wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 03:18 pm GMT

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)

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

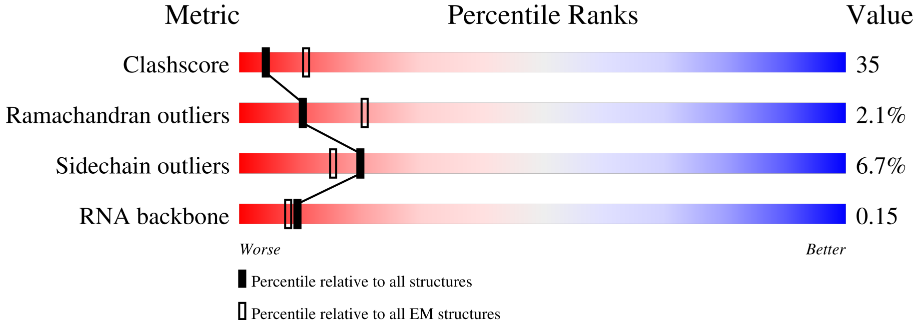
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

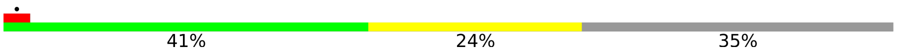
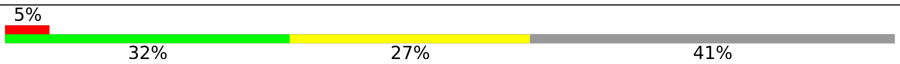
The reported resolution of this entry is 3.40 Å.

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

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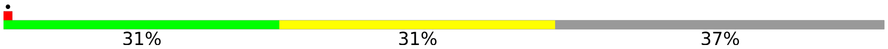
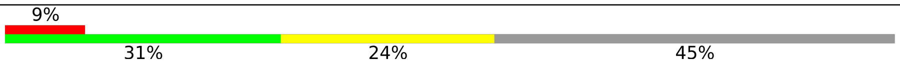
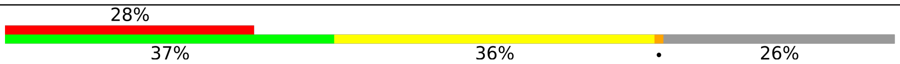
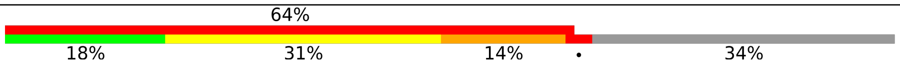
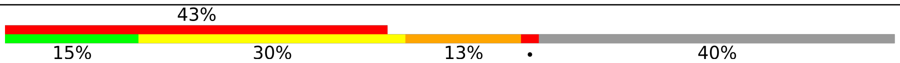
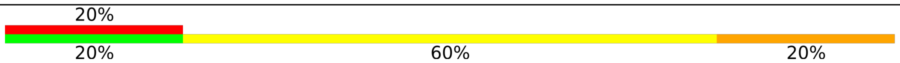
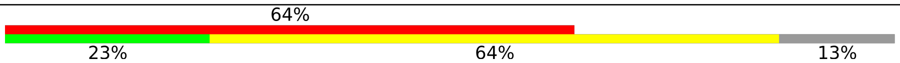
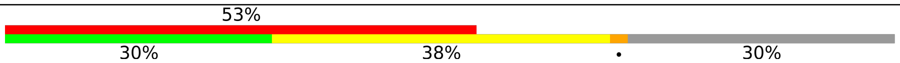
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	P	894	
17	Q	514	
18	R	507	
19	S	5	
20	T	47	
21	U	47	

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
			Total	C	N	O	S		
1	A	1459	11526	7281	2004	2180	61	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	1177	9350	5913	1639	1747	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	305	2423	1539	416	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	54	431	270	73	88	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	212	1735	1102	306	316	11	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	193	1526	985	262	274	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	131	1052	664	176	208	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	63	466	292	77	93	4	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	101	793	496	130	162	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	44	352	217	70	61	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	108	856	543	142	171	0	0

- 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 490 228 55 174 33	0	0

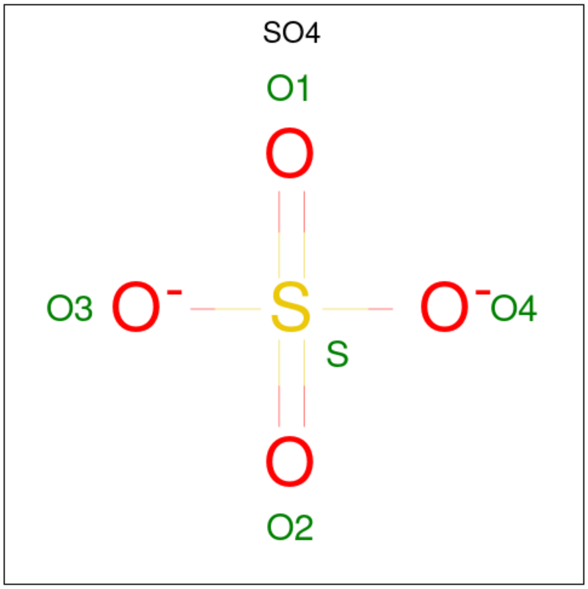
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 24 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

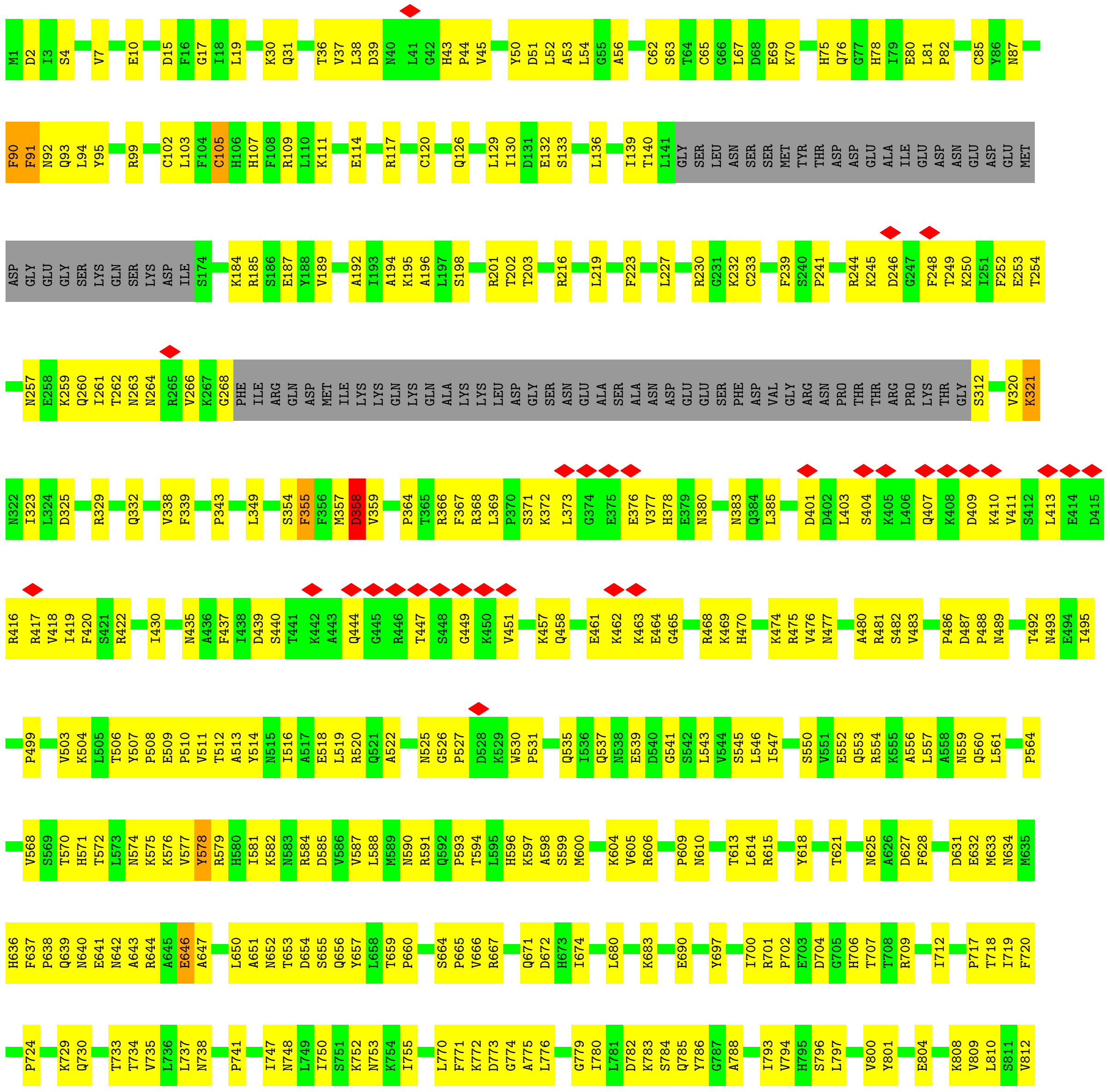


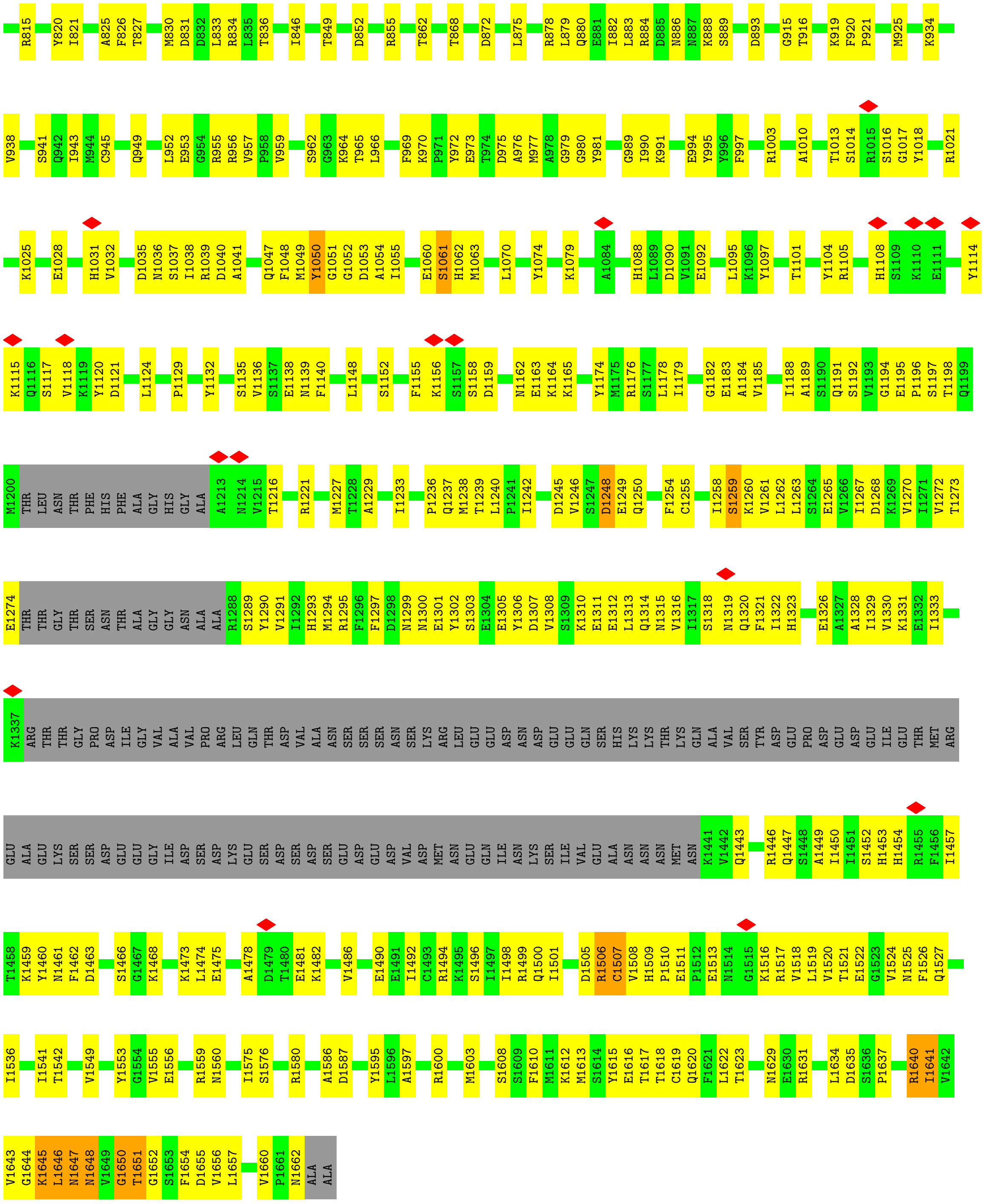
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total O S 5 4 1	0

3 Residue-property plots ⓘ

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

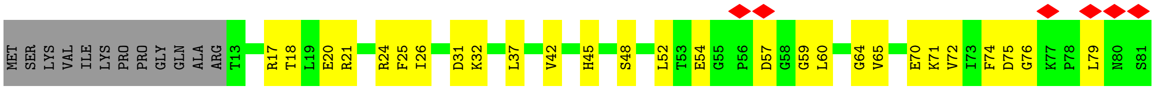
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

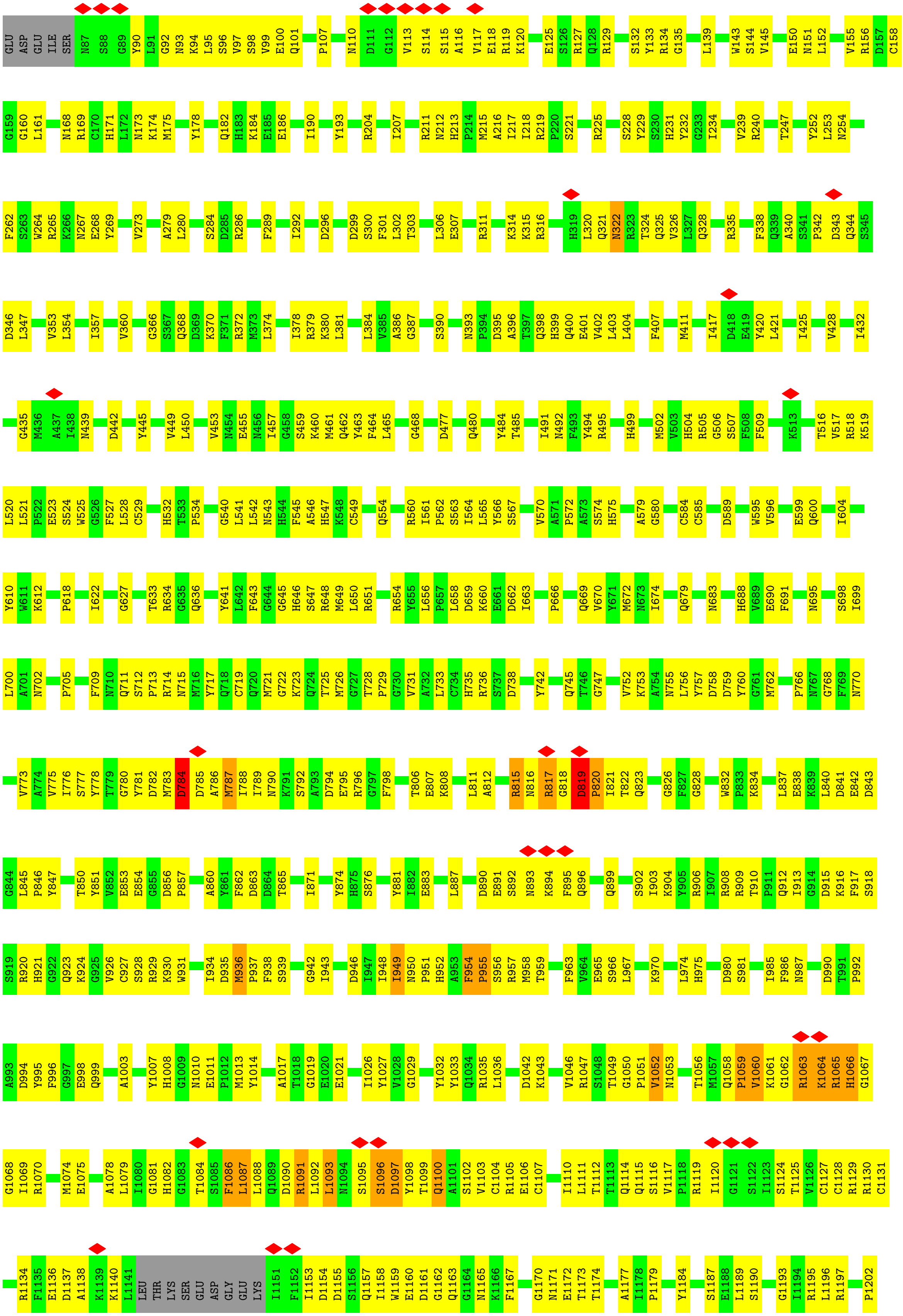




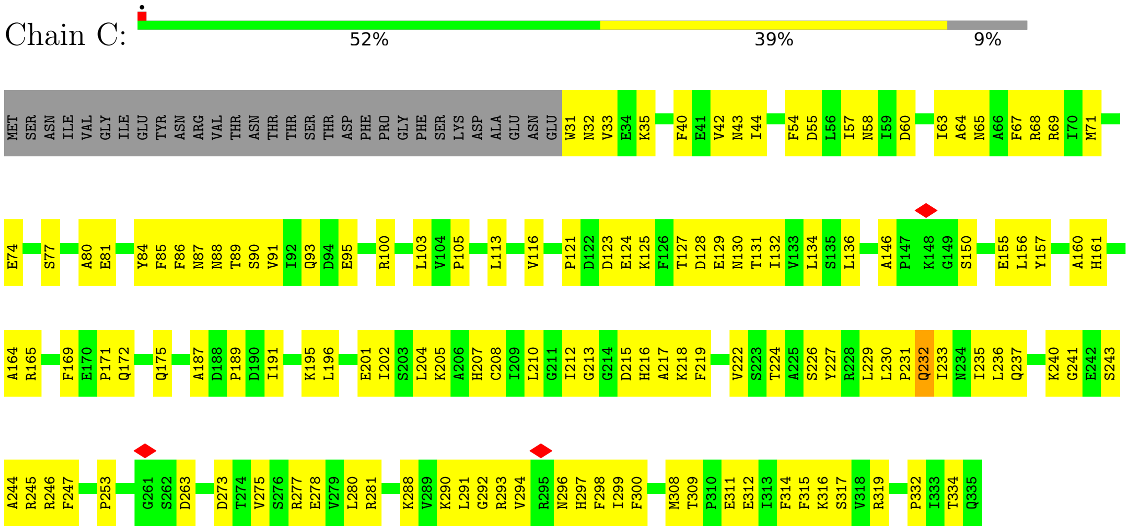
- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B:

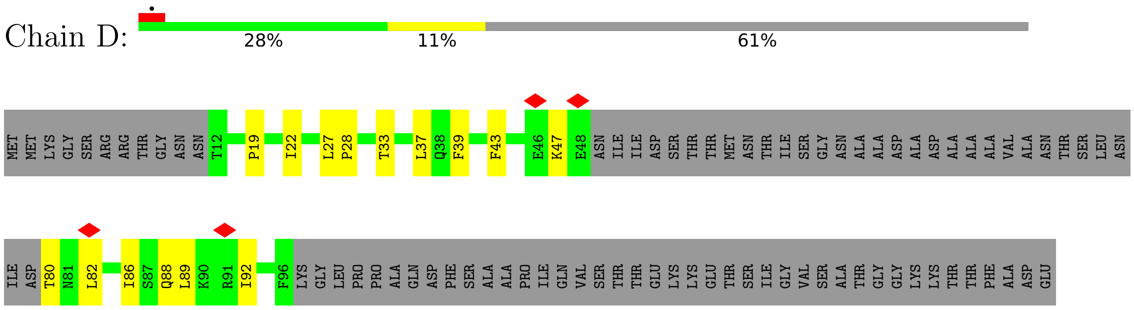



GLU ASP GLU ILE SER N87 S88 G89 Y90 L91 G92 N93 K94 L95 S96 V97 S98 V99 E100 Q101 P107 N110 D111 G112 V113 S114 S115 A116 V117 E118 R119 K120 E125 S126 R127 Q128 R129 S132 Y133 R134 G135 L139 W143 S144 V145 E150 N151 L152 V155 R156 D157 C158
G159 G160 L161 N168 R169 C170 H171 L172 N173 K174 M175 Y178 Q182 H183 K184 E185 E186 I190 Y193 R204 I207 R211 N212 H213 P214 M215 A216 I217 I218 R219 P220 S221 R225 S228 Y229 S230 H231 Y232 G233 I234 V239 R240 T247 Y252 L253 N254
F262 S263 W264 R265 K266 N267 E268 Y269 V273 A279 L280 S284 D285 R286 F289 I292 D296 D299 S300 F301 L302 T303 L306 E307 R311 K314 K315 R316 H319 L320 Q321 N322 R323 T324 Q325 V326 L327 Q328 R335 F338 Q339 A340 S341 P342 D343 Q344 S345
D346 L347 V353 L354 I357 V360 G366 S367 Q368 D369 K370 F371 R372 M373 L374 I378 R379 K380 L381 L384 V385 A386 G387 S390 N393 P394 D395 A396 T397 Q398 H399 Q400 E401 V402 L403 L404 F407 M411 I417 D418 E419 Y420 L421 I425 V428 I432
G435 M436 A437 I438 N439 D442 Y445 V449 L450 V453 N454 E455 N456 I457 G458 S459 K460 M461 Q462 Y463 F464 L465 G468 D477 Q480 Y484 T485 I491 N492 F493 Y494 R495 H499 M502 V503 H504 R505 G506 S507 F508 F509 K513 T516 V517 R518 K519
L520 L521 P522 E523 S524 W525 G526 F527 L528 C529 H532 T533 P534 G540 L541 L542 N543 H544 F545 A546 H547 K548 C549 Q554 R560 I561 P562 S563 I564 L565 Y566 S567 V570 A571 P572 A573 S574 H575 A579 G580 C584 C585 D589 W595 V596 E599 Q600 I604
Y610 W611 K612 P618 I622 G627 T633 R634 G635 Q636 Y641 L642 F643 G644 G645 H646 S647 R648 M649 L650 R651 R654 Y655 L656 P657 L658 D659 K660 E661 D662 I663 P666 Q669 V670 Y671 M672 N673 I674 Q679 N683 H688 V689 E690 F691 N695 S698 I699
L700 A701 N702 P705 F709 N710 Q711 S712 P713 R714 N715 M716 Y717 Q718 C719 Q720 M721 G722 K723 Q724 T725 M726 G727 T728 P729 G730 V731 A732 L733 C734 H735 R736 S737 D738 Y742 Q745 T746 G747 V752 K753 A754 N755 L756 Y757 D758 D759 Y760 G761 M762 P766 N767 G768 F769 N770
V773 A774 V775 I776 S777 Y778 T779 G780 Y781 D782 M783 D784 D785 A786 M787 I788 I789 N790 K791 S792 A793 D794 E795 R796 G797 F798 T806 E807 K808 L811 A812 R815 N816 R817 G818 D819 P820 I821 T822 Q823 G826 F827 G828 W832 P833 K834 L837 E838 K839 L840 D841 E842 D843
G844 L845 P846 Y847 T850 Y851 V852 E853 E854 G855 D856 P857 A860 Y861 F862 D863 D864 T865 I871 Y874 H875 S876 Y881 I882 E883 L887 D890 E891 S892 N893 K894 F895 Q896 Q899 S902 I903 K904 Y905 R906 I907 R908 R909 T910 P911 Q912 I913 G914 D915 K916 F917 S918
S919 R920 H921 G922 Q923 K924 G925 V926 C927 S928 R929 K930 W931 I934 D935 M936 P937 F938 S939 G942 I943 D946 I947 I948 I949 N950 P951 H952 A953 F954 P955 S956 R957 M958 T959 F963 V964 E965 S966 L967 K970 L974 H975 D980 S981 I985 F986 N987 D990 T991 P992
A993 D994 Y995 F996 G997 E998 Q999 A1003 Y1007 H1008 G1009 N1010 E1011 P1012 M1013 Y1014 A1017 T1018 G1019 E1020 E1021 I1026 Y1027 V1028 G1029 Y1032 Y1033 Q1034 R1035 L1036 D1042 K1043 V1046 R1047 S1048 T1049 G1050 P1051 V1052 N1053 T1056 M1057 Q1058 P1059 V1060 K1061 G1062 R1063 K1064 R1065 H1066 G1067
G1068 I1069 R1070 M1074 E1075 A1078 L1079 I1080 G1081 H1082 G1083 T1084 S1085 F1086 L1087 L1088 Q1089 D1090 R1091 L1092 L1093 N1094 S1095 S1096 D1097 Y1098 T1099 Q1100 A1101 S1102 V1103 C1104 R1105 E1106 C1107 I1110 L1111 T1112 T1113 Q1114 Q1115 S1116 V1117 P1118 R1119 I1120 G1121 S1122 I1123 S1124 T1125 V1126 C1127 C1128 R1129 R1130 C1131
R1134 F1135 E1136 D1137 A1138 K1139 K1140 L1141 LEU THR LYS SER GLU ASP GLY GLU LYS I1151 F1152 I1153 D1154 D1155 S1156 Q1157 I1158 W1159 E1160 D1161 G1162 Q1163 G1164 N1165 K1166 F1167 G1170 N1171 E1172 T1173 T1174 A1177 I1178 P1179 Y1184 S1187 E1188 L1189 S1190 G1193 I1194 R1195 L1196 R1197 P1202

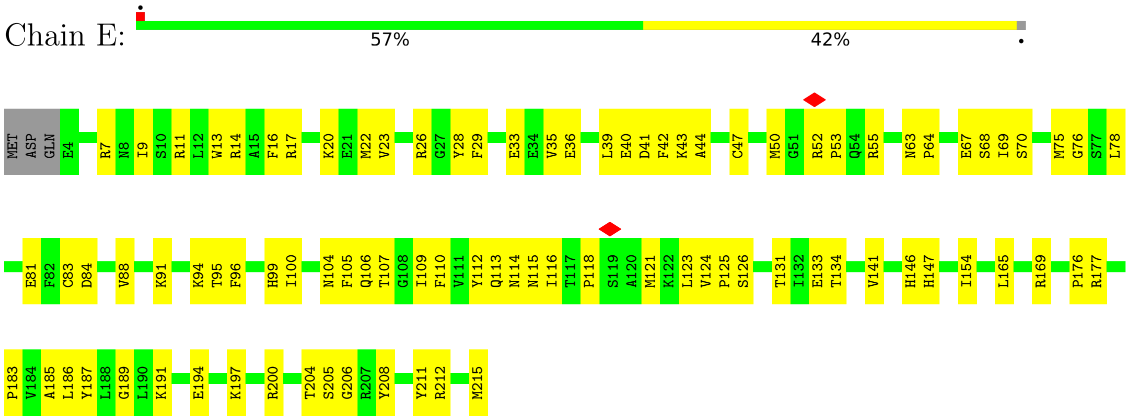
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



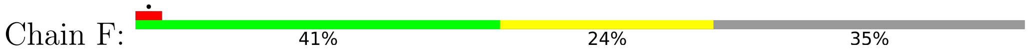
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

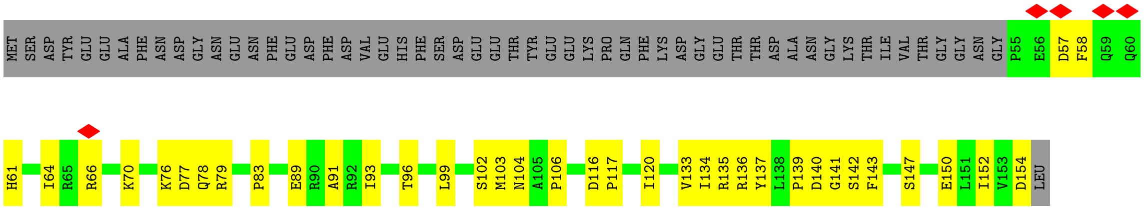


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

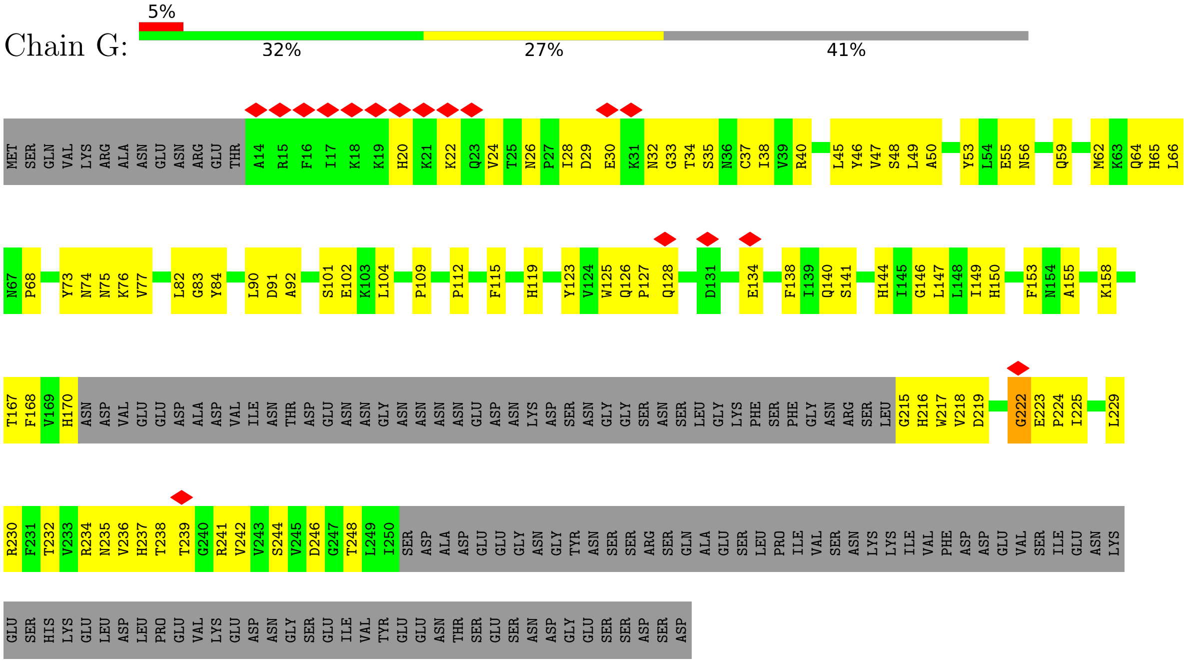


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

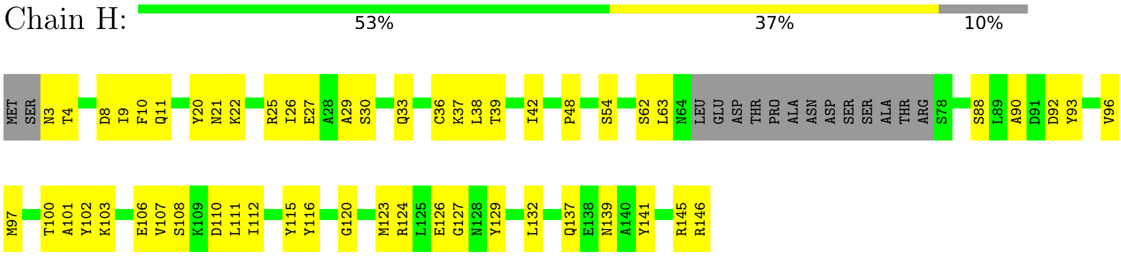




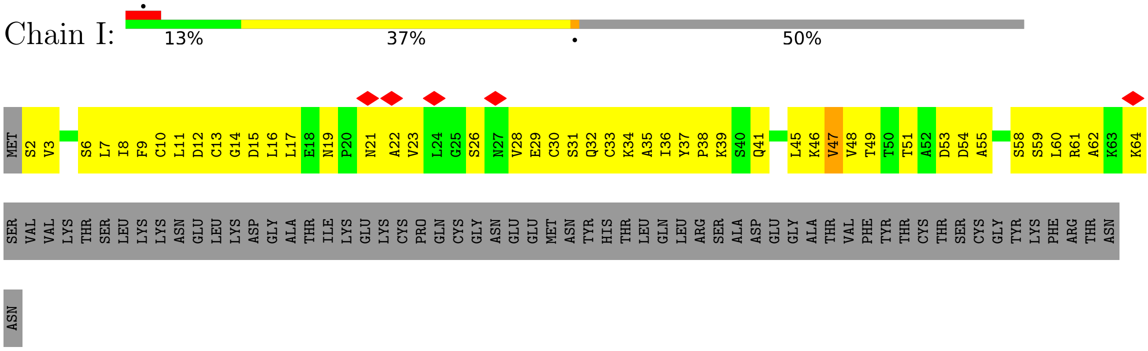
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



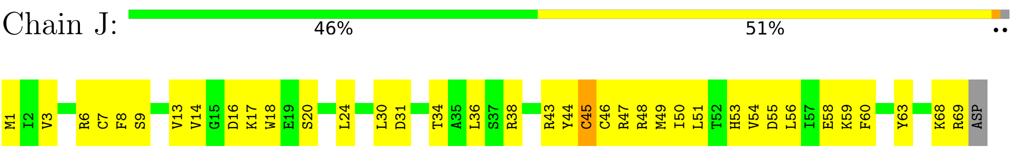
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



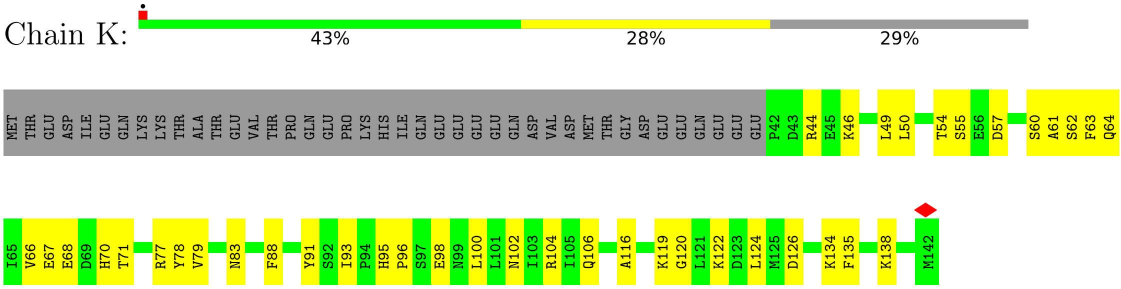
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



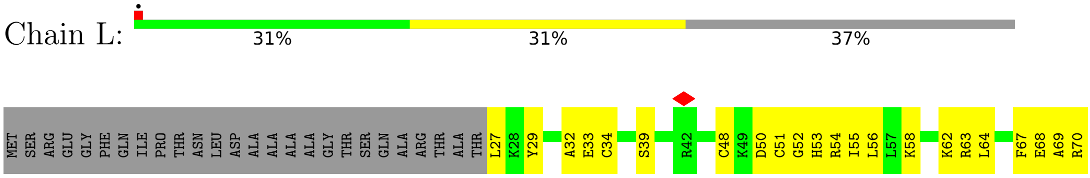
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



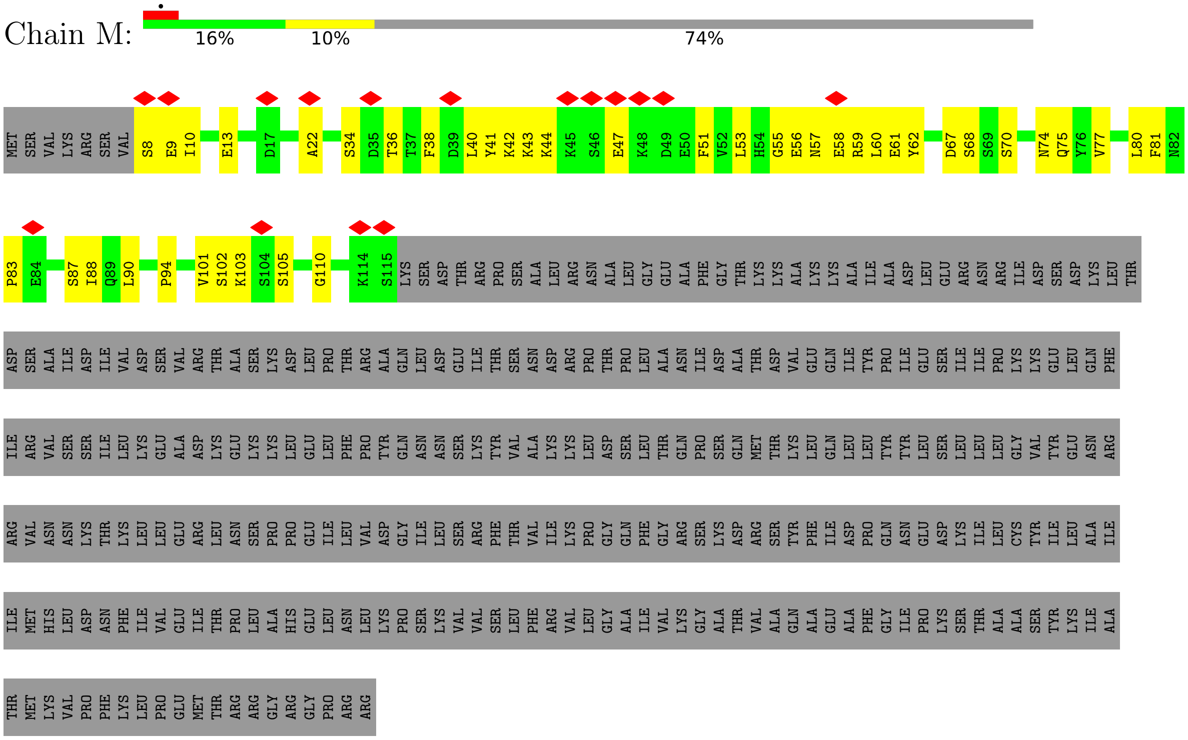
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



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

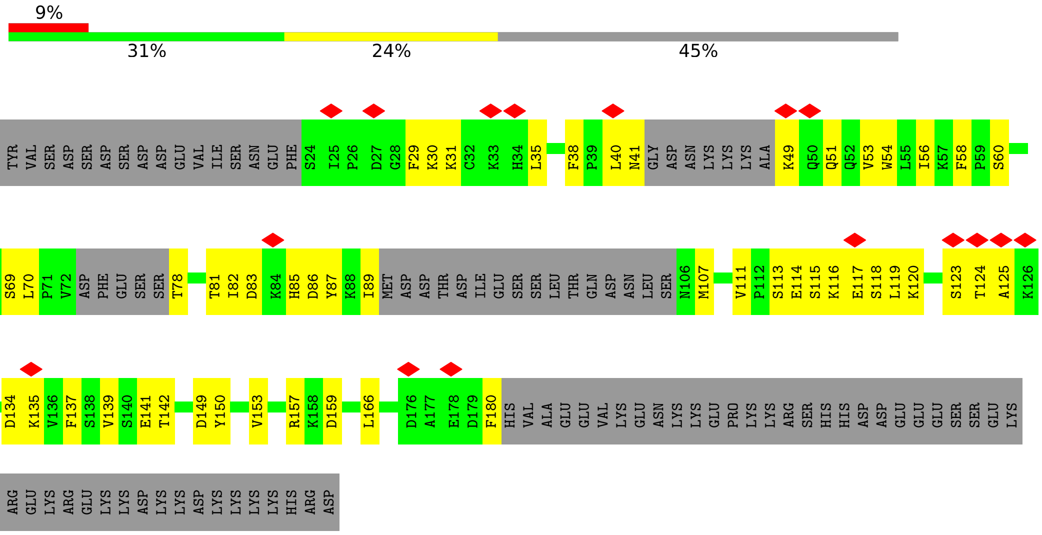


- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



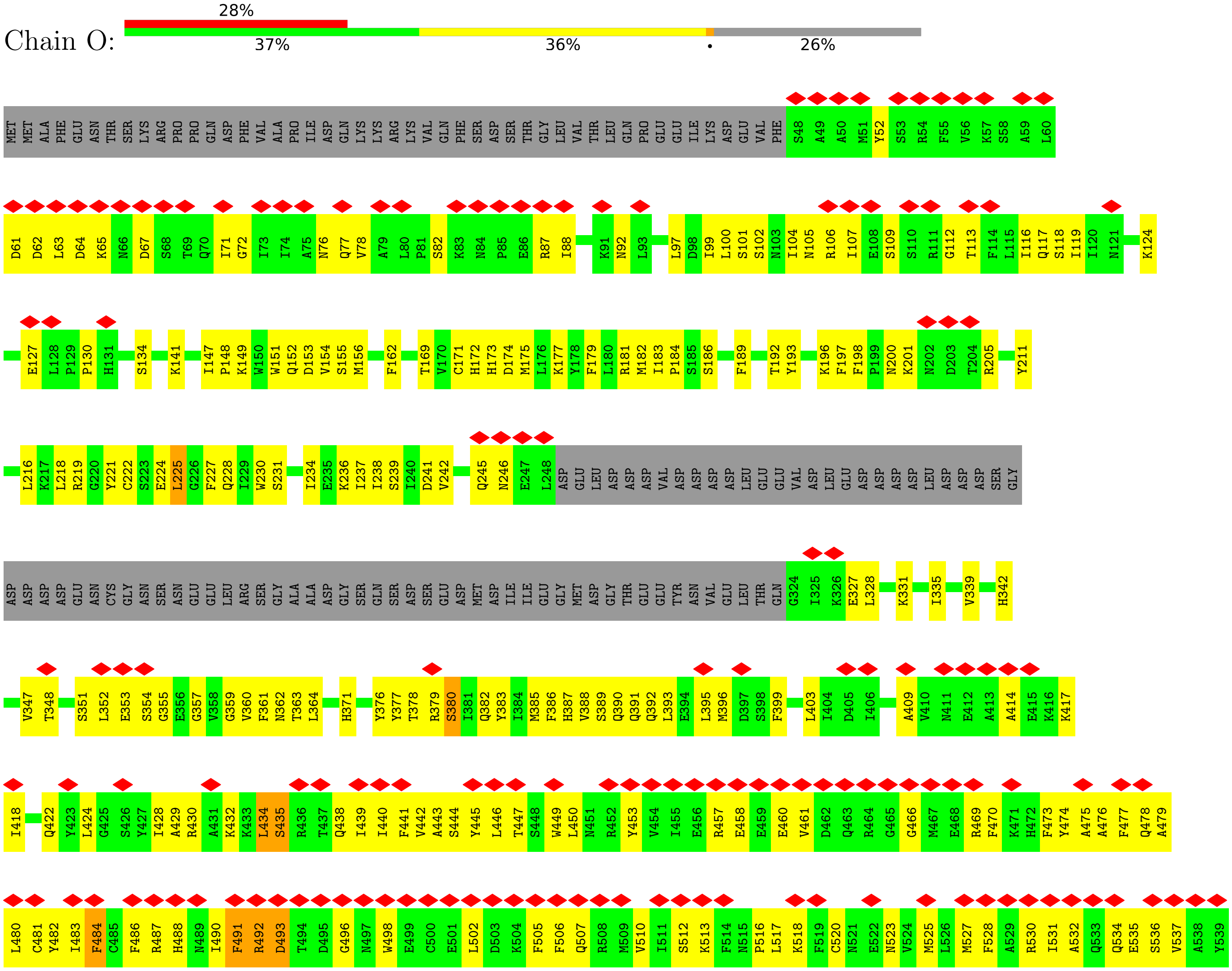
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

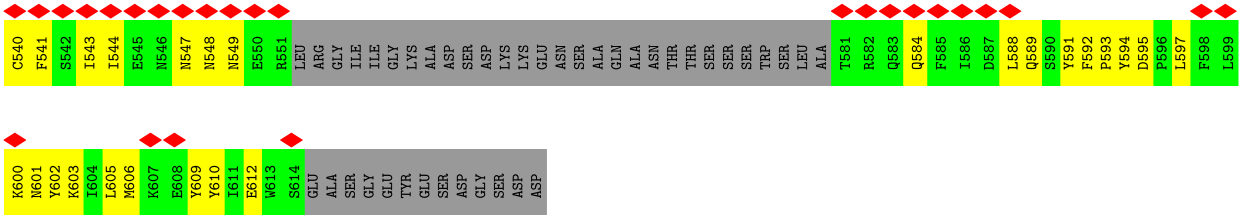
Chain N:



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

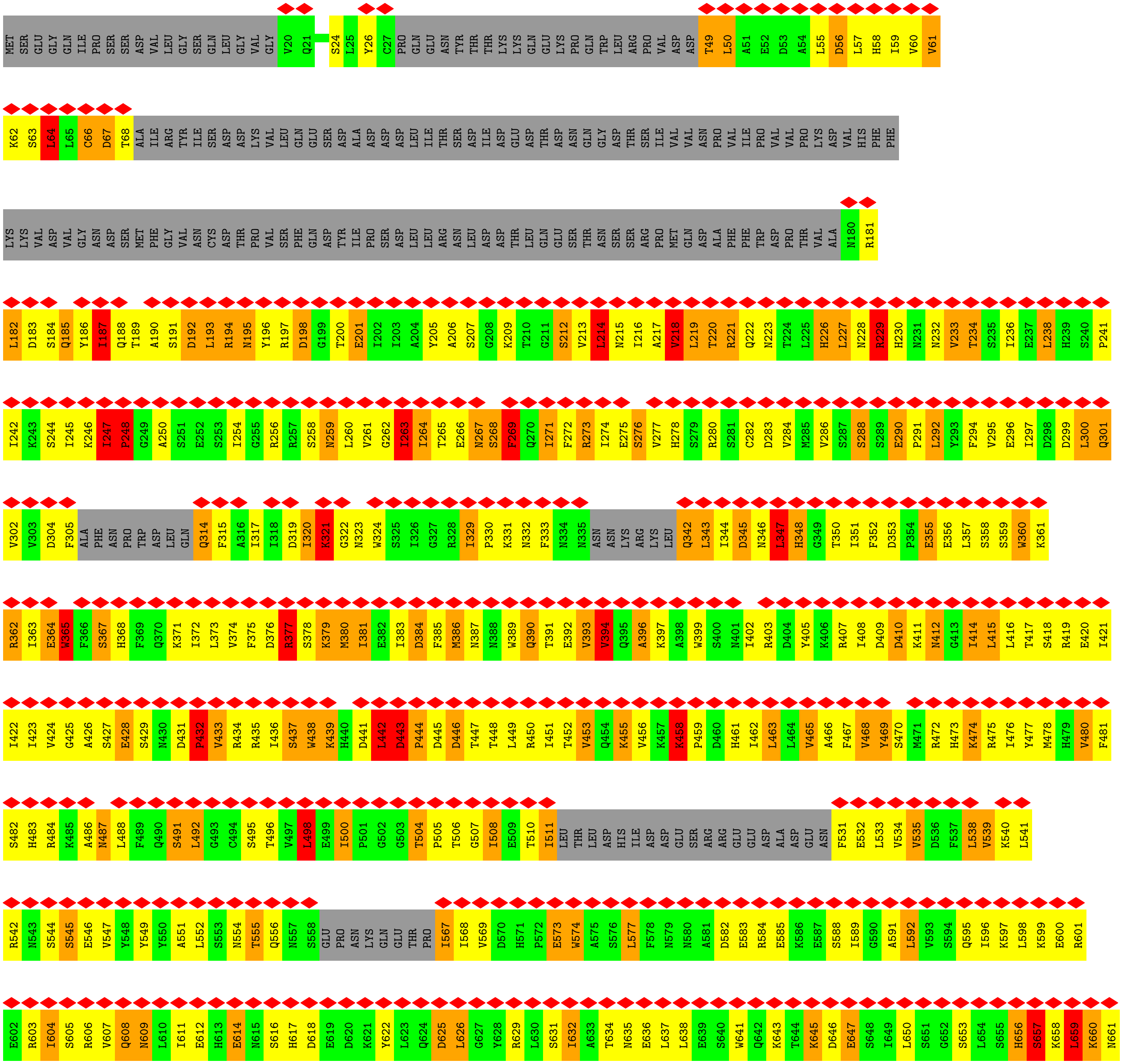
Chain O:

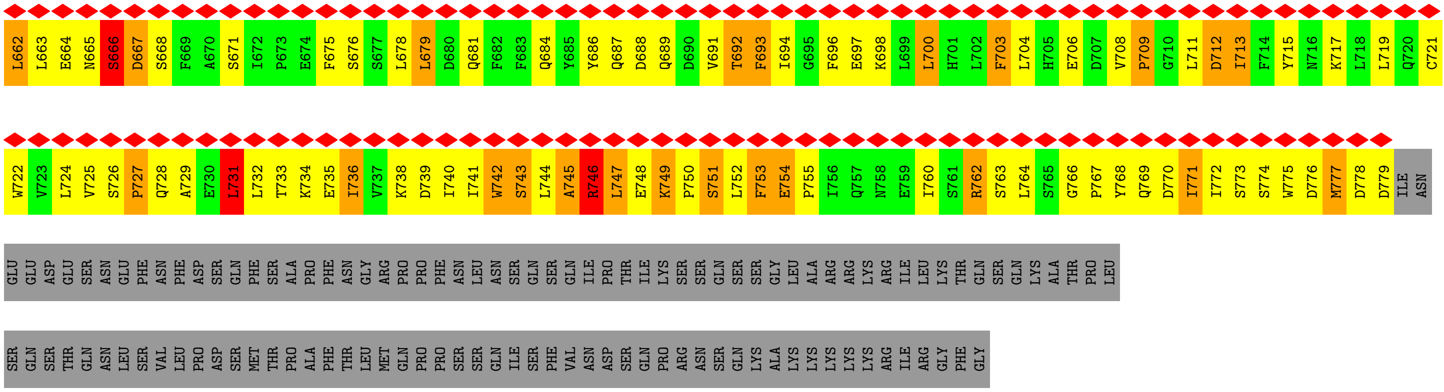




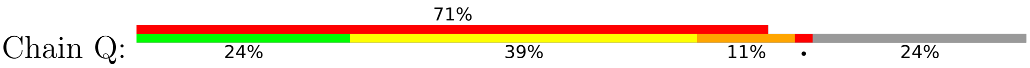
- Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

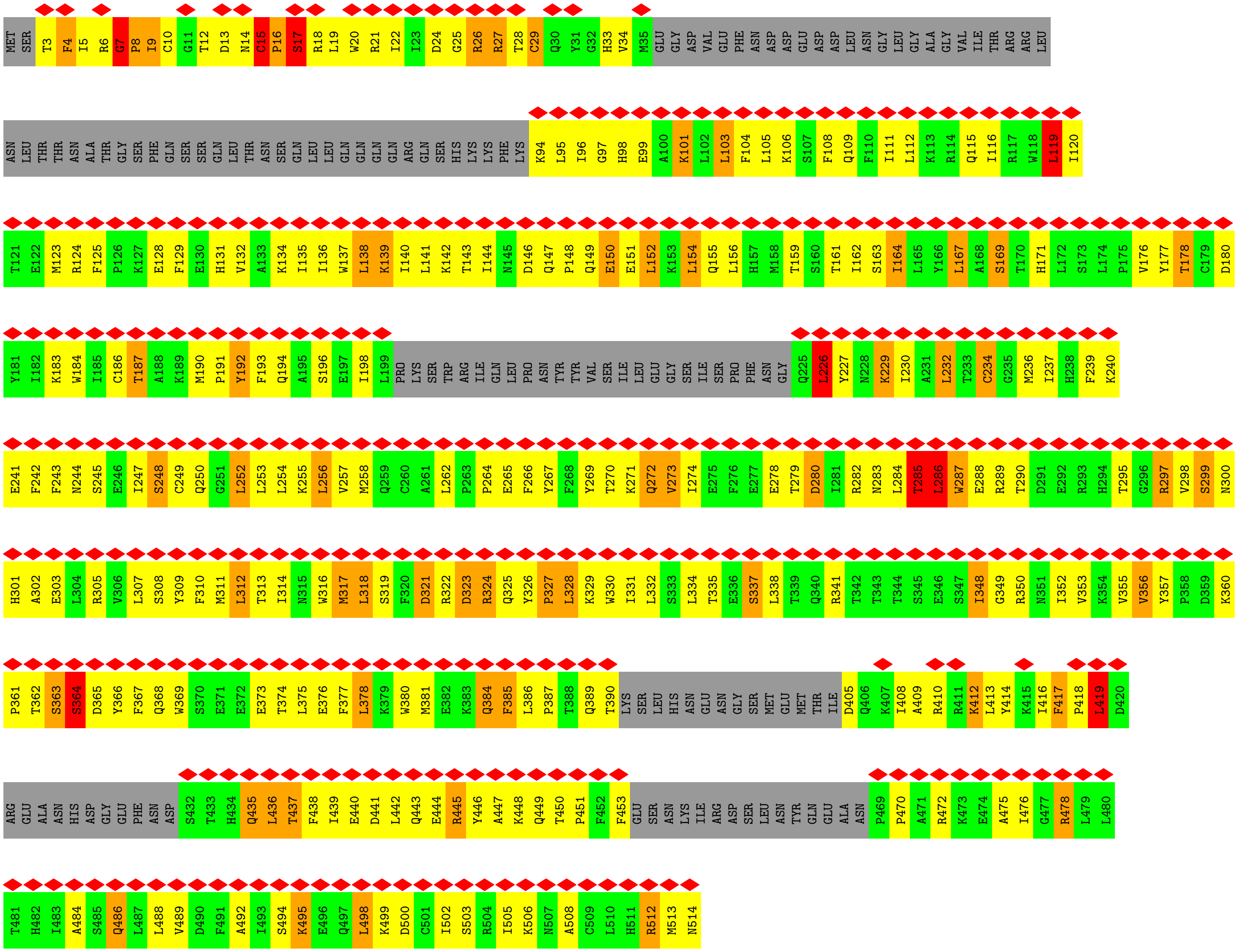
Chain P:



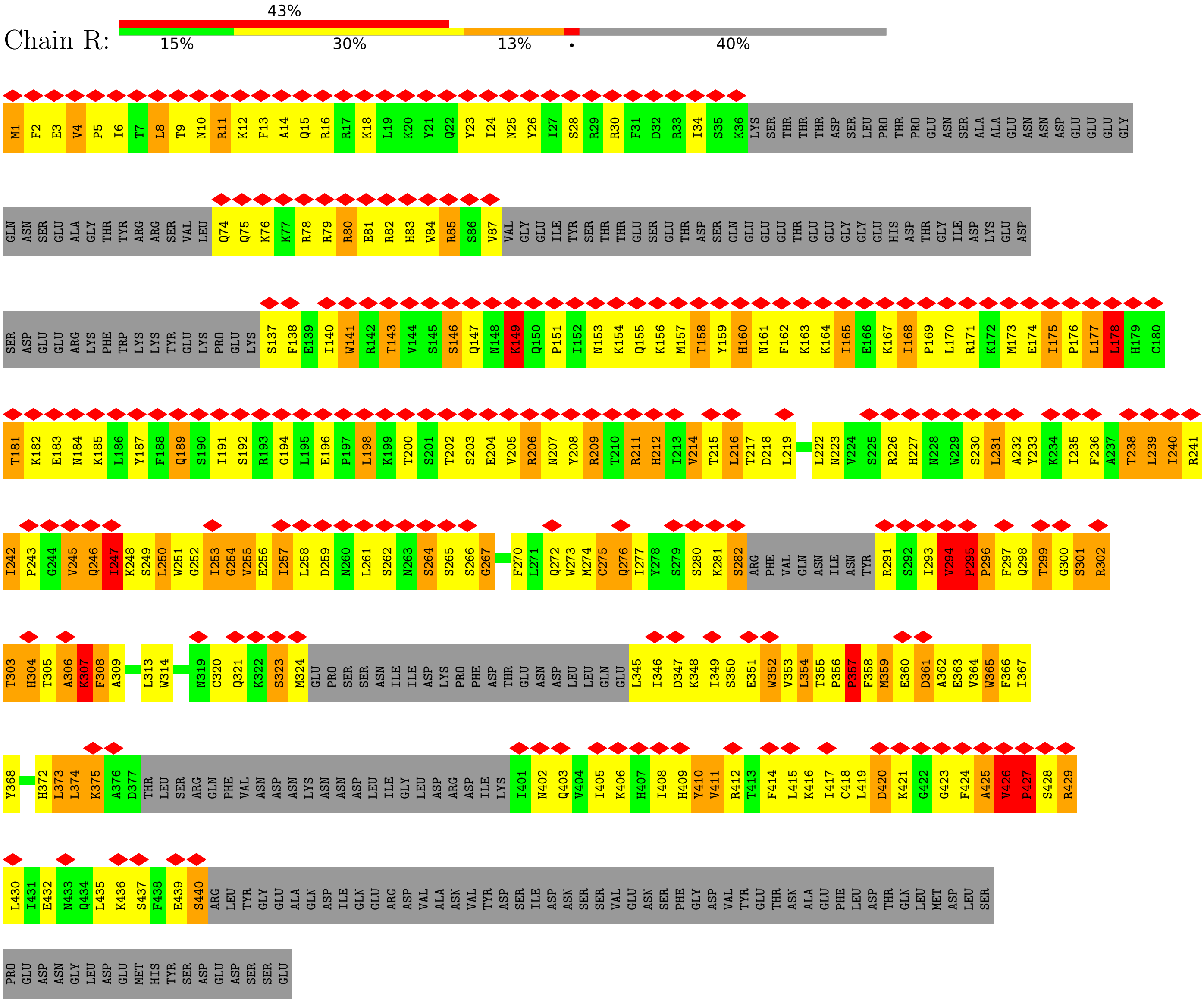


- Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7

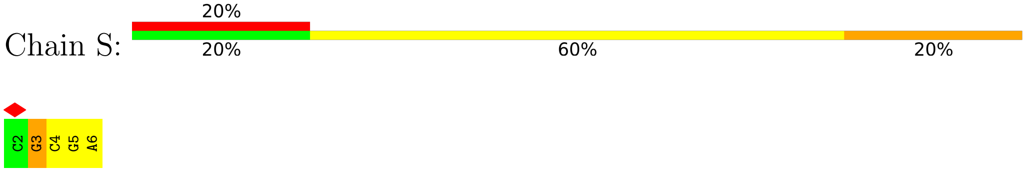




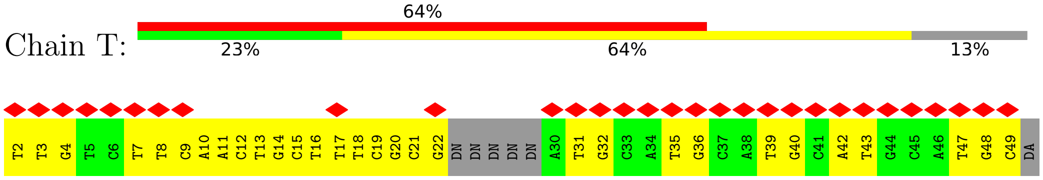
- Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11



- Molecule 19: product RNA

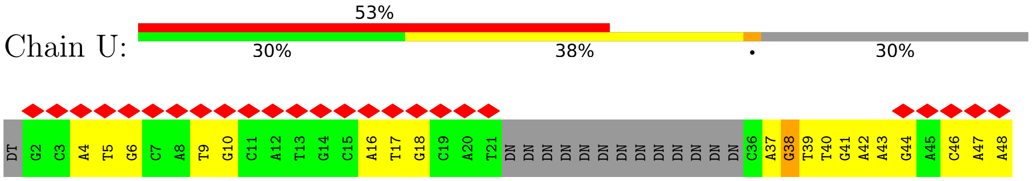


- Molecule 20: template DNA



- Molecule 21: non-template DNA

Chain U:


53%
30%
38%
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30%
DT
G2
C3
A4
T5
G6
C7
A8
T9
G10
C11
A12
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T17
G18
C19
A20
T21
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DN
DN
DN
DN
DN
DN
DN
DN
DN
C36
A37
G38
T39
T40
G41
A42
A43
G44
A45
C46
A47
A48

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 ($e^-/\text{Å}^2$)	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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11526	0	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%)	25	57
2	B	1171/1203 (97%)	1094 (93%)	61 (5%)	16 (1%)	11	37
3	C	303/335 (90%)	276 (91%)	26 (9%)	1 (0%)	41	72
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%)	9	34
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%)	22	55
16	P	573/894 (64%)	414 (72%)	113 (20%)	46 (8%)	1	6
17	Q	377/514 (73%)	311 (82%)	49 (13%)	17 (4%)	2	16
18	R	289/507 (57%)	219 (76%)	41 (14%)	29 (10%)	0	4
All	All	5787/7778 (74%)	5139 (89%)	526 (9%)	122 (2%)	10	30

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	819	ASP

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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%)	67	83
2	B	1030/1053 (98%)	1017 (99%)	13 (1%)	69	84
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%)	62	81
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%)	62	81
16	P	543/828 (66%)	374 (69%)	169 (31%)	0	1
17	Q	364/476 (76%)	293 (80%)	71 (20%)	1	4
18	R	286/474 (60%)	209 (73%)	77 (27%)	0	1
All	All	5296/6990 (76%)	4940 (93%)	356 (7%)	20	46

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 ⓘ

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

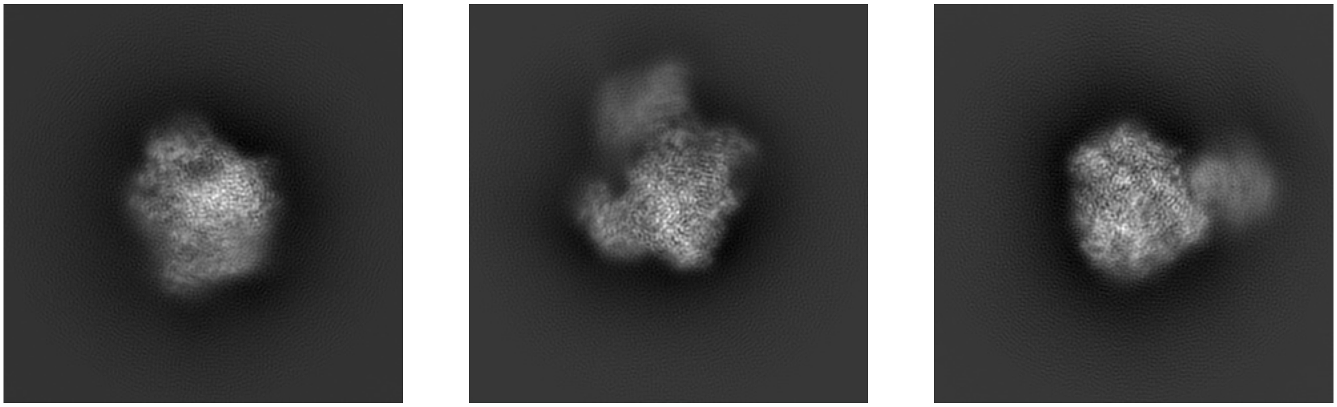
6 Map visualisation (i)

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

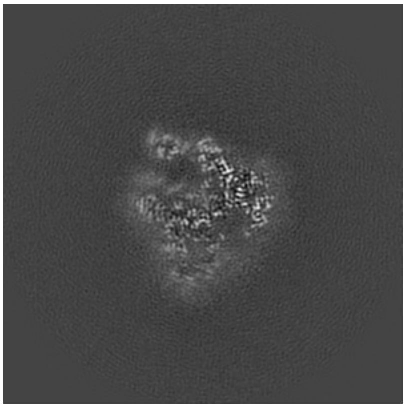


X Y Z

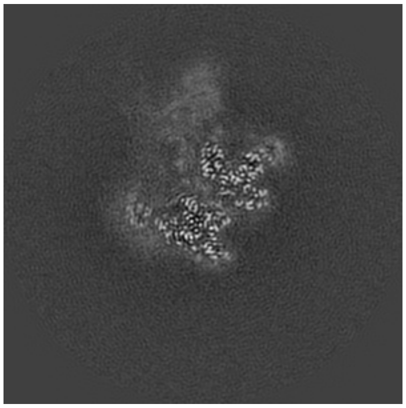
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

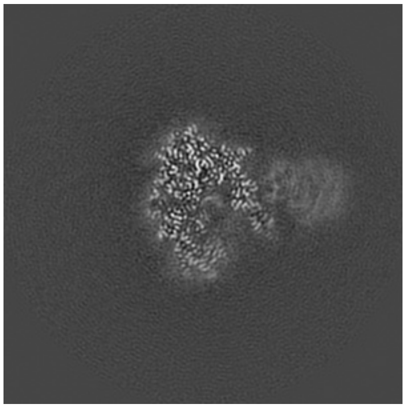
6.2.1 Primary map



X Index: 165



Y Index: 165

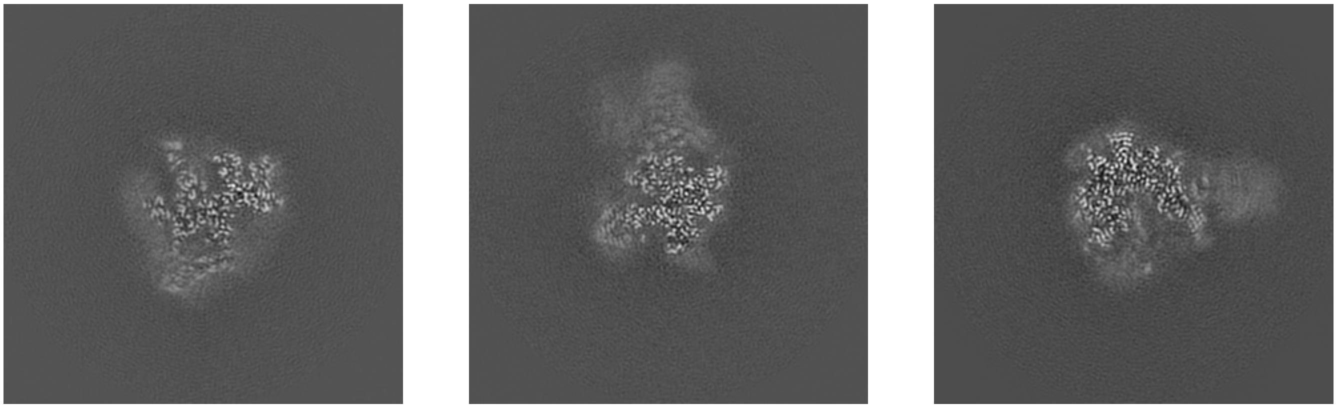


Z Index: 165

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

6.3 Largest variance slices

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 surface views

6.4.1 Primary map

X Y Z

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

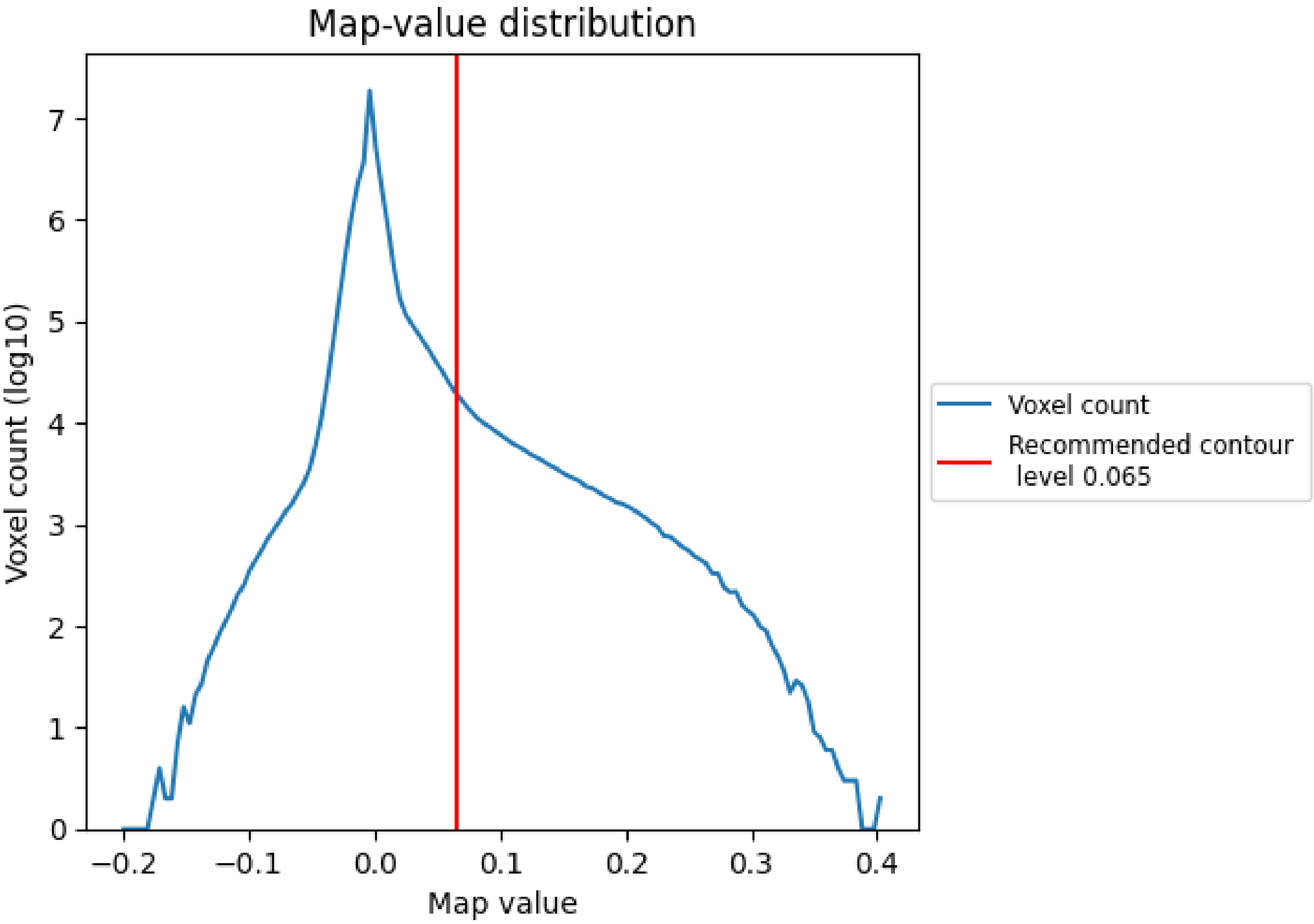
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

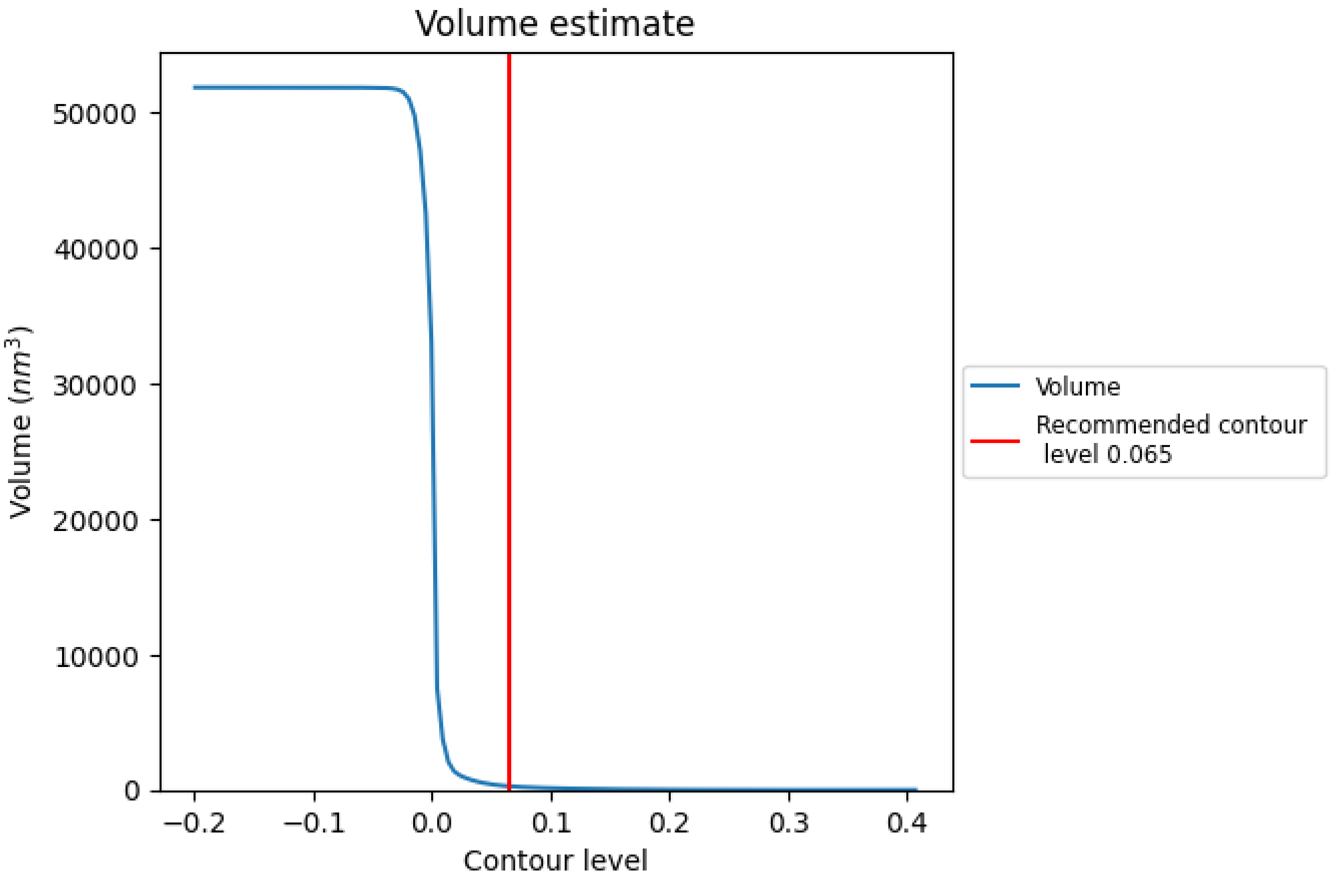
This section contains the results of statistical analysis of the map.

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.

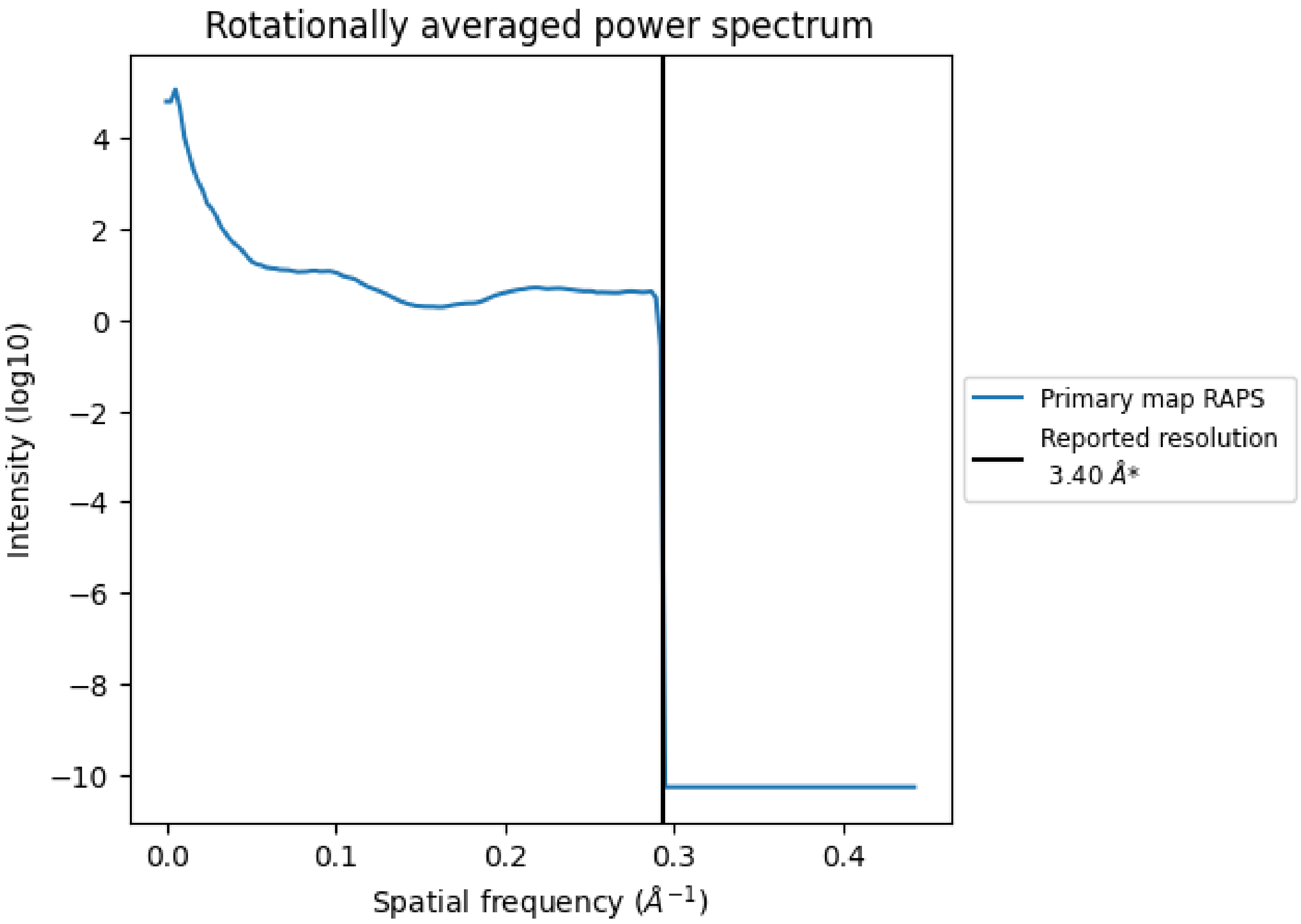
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 273 nm^3; 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}

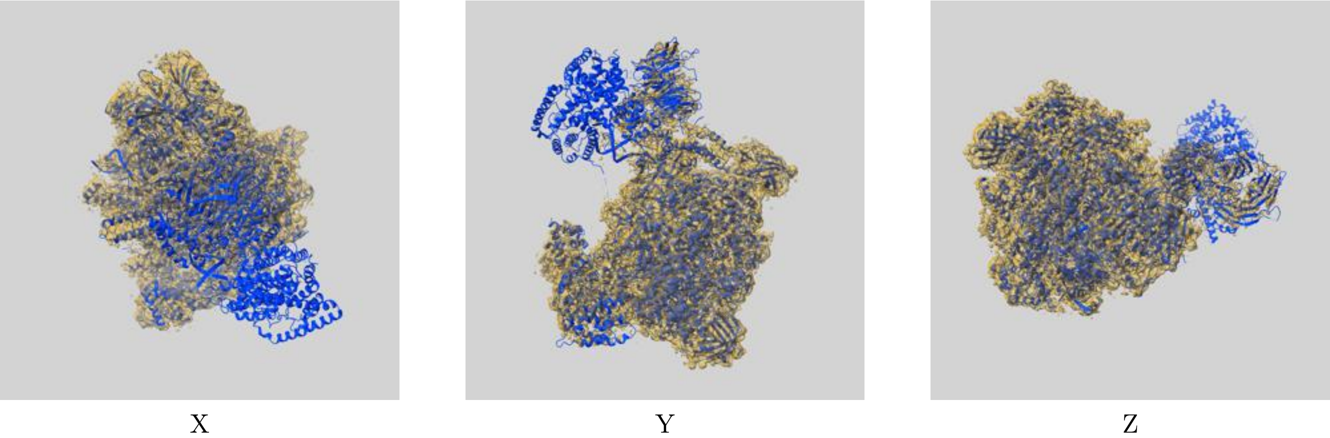
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

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 ⓘ

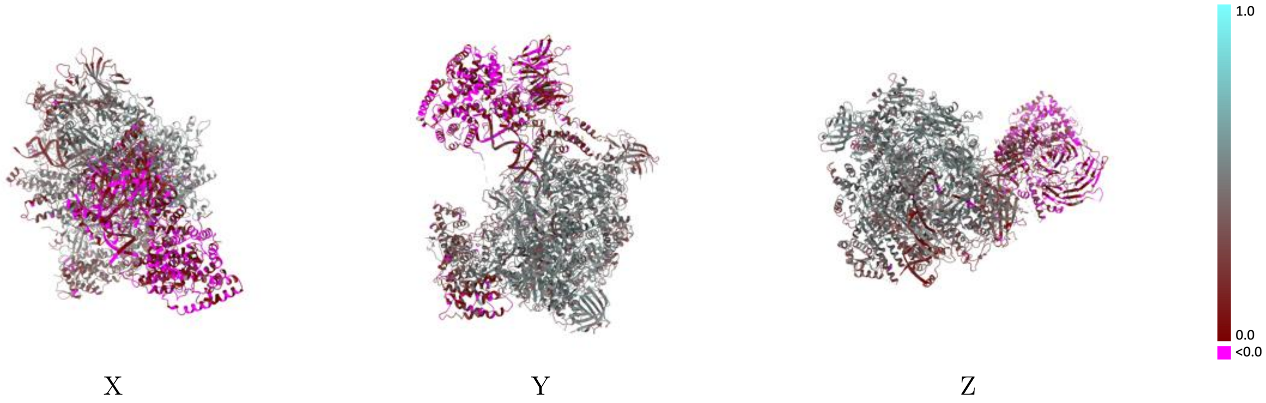

X

Y

Z

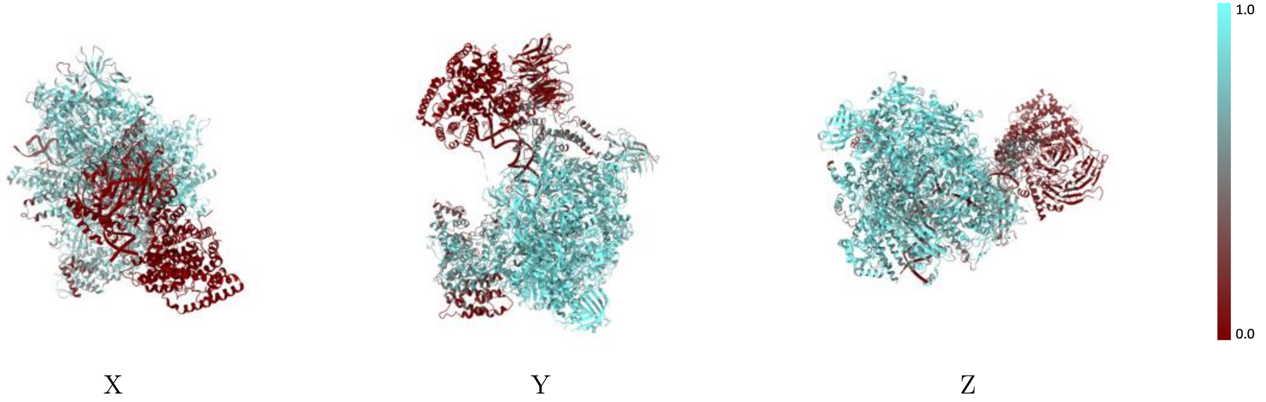
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



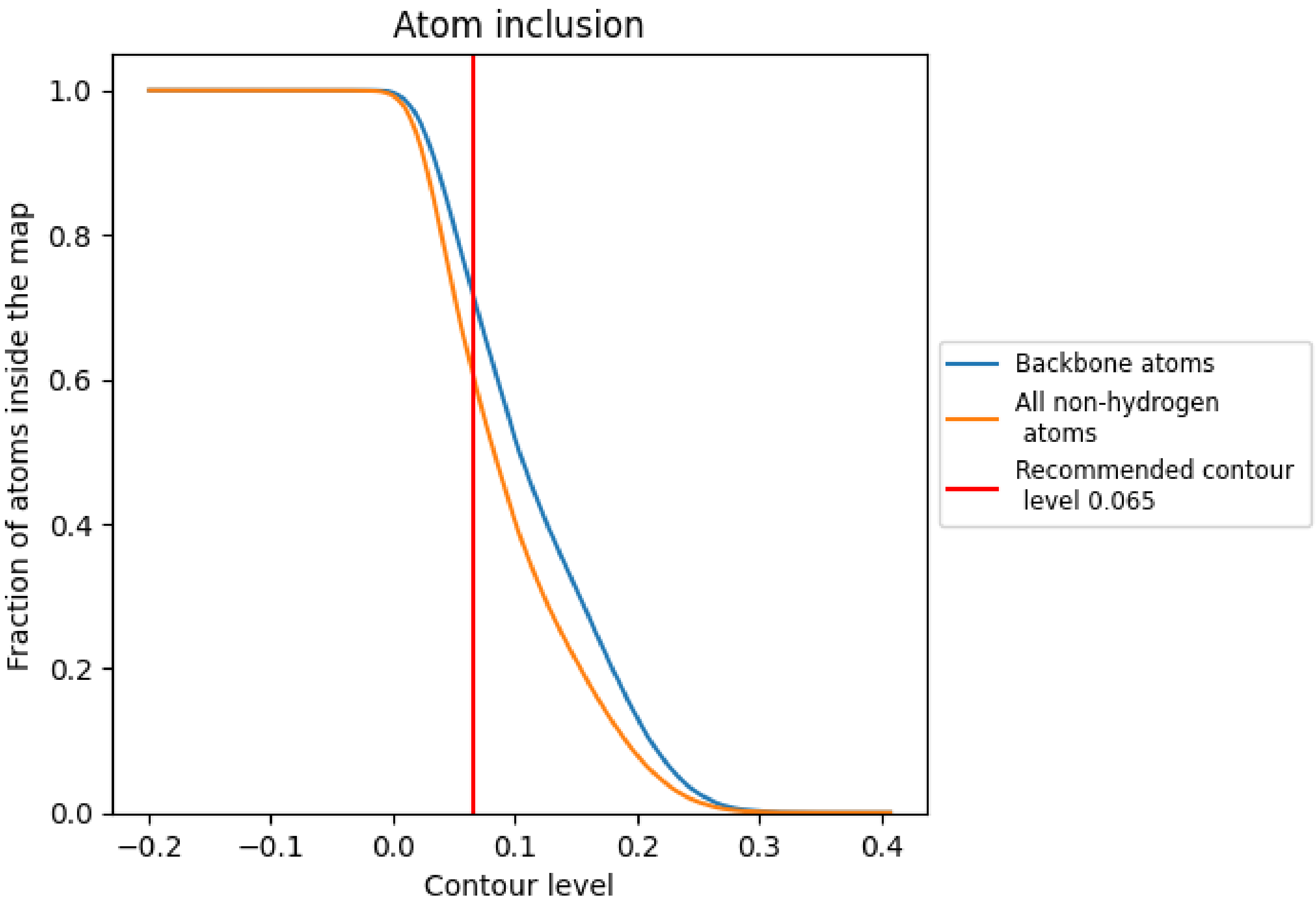
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 ⓘ



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	▬ 0.6108	▬ 0.3430
A	▬ 0.8017	▬ 0.4510
B	▬ 0.8256	▬ 0.4740
C	▬ 0.8764	▬ 0.4830
D	▬ 0.7377	▬ 0.4080
E	▬ 0.8304	▬ 0.4280
F	▬ 0.7965	▬ 0.4770
G	▬ 0.7098	▬ 0.3960
H	▬ 0.8801	▬ 0.4860
I	▬ 0.6875	▬ 0.3020
J	▬ 0.8967	▬ 0.5110
K	▬ 0.8431	▬ 0.4840
L	▬ 0.8382	▬ 0.4670
M	▬ 0.6355	▬ 0.3390
N	▬ 0.6268	▬ 0.3470
O	▬ 0.4817	▬ 0.2610
P	▬ 0.0552	▬ 0.0410
Q	▬ 0.0487	▬ 0.0480
R	▬ 0.2271	▬ 0.1240
S	▬ 0.4722	▬ 0.2280
T	▬ 0.2683	▬ 0.1150
U	▬ 0.2163	▬ 0.1170