SEE REMARK 999	UNP P32786
O	14	UNK	LYS	SEE REMARK 999	UNP P32786
O	15	UNK	SER	SEE REMARK 999	UNP P32786
O	16	UNK	LEU	SEE REMARK 999	UNP P32786
O	17	UNK	LEU	SEE REMARK 999	UNP P32786
O	18	UNK	CYS	SEE REMARK 999	UNP P32786
O	19	UNK	ASP	SEE REMARK 999	UNP P32786
O	20	UNK	THR	SEE REMARK 999	UNP P32786
O	21	UNK	ALA	SEE REMARK 999	UNP P32786
O	22	UNK	ILE	SEE REMARK 999	UNP P32786
O	23	UNK	ARG	SEE REMARK 999	UNP P32786
O	24	UNK	TYR	SEE REMARK 999	UNP P32786
O	25	UNK	ILE	SEE REMARK 999	UNP P32786
O	26	UNK	SER	SEE REMARK 999	UNP P32786
O	27	UNK	ASP	SEE REMARK 999	UNP P32786
O	28	UNK	ASP	SEE REMARK 999	UNP P32786
O	41	UNK	TYR	SEE REMARK 999	UNP P32786
O	42	UNK	ILE	SEE REMARK 999	UNP P32786
O	43	UNK	PRO	SEE REMARK 999	UNP P32786
O	44	UNK	SER	SEE REMARK 999	UNP P32786
O	45	UNK	ASP	SEE REMARK 999	UNP P32786

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Chain	Residue	Modelled	Actual	Comment	Reference
O	46	UNK	LEU	SEE REMARK 999	UNP P32786
O	47	UNK	LEU	SEE REMARK 999	UNP P32786
O	48	UNK	ARG	SEE REMARK 999	UNP P32786
O	49	UNK	ASN	SEE REMARK 999	UNP P32786
O	50	UNK	LEU	SEE REMARK 999	UNP P32786
O	51	UNK	ASP	SEE REMARK 999	UNP P32786
O	52	UNK	ASP	SEE REMARK 999	UNP P32786
O	53	UNK	THR	SEE REMARK 999	UNP P32786
O	54	UNK	LEU	SEE REMARK 999	UNP P32786
O	55	UNK	GLN	SEE REMARK 999	UNP P32786
O	56	UNK	GLU	SEE REMARK 999	UNP P32786
O	57	UNK	SER	SEE REMARK 999	UNP P32786
O	58	UNK	THR	SEE REMARK 999	UNP P32786
O	59	UNK	ASN	SEE REMARK 999	UNP P32786
O	60	UNK	SER	SEE REMARK 999	UNP P32786
O	61	UNK	SER	SEE REMARK 999	UNP P32786
O	62	UNK	ARG	SEE REMARK 999	UNP P32786
O	63	UNK	PRO	SEE REMARK 999	UNP P32786
O	64	UNK	MET	SEE REMARK 999	UNP P32786
O	65	UNK	GLN	SEE REMARK 999	UNP P32786
O	66	UNK	ASP	SEE REMARK 999	UNP P32786
O	67	UNK	ALA	SEE REMARK 999	UNP P32786

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	387	Total	C	N	O	S	0	0
			3238	2105	540	576	17		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	349	Total	C	N	O	S	0	0
			2923	1881	513	518	11		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	6	Total	C	N	O	P	0	0
			127	58	25	39	5		

- Molecule 19 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	45	Total	C	N	O	P	0	0
			935	447	174	270	44		

- Molecule 20 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	54	Total	C	N	O	P	0	0
			1082	522	177	330	53		

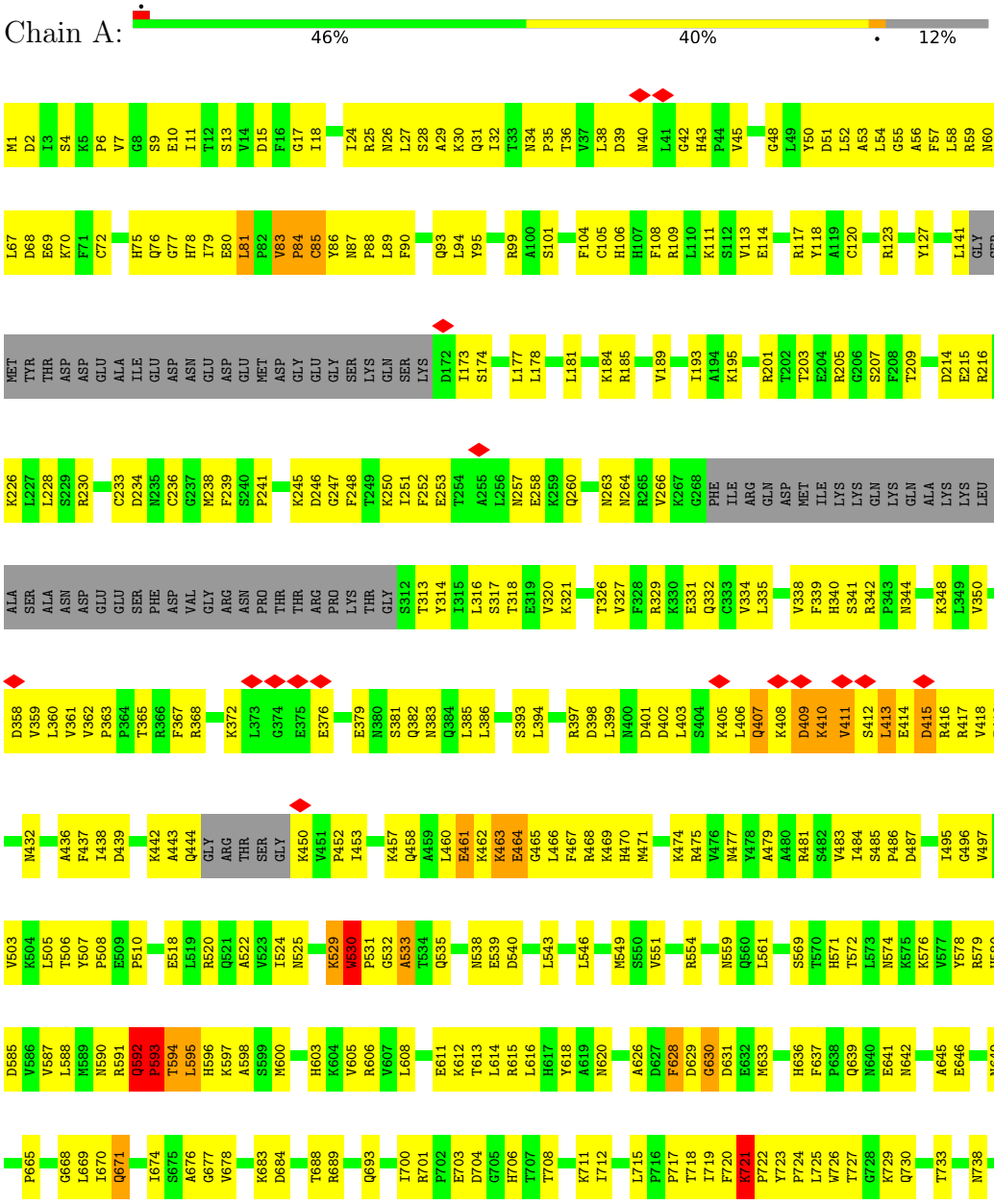
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

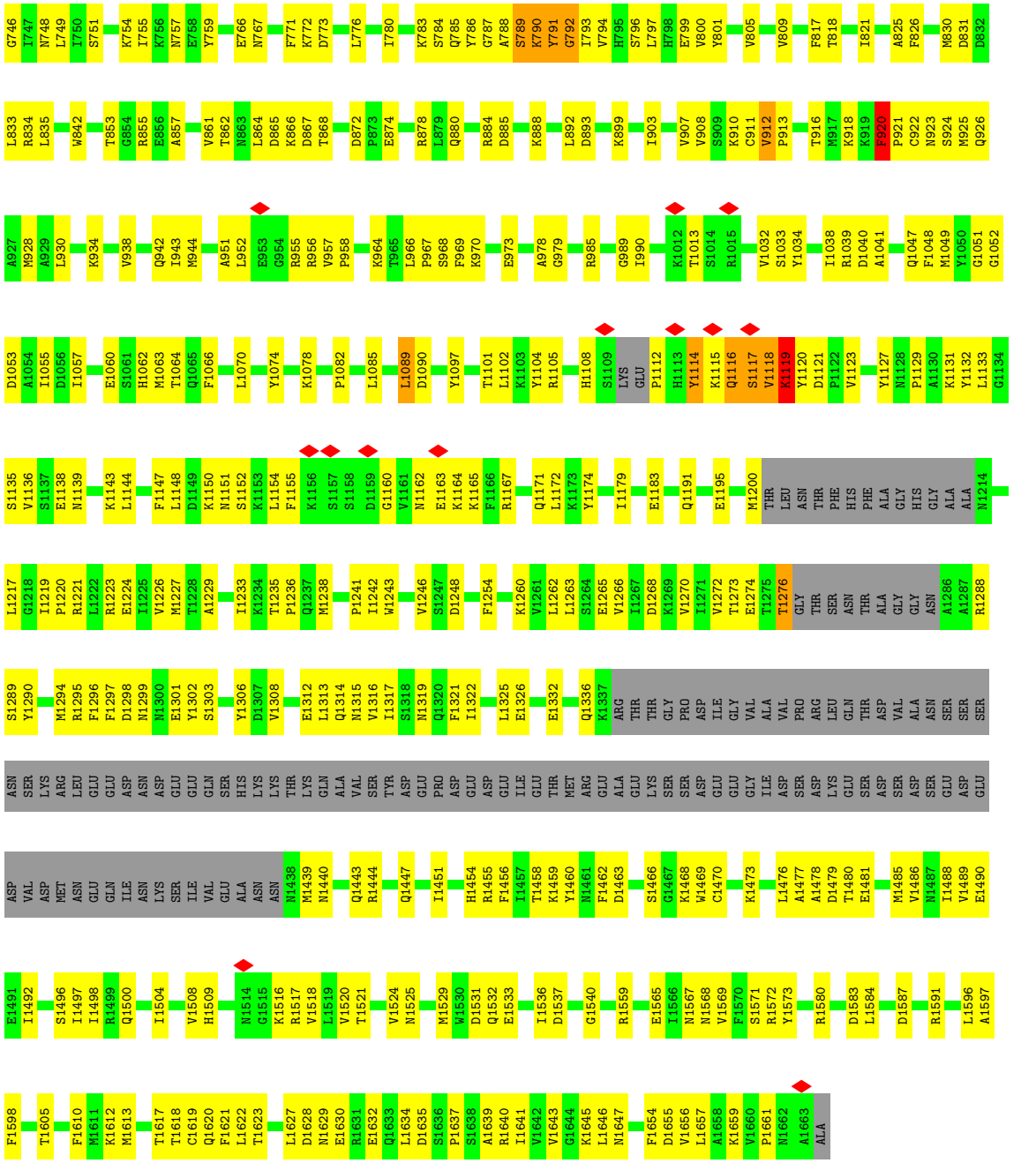
Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total	Zn	0
			2	2	
21	B	1	Total	Zn	0
			1	1	
21	I	1	Total	Zn	0
			1	1	
21	J	1	Total	Zn	0
			1	1	
21	L	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

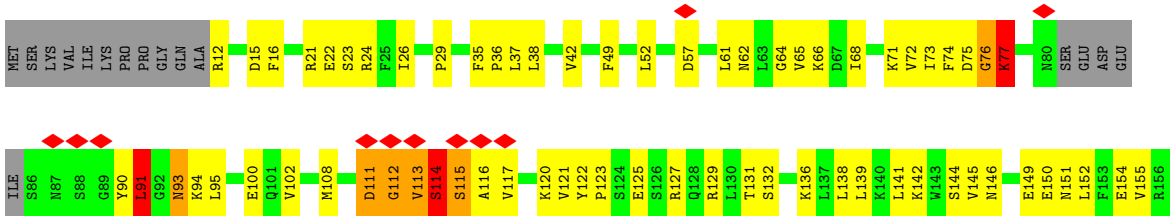
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

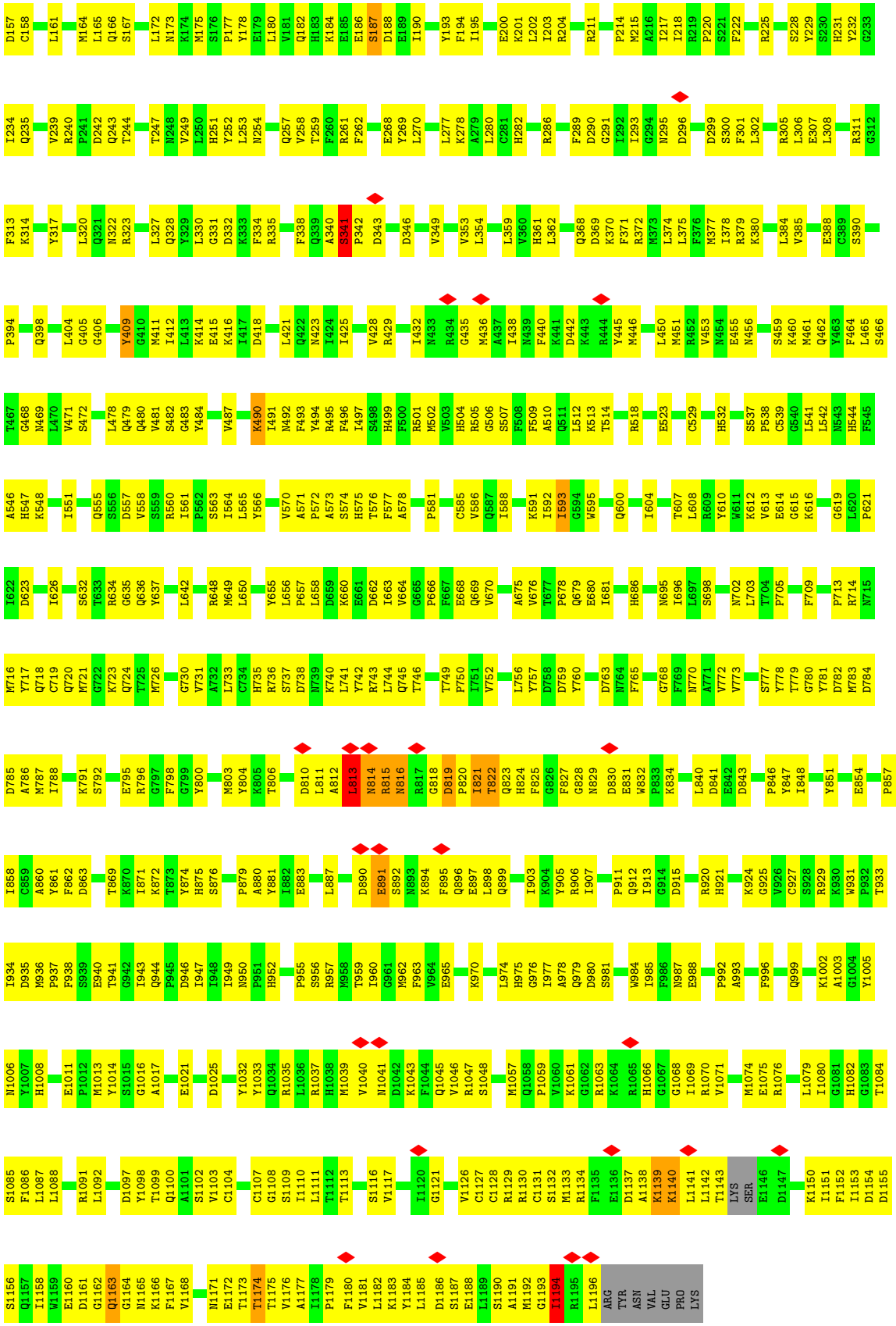




• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

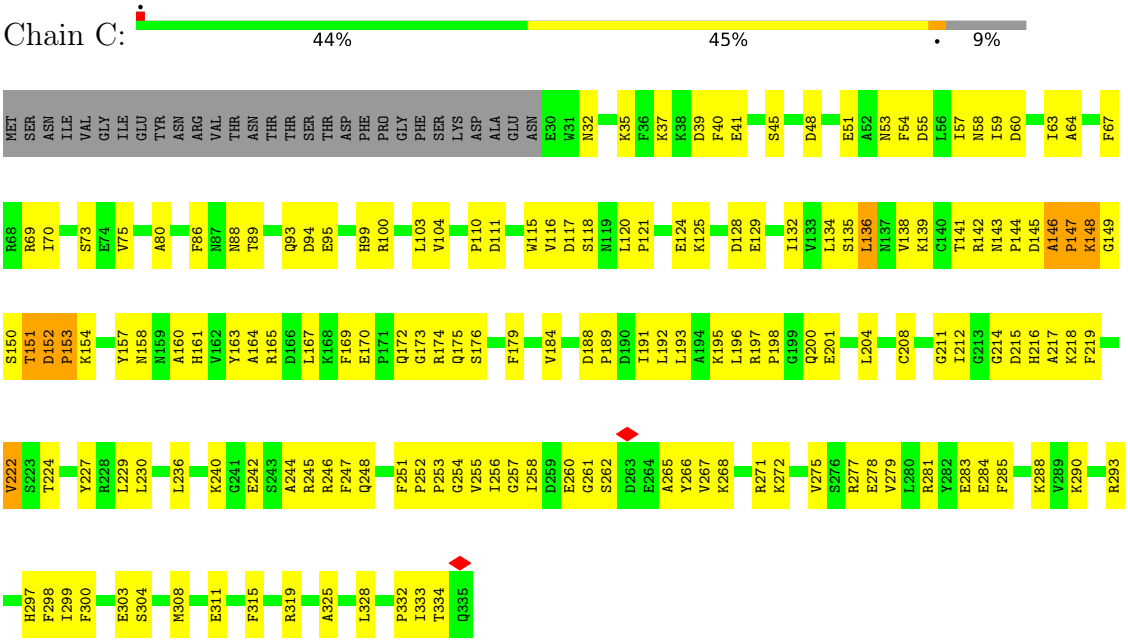
Chain B:





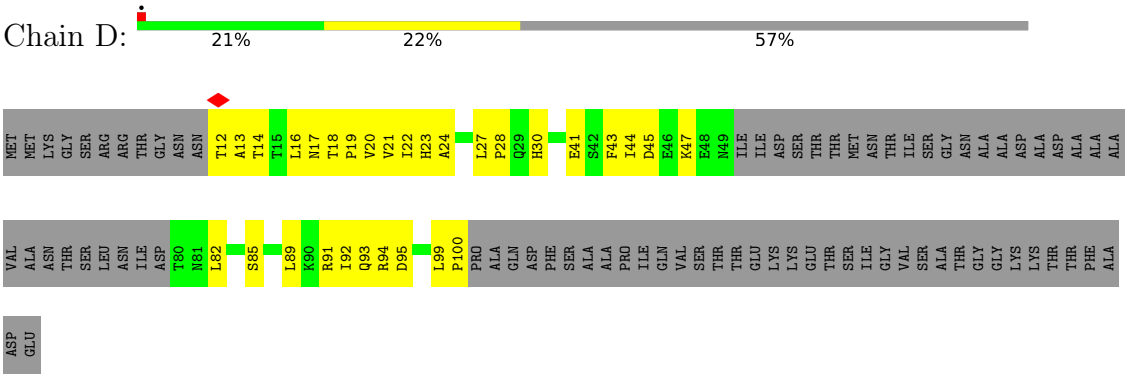
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



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

Chain D:

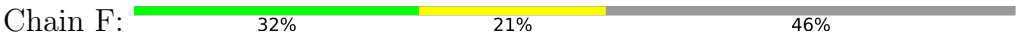


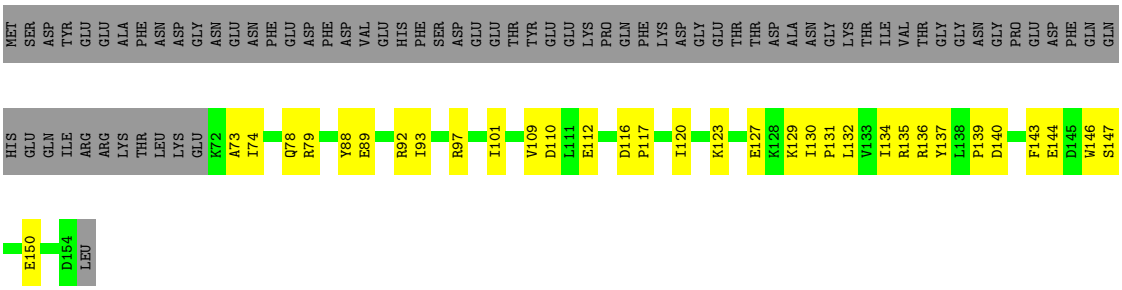
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

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

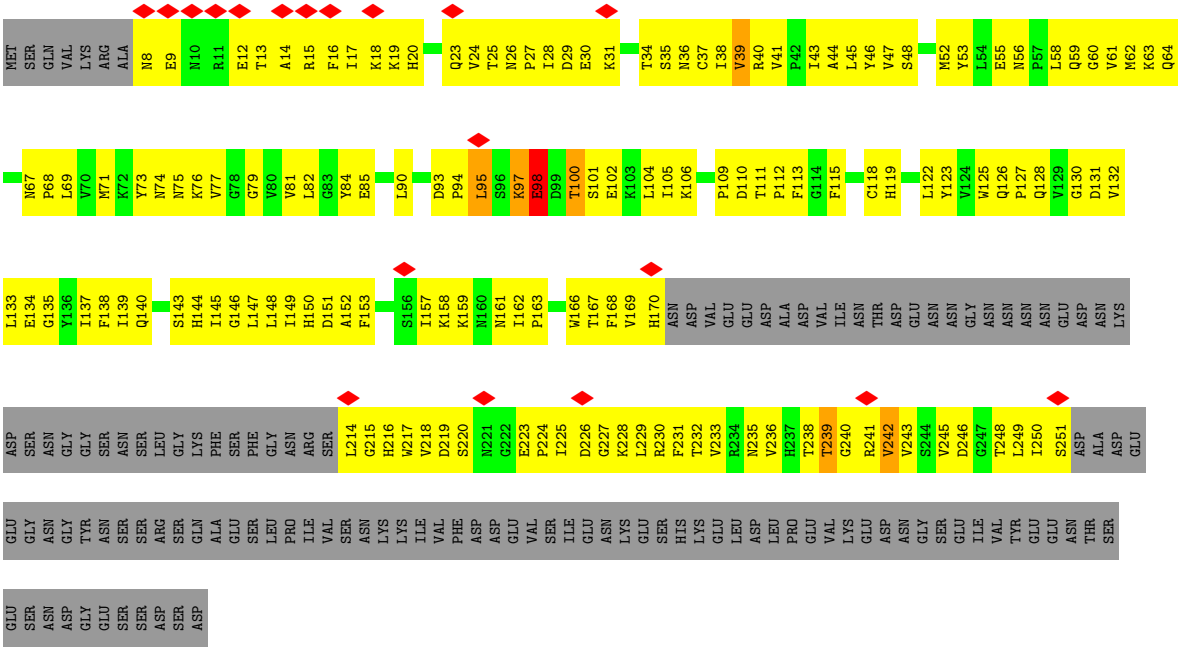
Chain F:





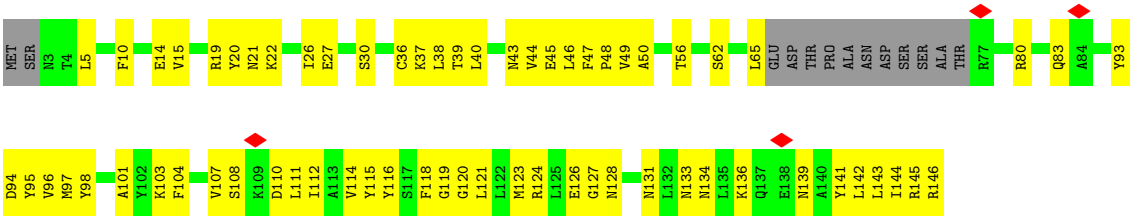
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G:



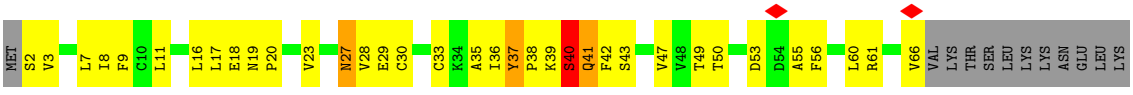
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:

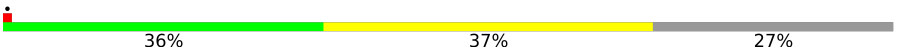


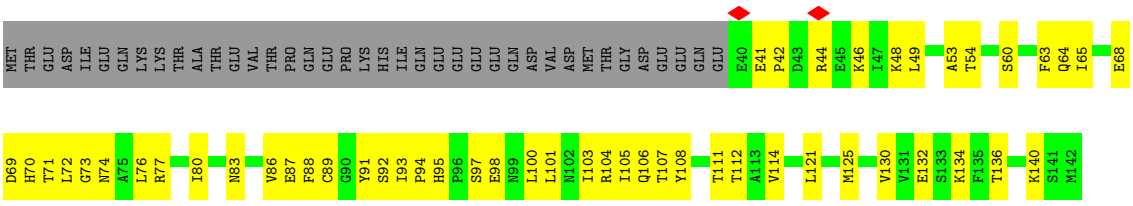
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

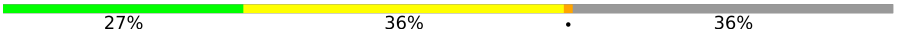
Chain K:

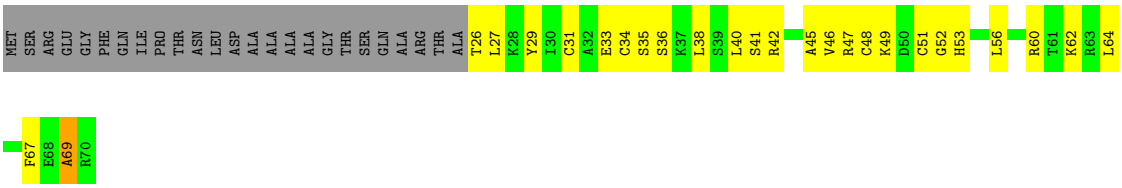




• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

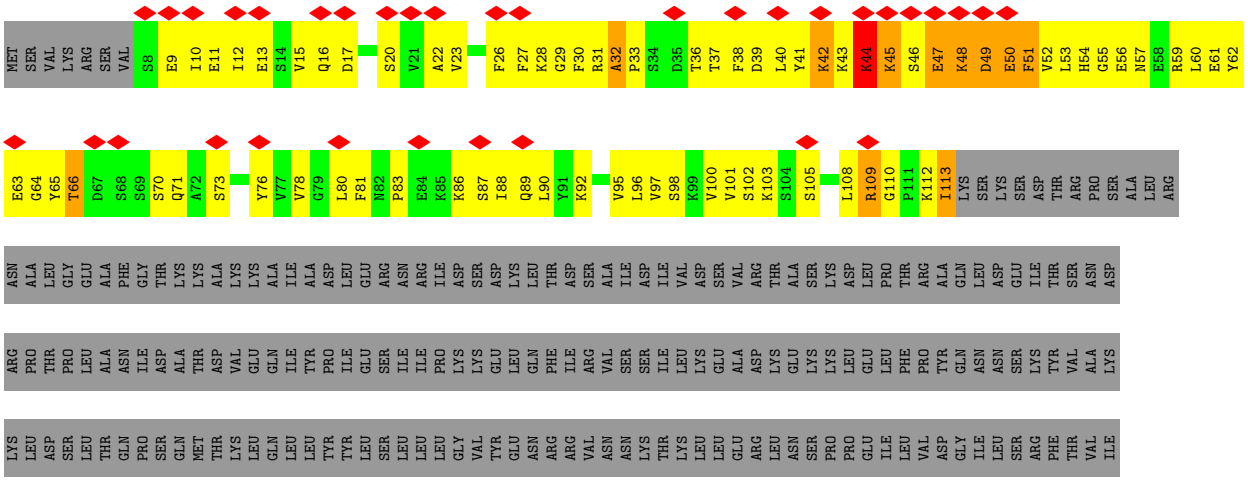
Chain L:

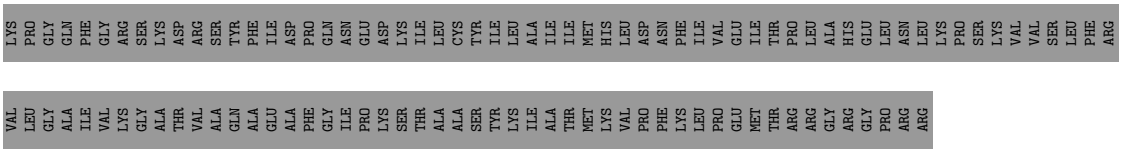




• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

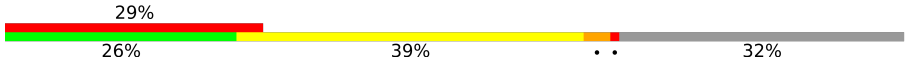
Chain M:

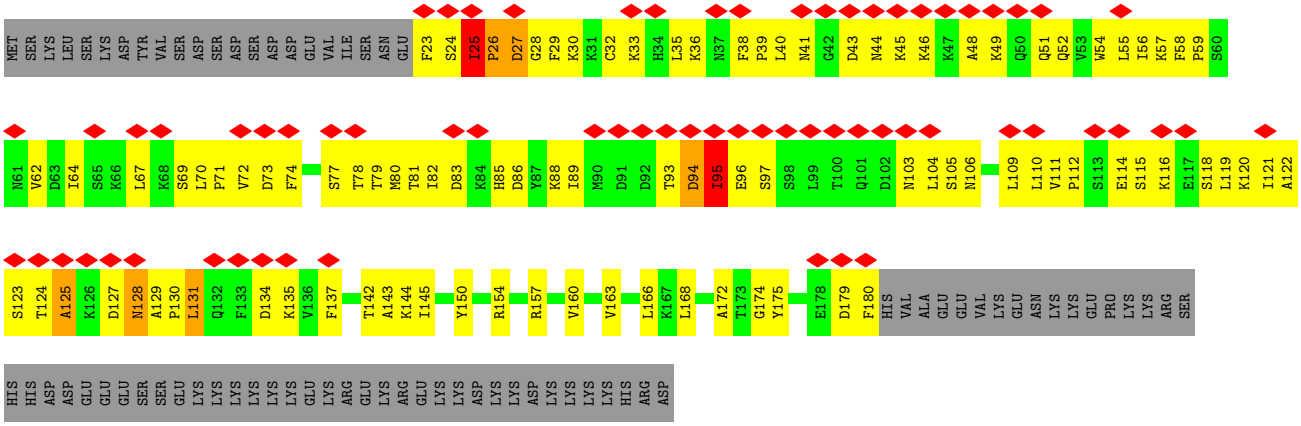




• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

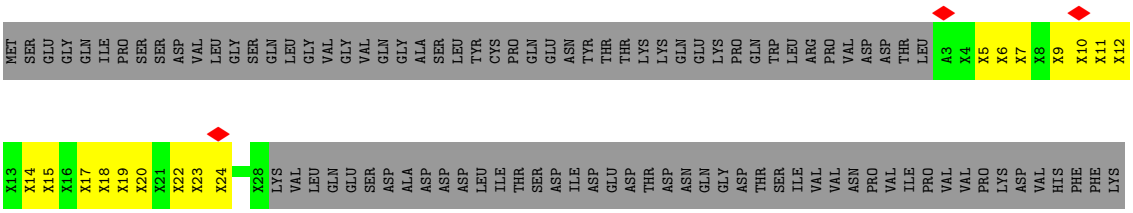
Chain N:

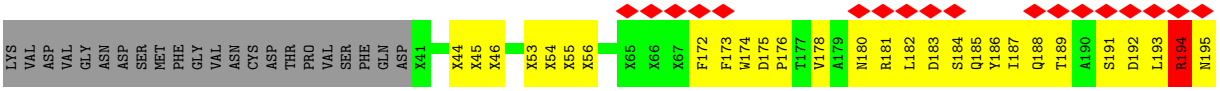


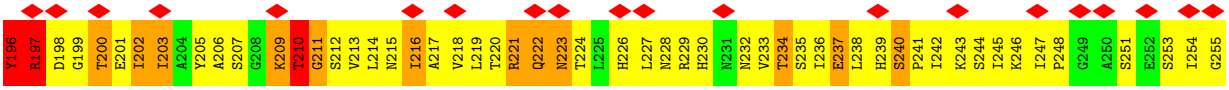


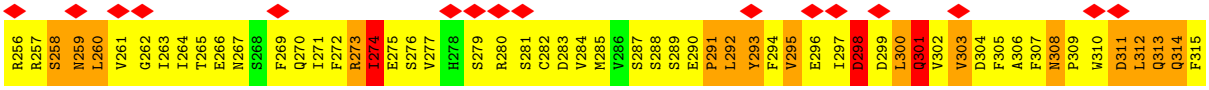
• Molecule 15: RNA polymerase I-specific transcription initiation factor RRN6

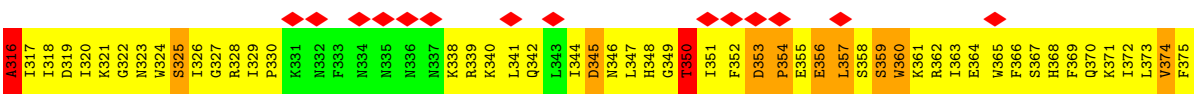
Chain O:

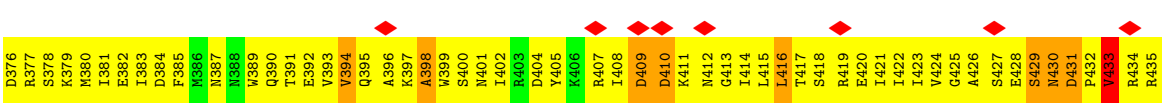


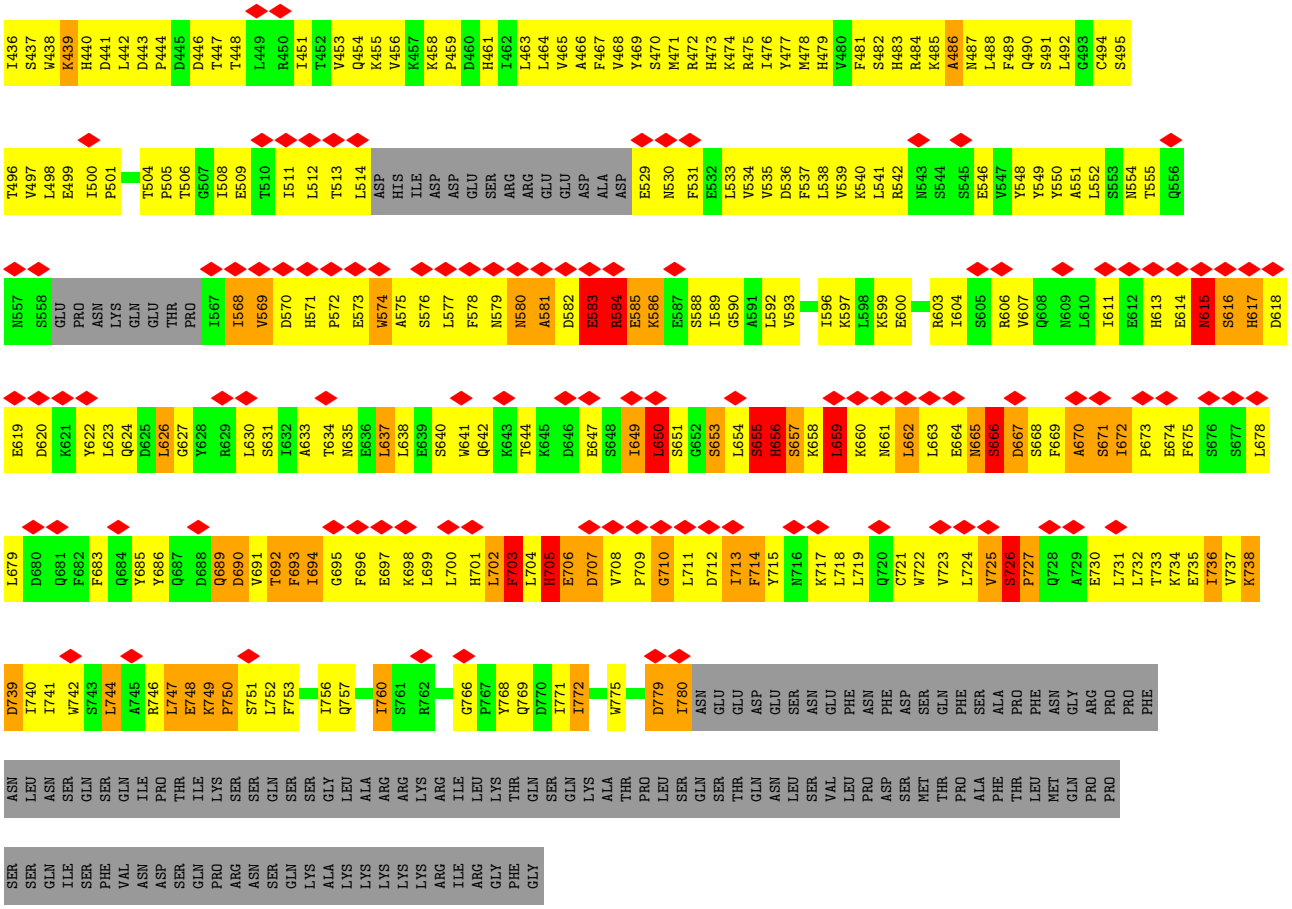






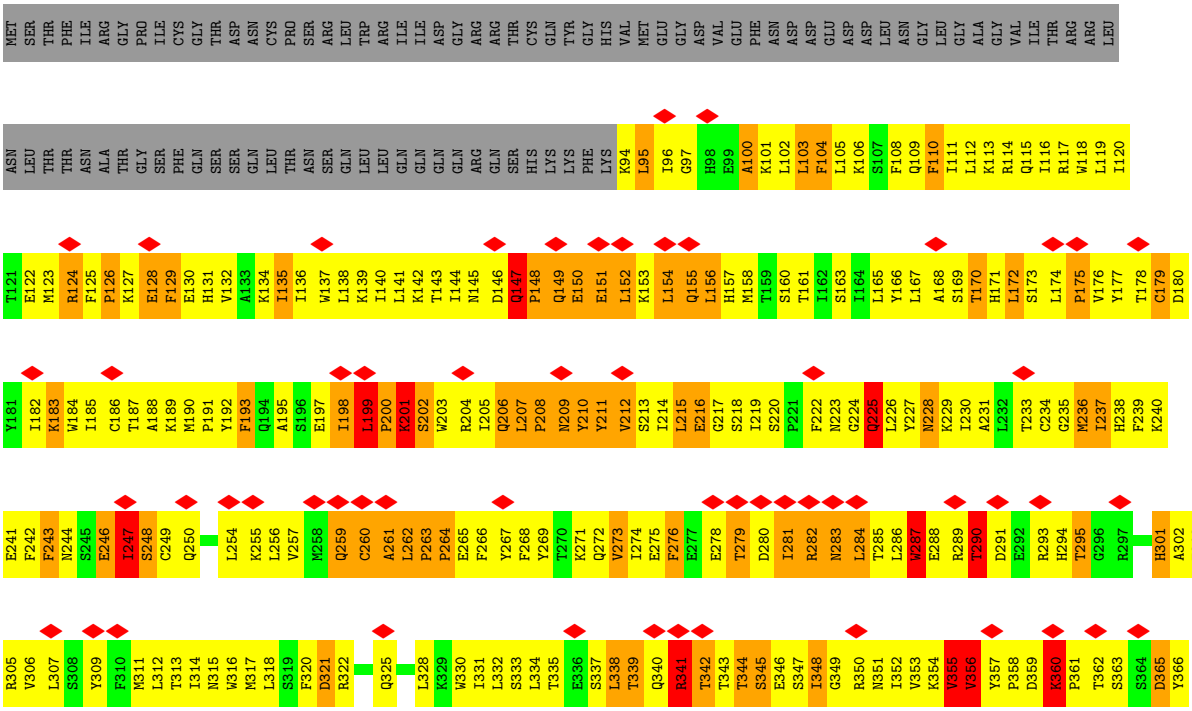


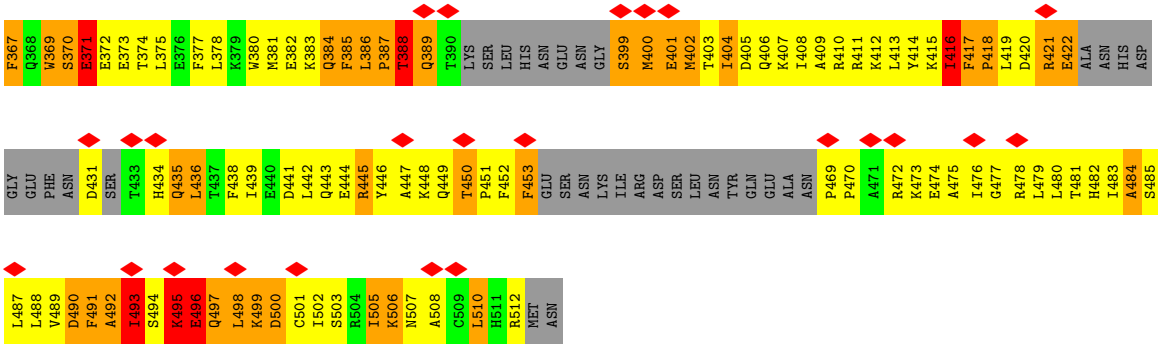




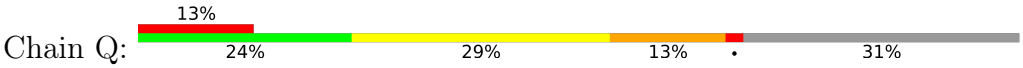
• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN7

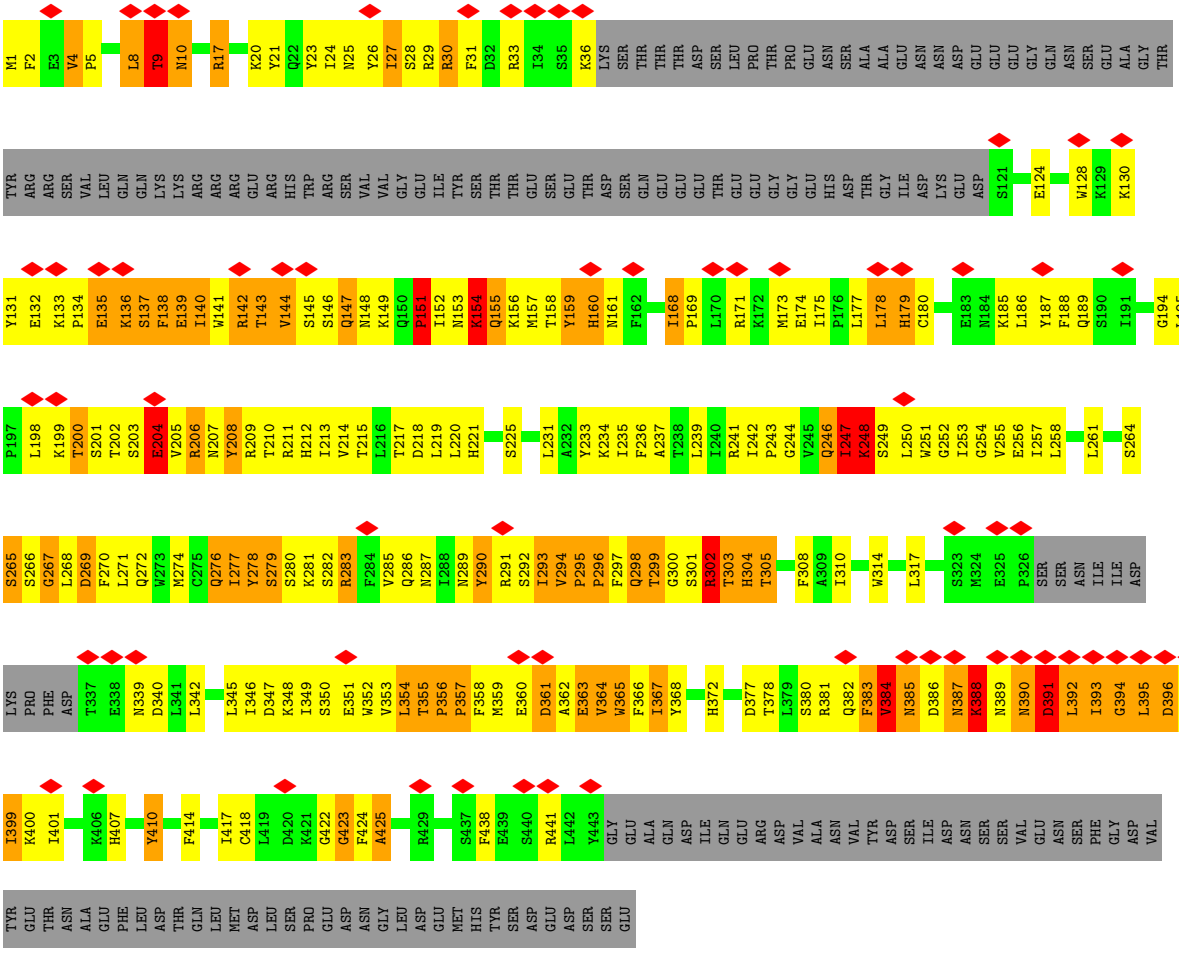
Chain P:



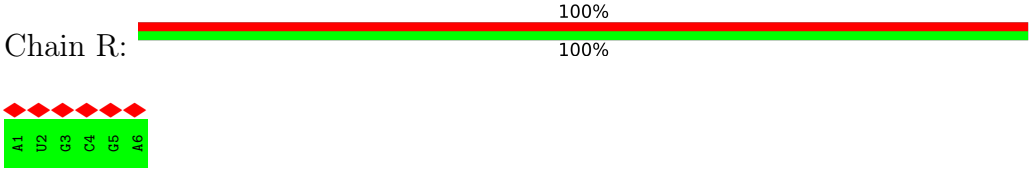


• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN11

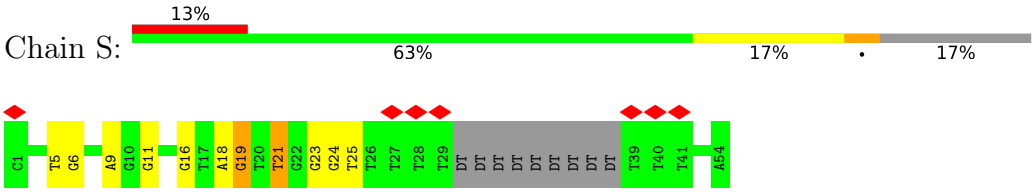




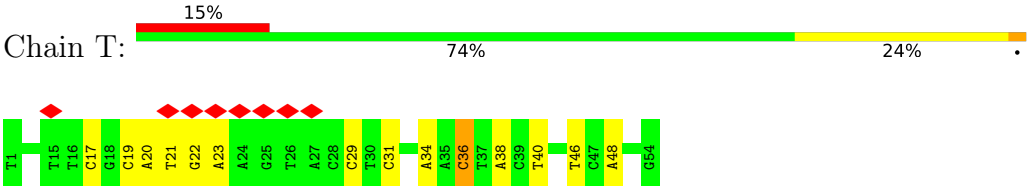
• Molecule 18: RNA



• Molecule 19: non-template strand DNA



• Molecule 20: template strand DNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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

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	0.29	1/11752 (0.0%)	0.53	1/15870 (0.0%)
2	B	0.31	0/9556	0.54	5/12916 (0.0%)
3	C	0.30	0/2484	0.54	1/3366 (0.0%)
4	D	0.25	0/473	0.46	0/641
5	E	0.28	0/1796	0.52	0/2416
6	F	0.27	0/682	0.49	0/922
7	G	0.26	0/1630	0.50	0/2216
8	H	0.30	0/1089	0.54	0/1474
9	I	0.27	0/485	0.67	0/657
10	J	0.32	0/578	0.58	0/775
11	K	0.28	0/822	0.51	0/1108
12	L	0.26	0/361	0.53	0/478
13	M	0.29	0/857	0.65	2/1151 (0.2%)
14	N	0.27	0/1279	0.58	0/1724
15	O	0.56	2/4906 (0.0%)	1.00	31/6645 (0.5%)
16	P	0.39	0/3316	1.08	30/4477 (0.7%)
17	Q	0.60	0/2990	1.03	13/4030 (0.3%)
18	R	0.34	0/142	0.99	0/220
19	S	0.75	0/1050	1.20	7/1621 (0.4%)
20	T	0.73	0/1206	1.26	9/1855 (0.5%)
All	All	0.39	3/47454 (0.0%)	0.74	99/64562 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	750	PRO	N-CD	7.11	1.57	1.47
1	A	593	PRO	N-CD	5.30	1.55	1.47
15	O	353	ASP	CA-C	5.23	1.66	1.52

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	199	LEU	N-CA-C	-9.72	84.76	111.00
20	T	22	DG	P-O3'-C3'	9.27	130.83	119.70
16	P	290	THR	N-CA-CB	8.88	127.17	110.30
19	S	19	DG	O4'-C1'-N9	-8.64	101.95	108.00
15	O	301	GLN	N-CA-C	-7.88	89.72	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11542	0	11625	1110	0
2	B	9351	0	9242	861	0
3	C	2432	0	2418	228	0
4	D	467	0	468	48	0
5	E	1760	0	1788	167	0
6	F	670	0	690	35	0
7	G	1592	0	1600	233	0
8	H	1071	0	1045	105	0
9	I	479	0	478	84	0
10	J	569	0	585	57	0
11	K	811	0	801	63	0
12	L	359	0	381	41	0
13	M	841	0	833	187	0
14	N	1254	0	1265	231	0
15	O	5063	0	4796	2307	0
16	P	3238	0	3263	1670	0
17	Q	2923	0	2969	1018	0
18	R	127	0	67	0	0
19	S	935	0	513	7	0
20	T	1082	0	615	21	0
21	A	2	0	0	2	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	46572	0	45442	7198	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 82.

The worst 5 of 7198 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)
16:P:419:LEU:HB3	17:Q:233:TYR:CZ	1.24	1.70
15:O:389:TRP:HZ3	17:Q:148:ASN:CA	1.05	1.68
16:P:104:PHE:CD1	16:P:211:TYR:HB2	1.22	1.67
2:B:155:VAL:HG21	17:Q:359:MET:SD	1.29	1.67
15:O:702:LEU:HD23	16:P:125:PHE:CZ	1.13	1.65

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	1445/1664 (87%)	1328 (92%)	92 (6%)	25 (2%)	9 43
2	B	1172/1203 (97%)	1081 (92%)	70 (6%)	21 (2%)	8 42
3	C	304/335 (91%)	283 (93%)	14 (5%)	7 (2%)	6 38
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100 100
5	E	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	29 66
6	F	81/155 (52%)	73 (90%)	7 (9%)	1 (1%)	13 50
7	G	197/326 (60%)	179 (91%)	15 (8%)	3 (2%)	10 46
8	H	129/146 (88%)	121 (94%)	8 (6%)	0	100 100
9	I	63/125 (50%)	52 (82%)	9 (14%)	2 (3%)	4 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	67/70 (96%)	60 (90%)	6 (9%)	1 (2%)	10 46
11	K	101/142 (71%)	94 (93%)	7 (7%)	0	100 100
12	L	43/70 (61%)	38 (88%)	4 (9%)	1 (2%)	6 38
13	M	104/415 (25%)	94 (90%)	8 (8%)	2 (2%)	8 42
14	N	156/233 (67%)	129 (83%)	21 (14%)	6 (4%)	3 29
15	O	581/894 (65%)	417 (72%)	108 (19%)	56 (10%)	0 10
16	P	378/514 (74%)	280 (74%)	46 (12%)	52 (14%)	0 4
17	Q	343/507 (68%)	236 (69%)	65 (19%)	42 (12%)	0 6
All	All	5432/7151 (76%)	4722 (87%)	490 (9%)	220 (4%)	5 27

5 of 220 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	LEU
1	A	530	TRP
1	A	533	ALA
1	A	592	GLN
1	A	594	THR

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	1292/1465 (88%)	1266 (98%)	26 (2%)	55 75
2	B	1030/1053 (98%)	1012 (98%)	18 (2%)	60 78
3	C	270/296 (91%)	268 (99%)	2 (1%)	84 91
4	D	56/116 (48%)	56 (100%)	0	100 100
5	E	197/197 (100%)	194 (98%)	3 (2%)	65 81
6	F	73/137 (53%)	73 (100%)	0	100 100
7	G	179/291 (62%)	171 (96%)	8 (4%)	27 57
8	H	117/128 (91%)	116 (99%)	1 (1%)	78 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	57/110 (52%)	54 (95%)	3 (5%)	22 54
10	J	64/65 (98%)	64 (100%)	0	100 100
11	K	93/130 (72%)	93 (100%)	0	100 100
12	L	40/57 (70%)	39 (98%)	1 (2%)	47 70
13	M	96/371 (26%)	86 (90%)	10 (10%)	7 30
14	N	146/220 (66%)	142 (97%)	4 (3%)	44 69
15	O	545/779 (70%)	483 (89%)	62 (11%)	5 28
16	P	362/476 (76%)	303 (84%)	59 (16%)	2 15
17	Q	331/474 (70%)	280 (85%)	51 (15%)	2 17
All	All	4948/6365 (78%)	4700 (95%)	248 (5%)	28 55

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	655	SER
17	Q	248	LYS
16	P	152	LEU
17	Q	246	GLN
17	Q	365	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	103	ASN
15	O	556	GLN
15	O	215	ASN
15	O	308	ASN
15	O	642	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	67:UNK	C	172:PHE	N	30.74

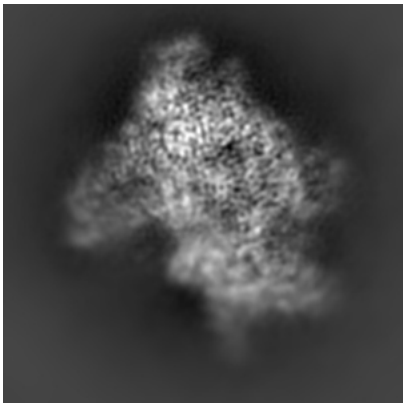
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8771. These allow visual inspection of the internal detail of the map and identification of artifacts.

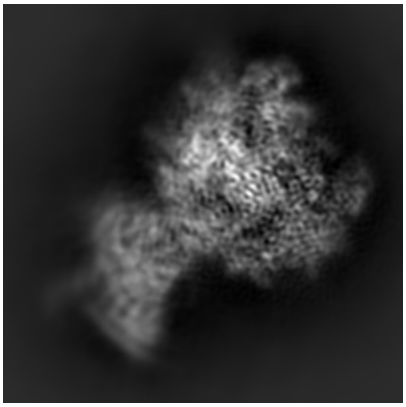
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

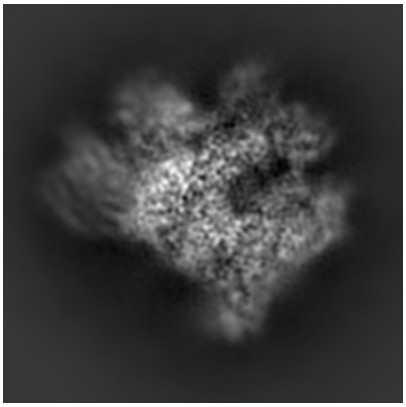
6.1.1 Primary map



X



Y

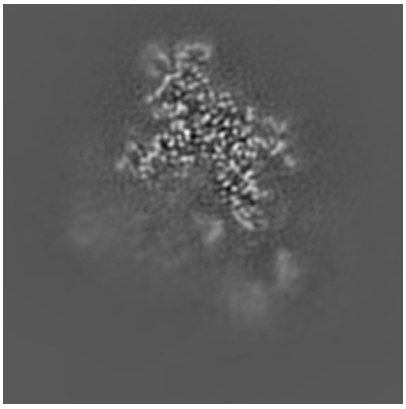


Z

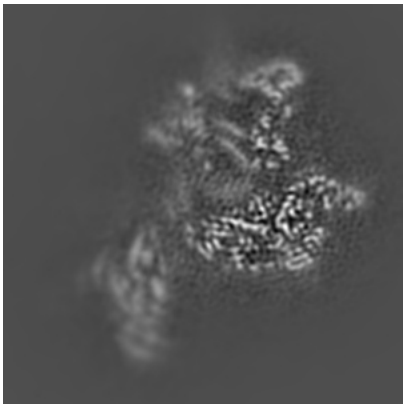
The images above show the map projected in three orthogonal directions.

6.2 Central slices

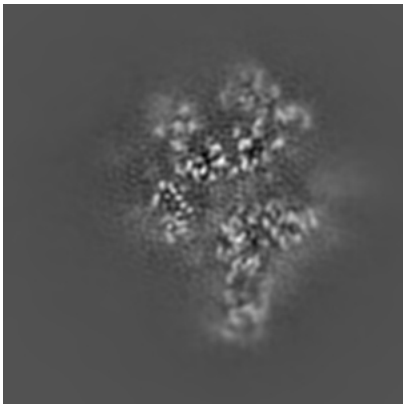
6.2.1 Primary map



X Index: 96



Y Index: 96

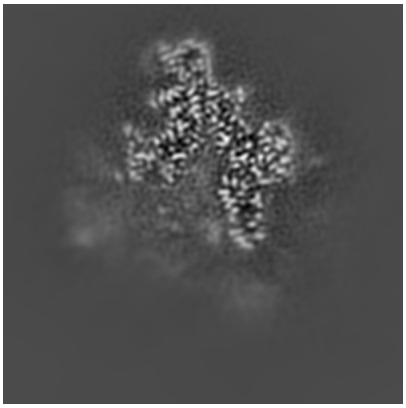


Z Index: 96

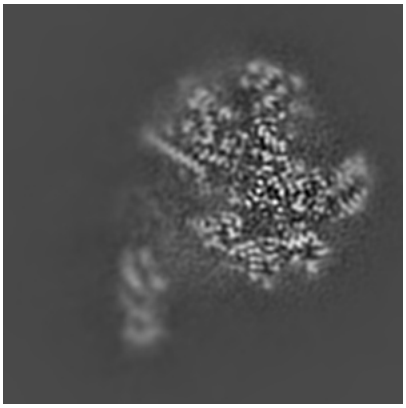
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

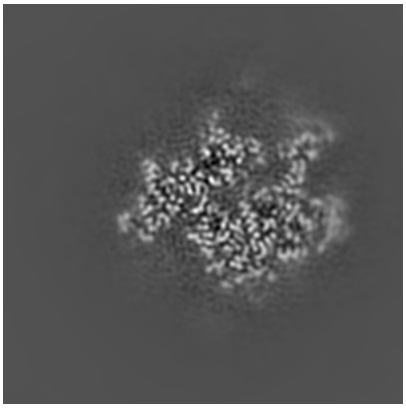
6.3.1 Primary map



X Index: 100



Y Index: 87

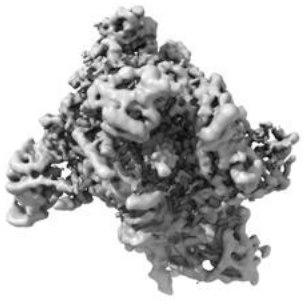


Z Index: 127

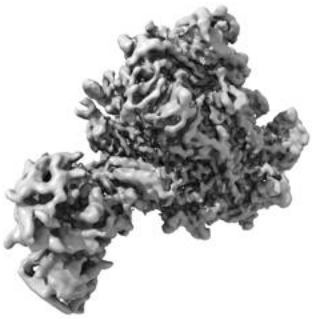
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

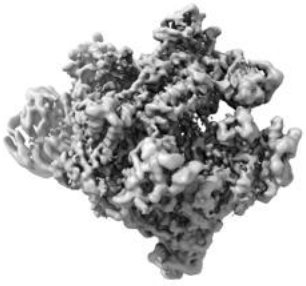
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

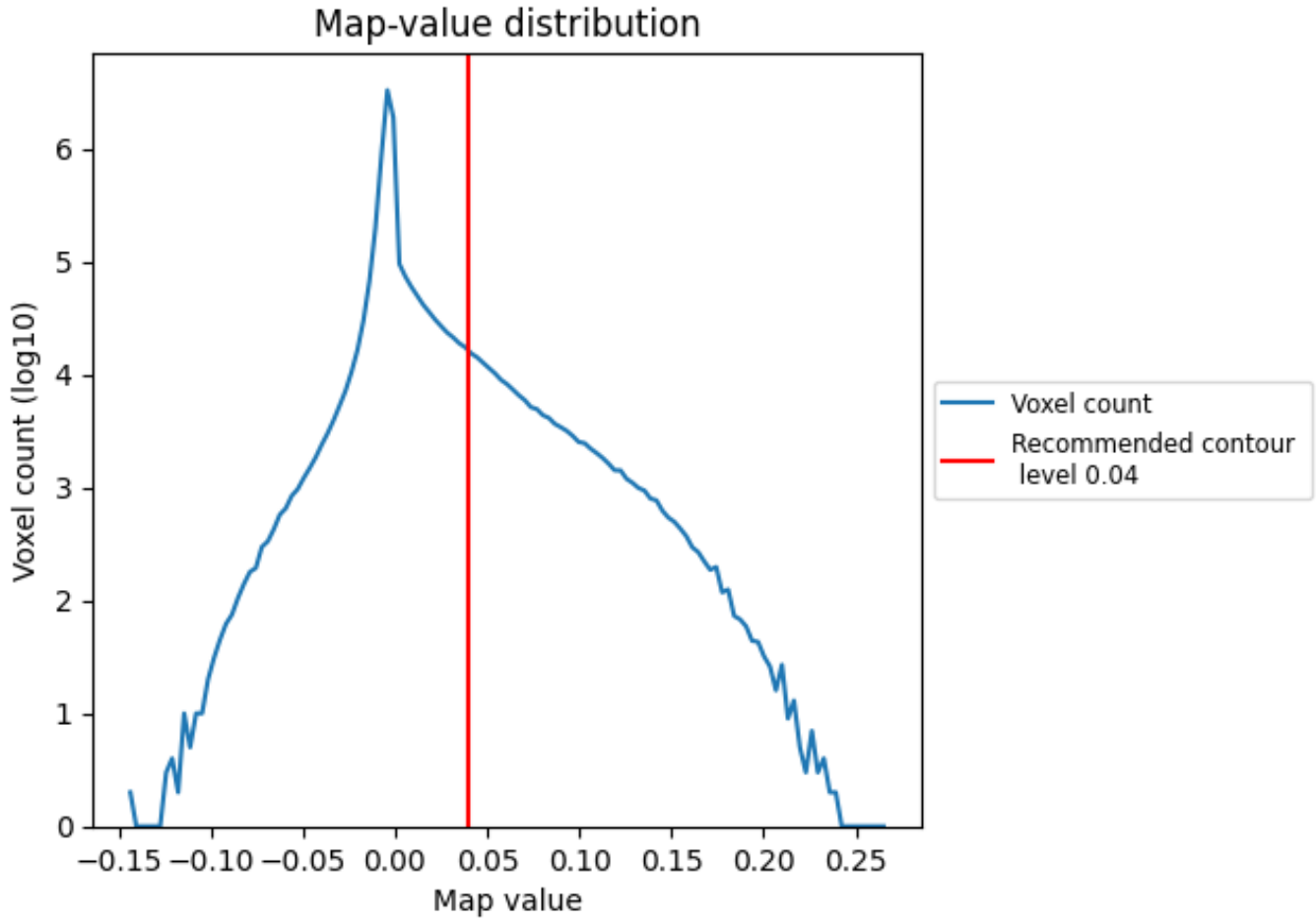
6.5 Mask visualisation (i)

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

7 Map analysis

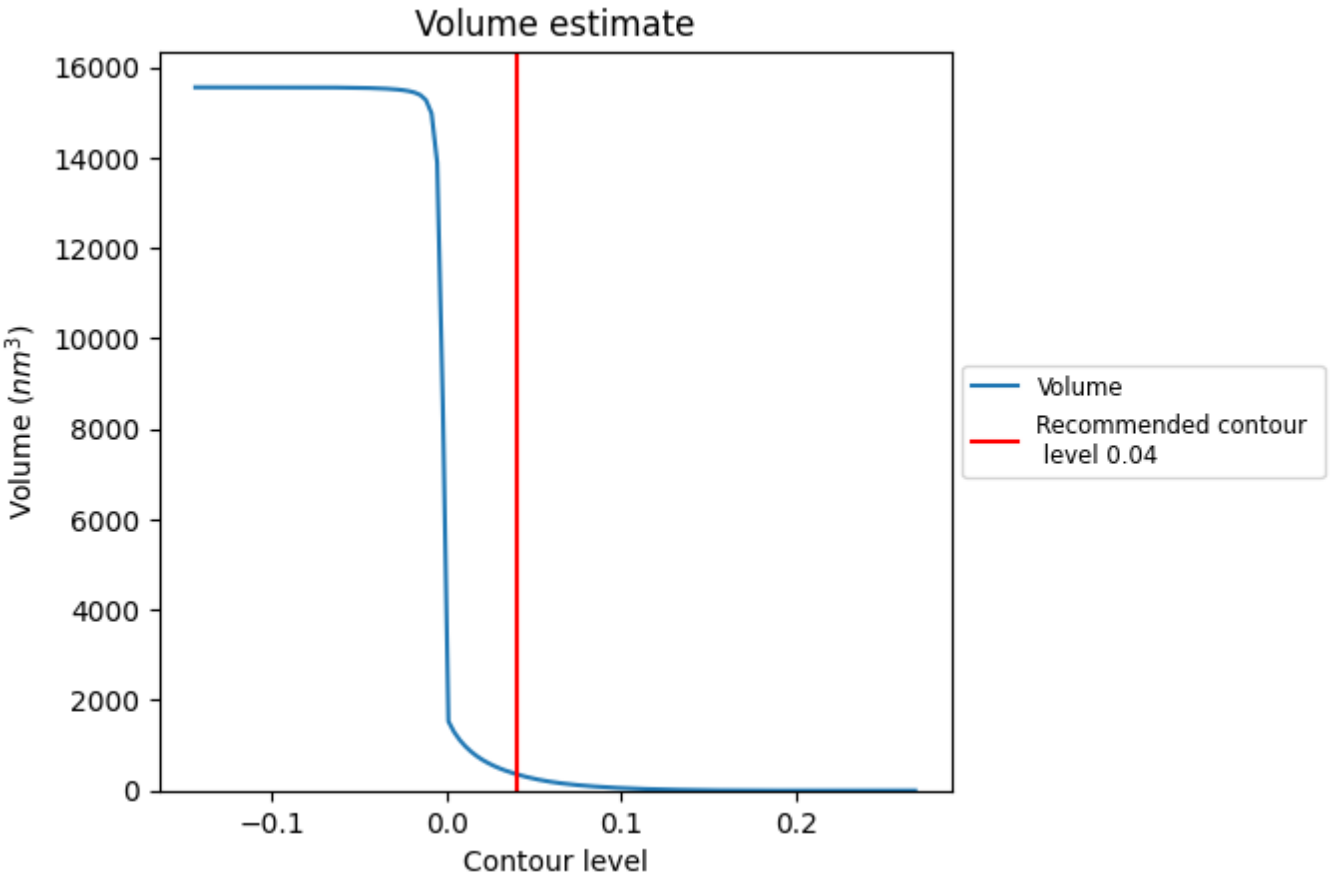
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

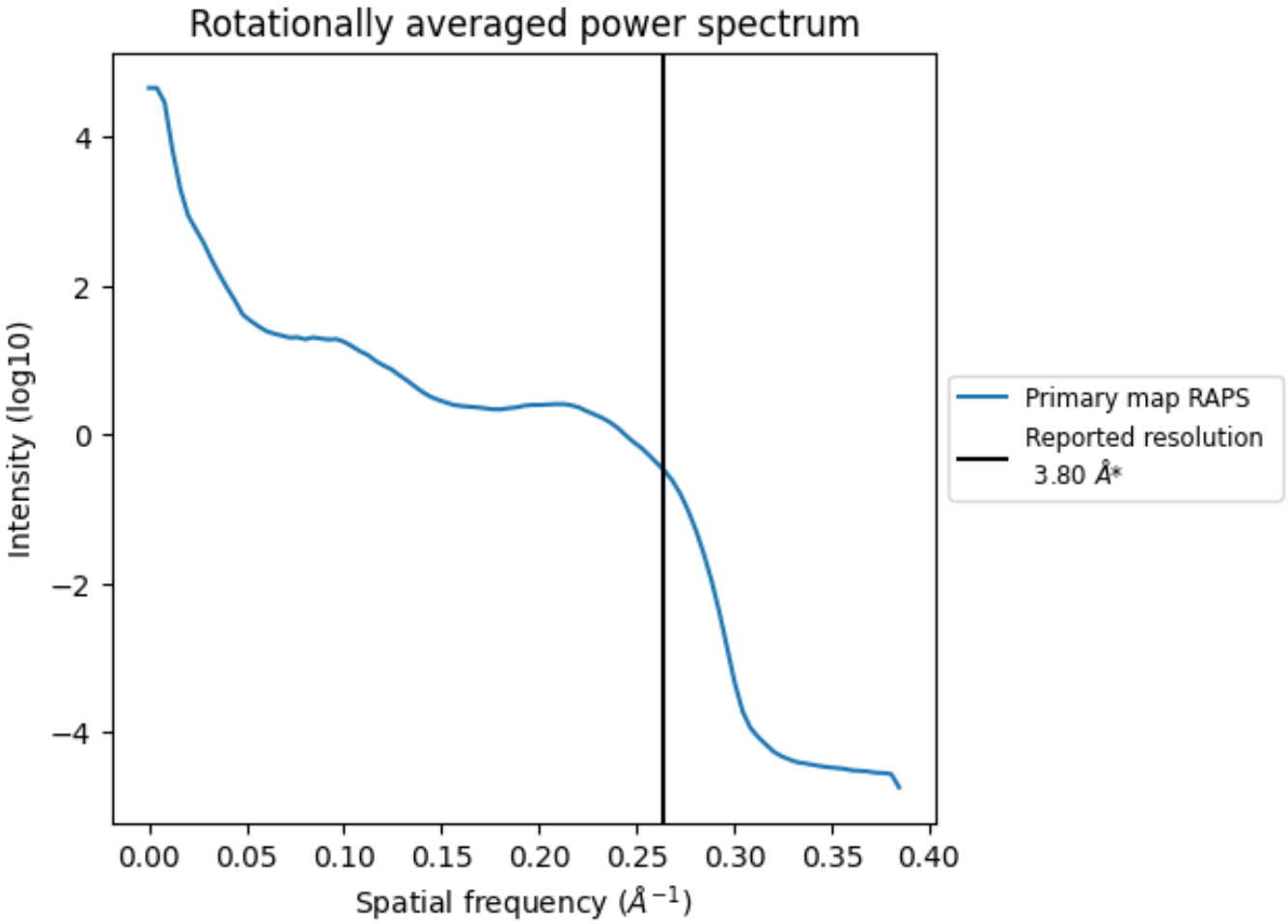
7.2 Volume estimate (i)



The volume at the recommended contour level is 363 nm^3; this corresponds to an approximate mass of 328 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)

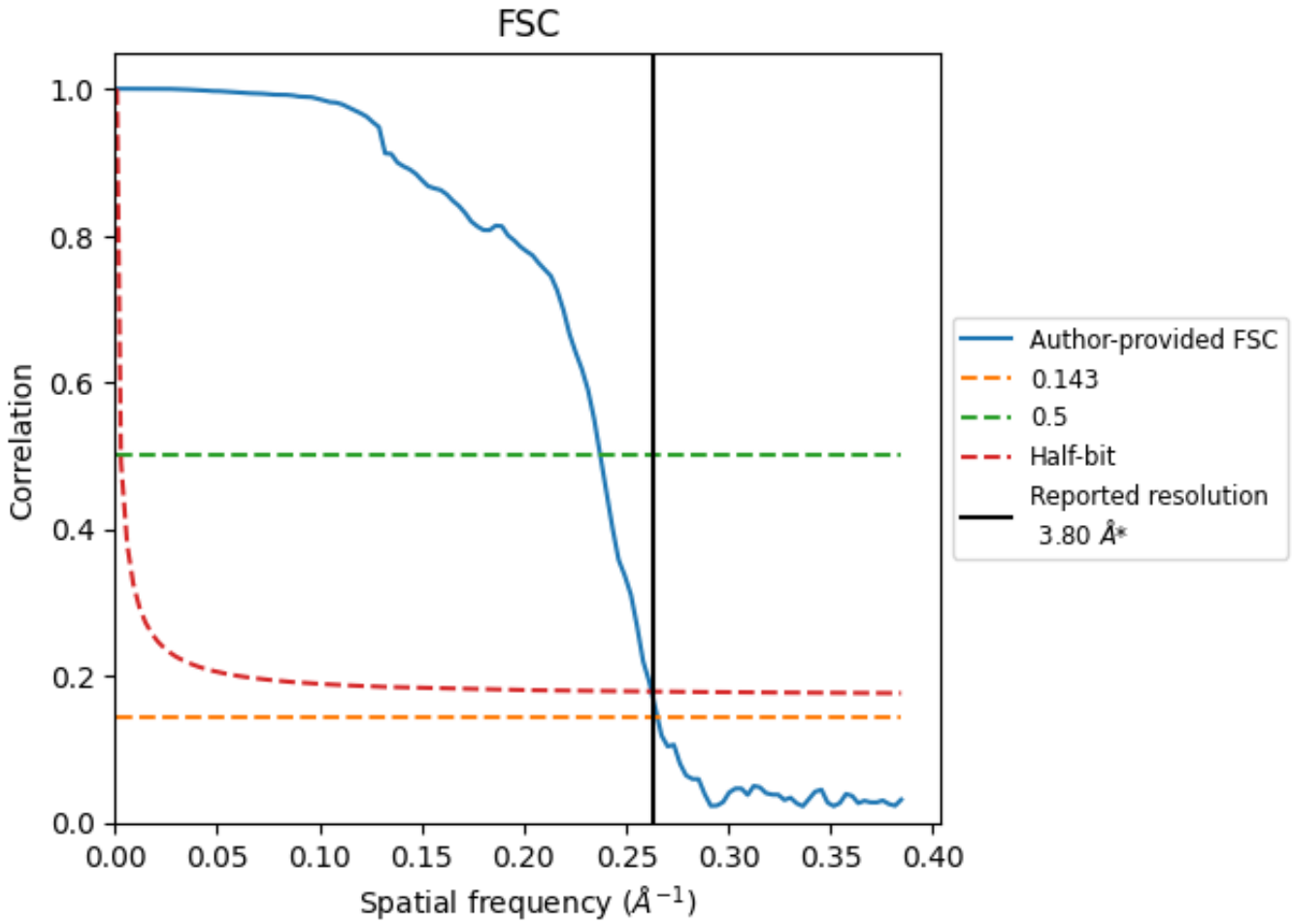


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

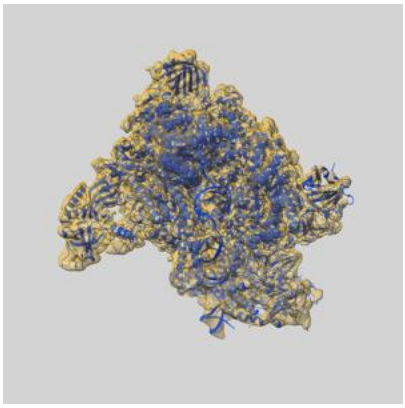
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.21	3.81
Unmasked-calculated*	-	-	-

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

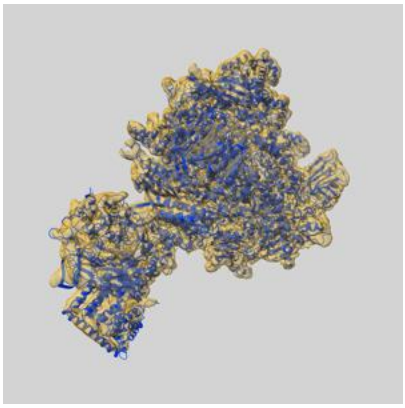
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8771 and PDB model 5W5Y. Per-residue inclusion information can be found in section 3 on page 9.

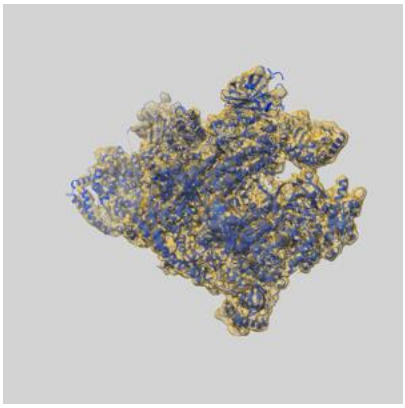
9.1 Map-model overlay



X



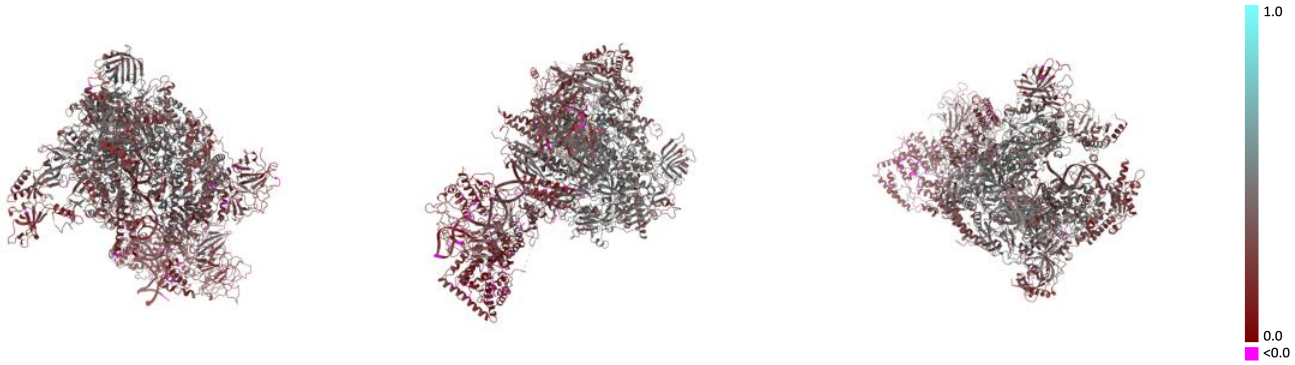
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

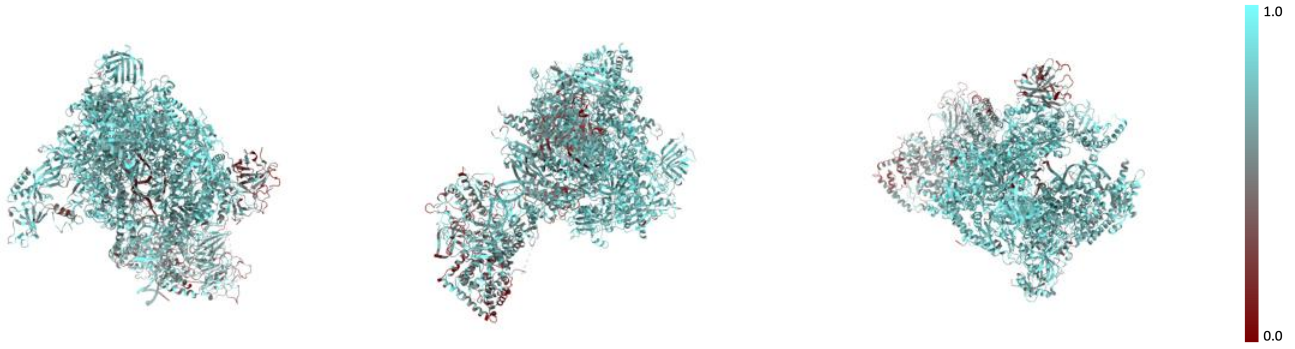
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

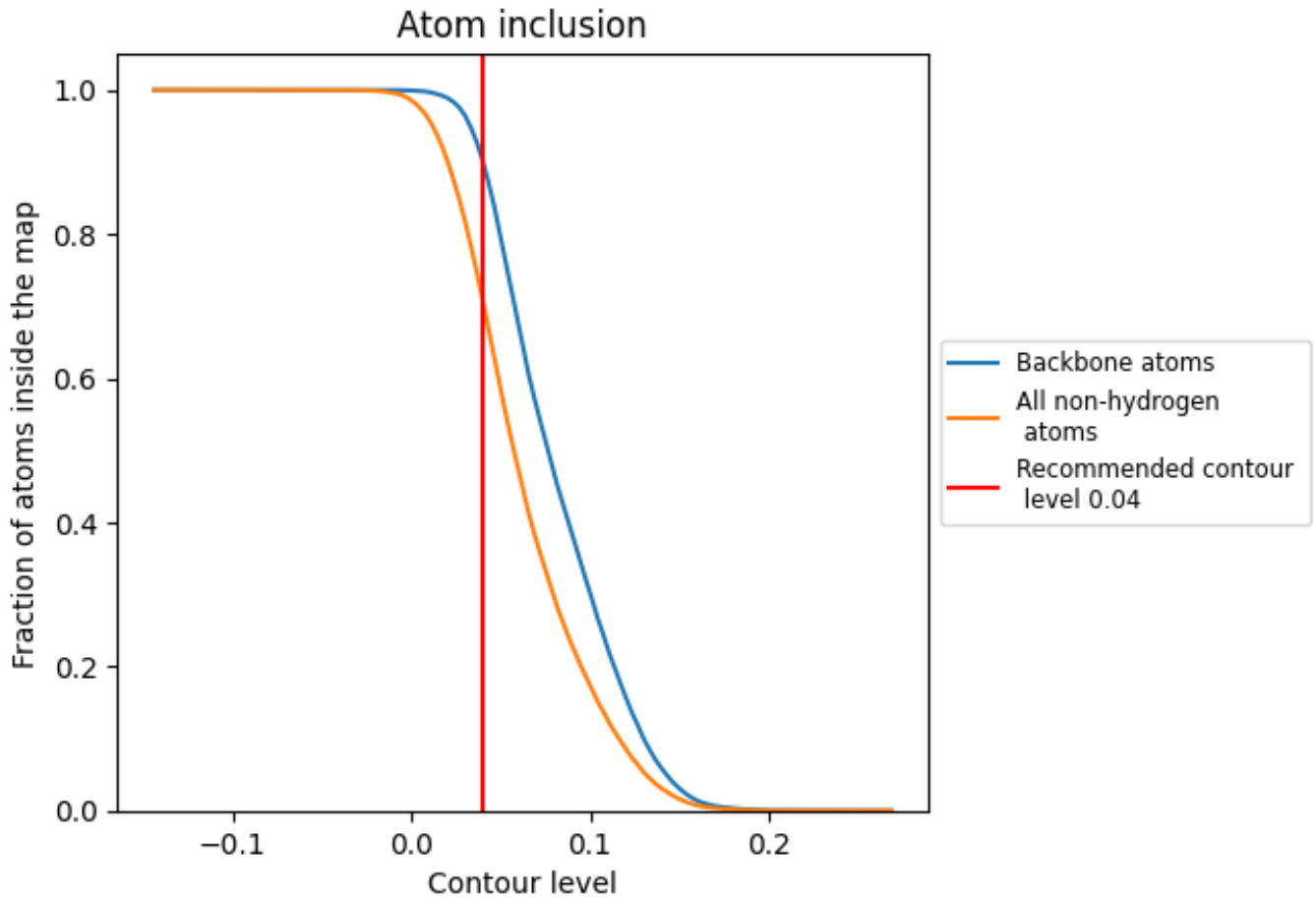
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 71% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.3370
A	0.7747	0.3930
B	0.7869	0.4230
C	0.8241	0.4090
D	0.7214	0.2800
E	0.7676	0.3390
F	0.8144	0.4130
G	0.7006	0.2810
H	0.7929	0.3880
I	0.7400	0.3380
J	0.8514	0.4560
K	0.7768	0.3950
L	0.7954	0.4100
M	0.4843	0.2730
N	0.4197	0.2770
O	0.5545	0.2150
P	0.5949	0.1900
Q	0.5874	0.2230
R	0.1260	0.2270
S	0.6781	0.2560
T	0.6359	0.2350