wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 11:58 pm GMT

PDB ID	:	6TED
EMDB ID	:	EMD-10480
Title	:	Structure of complete, activated transcription complex Pol II-DSIF-PAF-SPT6 uncovers allosteric elongation activation by RTF1
Authors	:	Vos, S.M.; Farnung, L.; Cramer, P.
Deposited on	:	2019-11-11
Resolution	:	3.10 Å(reported)
Based on initial models	:	4L1U, 6GMH, 6AFO

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

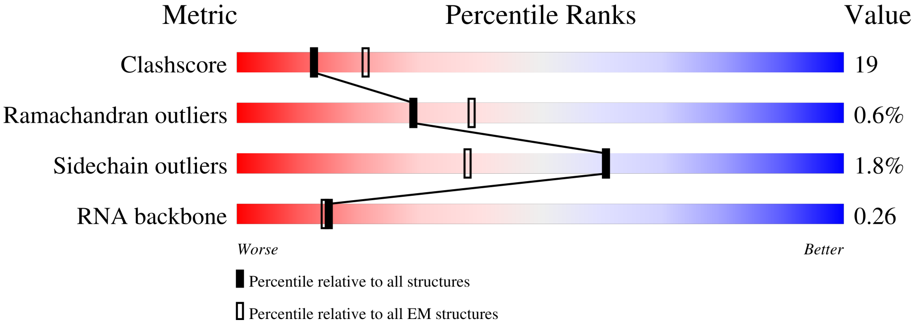
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

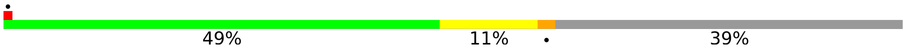
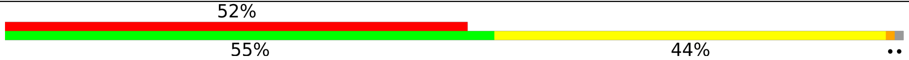
The reported resolution of this entry is 3.10 Å.

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	1984	
2	B	1251	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	

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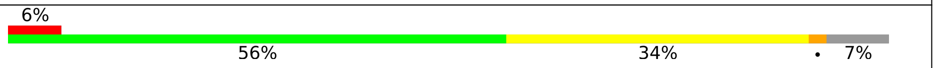
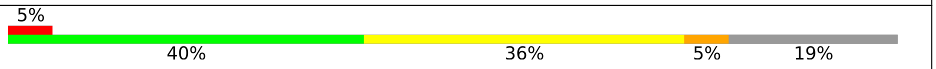
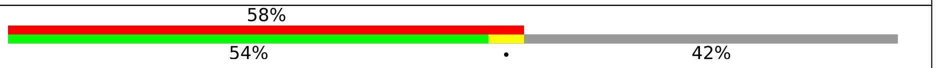
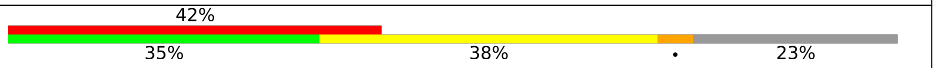
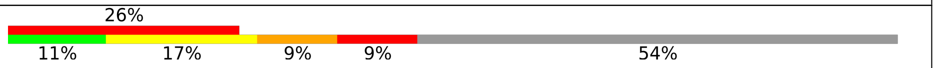
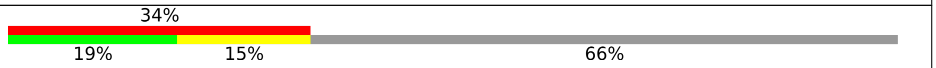
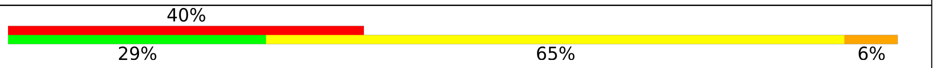
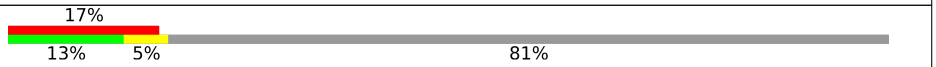
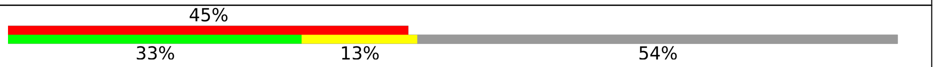
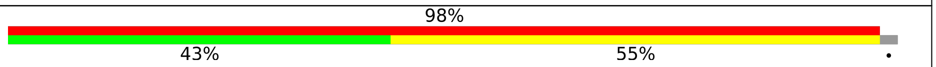
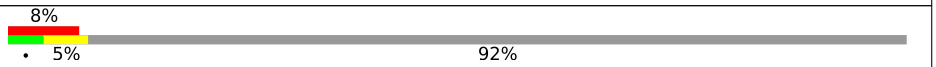
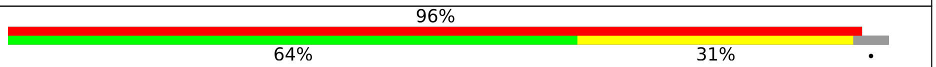
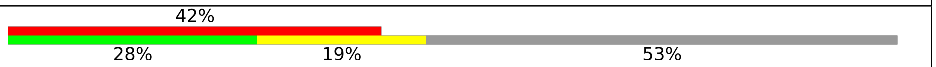
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	48	
15	P	46	
16	Q	1179	
17	R	713	
18	T	48	
19	U	666	
20	V	531	
21	W	305	
22	X	531	
23	Y	121	
24	Z	1087	

2 Entry composition ⓘ

There are 26 unique types of molecules in this entry. The entry contains 57142 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 subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	1426	11255	7074	2014	2095	2	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1122	8980	5684	1576	1656	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1004	630	170	200	4	0	0

- Molecule 5 is a protein called RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

- Molecule 7 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1333	866	214	245	8	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	149	1197	759	195	238	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	942	582	168	181	11	0	0

- Molecule 10 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	47	390	240	77	67	6	0	0

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	1002	4737	2583	1071	1076	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	37	773	361	158	217	37	0	0

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	P	21	452	202	87	142	21	0	0

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	890	7226	4579	1264	1352	31	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 17 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	244	1832	1148	340	337	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	T	48	974	462	168	296	48	0	0

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	125	852	534	151	166	1	0	0

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	244	1703	1061	305	333	4	0	0

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	300	2333	1483	392	454	4	0	0

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	X	43	353	220	69	64	0	0

- Molecule 23 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	116	911	570	159	173	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	510	Total 4023	C 2550	N 709	O 745	P 1	S 18	0	0

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total 2	Zn 2	0
25	B	1	Total 1	Zn 1	0
25	C	1	Total 1	Zn 1	0
25	I	2	Total 2	Zn 2	0
25	J	1	Total 1	Zn 1	0
25	L	1	Total 1	Zn 1	0
25	Y	1	Total 1	Zn 1	0

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

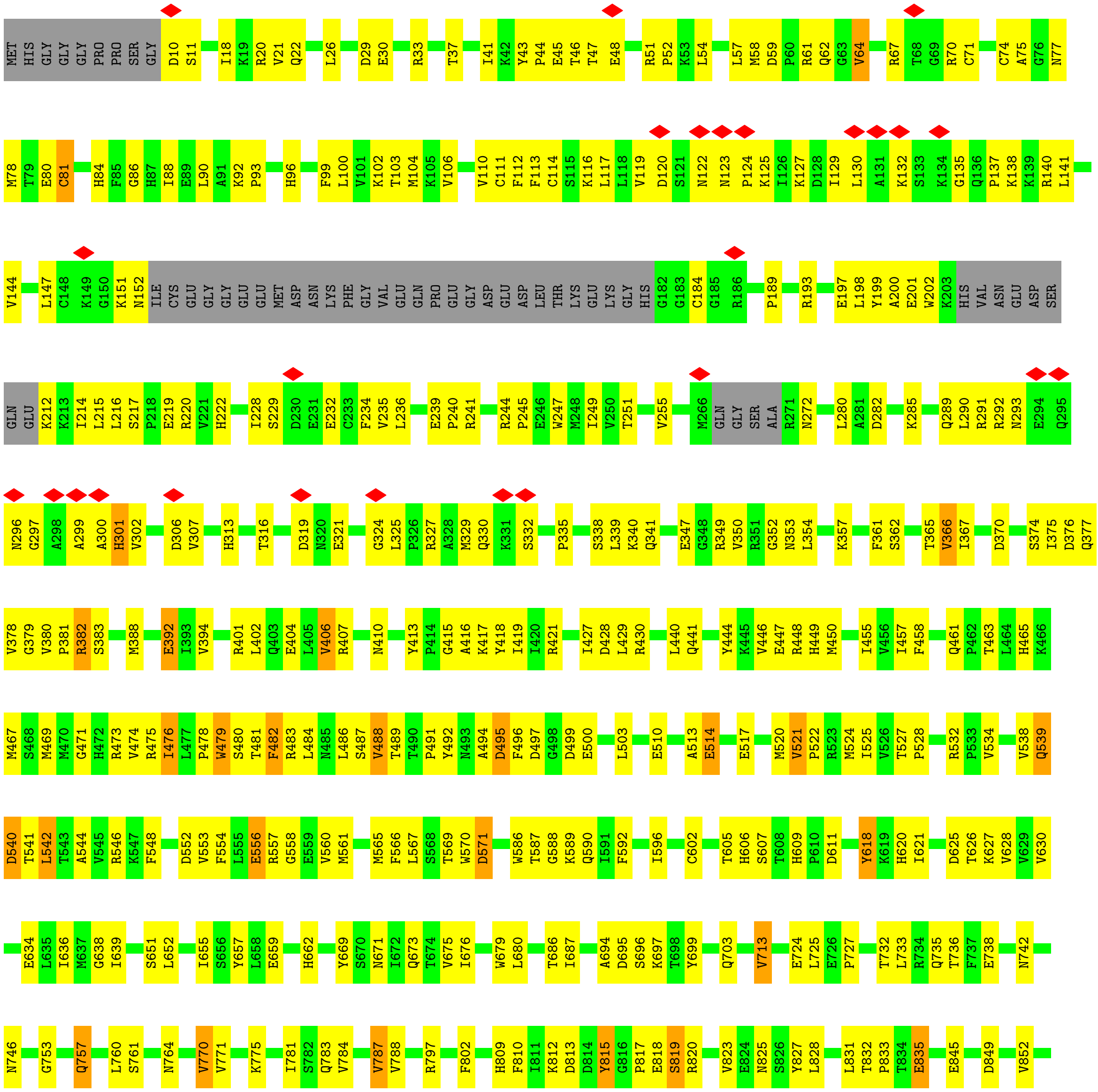
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total 1	Mg 1	0

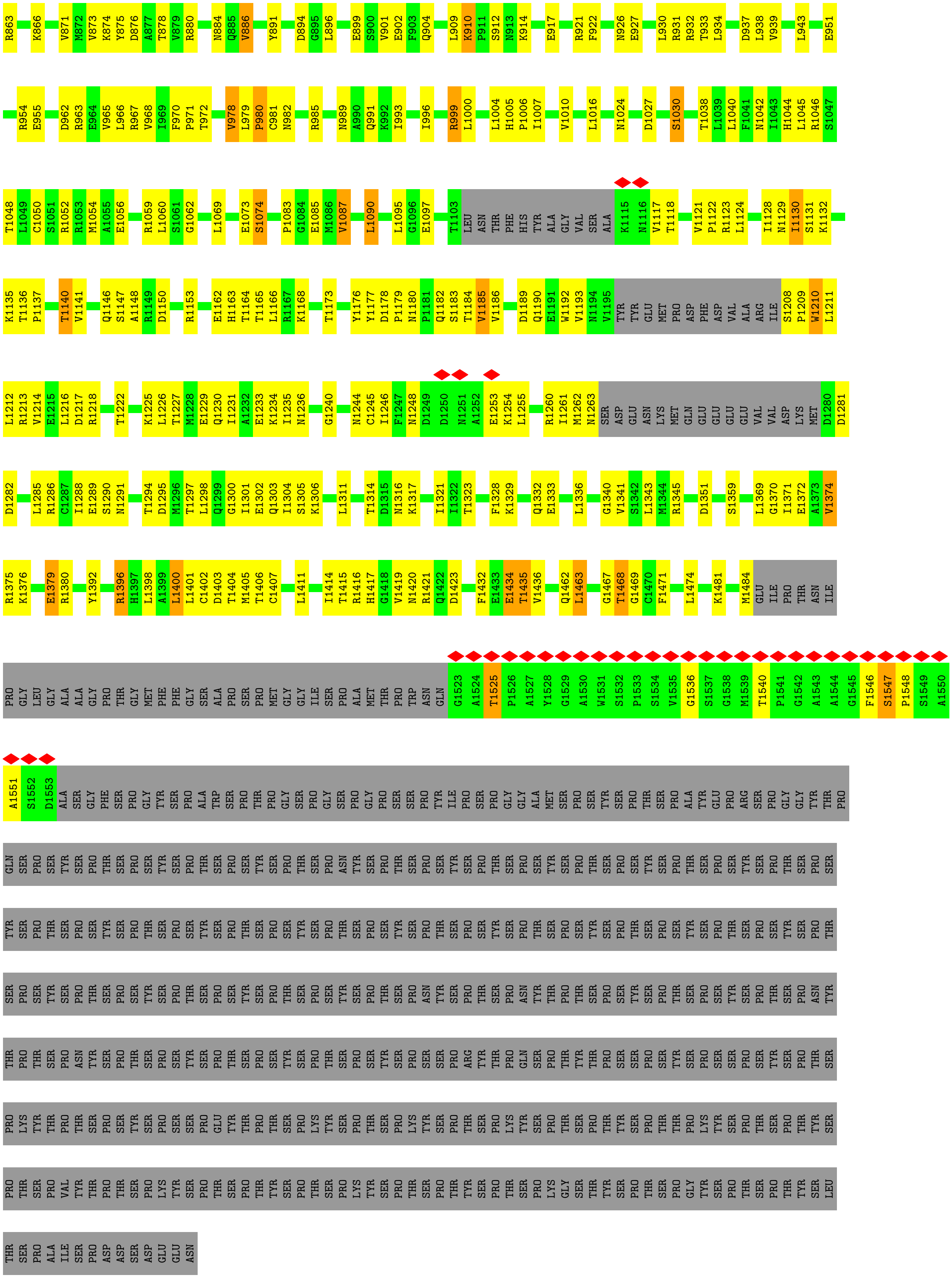
3 Residue-property plots ⓘ

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.

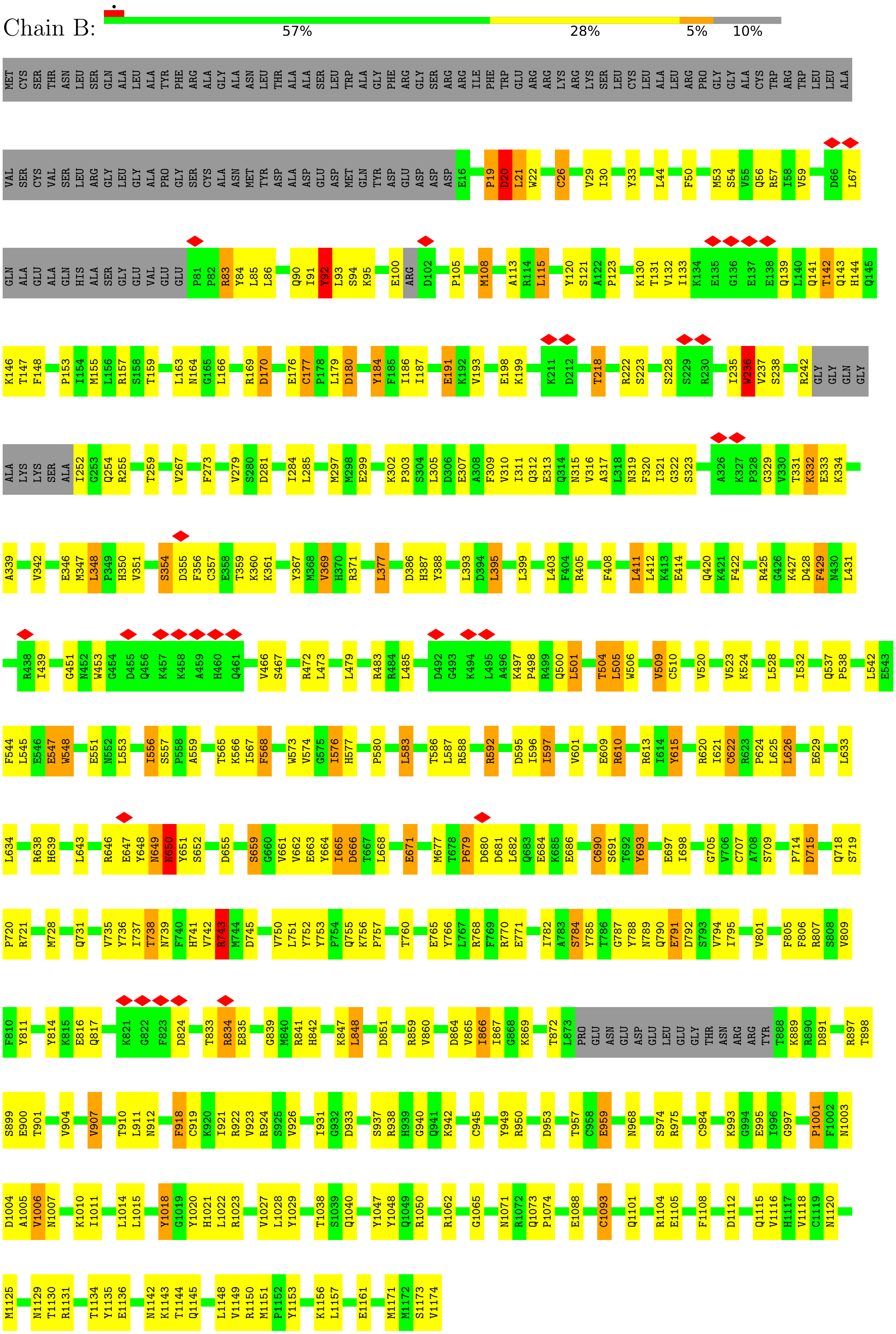
- Molecule 1: DNA-directed RNA polymerase subunit

Chain A:

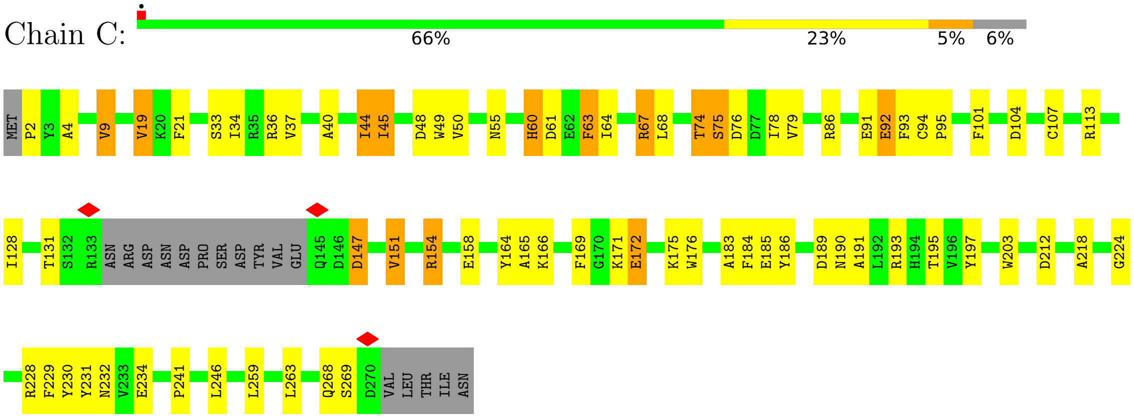




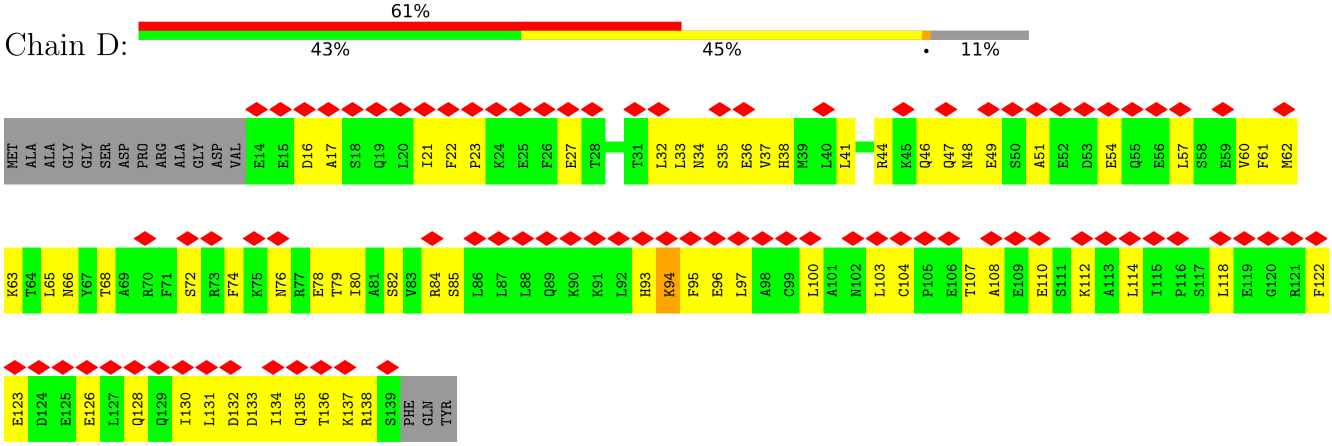
- Molecule 2: DNA-directed RNA polymerase subunit beta


Chain B:
57%
28%
5%
10%
MET CYS SER THR ASN LEU SER GLN ALA LEU ALA TYR PHE ARG ALA GLY ALA ASN LEU THR ALA ALA SER LEU TRP ALA GLY PHE ARG GLY SER ARG ARG ILE PHE TRP GLU ARG ARG LYS ARG LYS SER LEU CYS LEU ALA LEU ARG PRO GLY GLY ALA CYS TRP ARG TRP LEU LEU ALA
VAL SER CYS VAL SER LEU ARG GLY LEU GLY ALA PRO GLY SER CYS ALA ASN MET TYR ASP ALA ASP GLU SER GLU ASP MET GLN TYR ASP GLU ASP ASP ASP E16 P19 D20 L21 W22 C26 V29 I30 Y33 L44 F50 M53 S54 V55 Q56 R57 I58 V59 D66 L67
GLN ALA GLU ALA GLN HIS ALA SER GLY GLU VAL GLU GLU P81 P82 R83 Y84 L85 L86 Q90 I91 Y92 L93 S94 K95 E100 ARG D102 P105 M108 A113 R114 L115 Y120 S121 A122 P123 K130 T131 V132 I133 K134 E135 G136 E137 E138 Q139 L140 Q141 T142 Q143 H144 Q145
K146 T147 F148 P153 I154 M155 L156 R157 S158 T159 L163 N164 G165 L166 R169 D170 E176 C177 P178 L179 D180 Y184 F185 I186 I187 E191 K192 V193 E198 K199 K211 D212 T218 R222 S223 S228 S229 R230 I235 W236 V237 S238 R242 GLY GLY GLN GLY
ALA LYS LYS SER ALA I252 G253 Q254 R255 T259 V267 F273 V279 S280 D281 I284 L285 M297 M298 E299 K302 P303 S304 L305 D306 E307 A308 F309 V310 I311 Q312 E313 Q314 N315 V316 A317 L318 N319 F320 I321 G322 S323 A326 K327 P328 G329 V330 T331 K332 E333 K334
A339 V342 E346 M347 L348 P349 H350 V351 S354 D355 F356 C357 E358 T359 K360 K361 Y367 M368 V369 H370 R371 L377 D386 H387 Y388 L393 D394 L395 L399 L403 F404 R405 F408 L411 L412 K413 E414 Q420 K421 F422 R425 G426 K427 D428 F429 N430 L431
R438 I439 G451 N452 W453 G454 D455 Q456 K457 K458 A459 H460 Q461 V466 S467 R472 L473 L479 R483 R484 L485 D492 G493 K494 L495 A496 K497 P498 R499 Q500 L501 T504 L505 W506 V509 C510 V520 V523 K524 L528 I532 Q537 P538 L542 E543
F544 L545 E546 E547 W548 E551 N552 L553 I556 S557 P558 A559 T565 K566 I567 F568 W573 V574 G575 I576 H577 P580 L583 T586 L587 R588 R592 D595 I596 I597 V601 E609 R610 R613 I614 Y615 R620 I621 C622 R623 P624 L625 L626 E629 L633
L634 R638 H639 L643 R646 E647 Y648 N649 N650 Y651 S652 D655 S659 G660 V661 V662 E663 Y664 I665 D666 T667 L668 E671 M677 T678 P679 D680 D681 L682 Q683 E684 K685 E686 C690 S691 T692 Y693 E697 I698 G705 V706 C707 A708 S709 P714 D715 Q718 S719
P720 R721 M728 Q731 V735 Y736 I737 T738 N739 F740 H741 V742 R743 M744 D745 V750 L751 Y752 Y753 P754 Q755 K756 P757 T760 E765 Y766 L767 R768 F769 R770 E771 I782 A783 S784 Y785 T786 G787 Y788 N789 Q790 E791 D792 S793 V794 I795 V801 F805 F806 R807 S808 V809
F810 Y811 Y814 K815 E816 Q817 K821 G822 F823 D824 T833 R834 E835 G839 M840 R841 H842 K847 L848 D851 R859 V860 D864 V865 I866 I867 G868 K869 T872 L873 PRO GLU ASN GLU ASP GLU LEU GLU GLY THR ASN ARG ARG TYR T888 K889 R890 D891 R897 T898
S899 E900 T901 V904 V907 T910 L911 N912 F918 C919 K920 I921 R922 V923 R924 S925 V926 I931 G932 D933 S937 R938 H939 G940 Q941 K942 C945 Y949 R950 D953 T957 C958 E959 N968 S974 R975 C984 K993 G994 E995 I996 G997 P1001 F1002 N1003
D1004 A1005 V1006 N1007 K1010 I1011 L1014 L1015 Y1018 G1019 Y1020 H1021 L1022 R1023 V1027 L1028 Y1029 T1038 S1039 Q1040 Y1047 Y1048 Q1049 R1050 R1062 G1065 N1071 R1072 Q1073 P1074 E1088 C1093 Q1101 R1104 E1105 F1108 D1112 Q1115 V1116 H1117 V1118 C1119 N1120
M1125 N1129 T1130 R1131 T1134 Y1135 E1136 N1142 K1143 T1144 Q1145 L1148 V1149 R1150 M1151 P1152 Y1153 K1156 L1157 E1161 M1171 M1172 S1173 V1174

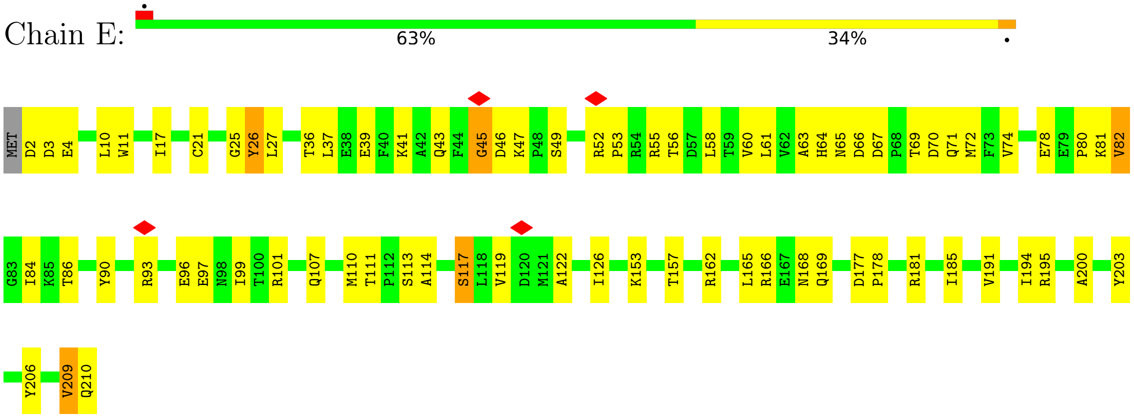
- Molecule 3: RNA polymerase II subunit C



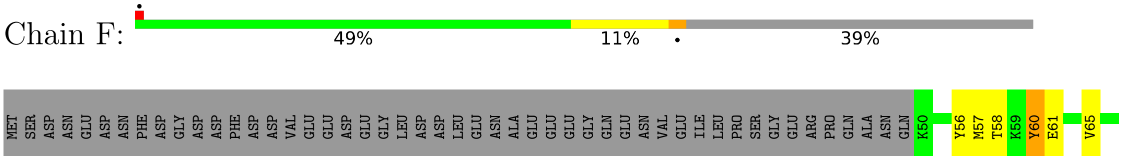
- Molecule 4: RNA polymerase II subunit D

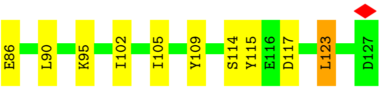


- Molecule 5: RNA polymerase II subunit E



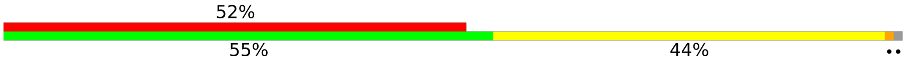
- Molecule 6: RNA polymerase II subunit F

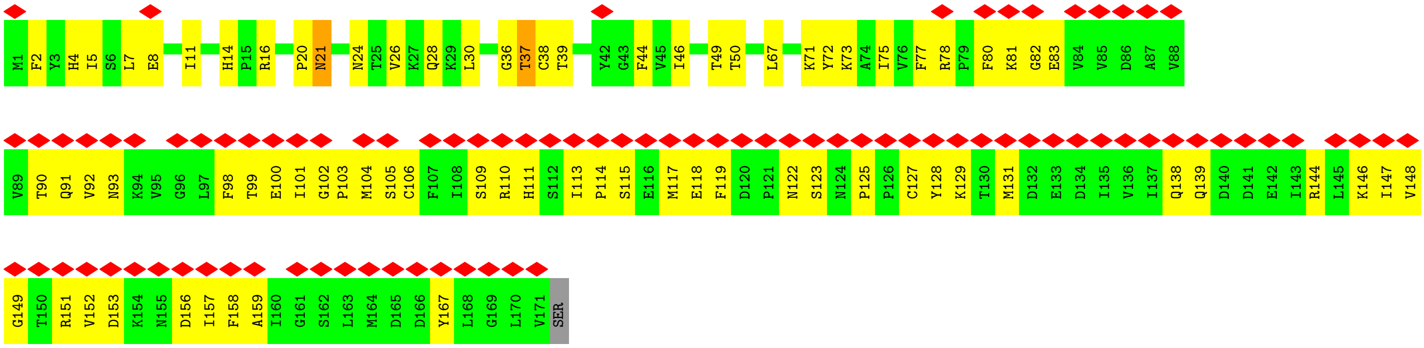




- Molecule 7: RNA polymerase II subunit G

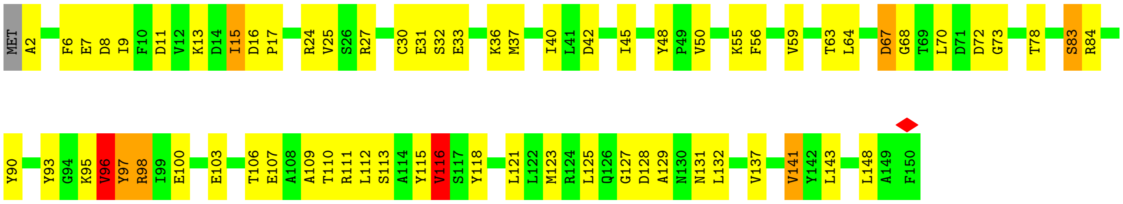
Chain G:





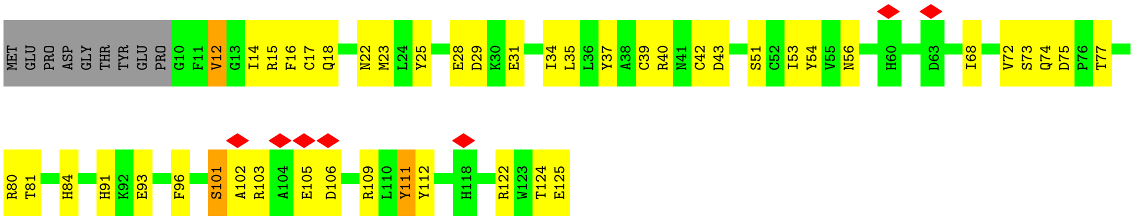
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



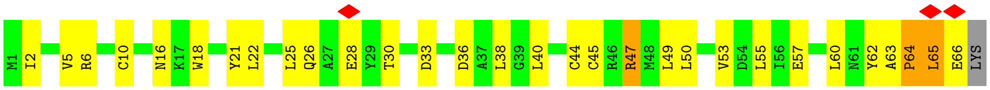
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:

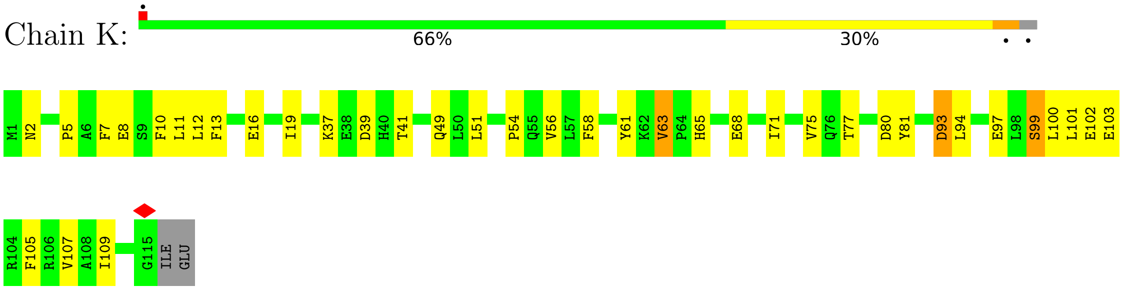


- Molecule 10: Uncharacterized protein

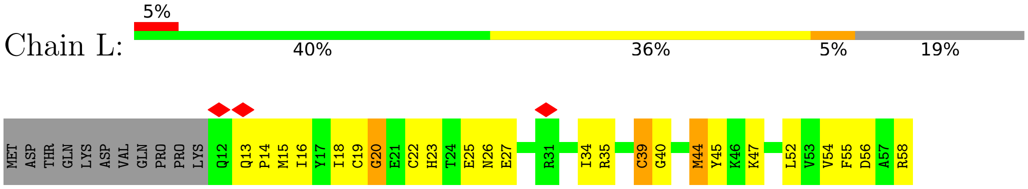
Chain J:



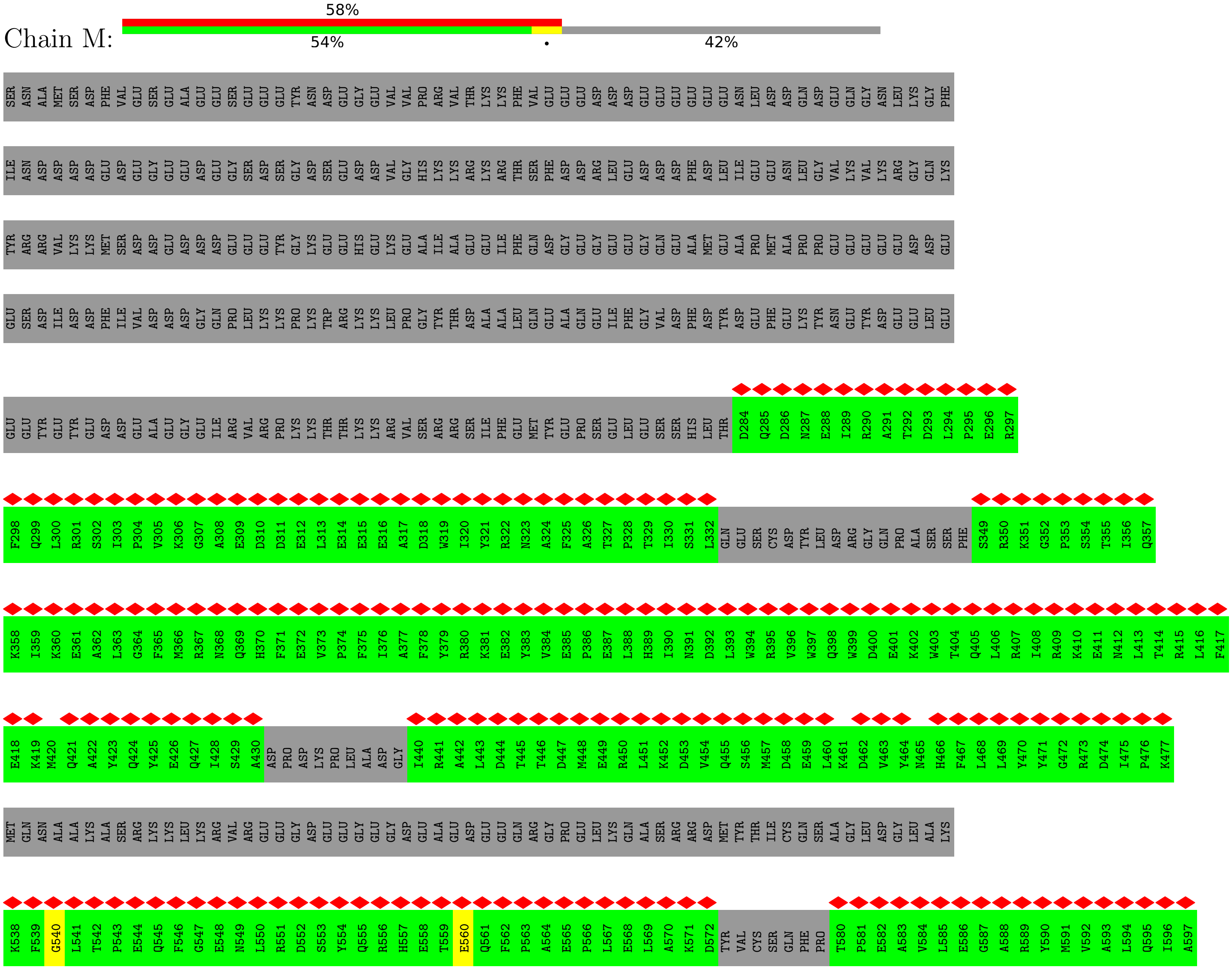
- Molecule 11: Uncharacterized protein

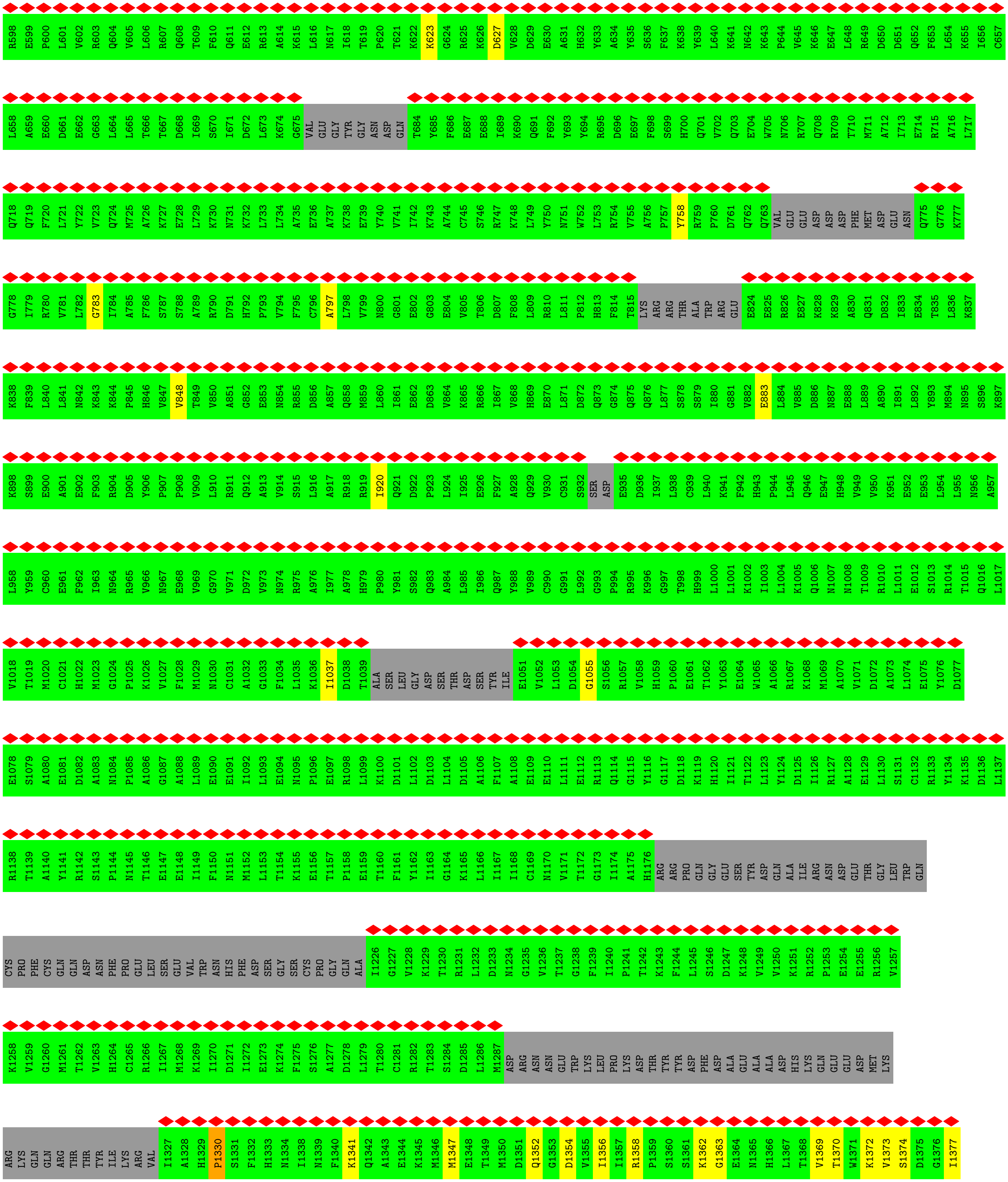


- Molecule 12: Uncharacterized protein



- Molecule 13: Transcription elongation factor SPT6

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Q718 Q719 F720 L721 Y722 V723 Q724 M725 A726 K727 E728 L729 K730 N731 K732 L733 L734 A735 E736 A737 K738 E739 Y740 V741 I742 K743 A744 C745 S746 R747 K748 L749 Y750 N751 W752 L753 R754 V755 A756 P757 Y758 R759 P760 D761 Q762 Q763 VAL GLU GLU ASP ASP ASP PHE MET ASP GLU ASN Q775 G776 K777
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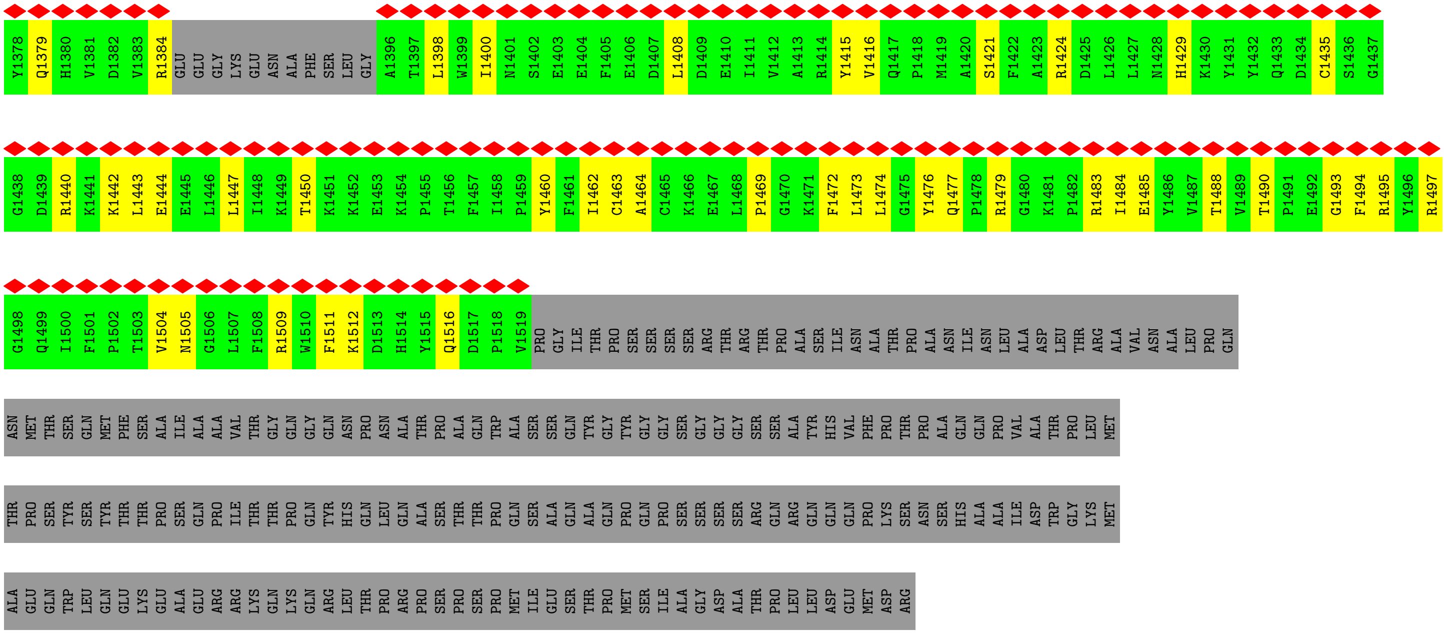
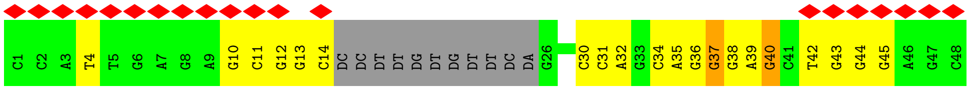
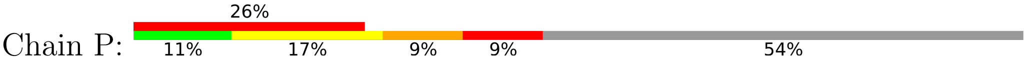
R1138 T1139 A1140 Y1141 R1142 S1143 P1144 N1145 T1146 E1147 E1148 I1149 F1150 N1151 M1152 L1153 T1154 K1155 E1156 T1157 P1158 E1159 T1160 F1161 Y1162 I1163 G1164 K1165 L1166 I1167 I1168 C1169 N1170 V1171 T1172 G1173 I1174 A1175 H1176 ARG ARG PRO GLN GLY GLU SER TYR ASP GLN ALA ILE ARG ASN ASP GLU THR GLY LEU TRP GLN
CYS PRO PHE CYS GLN GLN ASP ASN PHE PRO GLU LEU SER GLU VAL TRP ASN HIS PHE ASP SER GLY SER CYS PRO GLY GLN ALA I1226 G1227 V1228 K1229 T1230 R1231 L1232 D1233 N1234 G1235 V1236 T1237 G1238 F1239 I1240 P1241 T1242 K1243 F1244 L1245 S1246 D1247 K1248 V1249 V1250 K1251 R1252 P1253 E1254 E1255 R1256 V1257
K1258 V1259 G1260 M1261 T1262 V1263 H1264 C1265 R1266 I1267 M1268 K1269 I1270 D1271 I1272 E1273 K1274 F1275 S1276 A1277 D1278 L1279 T1280 C1281 R1282 T1283 S1284 D1285 L1286 M1287 ASP ARG ASN ASN GLU TRP LYS LEU PRO LYS ASP THR TYR TYR ASP PHE ASP ALA GLU ALA ALA ASP HIS LYS GLN GLU GLU ASP MET LYS
ARG LYS GLN GLN ARG THR THR TYR ILE LYS ARG VAL I1327 A1328 H1329 P1330 S1331 F1332 H1333 N1334 I1338 N1339 F1340 K1341 Q1342 A1343 E1344 K1345 M1346 M1347 E1348 T1349 M1350 D1351 Q1352 G1353 D1354 V1355 I1356 I1357 R1358 P1359 S1360 S1361 K1362 G1363 E1364 N1365 H1366 L1367 T1368 V1369 T1370 W1371 K1372 V1373 S1374 D1375 G1376 I1377

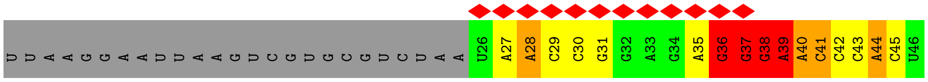


- Molecule 14: DNA (37-MER)

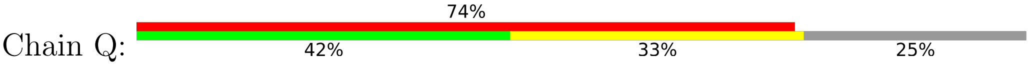


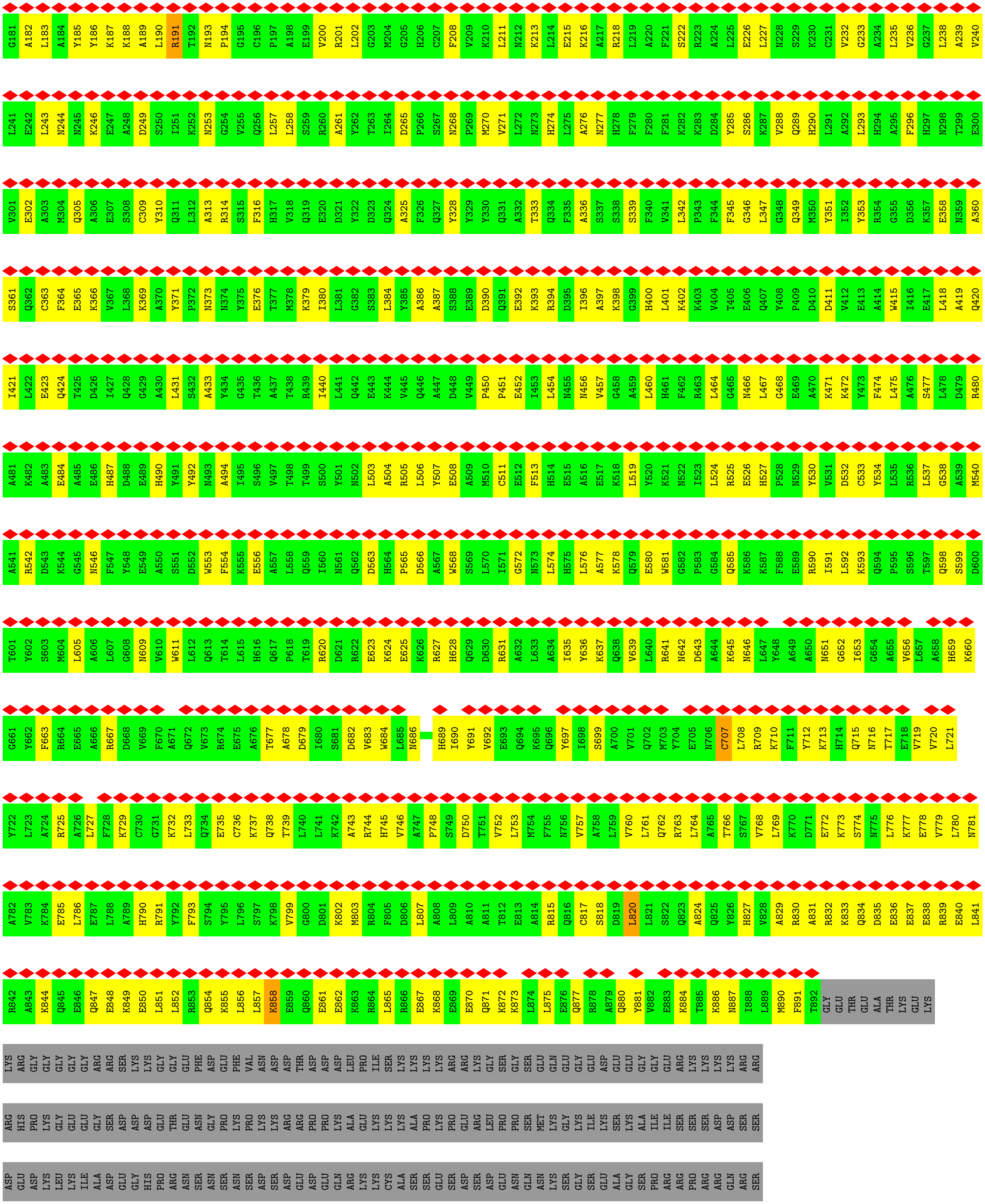
- Molecule 15: RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')





- Molecule 16: RNA polymerase-associated protein CTR9 homolog





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L241 E242 L243 N244 N245 K246 E247 A248 D249 S250 I251 K252 N253 G254 V255 Q256 L257 L258 S259 R260 A261 Y262 T263 I264 D265 P266 S267 N268 P269 M270 V271 L272 N273 H274 L275 A276 N277 H278 F279 F280 F281 K282 K283 D284 Y285 S286 K287 V288 Q289 H290 L291 A292 L293 H294 A295 F296 H297 N298 T299 E300

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I421 L422 E423 Q424 T425 D426 I427 Q428 G429 A430 L431 S432 A433 Y434 G435 T436 A437 T438 R439 I440 L441 Q442 E443 K444 V445 Q446 A447 D448 V449 P450 P451 E452 I453 L454 N455 N456 V457 G458 A459 L460 H461 F462 R463 L464 G465 N466 L467 G468 E469 A470 K471 K472 Y473 F474 L475 A476 S477 L478 D479 R480

A481 K482 A483 E484 A485 E486 H487 D488 E489 H490 Y491 Y492 N493 A494 I495 S496 V497 T498 T499 S500 Y501 N502 L503 A504 R505 L506 Y507 E508 A509 M510 C511 E512 F513 H514 E515 A516 E517 K518 L519 Y520 K521 N522 I523 L524 R525 E526 H527 P528 N529 Y530 V531 D532 C533 Y534 L535 R536 L537 G538 A539 M540

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T601 Y602 S603 M604 L605 A606 L607 G608 N609 V610 W611 L612 Q613 T614 L615 H616 Q617 P618 T619 R620 D621 R622 E623 K624 E625 K626 R627 H628 Q629 D630 R631 A632 L633 A634 I635 Y636 K637 Q638 V639 L640 R641 N642 D643 A644 K645 N646 L647 Y648 A649 A650 N651 G652 I653 G654 A655 V656 L657 A658 H659 K660

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Y722 L723 A724 R725 A726 L727 F728 K729 C730 G731 K732 L733 Q734 E735 C736 K737 Q738 T739 L740 L741 K742 A743 R744 H745 V746 A747 P748 S749 D750 T751 V752 L753 M754 F755 N756 V757 A758 L759 V760 L761 Q762 R763 L764 A765 T766 S767 V768 L769 K770 D771 E772 K773 S774 N775 L776 K777 E778 V779 L780 N781

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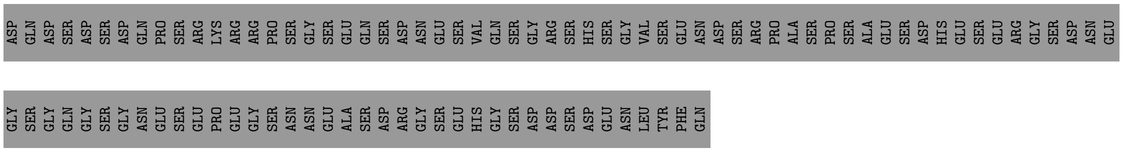
LYS ARG GLY GLY GLY GLY GLY ARG ARG SER LYS LYS GLY GLY GLU PHE ASP GLU PHE VAL ASN ASP ASP THR ASP ASP ASP LEU PRO ILE SER LYS LYS LYS LYS ARG ARG LYS GLY SER GLY SER GLU GLN GLU GLY GLU ASP GLU GLU GLY GLY GLU ARG LYS LYS LYS LYS ARG ARG

ARG HIS PRO LYS GLY GLU GLU GLY SER ASP ASP ASP GLU THR GLU ASN GLY PRO LYS PRO LYS LYS ARG ARG PRO PRO LYS ALA GLU LYS LYS LYS ALA PRO LYS PRO GLU ARG LEU PRO PRO SER MET LYS GLY LYS ILE LYS SER LYS ALA ILE ILE SER SER SER ASP ASP SER SER

ASP GLU ASP LYS LEU LYS ILE ALA ASP GLU GLY HIS PRO ARG ASN SER ASN SER ASN SER ASP SER ASP GLU ASP GLU GLN ARG LYS LYS CYS ALA SER SER GLU SER ASP SER ASP GLU ASN GLN ASN LYS SER GLY SER GLU ALA GLY SER PRO ARG ARG PRO ARG ARG GLN ARG SER



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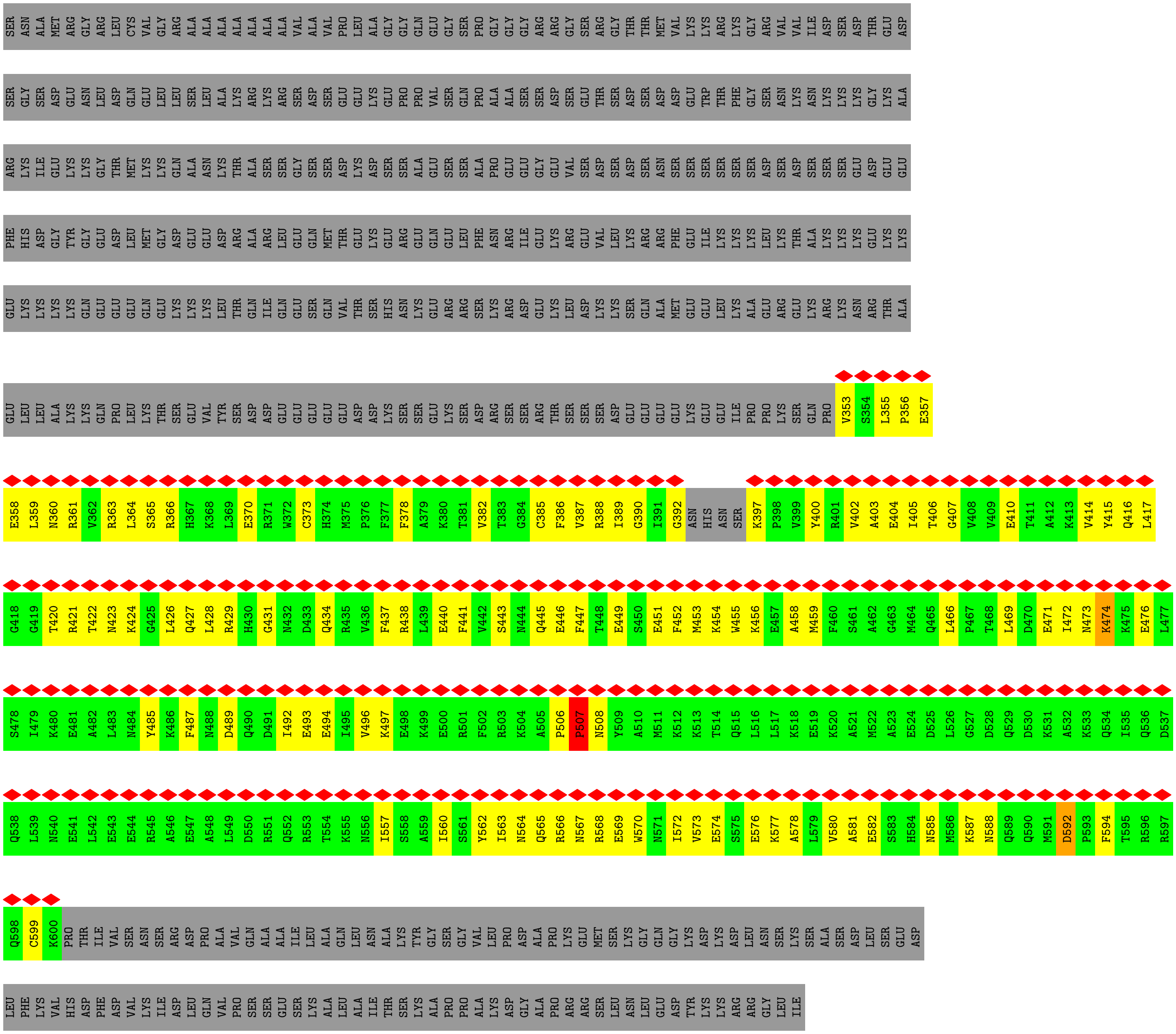
GLY SER GLY GLN GLY SER GLY ASN GLU SER GLU PRO GLU GLY SER ASN ASN GLU ALA SER ASP ARG GLY SER GLU HIS GLY SER ASP ASP SER ASP GLU ASN LEU TYR PHE GLN

- Molecule 17: RNA polymerase-associated protein RTF1 homolog

Chain R:



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SER GLY SER ASP GLU ASN LEU ASP GLN GLU LEU LEU SER LEU ALA LYS ARG LYS ARG SER ASP SER GLU GLU LYS GLU PRO PRO VAL SER GLN PRO ALA ALA SER SER ASP SER GLU THR SER ASP SER ASP ASP GLU TRP THR PHE GLY SER ASN LYS ASN LYS LYS LYS GLY LYS ALA

ARG LYS ILE GLU LYS LYS GLY THR MET LYS LYS GLN ALA ASN LYS THR ALA SER SER GLY SER SER ASP LYS ASP SER SER ALA GLU SER SER ALA PRO GLU GLU GLY GLU VAL SER ASP SER ASP SER ASN SER SER SER SER SER ASP SER ASP SER SER SER GLU ASP GLU GLU

PHE HIS ASP GLY TYR GLY GLU ASP LEU MET GLY ASP GLU GLU ASP ARG ALA ARG LEU GLU GLN MET THR GLU LYS GLU ARG GLU GLN GLU LEU PHE ASN ARG ILE GLU LYS ARG GLU VAL LEU LYS ARG ARG PHE GLU ILE LYS LYS LYS LEU LYS THR ALA LYS LYS LYS GLU LYS LYS

GLU LYS LYS LYS LYS GLN GLU GLU GLU GLN GLU LYS LYS LEU THR GLN ILE GLN GLU SER GLN VAL THR SER HIS ASN LYS GLU ARG ARG SER LYS ARG ASP GLU LYS LEU ASP LYS LYS SER GLN ALA MET GLU GLU LEU LYS ALA GLU ARG GLU LYS ARG LYS ASN ARG THR ALA

GLU LEU LEU ALA LYS LYS GLN PRO LEU LYS THR SER GLU VAL TYR SER ASP ASP GLU GLU GLU GLU GLU ASP ASP LYS SER SER GLU LYS SER ASP ARG SER SER ARG THR SER SER SER ASP GLU GLU GLU GLU LYS GLU GLU ILE PRO PRO LYS SER GLN PRO V353 S354 L355 P356 E357

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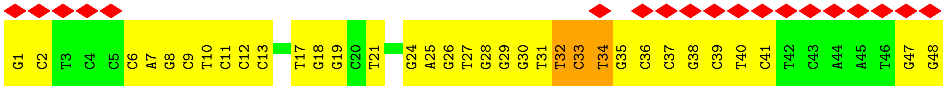
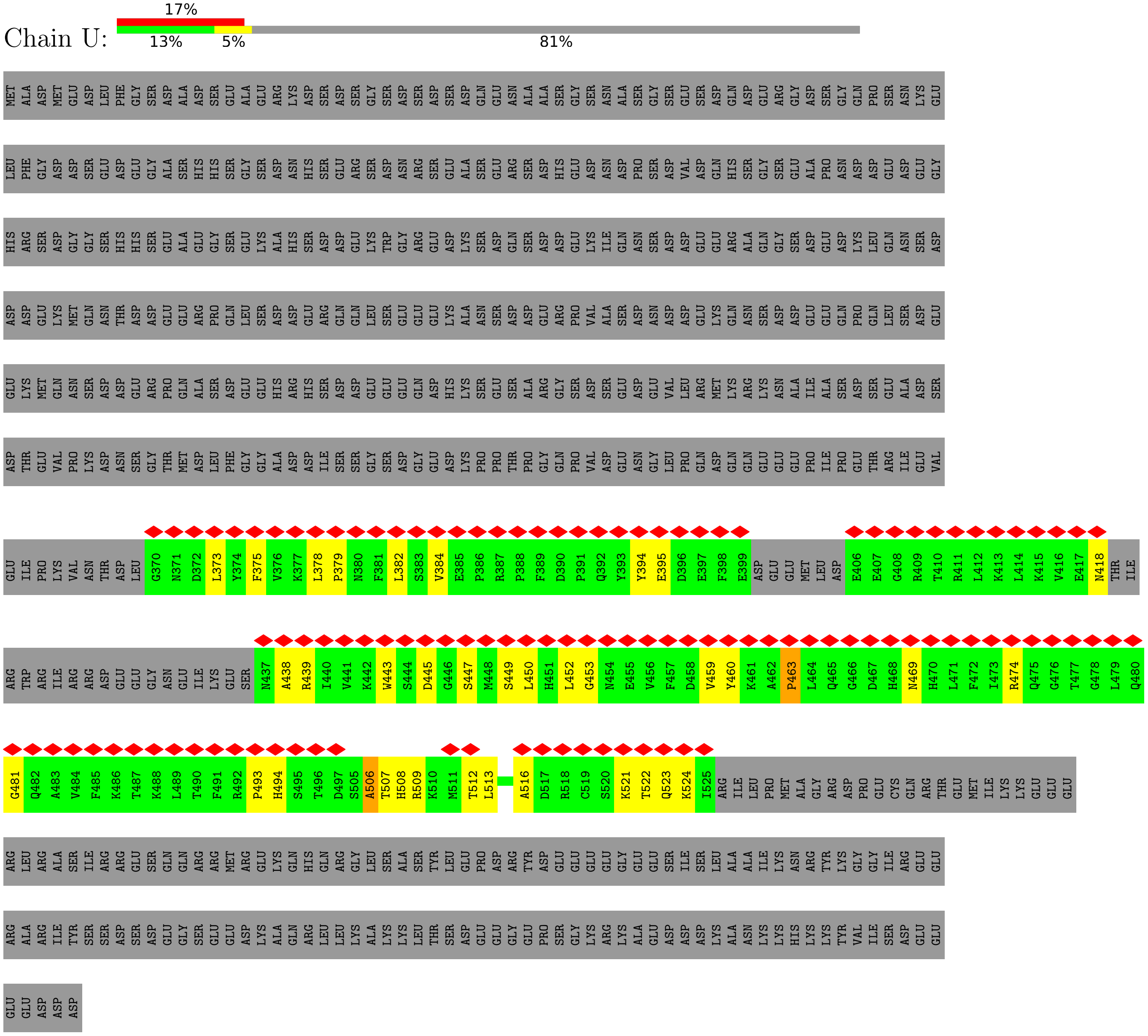
LEU PHE LYS VAL HIS ASP PHE ASP VAL LYS ILE ASP LEU GLN VAL PRO SER SER GLU SER LYS ALA LEU ALA ILE THR SER LYS ALA PRO PRO ALA LYS ASP GLY ALA PRO ARG ARG SER LEU ASN LEU GLU ASP TYR LYS LYS ARG ARG GLY LEU ILE

- Molecule 18: Template DNA

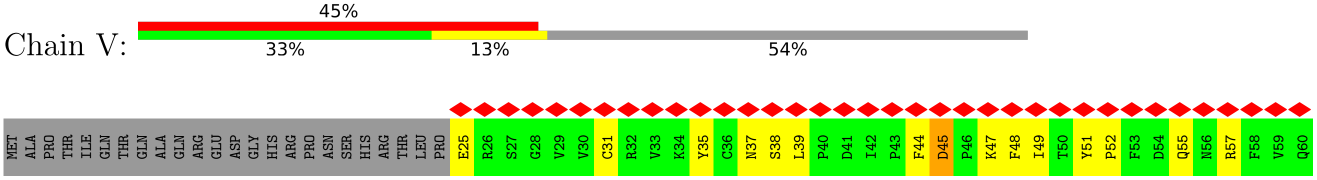
Chain T:

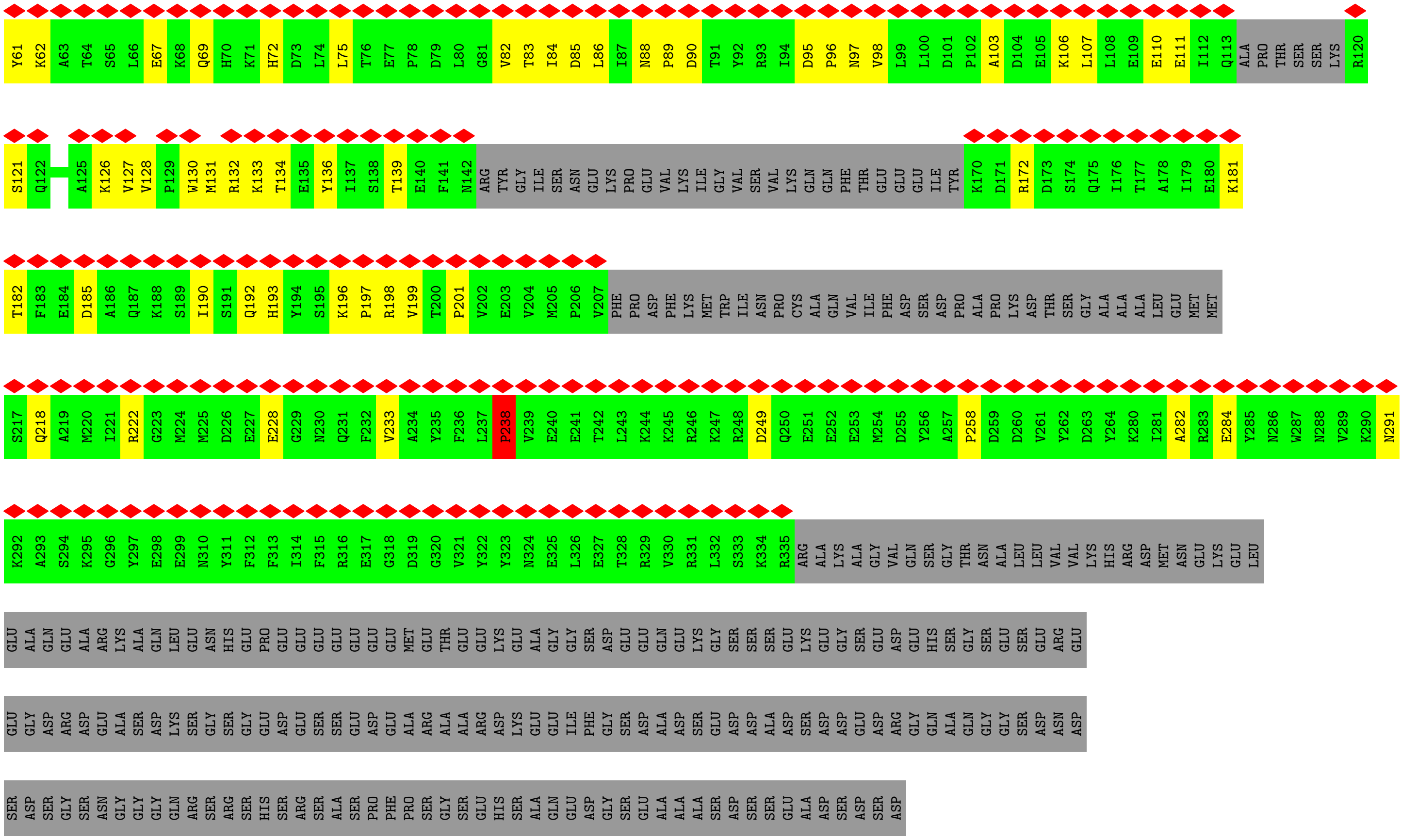


- Molecule 19: RNA polymerase-associated protein LEO1



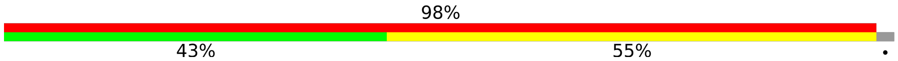
- Molecule 20: RNA polymerase II-associated factor 1 homolog



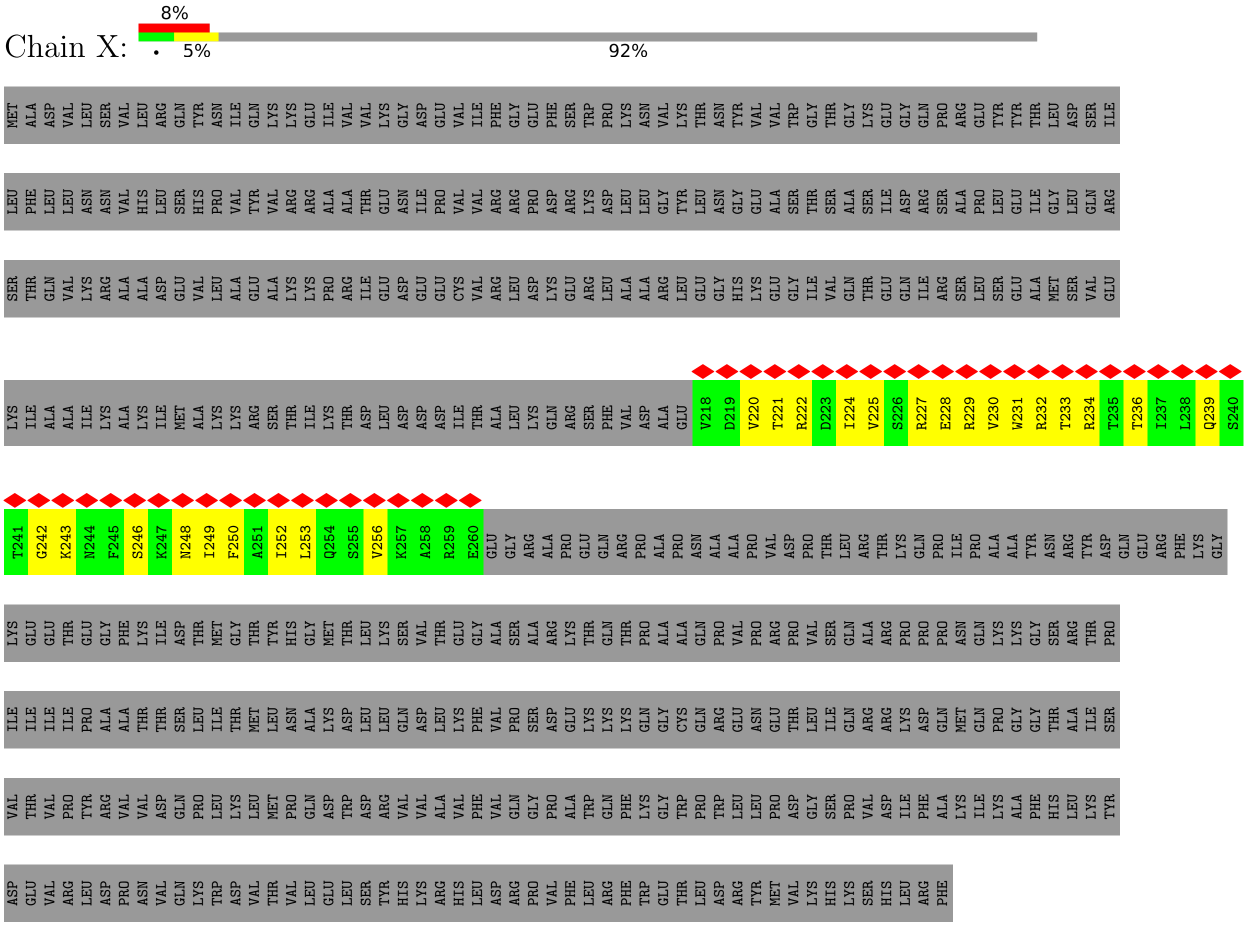


- Molecule 21: WD repeat-containing protein 61

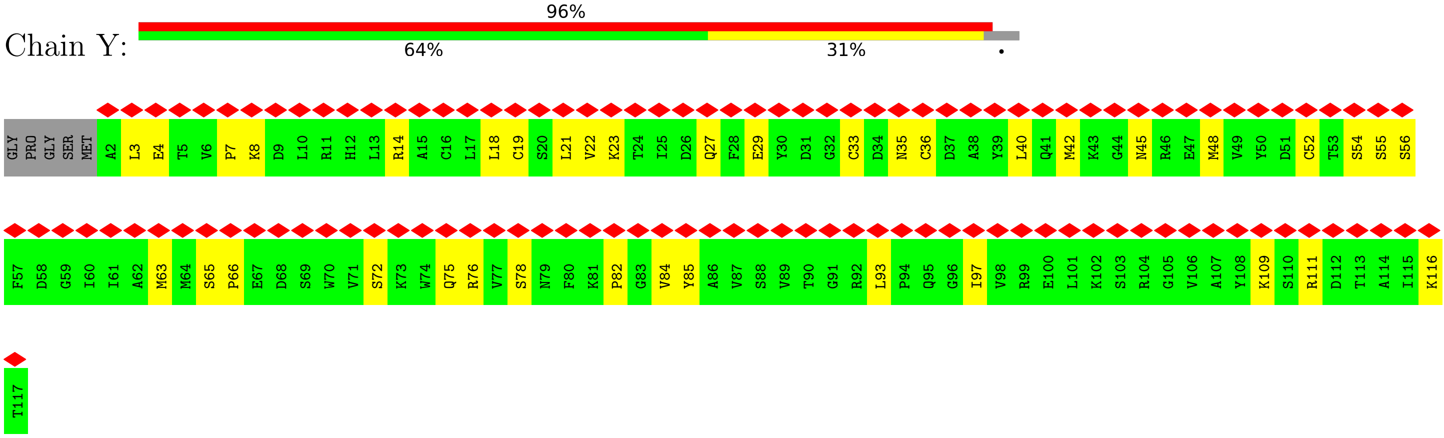
Chain W:



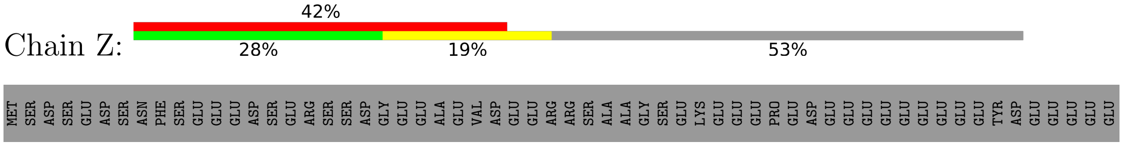
- Molecule 22: Parafibromin

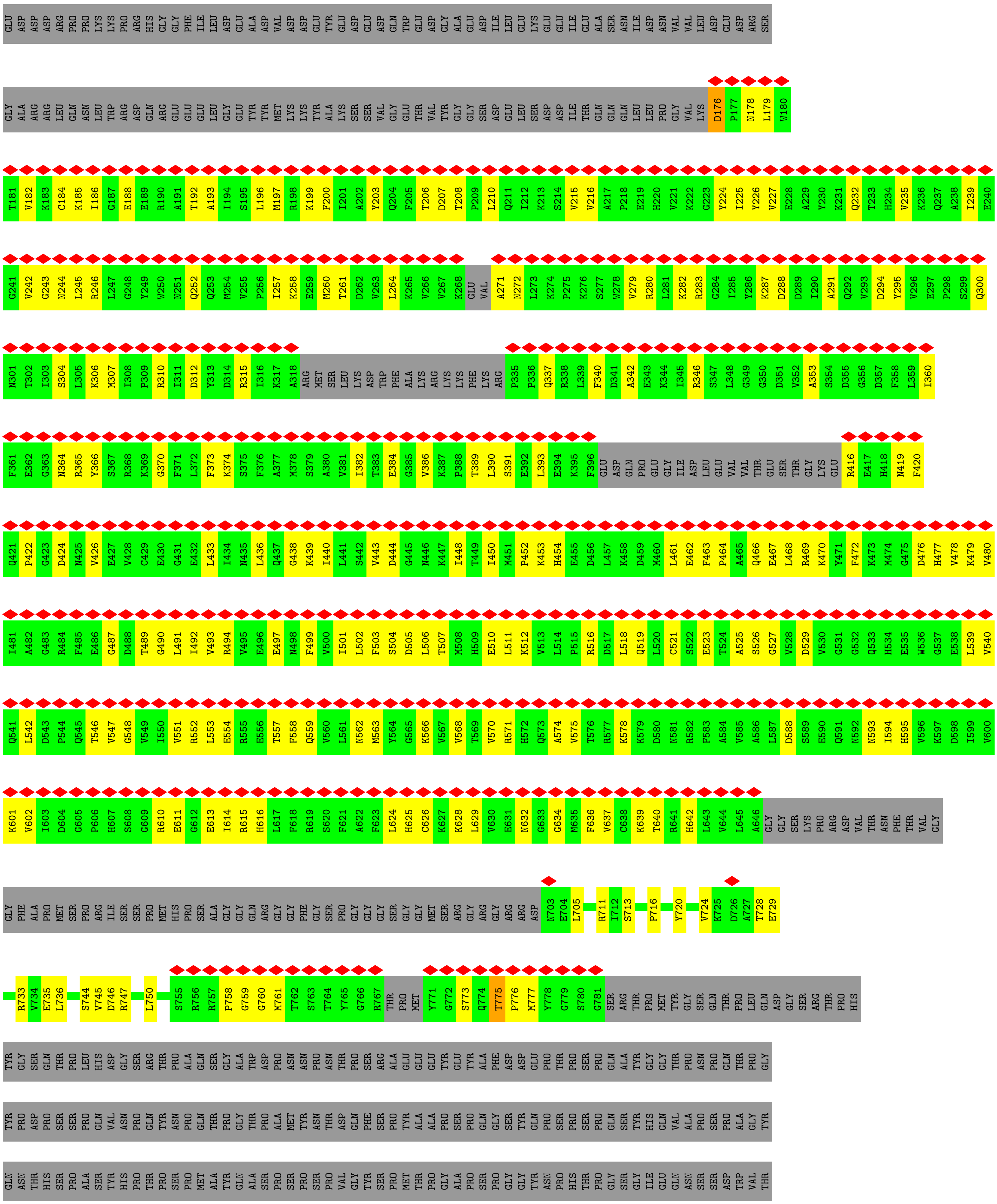


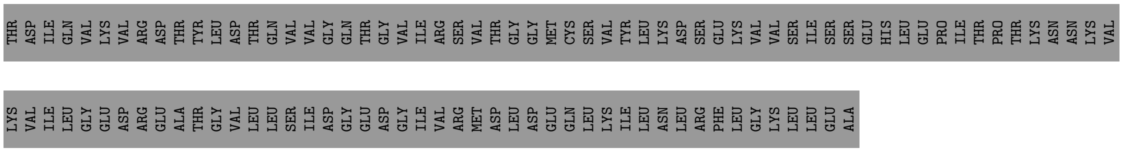
- Molecule 23: Transcription elongation factor SPT4



- Molecule 24: Transcription elongation factor SPT5




GLU ASP ASP ASP ARG PRO PRO LYS LYS PRO ARG HIS GLY GLY PHE ILE LEU ASP GLU ALA ASP VAL ASP ASP GLU TYR GLU ASP GLU ASP GLN TRP GLU ASP GLY ALA GLU ASP ILE LEU GLU LYS GLU GLU ILE THR GLU ALA SER ASN ILE ASP ASN VAL VAL LEU ASP GLU ASP ARG SER
GLY ALA ARG ARG LEU GLN ASN LEU TRP ARG ASP GLN ARG GLU GLU GLU LEU GLY GLU TYR TYR MET LYS LYS TYR ALA LYS SER SER VAL GLY GLU THR VAL TYR GLY GLY SER ASP GLU LEU SER ASP ASP ILE THR GLN GLN LEU LEU PRO GLY VAL LYS D176 P177 N178 L179 W180
T181 V182 K183 C184 K185 I186 G187 E188 E189 R190 A191 T192 A193 I194 S195 L196 M197 R198 K199 F200 I201 A202 Y203 Q204 F205 T206 D207 T208 P209 L210 Q211 I212 K213 S214 V215 V216 A217 P218 E219 H220 V221 K222 G223 Y224 I225 Y226 V227 E228 A229 Y230 K231 Q232 T233 H234 V235 K236 Q237 A238 I239 E240
G241 V242 G243 N244 L245 R246 L247 G248 Y249 W250 N251 Q252 Q253 M254 V255 P256 I257 K258 E259 M260 T261 D262 V263 L264 K265 V266 V267 K268 GLU VAL A271 N272 L273 K274 P275 K276 S277 W278 V279 R280 L281 K282 R283 G284 I285 Y286 K287 D288 D289 I290 A291 Q292 V293 D294 Y295 V296 E297 P298 S299 Q300
N301 T302 I303 S304 L305 K306 M307 I308 P309 R310 I311 D312 Y313 D314 R315 I316 K317 A318 ARG MET SER LEU LYS ASP TRP PHE ALA LYS ARG LYS LYS PHE LYS ARG P335 P336 Q337 R338 L339 F340 D341 A342 E343 K344 I345 R346 S347 L348 G349 G350 D351 V352 A353 S354 D355 G356 D357 F358 L359 I360
F361 E362 G363 N364 R365 Y366 S367 R368 K369 G370 F371 L372 F373 K374 S375 F376 A377 M378 S379 A380 V381 I382 T383 E384 G385 V386 K387 P388 T389 L390 S391 E392 L393 E394 K395 F396 GLU ASP GLN PRO GLU GLY ILE ASP LEU GLU VAL VAL THR GLU SER THR GLY LYS GLU R416 E417 H418 N419 F420
Q421 P422 G423 D424 N425 V426 E427 V428 C429 E430 G431 E432 L433 I434 N435 L436 Q437 G438 K439 I440 L441 S442 V443 D444 G445 N446 K447 I448 T449 I450 M451 P452 K453 H454 E455 D456 L457 K458 D459 M460 L461 E462 F463 P464 A465 Q466 E467 L468 R469 K470 Y471 F472 K473 M474 G475 D476 H477 V478 K479 V480
I481 A482 G483 R484 F485 E486 G487 D488 T489 G490 L491 I492 V493 R494 V495 E496 E497 N498 F499 V500 I501 L502 F503 S504 D505 L506 T507 M508 H509 E510 L511 K512 V513 L514 P515 R516 D517 L518 Q519 L520 C521 S522 E523 T524 A525 S526 G527 V528 D529 V530 G531 G532 Q533 H534 E535 W536 G537 E538 L539 V540
Q541 L542 D543 P544 Q545 T546 V547 G548 V549 I550 V551 R552 L553 E554 R555 E556 T557 F558 Q559 V560 L561 N562 M563 Y564 G565 K566 V567 V568 T569 V570 R571 H572 Q573 A574 V575 T576 R577 K578 K579 D580 N581 R582 F583 A584 V585 A586 L587 D588 S589 E590 Q591 N592 N593 I594 H595 V596 K597 D598 I599 V600
K601 V602 I603 D604 G605 P606 H607 S608 G609 R610 E611 G612 E613 I614 R615 H616 L617 F618 R619 S620 F621 A622 F623 L624 H625 C626 K627 K628 L629 V630 E631 N632 G633 G634 M635 F636 V637 C638 K639 T640 R641 H642 L643 V644 L645 A646 GLY GLY SER LYS PRO ARG ASP VAL THR ASN PHE THR VAL GLY
GLY PHE ALA PRO MET SER PRO ARG ILE SER SER PRO MET HIS PRO SER ALA GLY GLY GLN ARG GLY GLY PHE GLY SER PRO GLY GLY GLY SER GLY GLY MET SER ARG GLY ARG GLY ARG ARG ASP N703 E704 L705 R711 I712 S713 P716 Y720 V724 K725 D726 A727 T728 E729
R733 V734 E735 L736 S744 V745 D746 R747 L750 S755 R756 R757 P758 G759 G760 M761 T762 S763 T764 Y765 G766 R767 THR PRO MET Y771 G772 S773 Q774 T775 P776 M777 Y778 G779 S780 G781 SER ARG THR PRO MET TYR GLY SER GLN THR PRO LEU GLN ASP GLY SER ARG THR PRO HIS
TYR GLY SER GLN THR PRO LEU HIS ASP GLY SER ARG THR PRO ALA GLN SER GLY ALA TRP ASP PRO ASN ASN PRO ASN THR PRO SER ARG ALA GLU GLU GLU TYR GLU TYR ALA PHE ASP ASP GLU PRO THR PRO SER PRO GLN ALA TYR GLY GLY THR PRO ASN PRO GLN THR PRO GLY
TYR PRO ASP PRO SER SER PRO GLN VAL ASN PRO GLN TYR ASN PRO GLN THR PRO GLY THR PRO ALA MET TYR ASN THR ASP GLN PHE SER PRO TYR ALA ALA PRO SER PRO GLN GLY SER TYR GLN PRO SER PRO SER PRO GLN SER TYR HIS GLN VAL ALA PRO SER PRO ALA GLY TYR
GLN ASN THR HIS SER PRO ALA SER TYR HIS PRO THR PRO SER PRO MET ALA TYR GLN ALA SER PRO SER PRO SER PRO VAL GLY TYR SER PRO MET THR PRO GLY ALA PRO SER PRO GLY GLY TYR ASN PRO HIS THR PRO GLY SER GLY ILE GLU GLN ASN SER SER ASP TRP VAL THR


THR ASP ILE GLN VAL LYS VAL ARG ASP THR TYR LEU ASP THR GLN VAL VAL GLY GLN THR GLY VAL ILE ARG SER VAL THR GLY GLY MET CYS SER VAL TYR LEU LYS ASP SER GLU LYS VAL VAL SER ILE SER SER GLU HIS LEU GLU PRO ILE THR PRO THR LYS ASN ASN LYS VAL
LYS VAL ILE LEU GLY GLU ASP ARG GLU ALA THR GLY VAL LEU LEU SER ILE ASP GLY GLU ASP GLY ILE VAL ARG MET ASP LEU ASP GLU GLN LEU LYS ILE LEU ASN LEU ARG PHE LEU GLY LYS LEU LEU GLU ALA

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	446195	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPO, SEP, 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	1.40	97/11437 (0.8%)	0.89	18/15433 (0.1%)
2	B	1.63	126/9158 (1.4%)	0.97	28/12360 (0.2%)
3	C	1.77	44/2115 (2.1%)	0.96	7/2873 (0.2%)
4	D	0.42	0/1017	0.51	0/1368
5	E	1.29	10/1751 (0.6%)	0.81	1/2366 (0.0%)
6	F	1.69	9/636 (1.4%)	0.89	0/859
7	G	0.75	0/1364	0.62	0/1853
8	H	1.78	31/1219 (2.5%)	0.92	1/1644 (0.1%)
9	I	1.25	4/964 (0.4%)	0.79	0/1305
10	J	1.82	9/533 (1.7%)	1.03	3/719 (0.4%)
11	K	1.68	8/939 (0.9%)	0.92	2/1271 (0.2%)
12	L	1.57	5/395 (1.3%)	1.00	2/525 (0.4%)
13	M	0.26	0/4763	0.48	1/6084 (0.0%)
14	N	0.98	1/870 (0.1%)	0.87	1/1341 (0.1%)
15	P	1.34	3/506 (0.6%)	1.82	22/787 (2.8%)
16	Q	0.36	0/7365	0.51	0/9927
17	R	0.39	0/1860	0.56	2/2509 (0.1%)
18	T	1.68	11/1087 (1.0%)	1.13	6/1674 (0.4%)
19	U	0.34	0/864	0.58	2/1173 (0.2%)
20	V	0.32	0/1728	0.52	2/2357 (0.1%)
21	W	0.37	0/2392	0.53	0/3257
22	X	0.34	0/356	0.52	0/478
23	Y	0.27	0/927	0.48	0/1250
24	Z	0.45	0/4081	0.55	1/5493 (0.0%)
All	All	1.15	358/58327 (0.6%)	0.79	99/78906 (0.1%)

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
1	A	0	2
2	B	0	3
17	R	0	1
All	All	0	6

The worst 5 of 358 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	791	GLU	CA-CB	-15.42	1.20	1.53
2	B	94	SER	C-N	-11.45	1.07	1.34
8	H	116	VAL	CB-CG1	-9.52	1.32	1.52
2	B	690	CYS	CB-SG	-8.84	1.67	1.82
2	B	1047	TYR	CD1-CE1	-8.57	1.26	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	40	A	C8-N9-C4	-13.77	100.29	105.80
15	P	40	A	N7-C8-N9	12.63	120.11	113.80
15	P	41	C	C6-N1-C2	-11.07	115.87	120.30
3	C	224	GLY	C-N-CA	10.22	147.25	121.70
15	P	40	A	C5-N7-C8	-9.32	99.24	103.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1434	GLU	Peptide
1	A	910	LYS	Peptide
2	B	20	ASP	Peptide
2	B	547	GLU	Peptide
2	B	686	GLU	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	11255	0	11374	435	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8980	0	9017	295	0
3	C	2072	0	2019	45	0
4	D	1004	0	980	55	0
5	E	1720	0	1737	73	0
6	F	626	0	657	11	0
7	G	1333	0	1321	80	0
8	H	1197	0	1156	44	0
9	I	942	0	873	38	0
10	J	524	0	541	19	0
11	K	920	0	942	28	0
12	L	390	0	397	13	0
13	M	4737	0	2262	46	0
14	N	773	0	412	38	0
15	P	452	0	229	24	0
16	Q	7226	0	7169	355	0
17	R	1832	0	1687	114	0
18	T	974	0	541	39	0
19	U	852	0	668	31	0
20	V	1703	0	1426	85	0
21	W	2333	0	2246	155	0
22	X	353	0	371	28	0
23	Y	911	0	908	27	0
24	Z	4023	0	4035	181	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	Y	1	0	0	0	0
26	A	1	0	0	0	0
All	All	57142	0	52968	2040	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 19.

The worst 5 of 2040 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)
8:H:37:MET:HE2	8:H:127:GLY:HA3	1.42	0.99
2:B:953:ASP:OD1	3:C:36:ARG:NH2	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:HIS:HD1	1:A:626:THR:HG1	1.04	0.94
16:Q:505:ARG:HH21	20:V:44:PHE:HB2	1.32	0.93
1:A:904:GLN:NE2	1:A:981:CYS:O	2.01	0.91

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	1408/1984 (71%)	1281 (91%)	117 (8%)	10 (1%)	22	57
2	B	1112/1251 (89%)	998 (90%)	105 (9%)	9 (1%)	19	54
3	C	254/275 (92%)	232 (91%)	19 (8%)	3 (1%)	13	44
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	29	64
6	F	76/127 (60%)	70 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
8	H	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	22	57
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	60 (94%)	2 (3%)	2 (3%)	4	23
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
13	M	976/1729 (56%)	903 (92%)	72 (7%)	1 (0%)	51	83
16	Q	888/1179 (75%)	836 (94%)	52 (6%)	0	100	100
17	R	240/713 (34%)	225 (94%)	14 (6%)	1 (0%)	34	69
19	U	117/666 (18%)	88 (75%)	21 (18%)	8 (7%)	1	7
20	V	234/531 (44%)	199 (85%)	31 (13%)	4 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	298/305 (98%)	268 (90%)	30 (10%)	0	100	100
22	X	41/531 (8%)	41 (100%)	0	0	100	100
23	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100	100
24	Z	497/1087 (46%)	460 (93%)	36 (7%)	1 (0%)	47	79
All	All	7238/11540 (63%)	6624 (92%)	573 (8%)	41 (1%)	29	59

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
1	A	1185	VAL
1	A	1468	THR
2	B	19	PRO
3	C	93	PHE

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	1245/1761 (71%)	1226 (98%)	19 (2%)	65	85
2	B	986/1084 (91%)	949 (96%)	37 (4%)	33	66
3	C	235/252 (93%)	228 (97%)	7 (3%)	41	71
4	D	109/126 (86%)	108 (99%)	1 (1%)	78	91
5	E	191/192 (100%)	189 (99%)	2 (1%)	76	90
6	F	68/111 (61%)	67 (98%)	1 (2%)	65	85
7	G	146/153 (95%)	143 (98%)	3 (2%)	53	79
8	H	130/131 (99%)	122 (94%)	8 (6%)	18	49
9	I	104/112 (93%)	101 (97%)	3 (3%)	42	72
10	J	55/56 (98%)	54 (98%)	1 (2%)	59	82
11	K	104/106 (98%)	103 (99%)	1 (1%)	76	90
12	L	43/55 (78%)	40 (93%)	3 (7%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	154/1524 (10%)	154 (100%)	0	100	100
16	Q	761/1011 (75%)	755 (99%)	6 (1%)	81	92
17	R	168/625 (27%)	166 (99%)	2 (1%)	71	88
19	U	63/590 (11%)	63 (100%)	0	100	100
20	V	144/462 (31%)	141 (98%)	3 (2%)	53	79
21	W	255/260 (98%)	254 (100%)	1 (0%)	91	96
22	X	40/467 (9%)	40 (100%)	0	100	100
23	Y	102/105 (97%)	102 (100%)	0	100	100
24	Z	434/939 (46%)	432 (100%)	2 (0%)	88	94
All	All	5537/10122 (55%)	5437 (98%)	100 (2%)	61	82

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	63	PHE
8	H	67	ASP
24	Z	720	TYR
3	C	75	SER
5	E	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
16	Q	359	ASN
16	Q	887	ASN
16	Q	407	GLN
16	Q	585	GLN
17	R	585	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/46 (43%)	7 (35%)	3 (15%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	29	C
15	P	30	C
15	P	31	G
15	P	36	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	36	G
15	P	38	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	TPO	Z	775	24	8,10,11	1.54	1 (12%)	10,14,16	1.99	1 (10%)
1	TPO	A	1525	1	8,10,11	1.60	1 (12%)	10,14,16	1.83	1 (10%)
1	SEP	A	1547	1	8,9,10	1.49	1 (12%)	8,12,14	1.39	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	TPO	Z	775	24	-	1/9/11/13	-
1	TPO	A	1525	1	-	4/9/11/13	-
1	SEP	A	1547	1	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	P-O1P	3.41	1.61	1.50
24	Z	775	TPO	P-O1P	3.34	1.61	1.50
1	A	1547	SEP	P-O1P	3.25	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Z	775	TPO	P-OG1-CB	-5.85	105.53	123.21
1	A	1525	TPO	P-OG1-CB	-4.96	108.22	123.21
1	A	1547	SEP	P-OG-CB	-2.69	110.89	118.30
1	A	1547	SEP	OG-CB-CA	2.01	110.10	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	N-CA-CB-CG2
1	A	1525	TPO	N-CA-CB-OG1
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	C-CA-CB-CG2
1	A	1525	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	2	0
1	A	1525	TPO	1	0
1	A	1547	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3
19	U	1
20	V	1
13	M	1
1	A	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	25.86
1	V	299:GLU	C	310:ASN	N	12.74
1	M	1334:ASN	C	1338:ILE	N	5.29
1	B	755:GLN	C	756:LYS	N	1.18
1	B	108:MET	C	109:MET	N	1.17

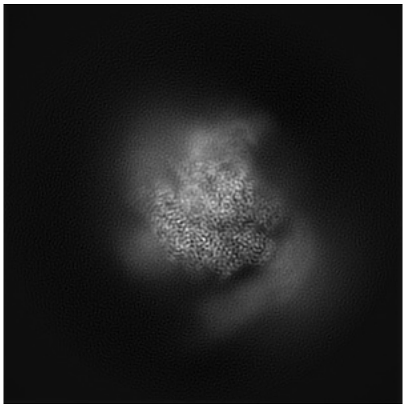
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10480. These allow visual inspection of the internal detail of the map and identification of artifacts.

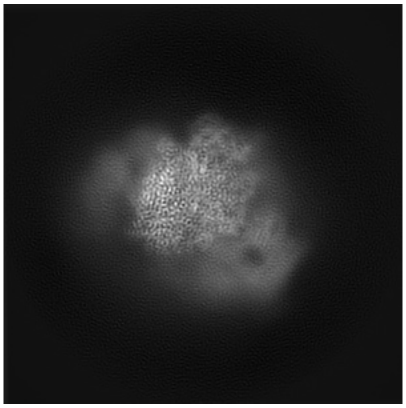
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

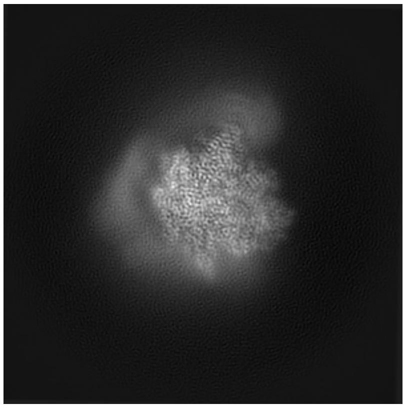
6.1.1 Primary map



X

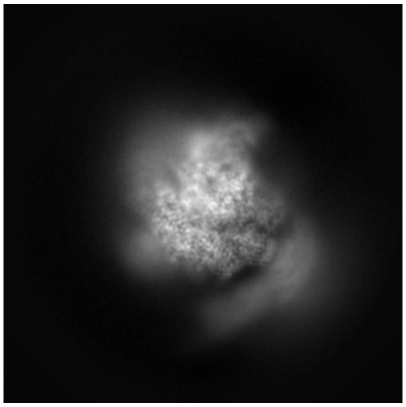


Y

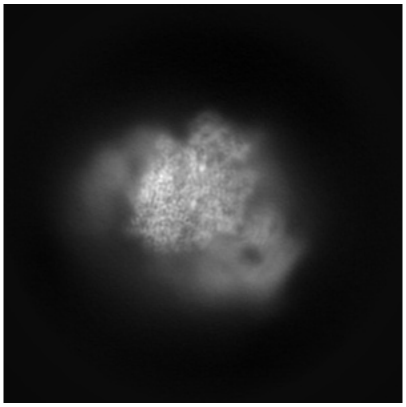


Z

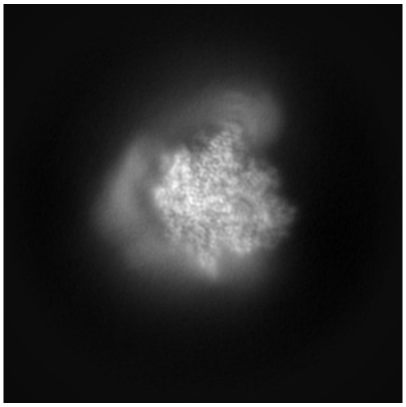
6.1.2 Raw map



X



Y

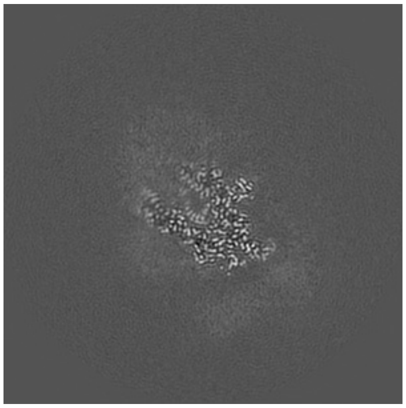


Z

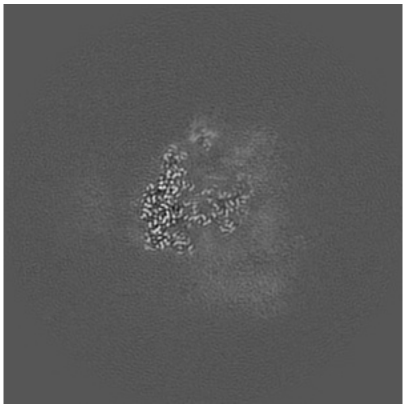
The images above show the map projected in three orthogonal directions.

6.2 Central slices

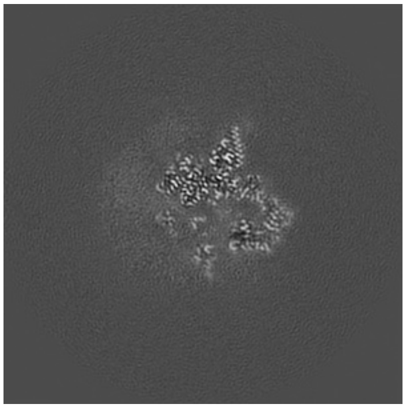
6.2.1 Primary map



X Index: 180

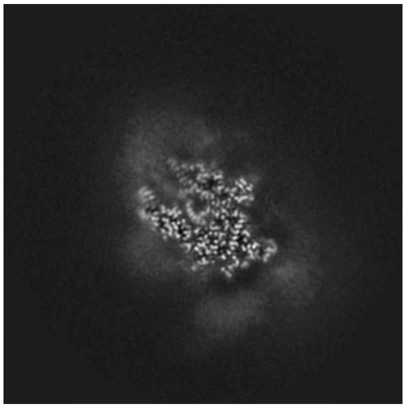


Y Index: 180

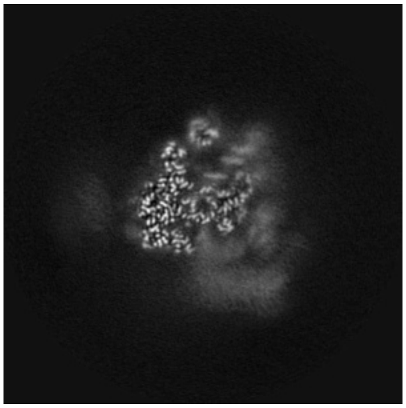


Z Index: 180

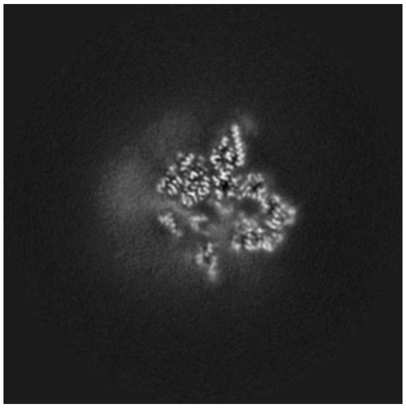
6.2.2 Raw map



X Index: 180



Y Index: 180

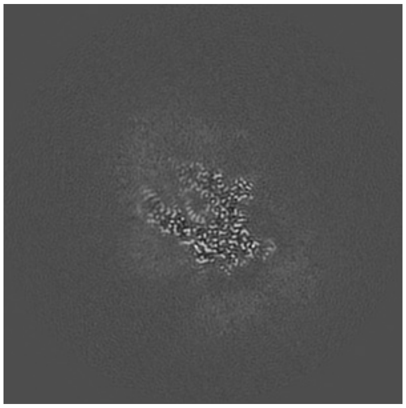


Z Index: 180

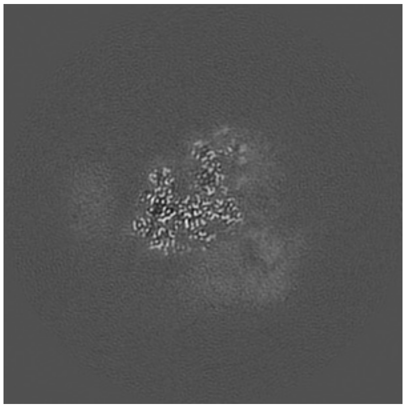
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

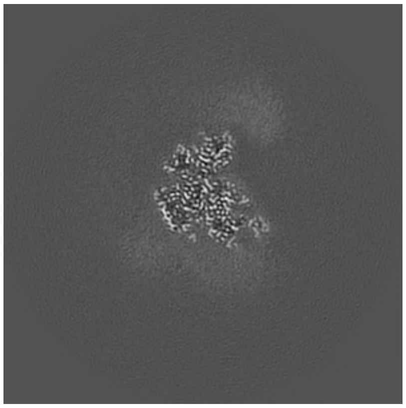
6.3.1 Primary map



X Index: 179

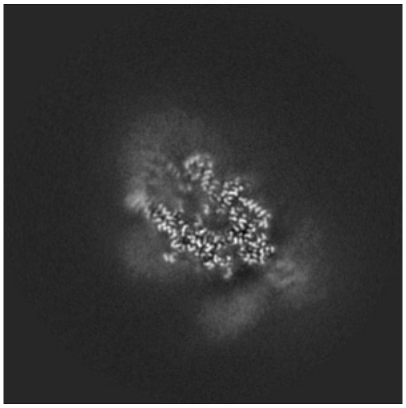


Y Index: 193

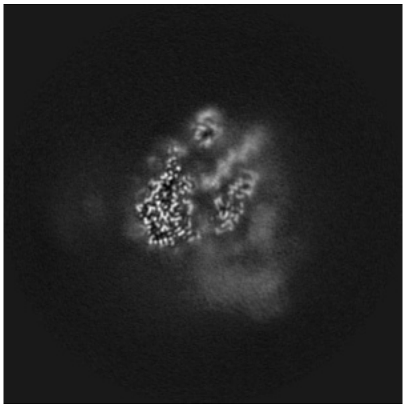


Z Index: 143

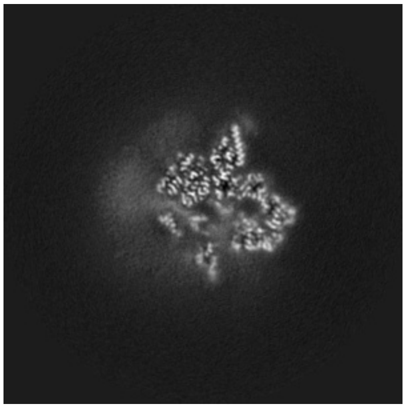
6.3.2 Raw map



X Index: 189



Y Index: 174



Z Index: 180

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

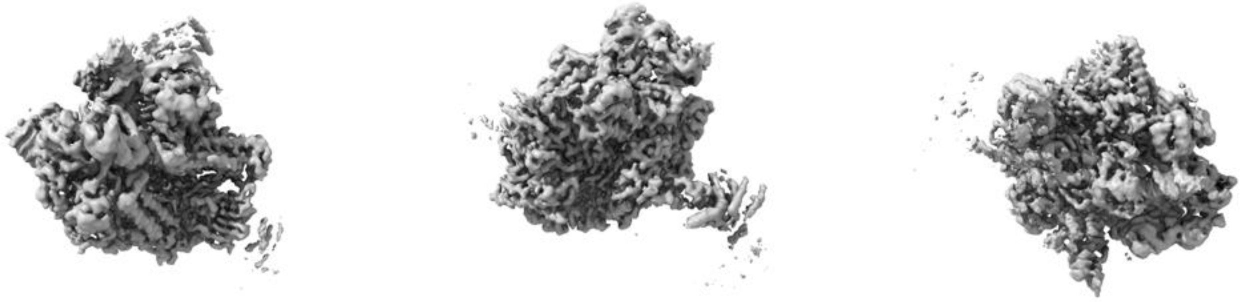
6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

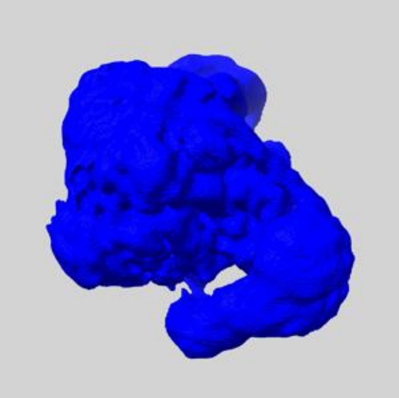
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

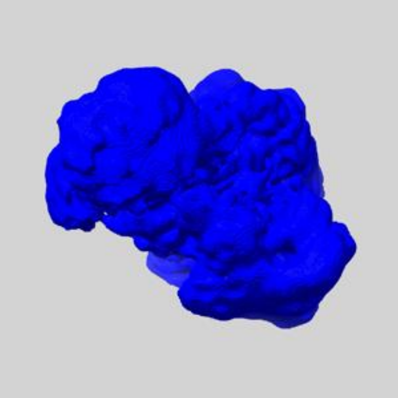
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

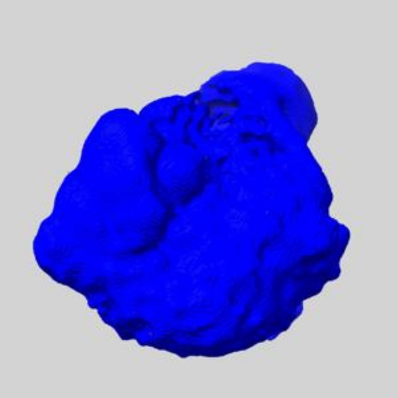
6.5.1 emd_10480_msk_1.map



X

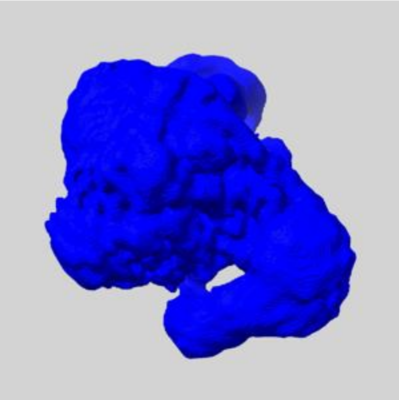


Y

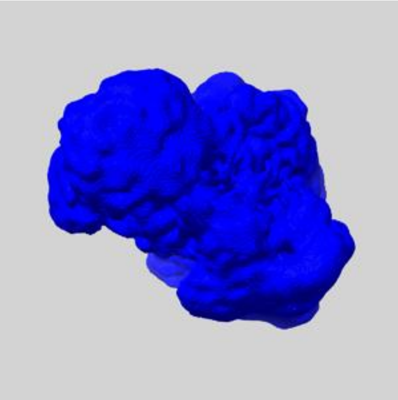


Z

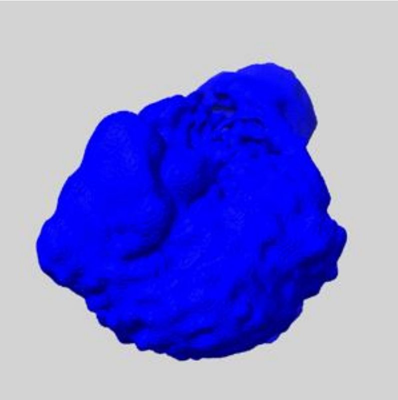
6.5.2 emd_10480_msk_2.map



X



Y

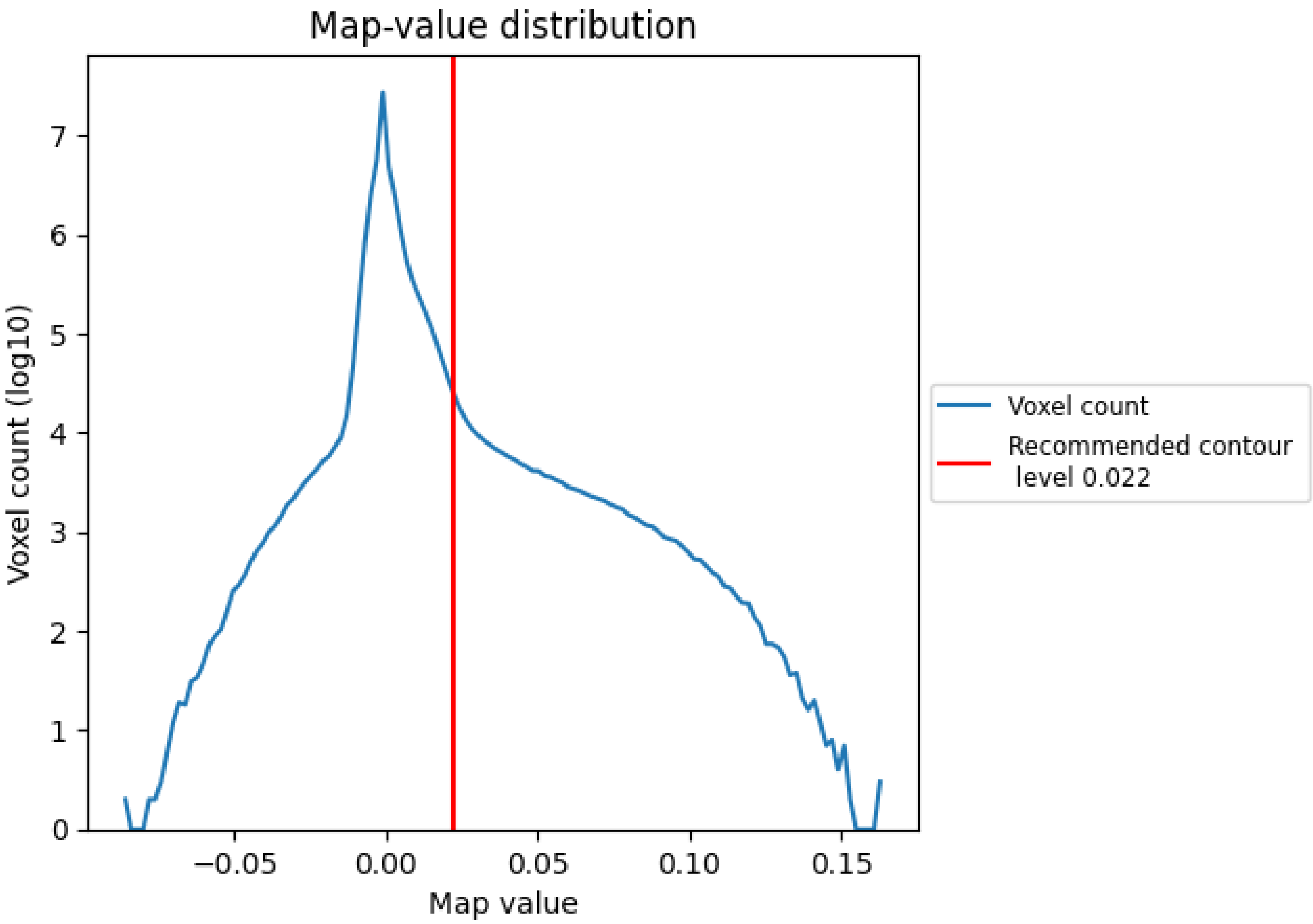


Z

7 Map analysis ⓘ

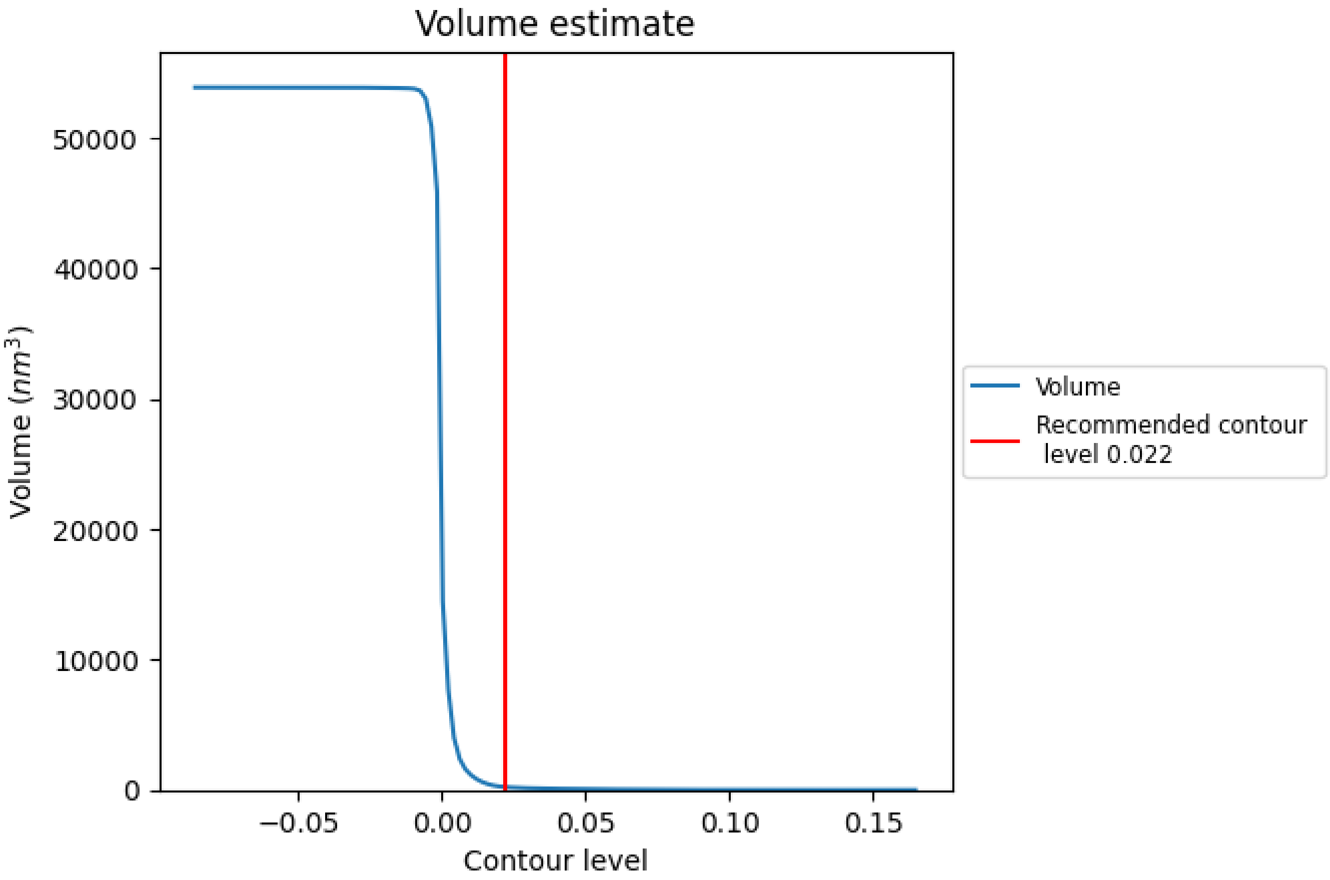
This section contains the results of statistical analysis of the map.

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.

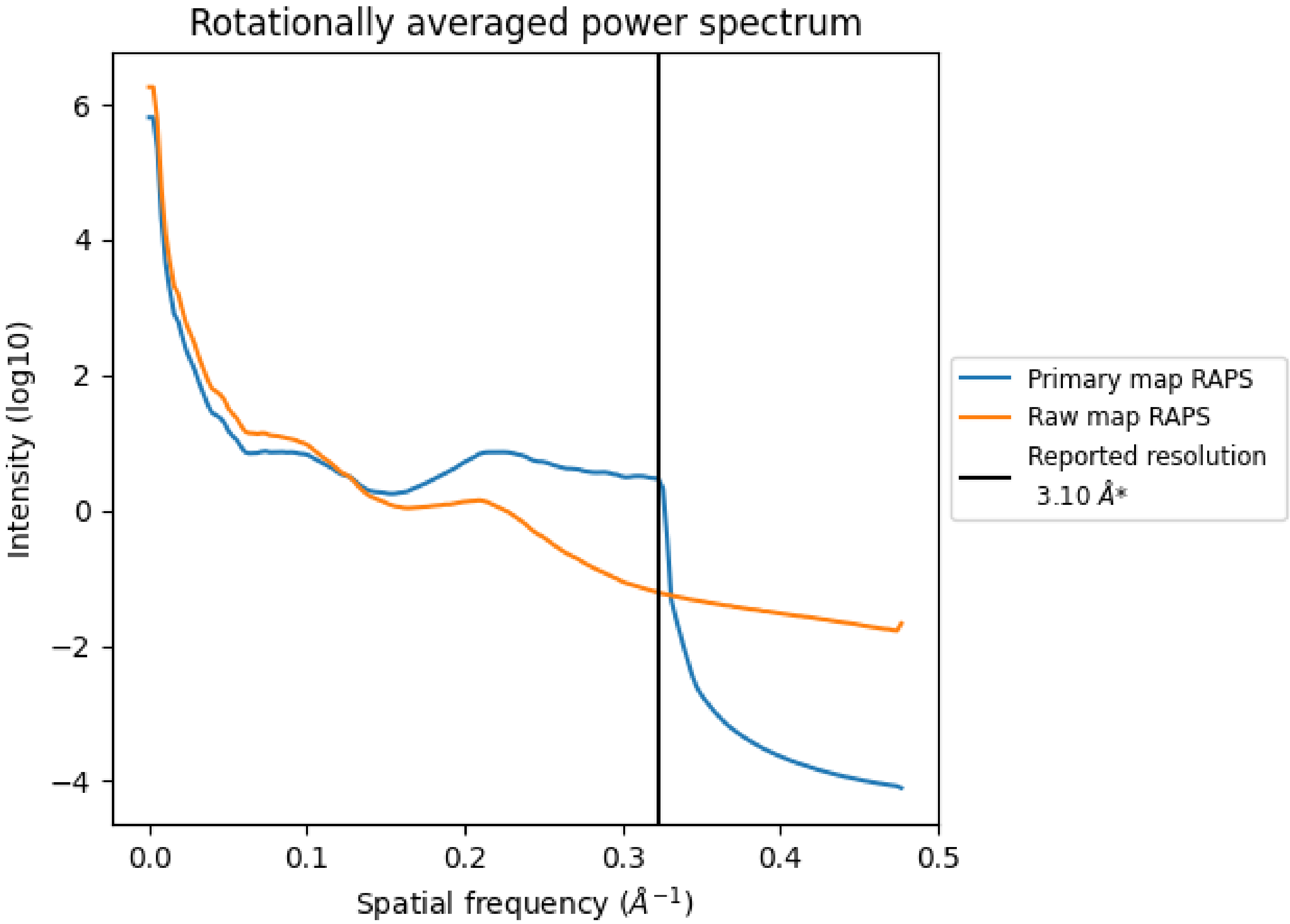
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 223 nm^3; this corresponds to an approximate mass of 202 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 ⓘ

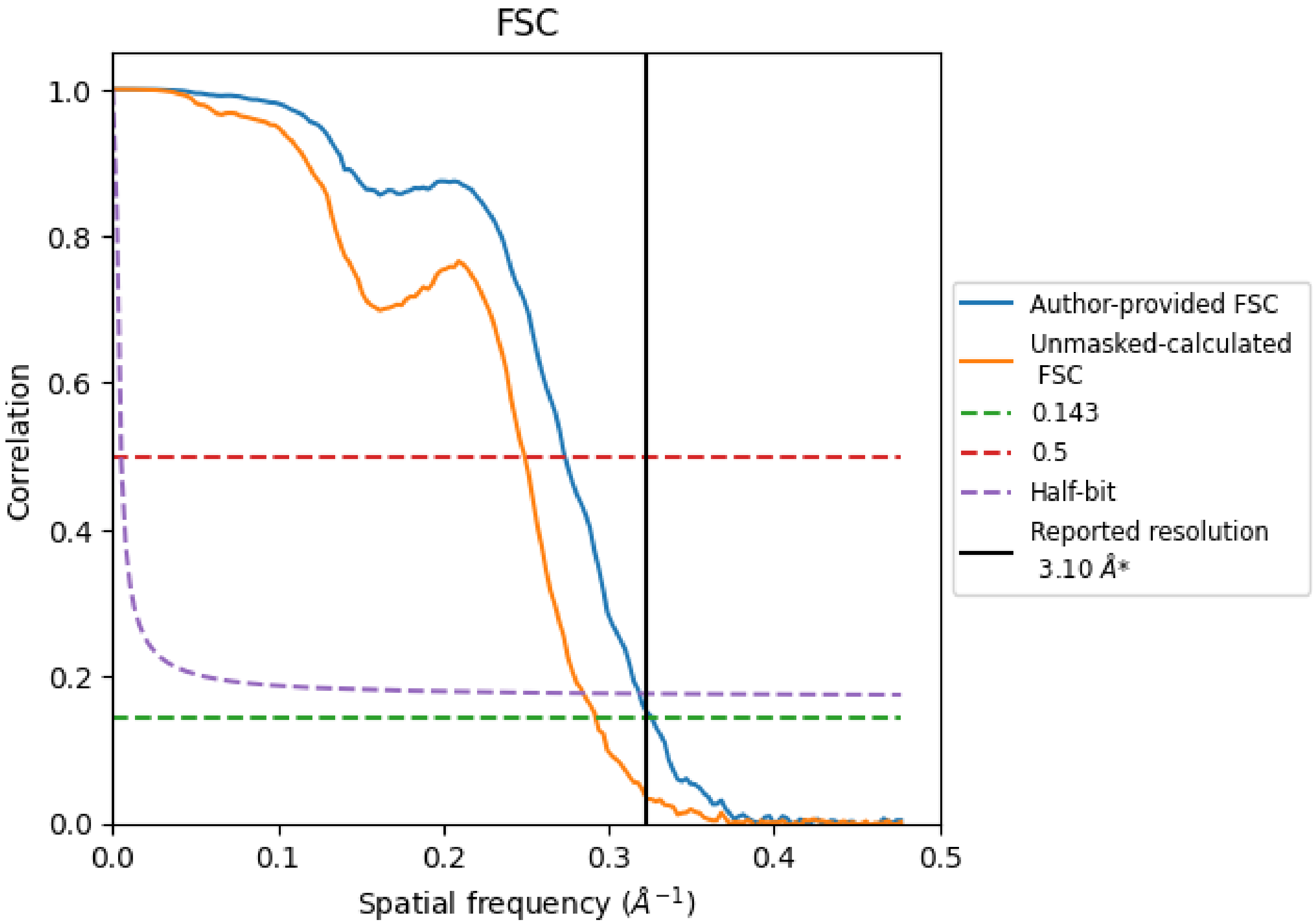


*Reported resolution corresponds to spatial frequency of 0.323 $\AA^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates ⓘ

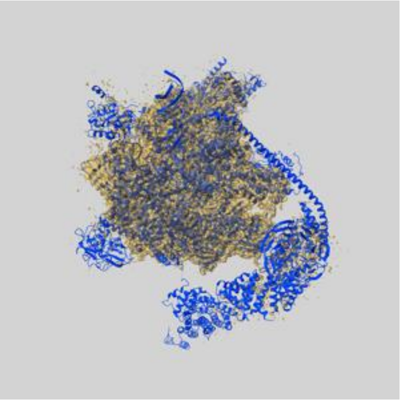
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.66	3.14
Unmasked-calculated*	3.42	4.01	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.1 by more than 10 %

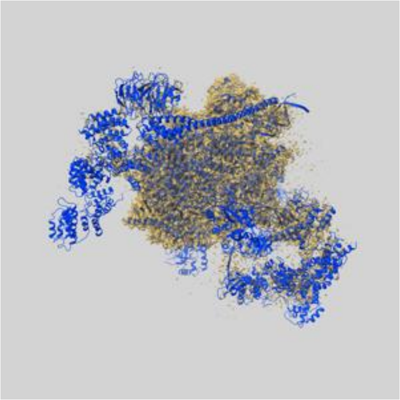
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10480 and PDB model 6TED. Per-residue inclusion information can be found in section 3 on page 9.

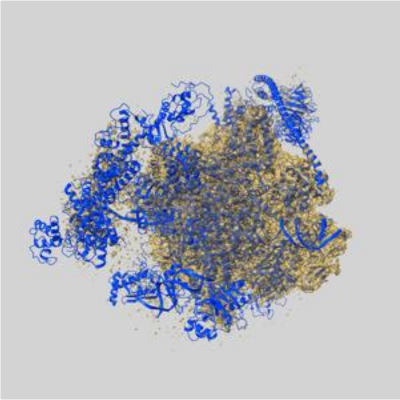
9.1 Map-model overlay ⓘ



X



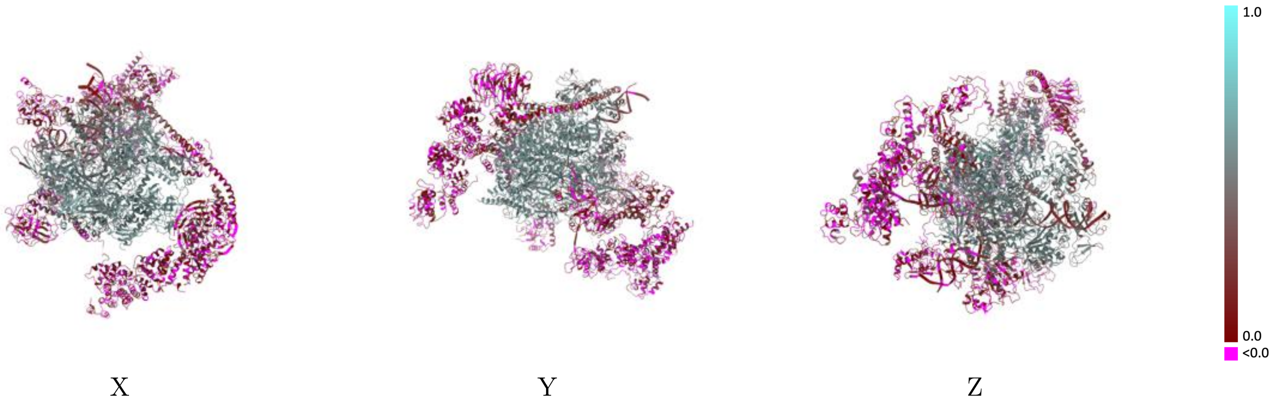
Y



Z

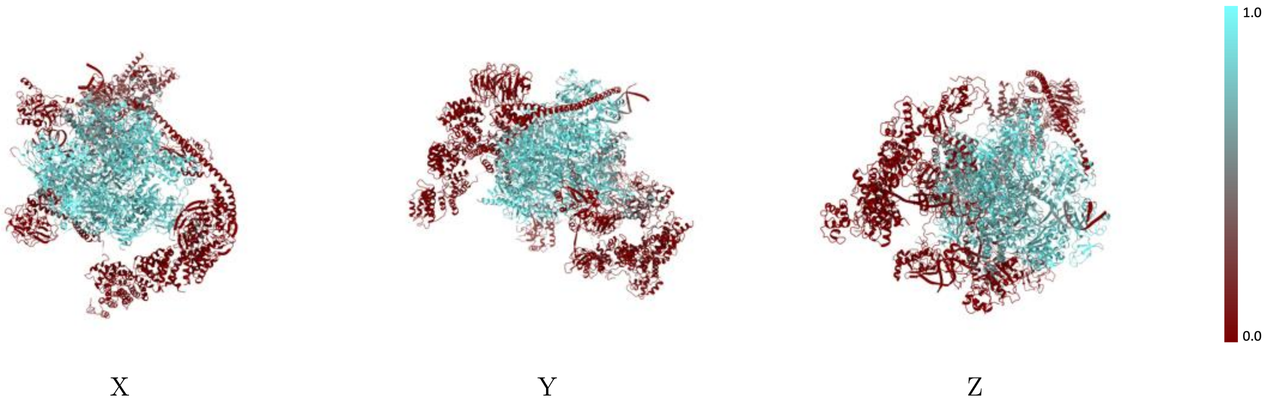
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



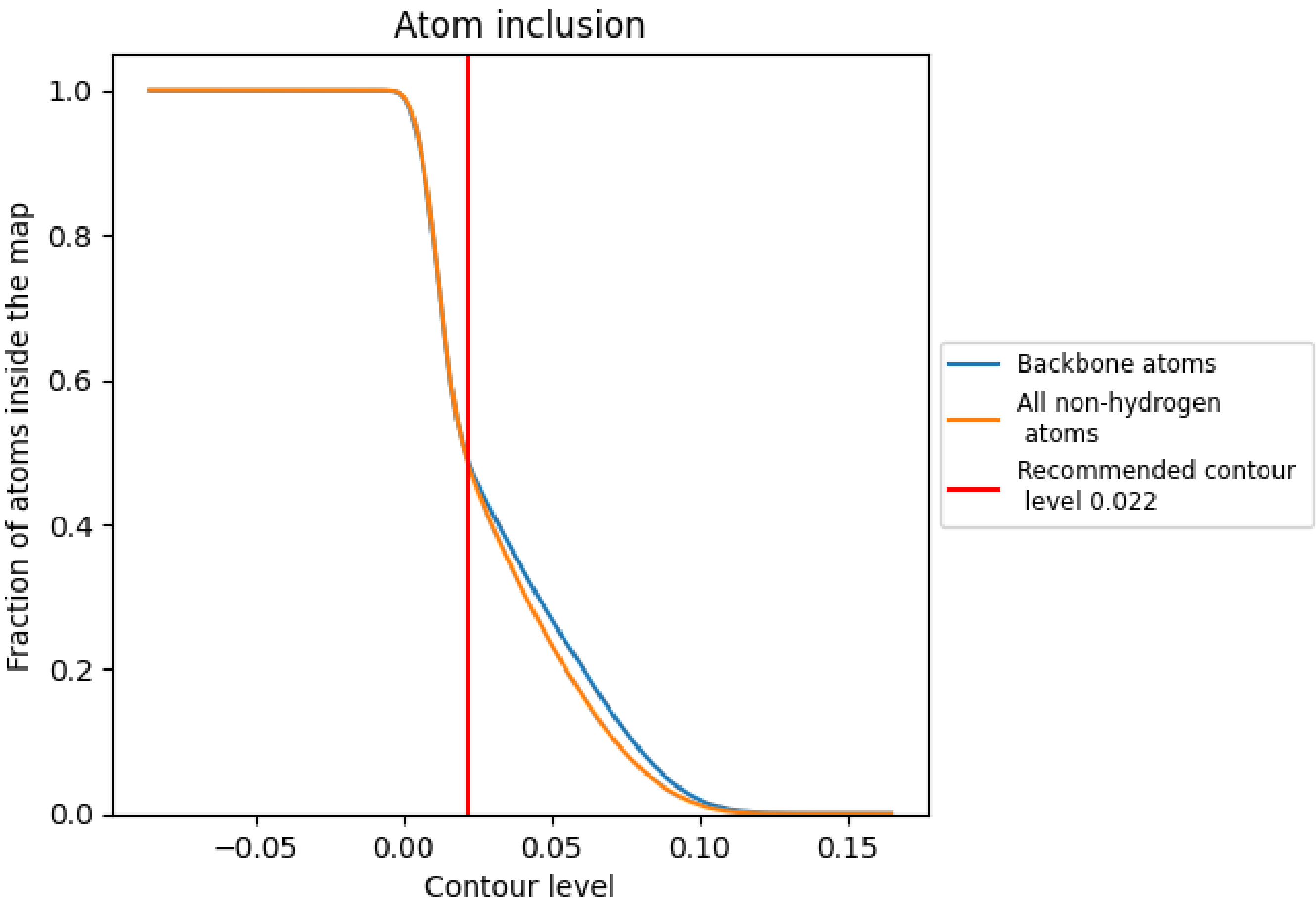
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion ⓘ



At the recommended contour level, 48% of all backbone atoms, 48% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4806	0.3380
A	0.8491	0.5370
B	0.8820	0.5560
C	0.9108	0.5800
D	0.2725	0.1850
E	0.8535	0.5210
F	0.8962	0.5740
G	0.4391	0.3110
H	0.8513	0.5590
I	0.8472	0.5110
J	0.9180	0.5730
K	0.9211	0.5890
L	0.8480	0.5090
M	0.0153	0.0750
N	0.3467	0.2200
P	0.4248	0.2780
Q	0.0282	0.1020
R	0.0117	0.0880
T	0.5195	0.3100
U	0.0548	0.1140
V	0.0256	0.1270
W	0.0109	0.0430
X	0.0235	0.1060
Y	0.0056	0.0770
Z	0.0993	0.1660