



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 03:01 pm BST

PDB ID : 5N61
EMDB ID : EMD-3593
Title : RNA polymerase I initially transcribing complex
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : 2017-02-14
Resolution : 3.40 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.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

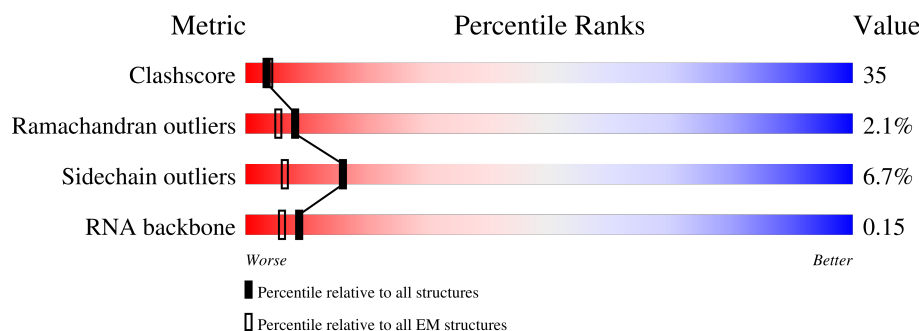
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	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	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	

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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	627	
16	P	894	
17	Q	514	
18	R	507	
19	S	5	
20	T	47	
21	U	47	

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
24	SO4	B	1301	-	-	X	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 48547 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 polymerase I subunit RPA14.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	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	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	63	Total	C	N	O	S	0	0
			466	292	77	93	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	101	Total	C	N	O	S	0	0
			793	496	130	162	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	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	129	Total	C	N	O	S	0	0
			1029	665	170	191	3		

- 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 protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	587	Total	C	N	O	S	0	0
			4764	3030	811	912	11		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	389	Total	C	N	O	S	0	0
			3254	2110	552	572	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	303	Total	C	N	O	S	0	0
			2535	1634	456	434	11		

- Molecule 19 is a RNA chain called product RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	5	Total	C	N	O	P	0	0
			108	48	21	34	5		

- Molecule 20 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	41	Total	C	N	O	P	0	0
			641	304	66	231	40		

- Molecule 21 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	33	Total	C	N	O	P	0	0
			490	228	55	174	33		

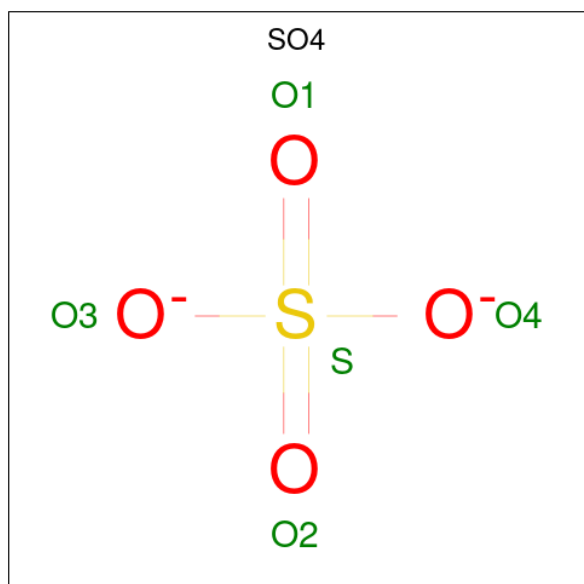
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

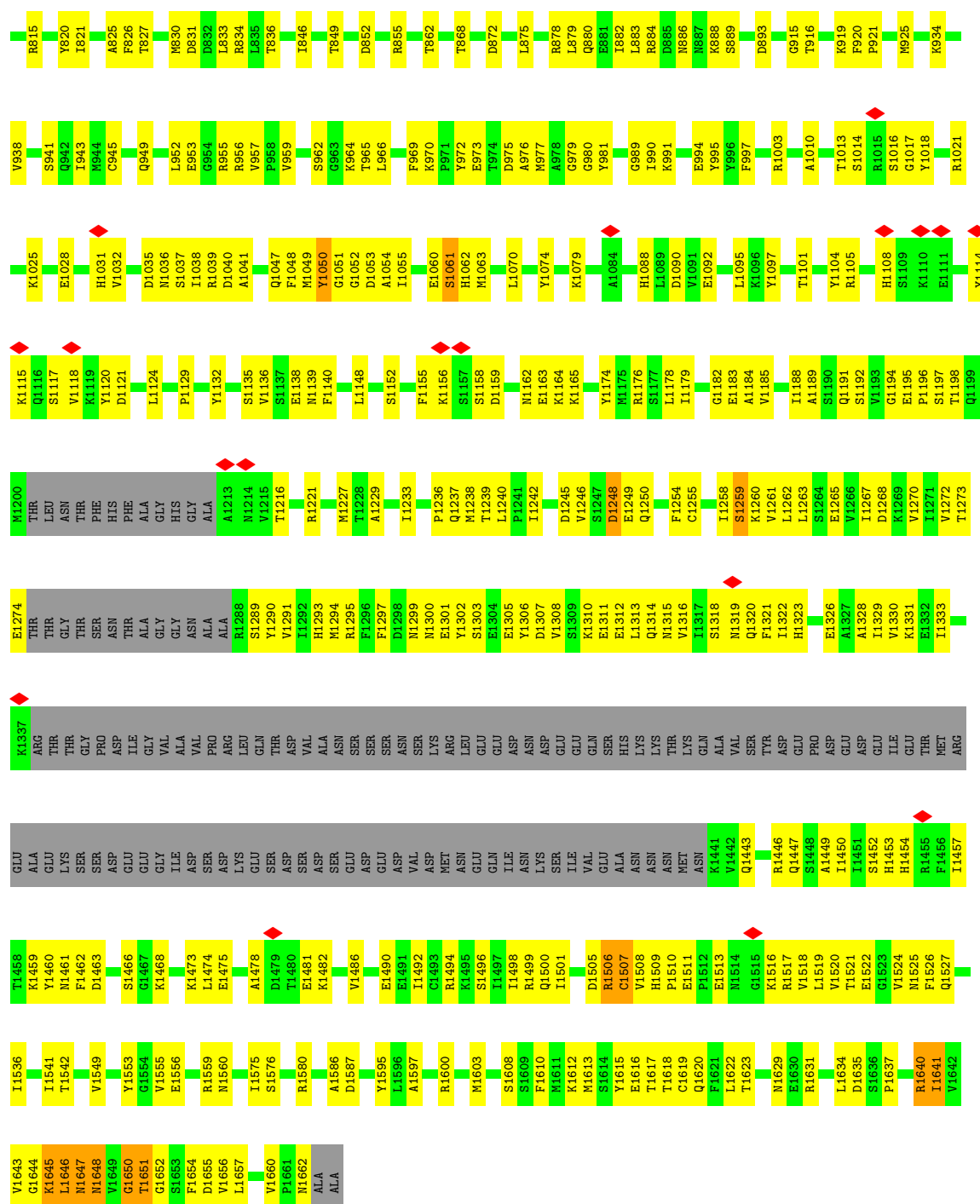
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 24 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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



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

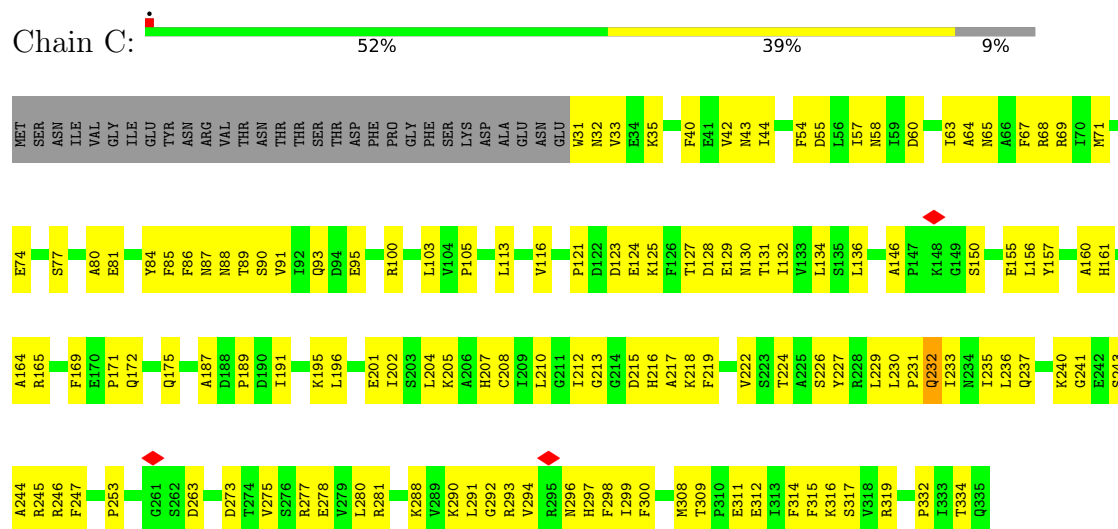
Chain B: 50% 46%



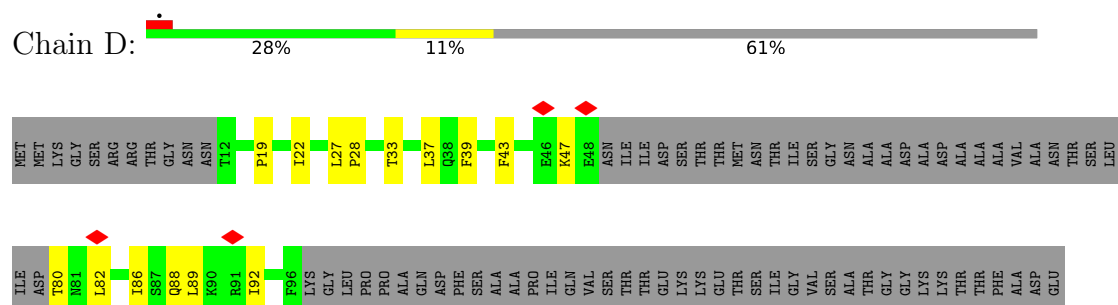




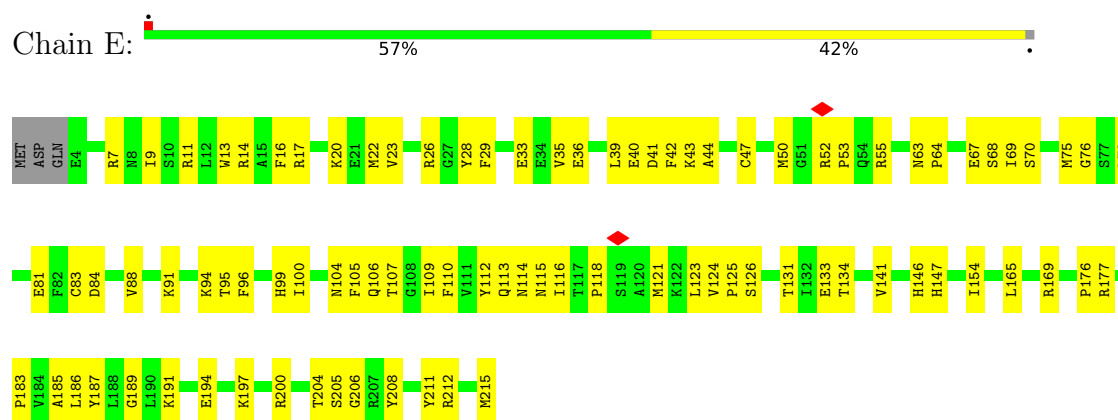
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



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



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

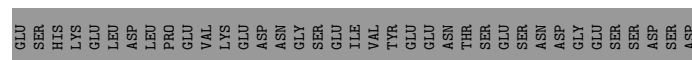
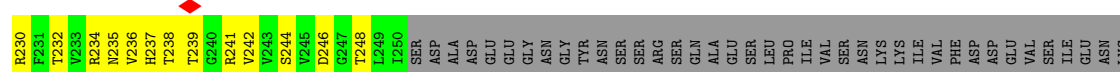
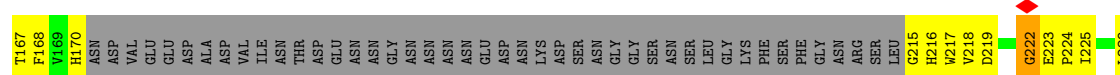
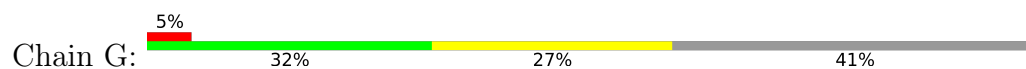


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2





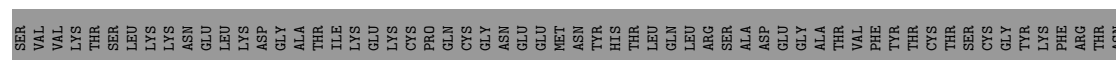
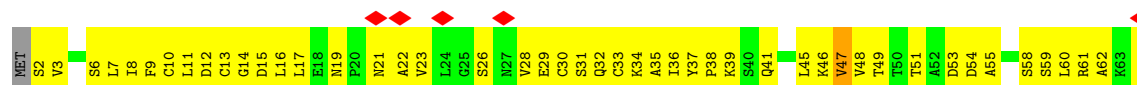
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43



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



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



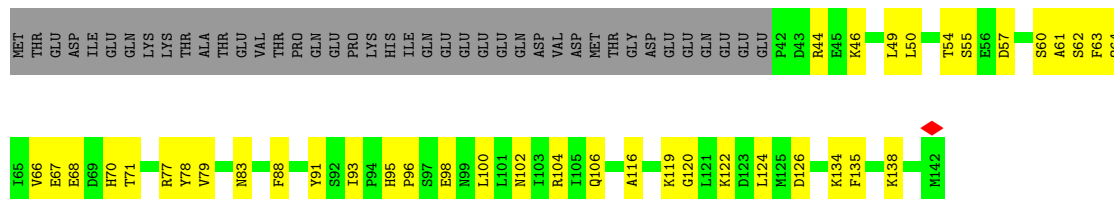
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



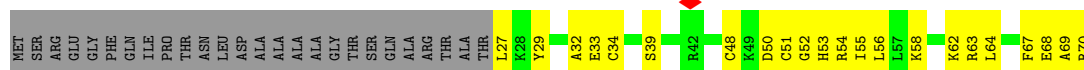
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 



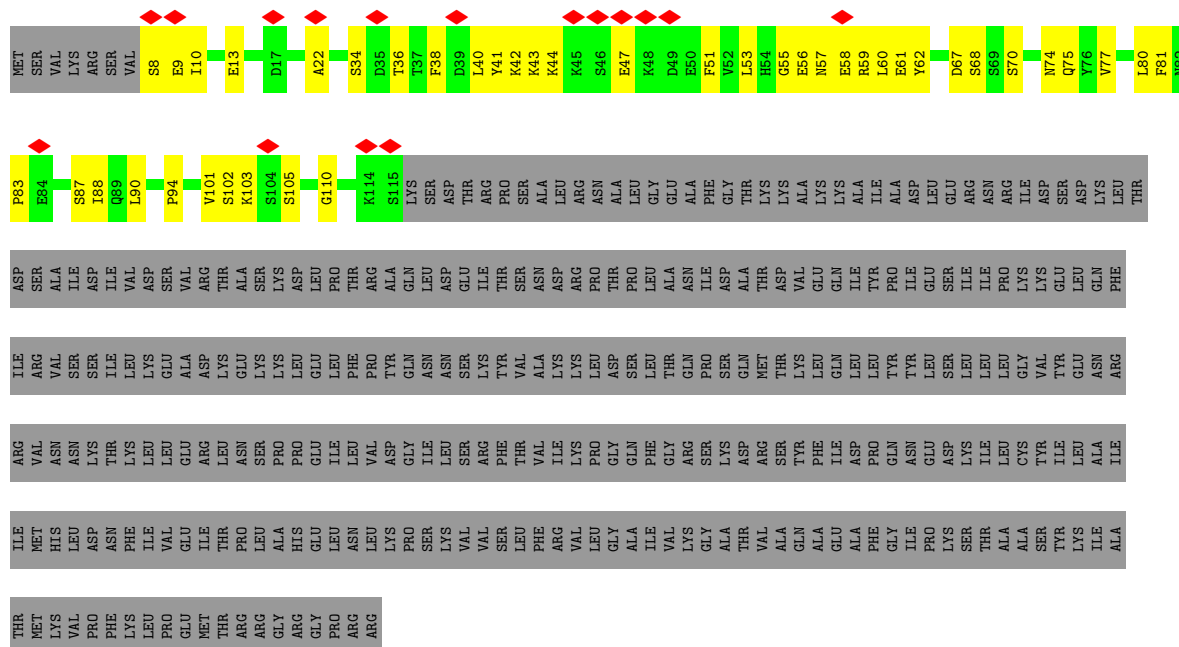
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 

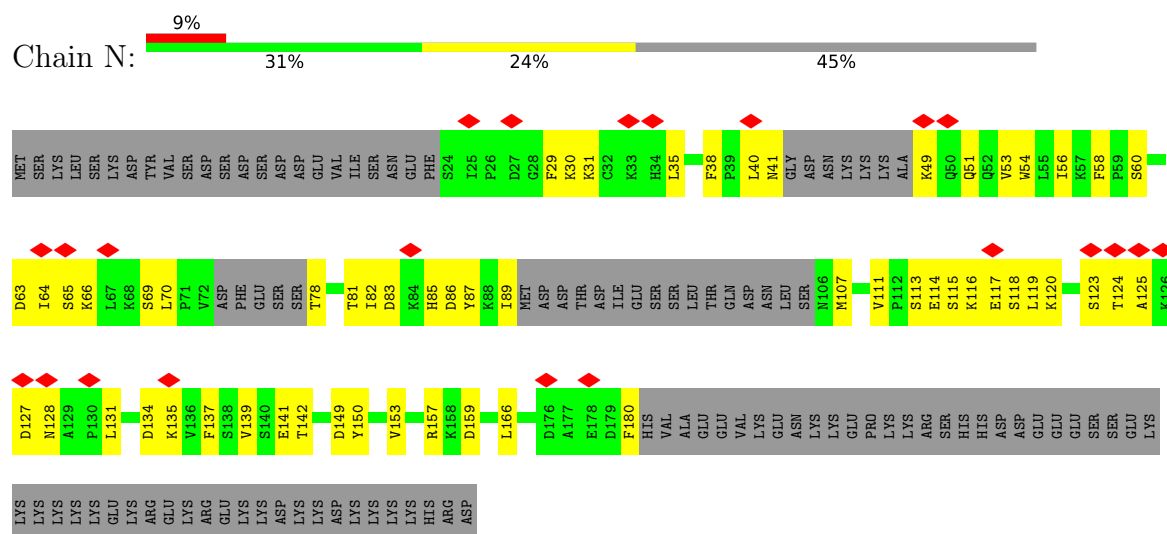


- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

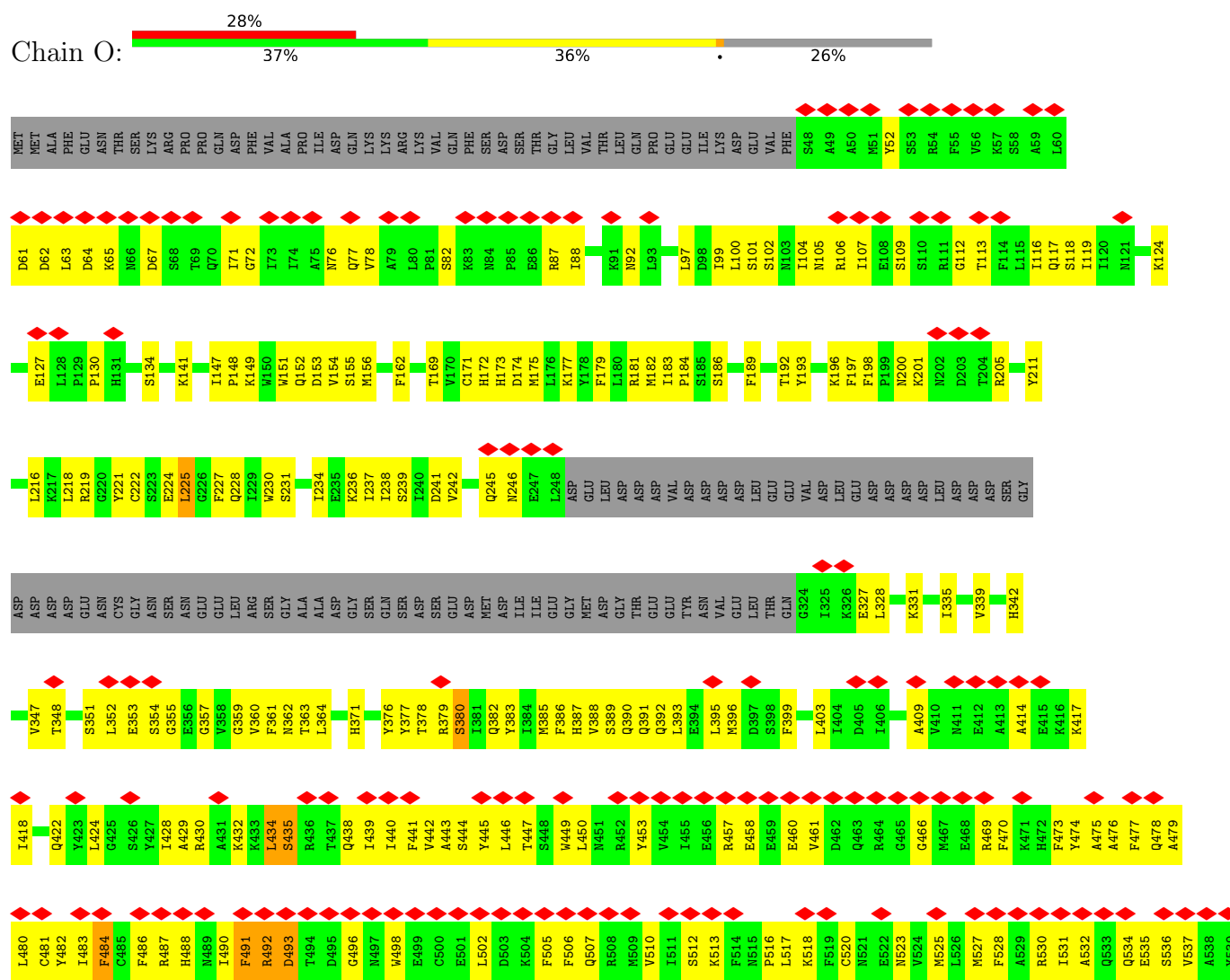
Chain M: 

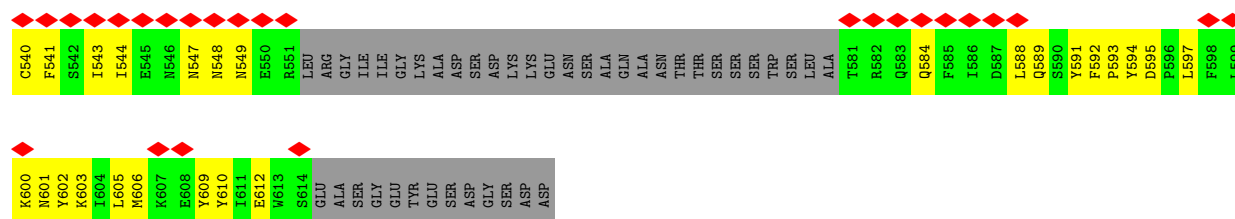


- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

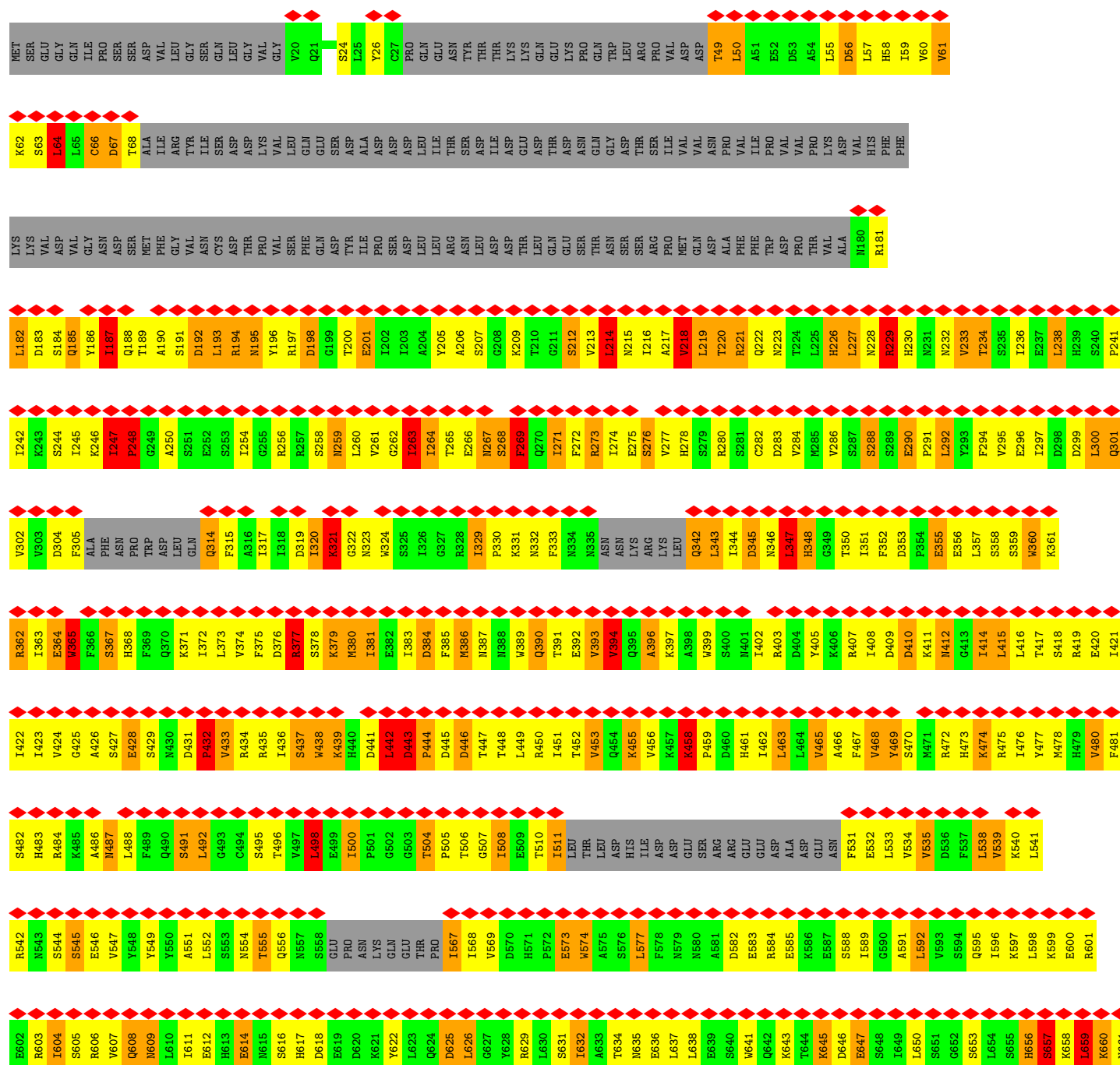


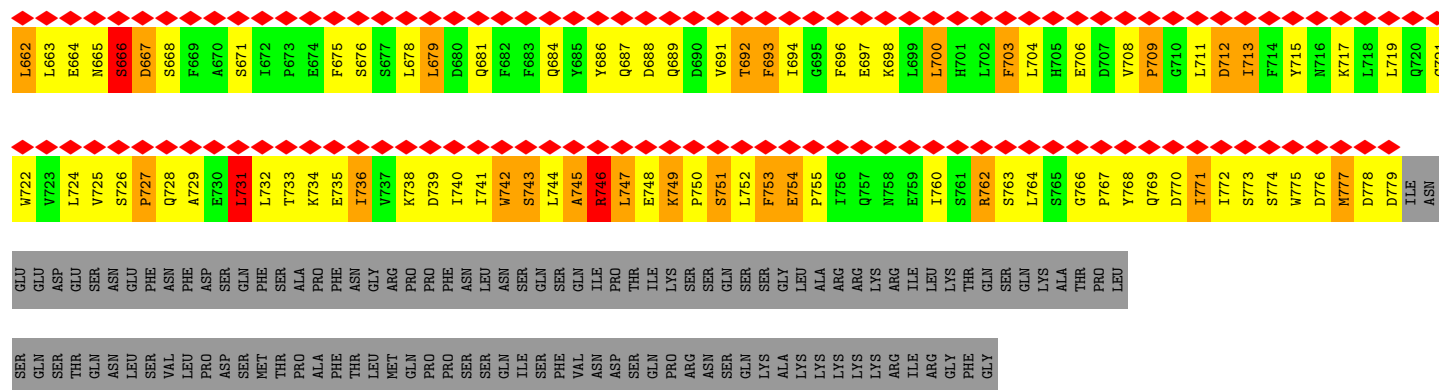
- Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3



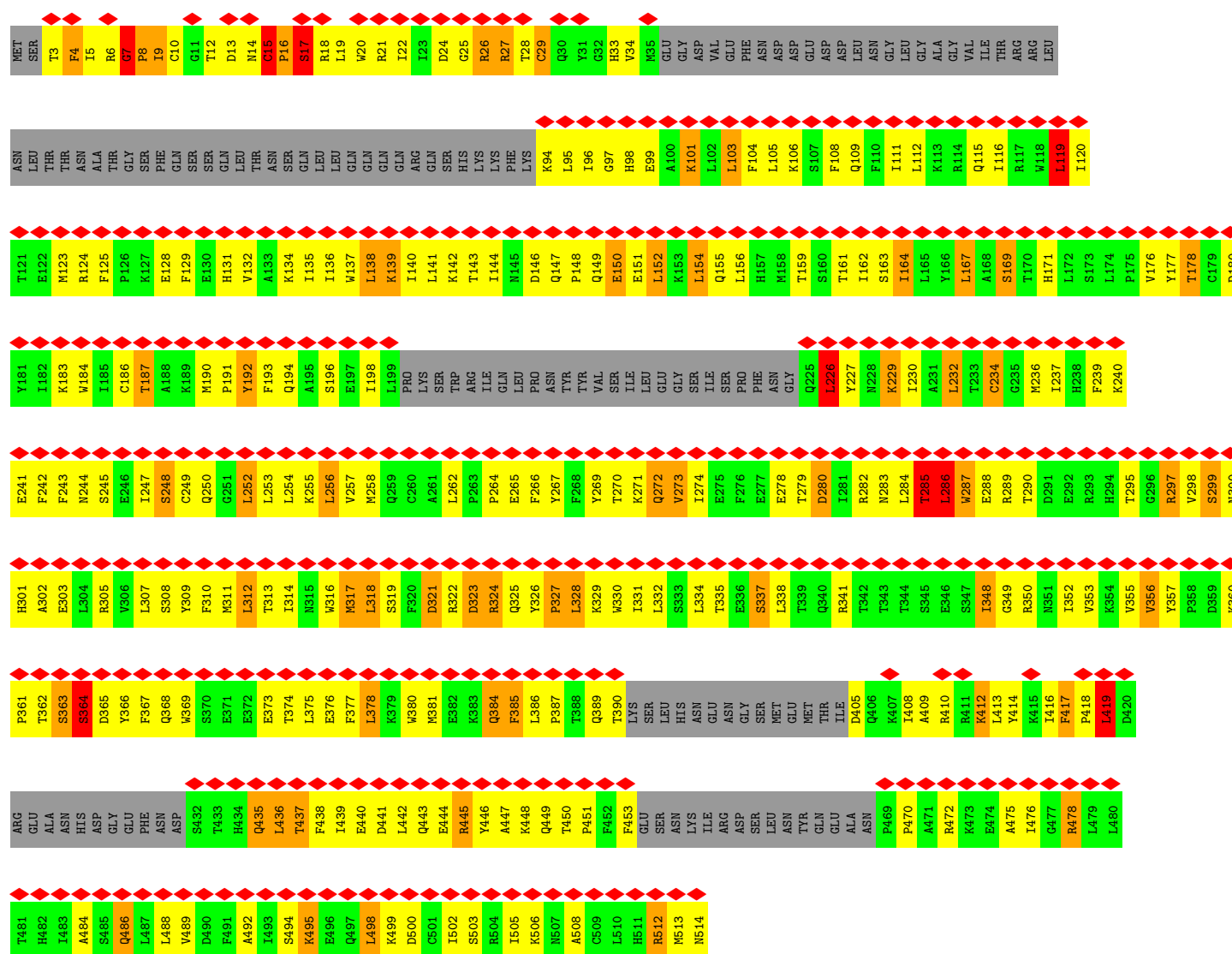
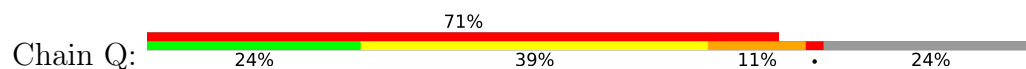


• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

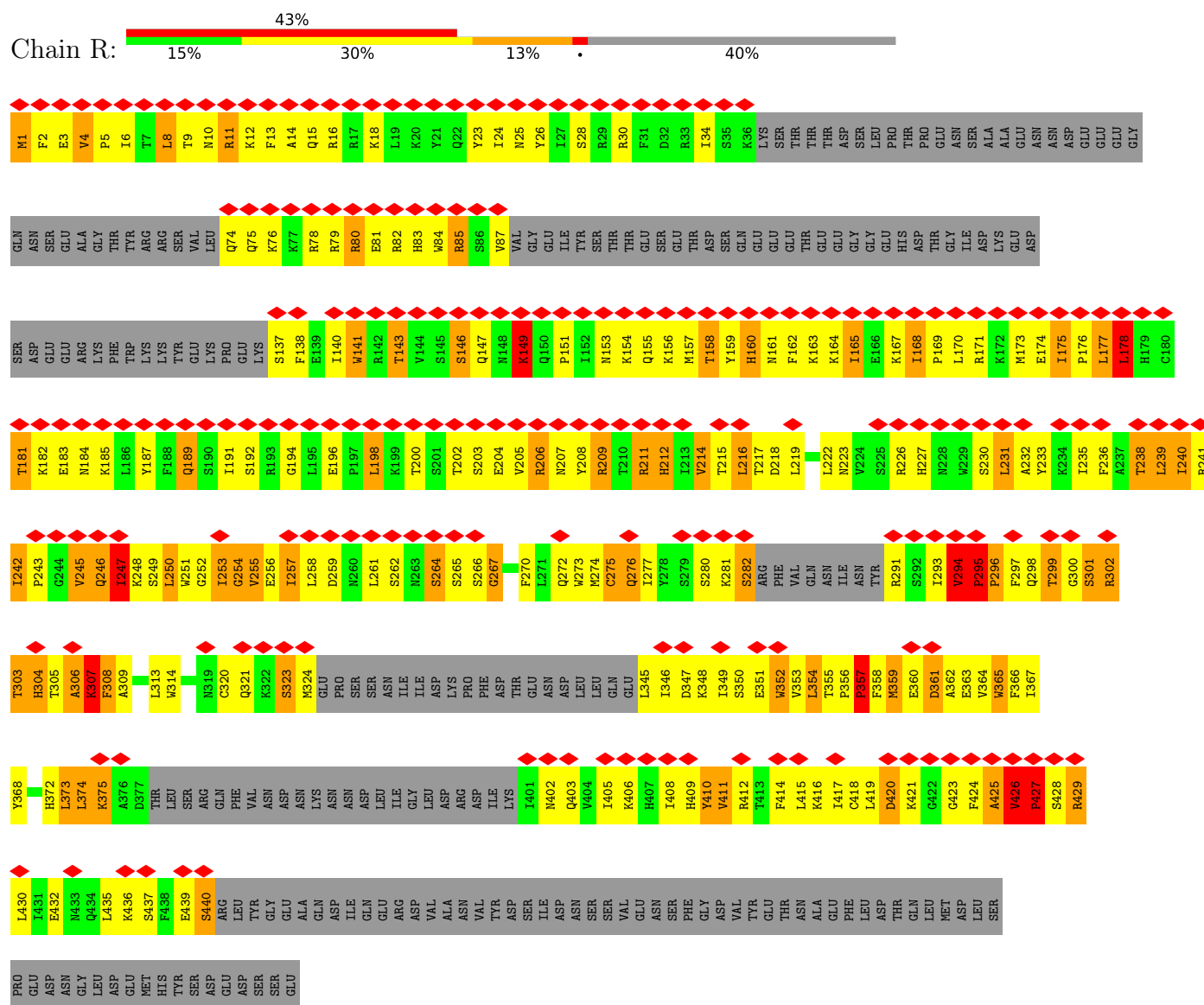




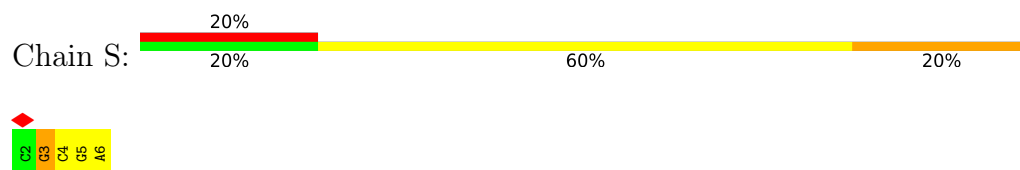
• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7



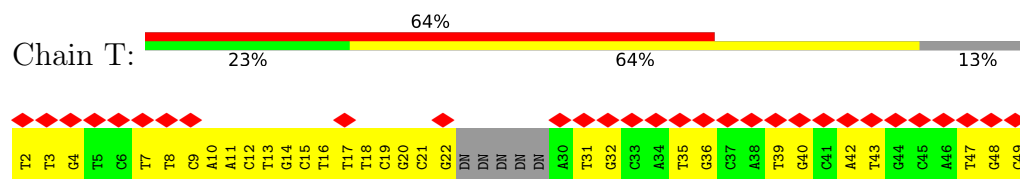
• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11



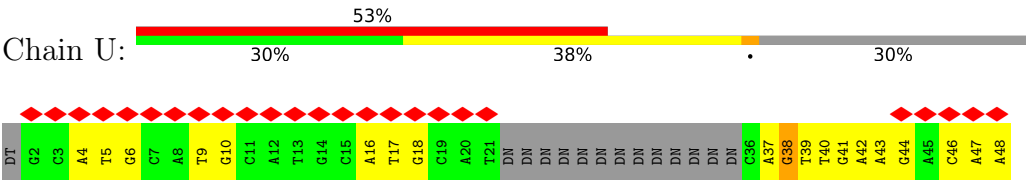
- Molecule 19: product RNA



- Molecule 20: template DNA



- Molecule 21: non-template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345000	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.407	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	372.9, 372.9, 372.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	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, SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/11738	0.53	0/15851
2	B	0.52	0/9557	0.59	1/12918 (0.0%)
3	C	0.53	0/2475	0.54	0/3354
4	D	0.36	0/436	0.45	0/591
5	E	0.45	0/1771	0.49	0/2383
6	F	0.49	0/838	0.54	0/1129
7	G	0.42	0/1564	0.51	1/2127 (0.0%)
8	H	0.54	0/1070	0.55	0/1449
9	I	0.38	0/472	0.56	0/639
10	J	0.56	0/578	0.57	0/775
11	K	0.53	0/804	0.55	0/1083
12	L	0.52	0/354	0.57	0/468
13	M	0.41	0/872	0.51	0/1170
14	N	0.35	0/1049	0.50	0/1411
15	O	0.34	0/3897	0.44	0/5268
16	P	0.61	1/4857 (0.0%)	0.88	12/6572 (0.2%)
17	Q	0.65	2/3330 (0.1%)	0.91	9/4492 (0.2%)
18	R	0.52	0/2591	0.75	2/3483 (0.1%)
19	S	0.28	0/120	0.61	0/185
20	T	0.53	0/707	0.83	0/1076
21	U	0.67	1/543 (0.2%)	0.95	0/823
All	All	0.51	4/49623 (0.0%)	0.63	25/67247 (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
16	P	0	18
17	Q	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	10
All	All	0	39

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	323	ASP	C-N	19.90	1.79	1.34
17	Q	356	VAL	C-N	-7.09	1.17	1.34
21	U	38	DG	C1'-N9	-6.35	1.38	1.47
16	P	247	ILE	C-N	5.97	1.45	1.34

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	819	ASP	C-N-CD	-28.25	58.44	120.60
17	Q	323	ASP	O-C-N	21.78	157.54	122.70
17	Q	323	ASP	CA-C-N	-17.00	79.80	117.20
17	Q	7	GLY	C-N-CD	-15.29	86.97	120.60
17	Q	323	ASP	C-N-CA	-14.08	86.50	121.70

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	P	218	VAL	Peptide
16	P	234	THR	Peptide
16	P	247	ILE	Peptide
16	P	256	ARG	Peptide
16	P	258	SER	Peptide

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	11526	0	11612	862	0
2	B	9350	0	9231	839	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2423	0	2412	122	0
4	D	431	0	428	16	0
5	E	1735	0	1764	70	0
6	F	823	0	841	52	0
7	G	1526	0	1540	73	0
8	H	1052	0	1021	42	0
9	I	466	0	466	55	0
10	J	569	0	585	45	0
11	K	793	0	790	41	0
12	L	352	0	375	22	0
13	M	856	0	855	46	0
14	N	1029	0	1061	57	0
15	O	3811	0	3802	243	0
16	P	4764	0	4711	528	0
17	Q	3254	0	3296	484	0
18	R	2535	0	2594	459	0
19	S	108	0	53	19	0
20	T	641	0	362	130	0
21	U	490	0	267	45	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	Q	1	0	0	0	0
23	A	1	0	0	0	0
24	B	5	0	0	2	0
All	All	48547	0	48066	3403	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 35.

The worst 5 of 3403 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)
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.66
2:B:116:ALA:H	18:R:282:SER:CB	1.05	1.65
17:Q:12:THR:HG21	17:Q:33:HIS:CE1	1.12	1.62
16:P:725:VAL:HG21	17:Q:446:TYR:CD1	1.14	1.60
17:Q:356:VAL:HG21	18:R:208:TYR:CD2	1.09	1.59

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%)	1307 (90%)	131 (9%)	9 (1%)	22	50
2	B	1171/1203 (97%)	1094 (93%)	61 (5%)	16 (1%)	9	31
3	C	303/335 (90%)	276 (91%)	26 (9%)	1 (0%)	37	66
4	D	50/137 (36%)	48 (96%)	2 (4%)	0	100	100
5	E	210/215 (98%)	199 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	92 (94%)	6 (6%)	0	100	100
7	G	189/326 (58%)	180 (95%)	9 (5%)	0	100	100
8	H	127/146 (87%)	123 (97%)	4 (3%)	0	100	100
9	I	61/125 (49%)	52 (85%)	8 (13%)	1 (2%)	8	29
10	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
13	M	106/415 (26%)	101 (95%)	5 (5%)	0	100	100
14	N	121/233 (52%)	112 (93%)	9 (7%)	0	100	100
15	O	457/627 (73%)	418 (92%)	36 (8%)	3 (1%)	19	47
16	P	573/894 (64%)	414 (72%)	113 (20%)	46 (8%)	1	5
17	Q	377/514 (73%)	311 (82%)	49 (13%)	17 (4%)	2	13
18	R	289/507 (57%)	219 (76%)	41 (14%)	29 (10%)	0	3
All	All	5787/7778 (74%)	5139 (89%)	526 (9%)	122 (2%)	8	24

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	819	ASP

Continued on next page...

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Mol	Chain	Res	Type
2	B	820	PRO
2	B	954	PHE
2	B	1097	ASP
15	O	493	ASP

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%)	1271 (99%)	18 (1%)	62	77
2	B	1030/1053 (98%)	1017 (99%)	13 (1%)	65	78
3	C	269/296 (91%)	269 (100%)	0	100	100
4	D	52/116 (45%)	52 (100%)	0	100	100
5	E	194/197 (98%)	194 (100%)	0	100	100
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	171/291 (59%)	171 (100%)	0	100	100
8	H	115/128 (90%)	115 (100%)	0	100	100
9	I	55/110 (50%)	55 (100%)	0	100	100
10	J	64/65 (98%)	63 (98%)	1 (2%)	58	75
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
13	M	98/371 (26%)	98 (100%)	0	100	100
14	N	119/220 (54%)	119 (100%)	0	100	100
15	O	427/576 (74%)	420 (98%)	7 (2%)	58	75
16	P	543/828 (66%)	374 (69%)	169 (31%)	0	1
17	Q	364/476 (76%)	293 (80%)	71 (20%)	1	3
18	R	286/474 (60%)	209 (73%)	77 (27%)	0	1
All	All	5296/6990 (76%)	4940 (93%)	356 (7%)	16	38

5 of 356 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	192	TYR
18	R	85	ARG
17	Q	252	LEU
17	Q	378	LEU
18	R	181	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	117	GLN
17	Q	368	GLN
15	O	362	ASN
16	P	223	ASN
18	R	207	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S	3	G

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 9 ligands modelled in this entry, 8 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	$\# Z > 2$
24	SO4	B	1301	-	4,4,4	0.17	0	6,6,6	0.07	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
24	B	1301	SO4	2	0

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
17	Q	2
18	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	206:ARG	C	207:ASN	N	2.76
1	Q	323:ASP	C	324:ARG	N	1.79
1	Q	356:VAL	C	357:TYR	N	1.17

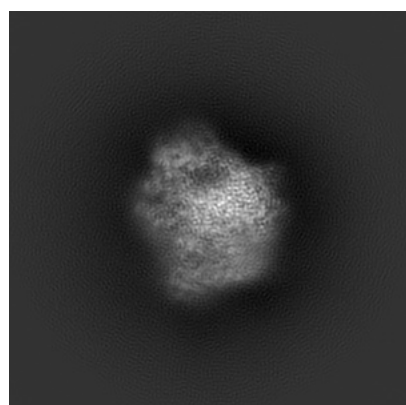
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3593. These allow visual inspection of the internal detail of the map and identification of artifacts.

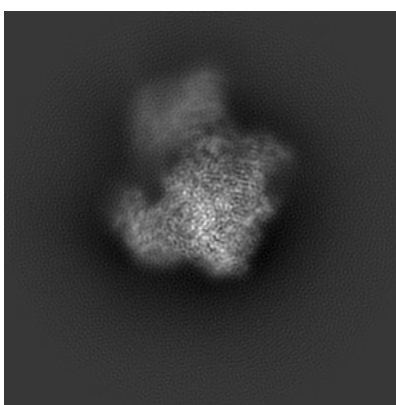
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

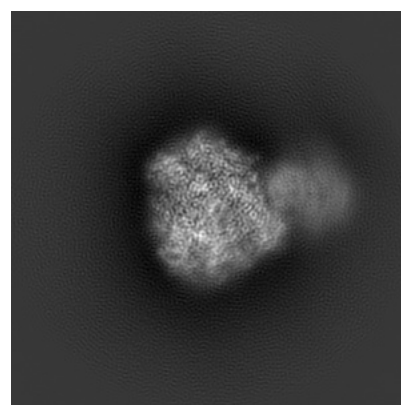
6.1.1 Primary map



X



Y

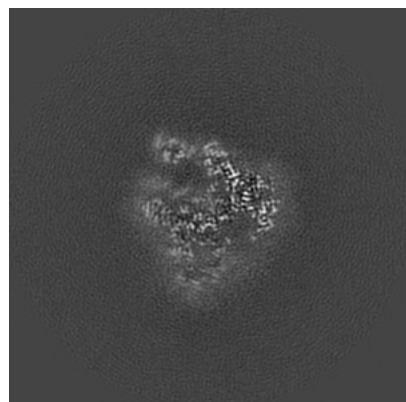


Z

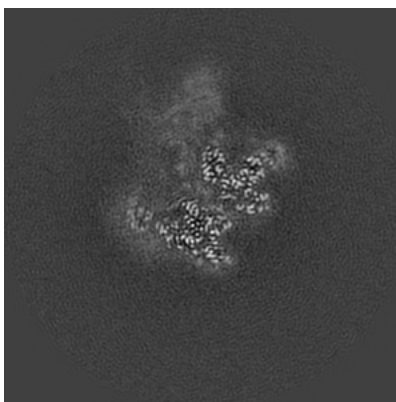
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

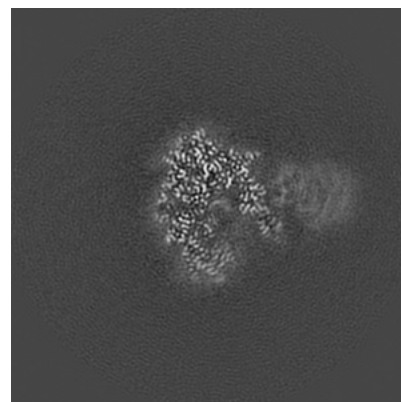
6.2.1 Primary map



X Index: 165



Y Index: 165

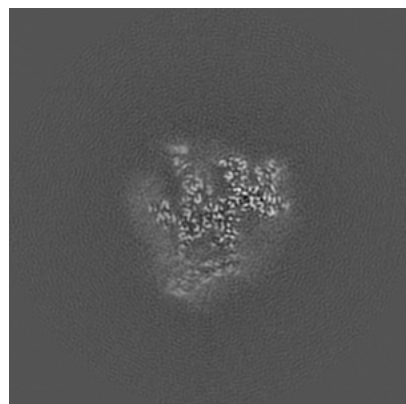


Z Index: 165

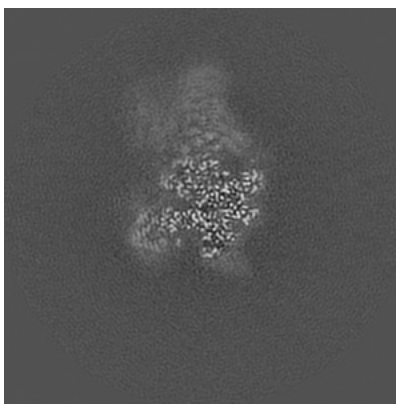
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

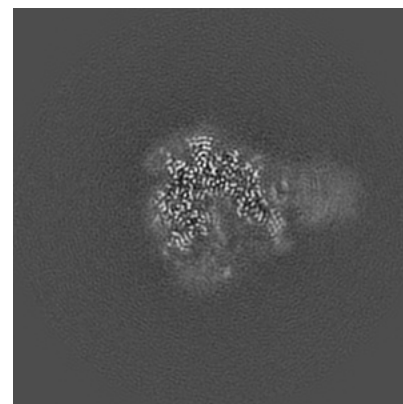
6.3.1 Primary map



X Index: 157



Y Index: 182

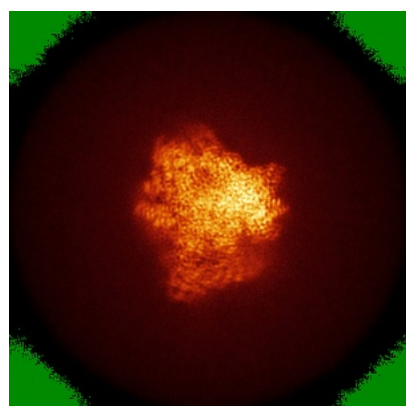


Z Index: 172

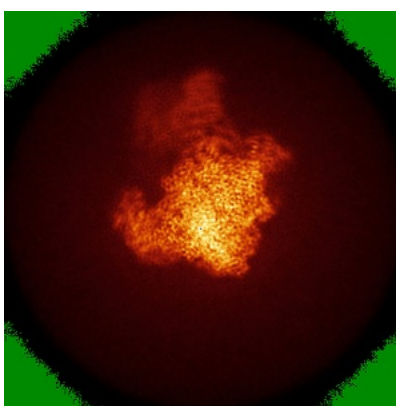
The images above show the largest variance slices of the map in three orthogonal directions.

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

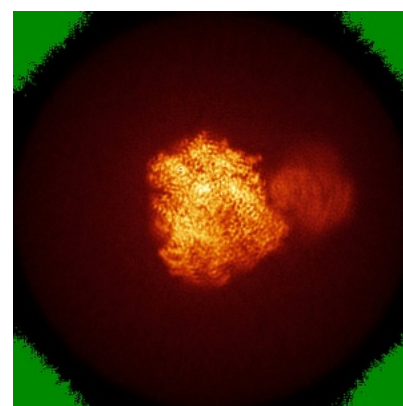
6.4.1 Primary map



X



Y

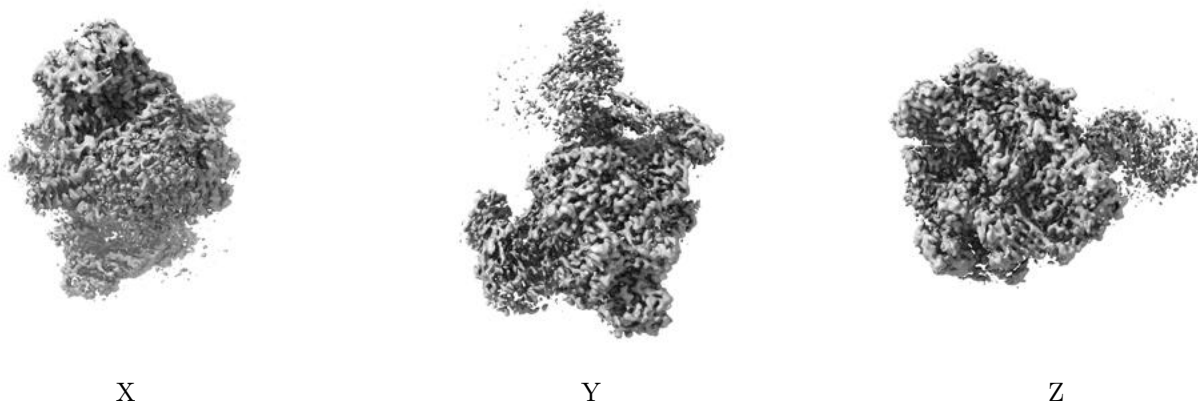


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

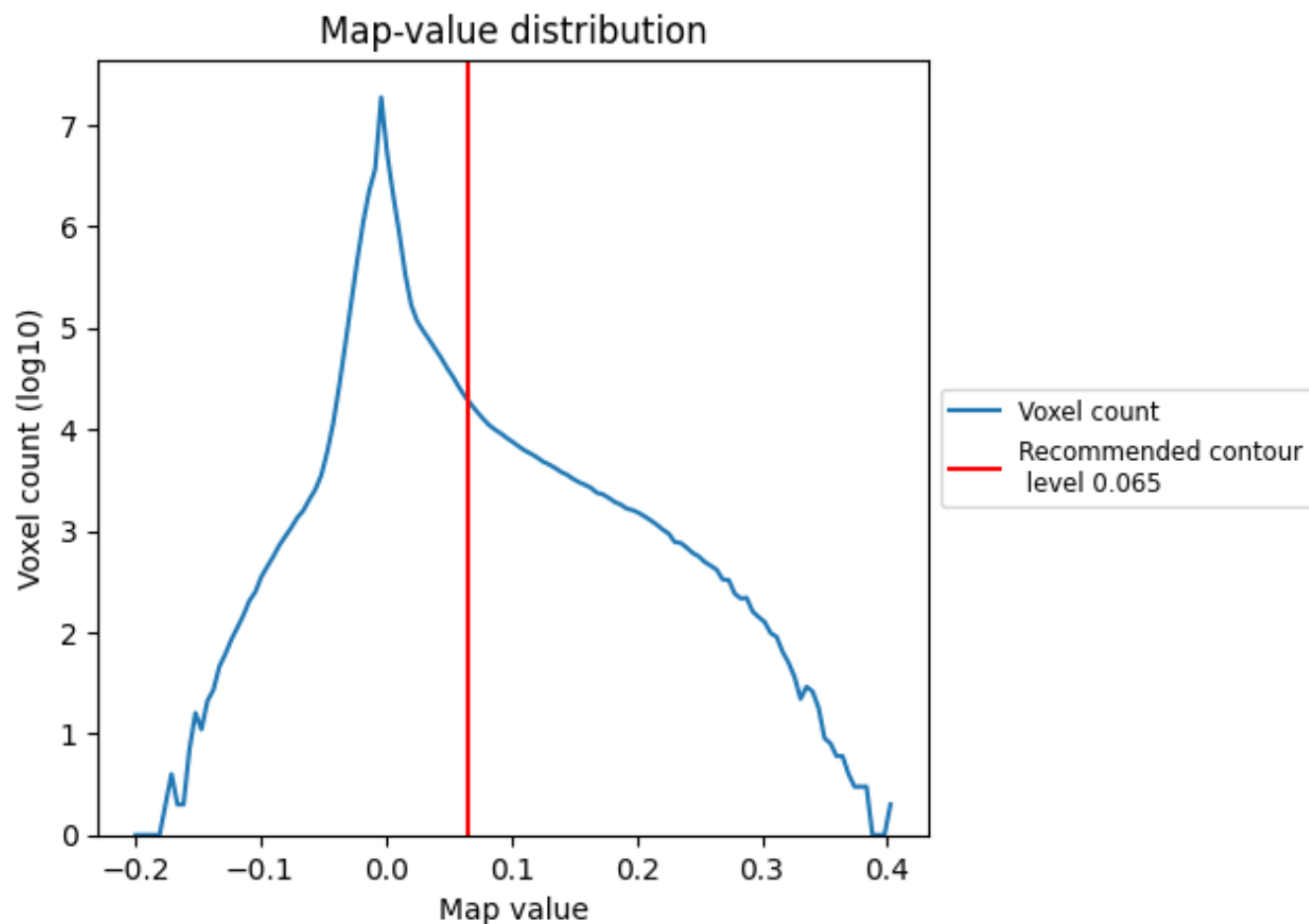
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

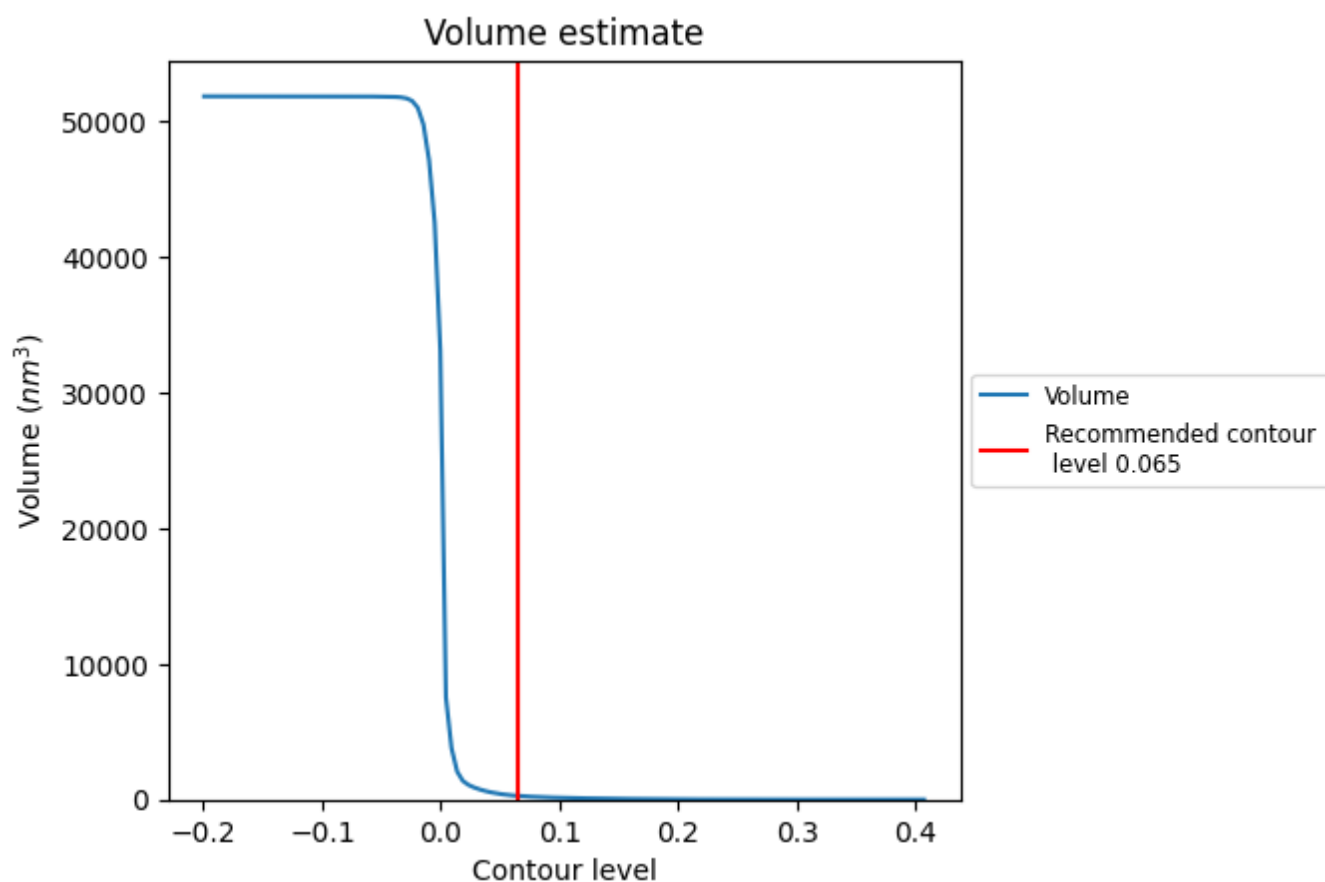
This section contains the results of statistical analysis of the map.

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.

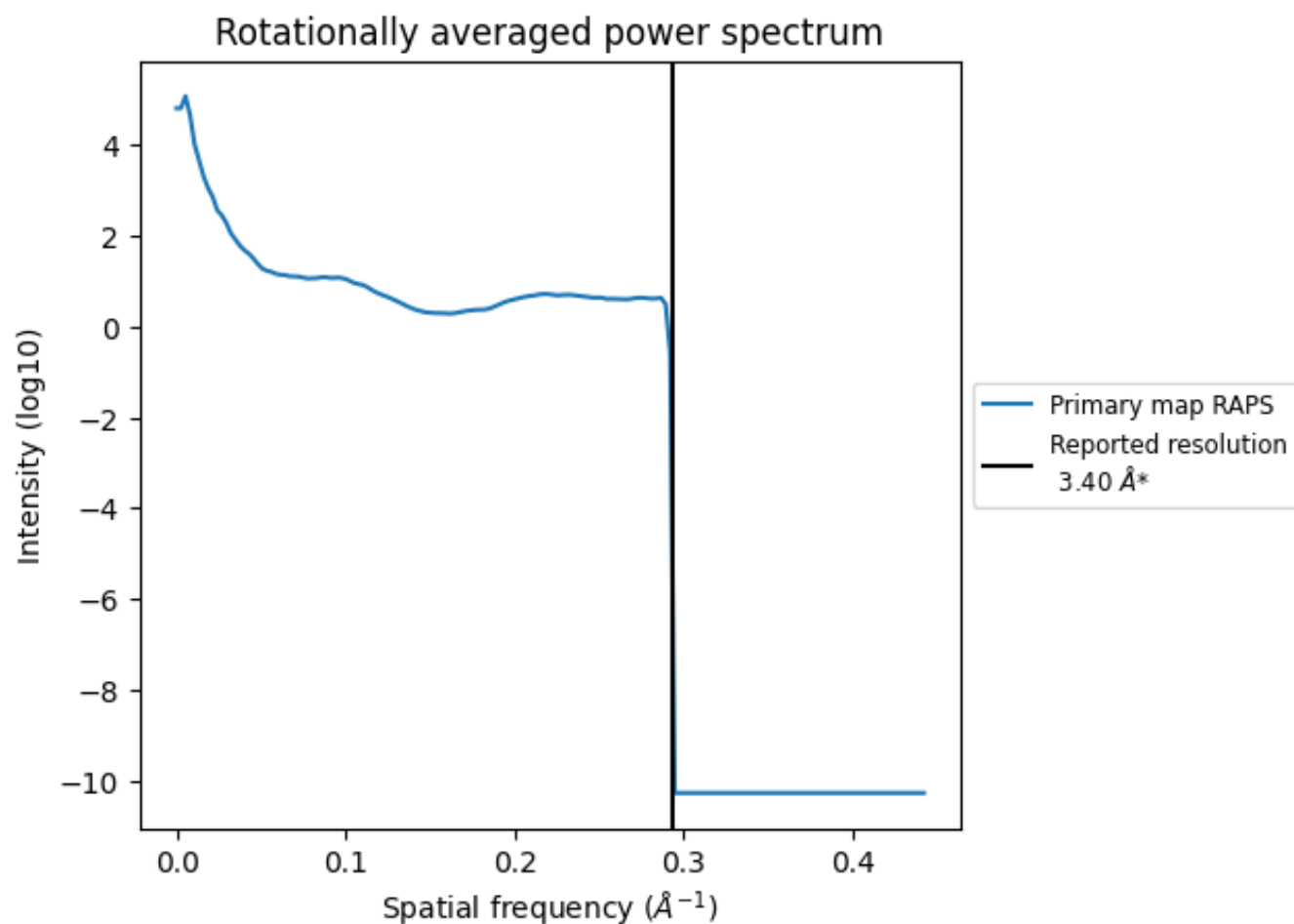
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 246 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 0.294 Å⁻¹

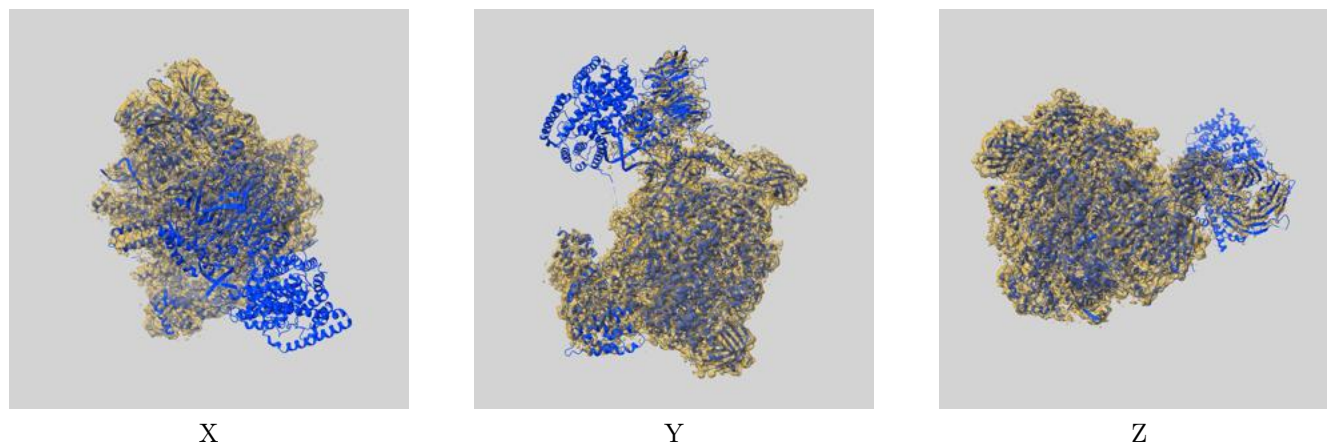
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

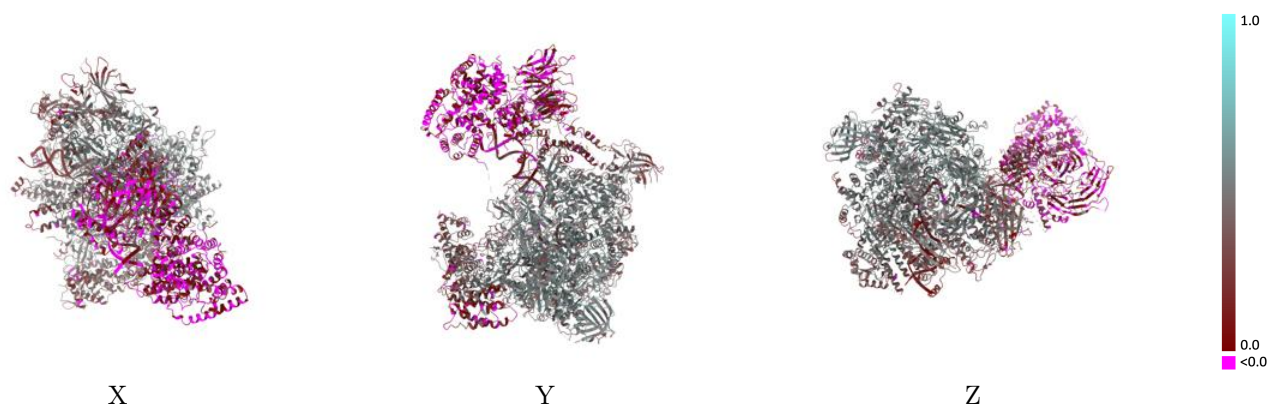
This section contains information regarding the fit between EMDB map EMD-3593 and PDB model 5N61. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



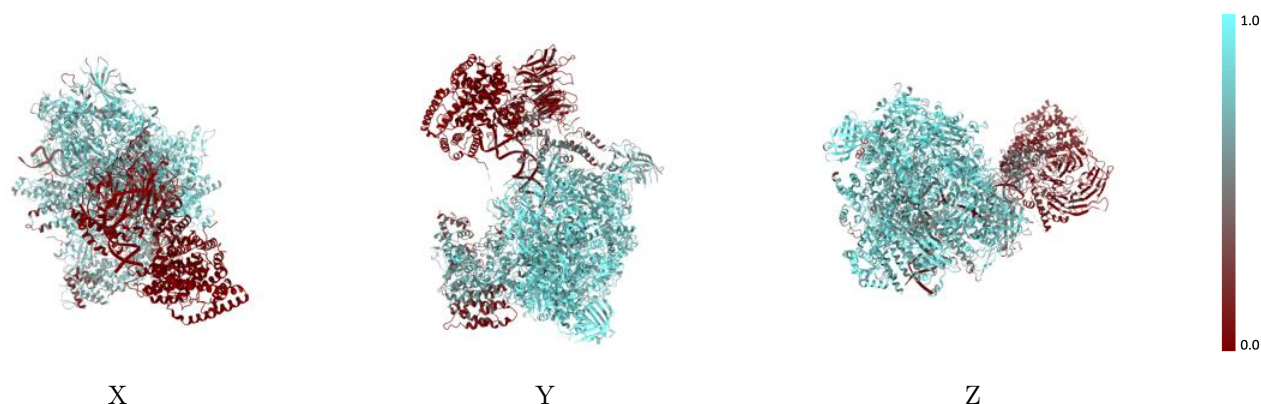
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



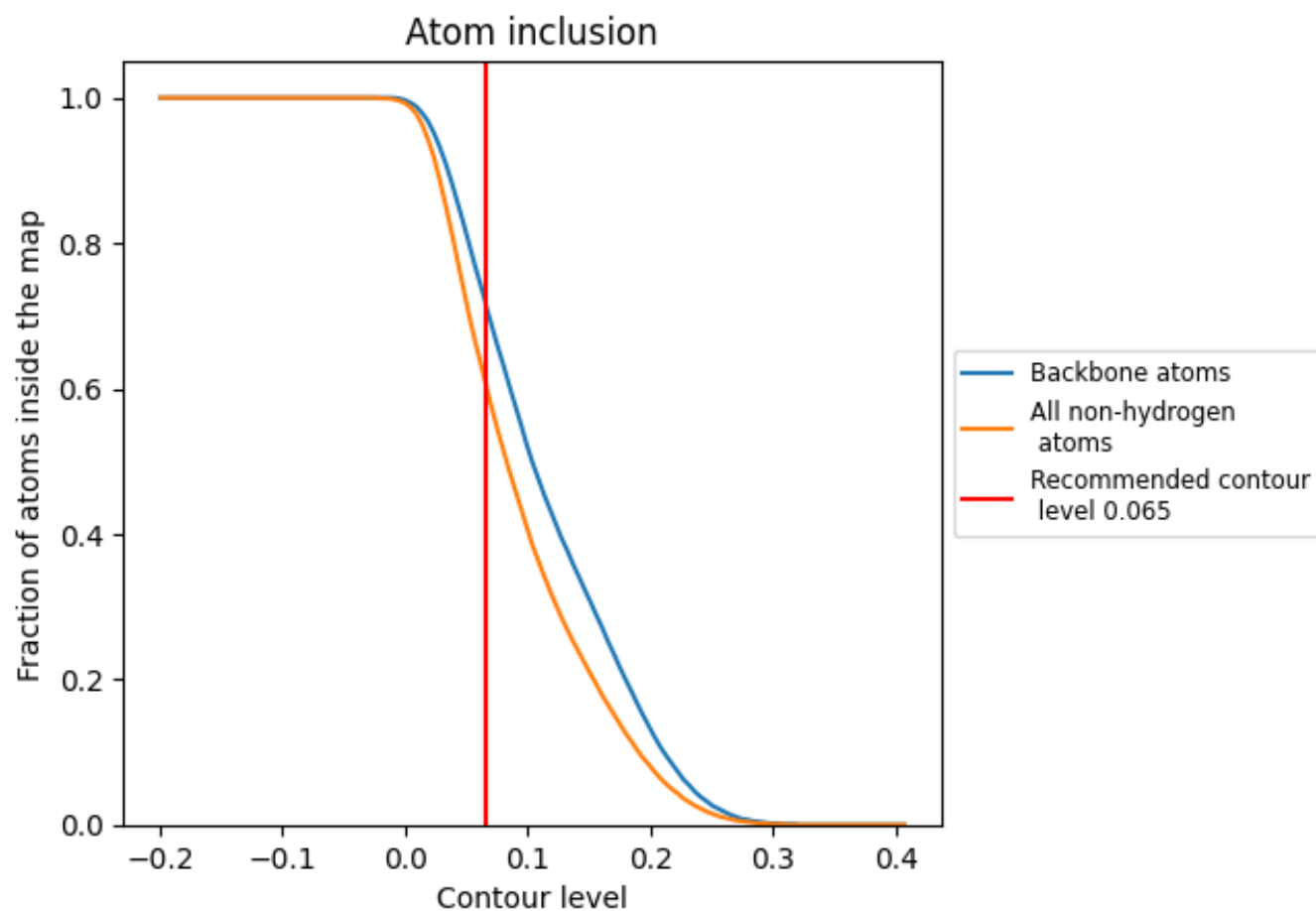
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.3430
A	 0.8020	 0.4510
B	 0.8260	 0.4740
C	 0.8760	 0.4830
D	 0.7380	 0.4080
E	 0.8300	 0.4280
F	 0.7960	 0.4770
G	 0.7100	 0.3960
H	 0.8800	 0.4860
I	 0.6880	 0.3020
J	 0.8970	 0.5110
K	 0.8430	 0.4840
L	 0.8380	 0.4670
M	 0.6350	 0.3390
N	 0.6270	 0.3470
O	 0.4820	 0.2610
P	 0.0550	 0.0410
Q	 0.0490	 0.0480
R	 0.2270	 0.1240
S	 0.4720	 0.2280
T	 0.2680	 0.1150
U	 0.2160	 0.1170

