wwPDB EM Validation Summary Report

Oct 13, 2024 – 11:47 AM EDT

PDB ID	:	7UNC
EMDB ID	:	EMD-26620
Title	:	Pol II-DSIF-SPT6-PAF1c-TFIIS complex with rewrapped nucleosome
Authors	:	Filipovski, M.; Vos, S.M.; Farnung, L.
Deposited on	:	2022-04-10
Resolution	:	3.00 Å(reported)
Based on initial models	:	3LZ0, 6TED

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

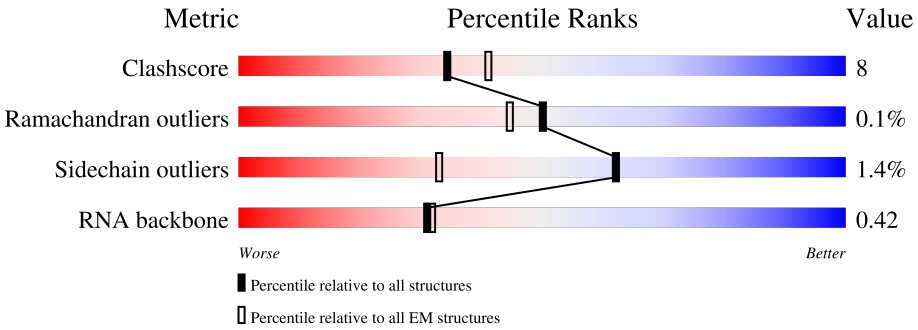
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	58% 13% 28%
2	B	1251	75% 14% 11%
3	C	275	83% 11% 6%
4	D	184	66% 32%
5	E	210	79% 20%
6	F	127	54% 7% 39%
7	G	172	86% 12%

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Mol	Chain	Length	Quality of chain
8	H	150	88% 11%
9	I	125	71% 22% 7%
10	J	67	79% 18%
11	K	117	79% 19%
12	L	58	71% 9% 19%
13	M	1729	31% 57% 42%
14	N	209	8% 48% 11% 33%
15	O	304	36% 51% 47%
16	P	16	56% 19% 19% 6%
17	Q	1179	24% 75% 25%
18	R	713	26% 34% 66%
19	T	215	19% 45% 9% 28%
20	U	666	15% 15% 84%
21	V	531	32% 45% 54%
22	W	305	98%
23	X	531	8% 92%
24	Z	1087	6% 23% 5% 72%
25	a	136	71% 29%
25	e	136	71% 29%
26	b	103	80% 19%
26	f	103	76% 24%
27	c	130	79% 21%
27	g	130	81% 19%
28	d	123	76% 23%
28	h	123	75% 24%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 105742 atoms, of which 48112 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	H	N	O	P	S		
1	A	1426	22643	7074	11388	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	H	N	O	S		
2	B	1117	17949	5665	9002	1571	1647	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	258	4096	1300	2024	356	410	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	126	1985	630	981	170	200	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	209	3458	1089	1738	300	323	8	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	H	N	O	S		
6	F	78	1284	401	658	106	114	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2654	866	1321	214	245	8		

- Molecule 8 is a protein called RPB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	149	Total	C	H	N	O	S	0	0
			2354	759	1157	195	238	5		

- Molecule 9 is a protein called RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	116	Total	C	H	N	O	S	0	0
			1822	582	880	168	181	11		

- Molecule 10 is a protein called RPB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O	S	0	0
			1068	339	544	88	91	6		

- Molecule 11 is a protein called RPB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	47	Total	C	H	N	O	S	0	0
			803	246	406	77	68	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1002	Total	C	H	N	O	0	0
			5267	2004	1259	1002	1002		

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 Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	140	Total	C	H	N	O	P	0	0
			4480	1376	1594	490	880	140		

- Molecule 15 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	161	Total	C	N	O	0	0
			645	322	161	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP P23193
O	-1	ASN	-	expression tag	UNP P23193
O	0	ALA	-	expression tag	UNP P23193

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	16	Total	C	H	N	O	P	0	0
			502	148	170	49	119	16		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	H	N	O	0	0
			5356	1780	1796	890	890		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	244	Total	C	H	N	O	0	0
			1467	488	491	244	244		

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 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	155	Total	C	H	N	O	P	0	0
			4885	1498	1719	629	884	155		

- Molecule 20 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	104	Total	C	H	N	O	0	0
			626	208	210	104	104		

- Molecule 21 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	244	Total	C	H	N	O	0	0
			1457	488	481	244	244		

- Molecule 22 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	300	Total	C	H	N	O	0	0
			1817	600	617	300	300		

- Molecule 23 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	43	Total	C	H	N	O	0	0
			259	86	87	43	43		

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

Mol	Chain	Residues	Atoms							AltConf	Trace
24	Z	307	Total	C	H	N	O	P	S	0	0
			4751	1495	2363	430	450	1	12		

- Molecule 25 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	a	97	Total	C	H	N	O	S	0	0
			1643	506	841	155	138	3		
25	e	97	Total	C	H	N	O	S	0	0
			1640	504	839	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	engineered mutation	UNP P84233
e	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 26 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	b	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
26	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

- Molecule 27 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	103	Total	C	H	N	O	0	0
			1642	501	847	155	139		
27	g	105	Total	C	H	N	O	0	0
			1674	510	865	158	141		

- Molecule 28 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	d	95	Total	C	H	N	O	S	0	0
			1519	469	774	134	140	2		
28	h	93	Total	C	H	N	O	S	0	0
			1474	457	748	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total	Zn	0
			2	2	
29	B	1	Total	Zn	0
			1	1	
29	C	1	Total	Zn	0
			1	1	
29	I	2	Total	Zn	0
			2	2	
29	J	1	Total	Zn	0
			1	1	
29	R	1	Total	Zn	0
			1	1	

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

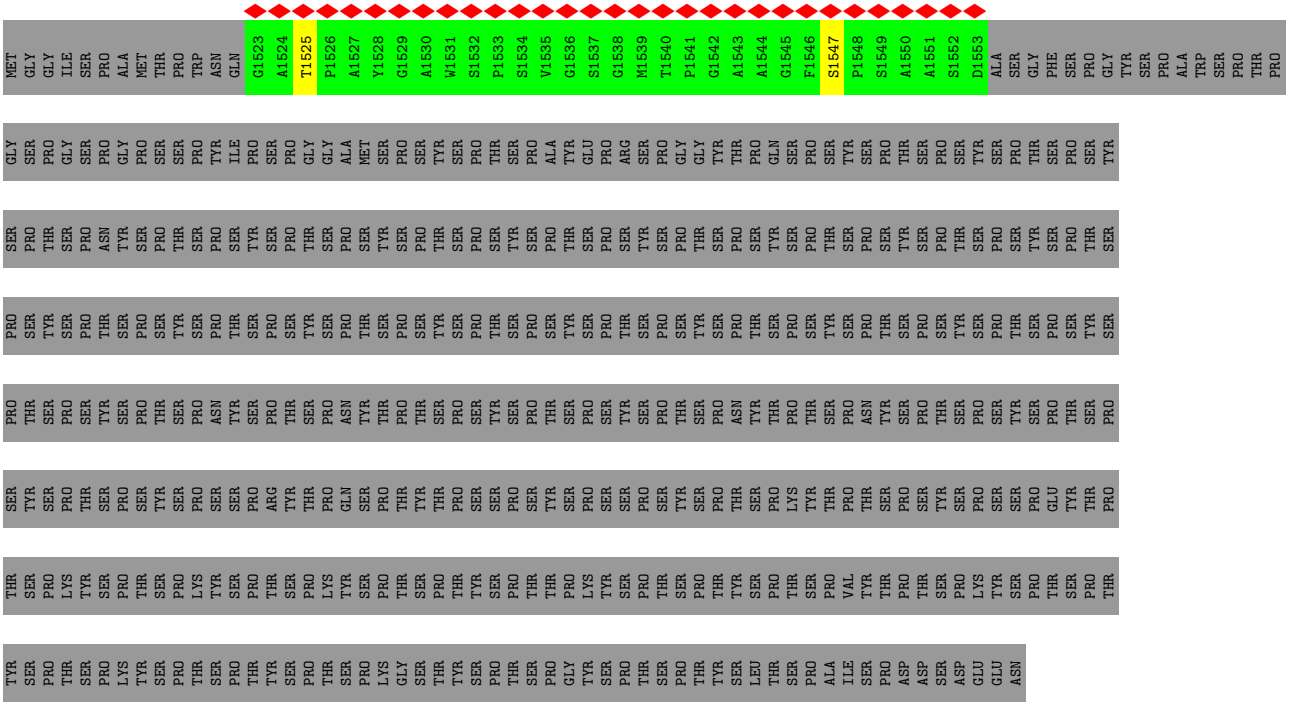
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

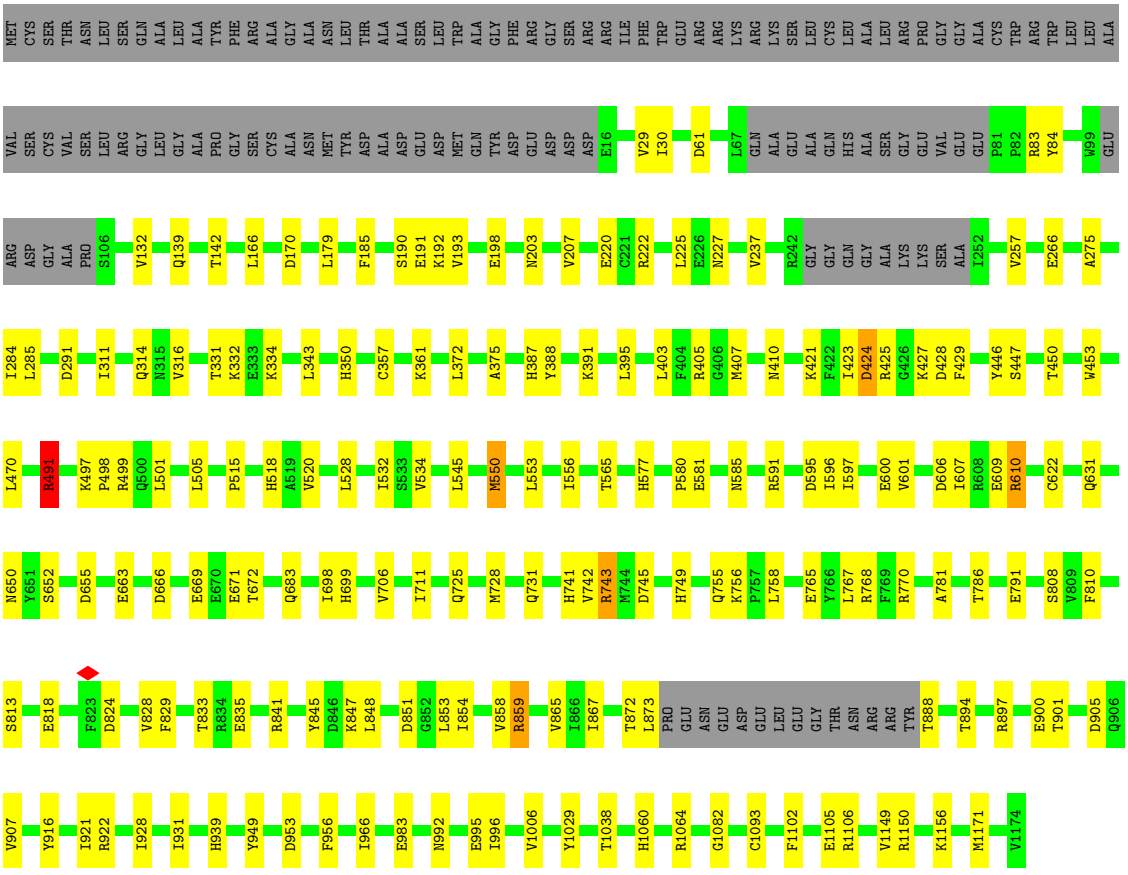
- Molecule 1: DNA-directed RNA polymerase subunit

Chain A:



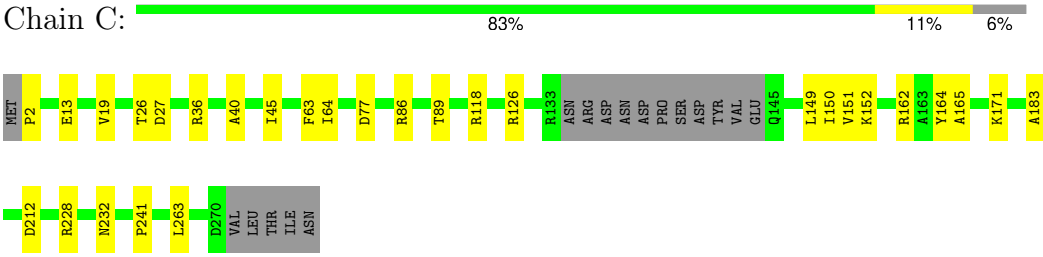
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



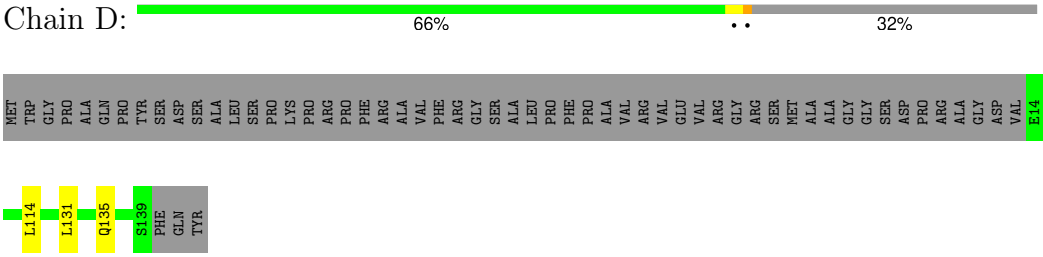
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



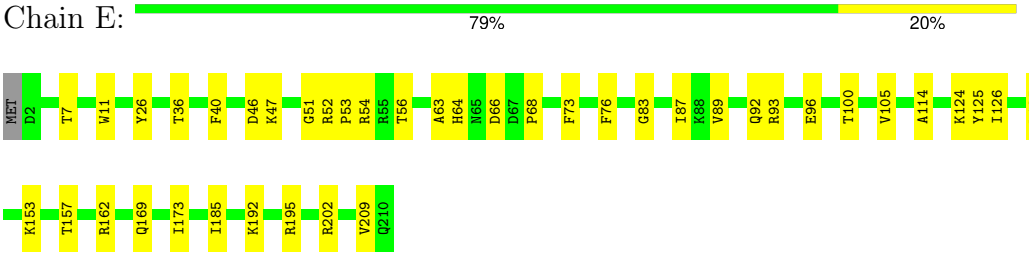
• Molecule 4: RPOL4c domain-containing protein

Chain D:



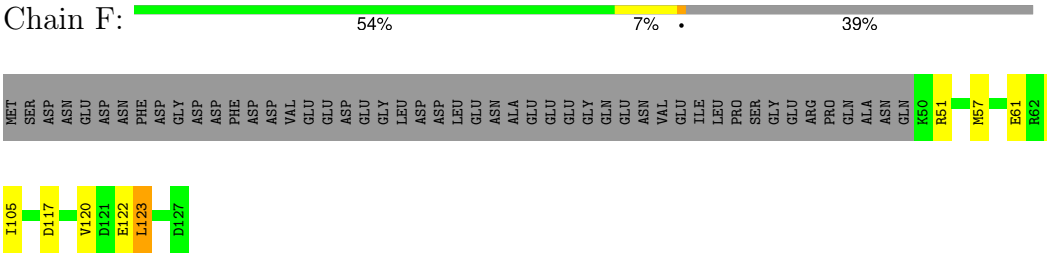
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:



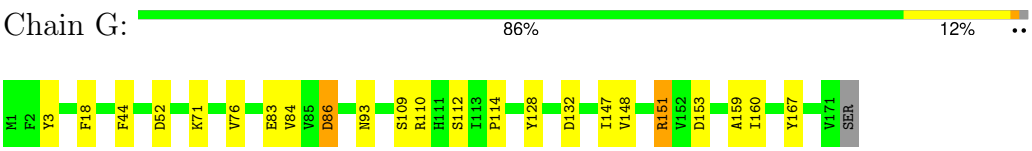
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



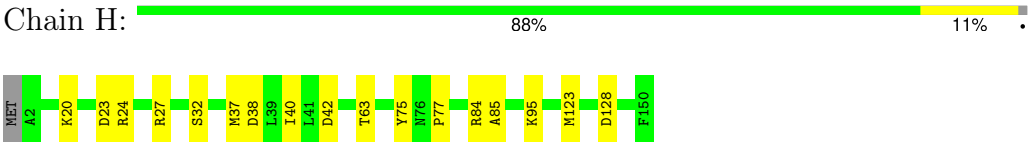
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



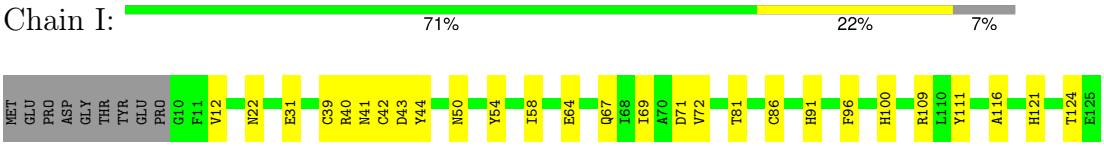
• Molecule 8: RPB8

Chain H:



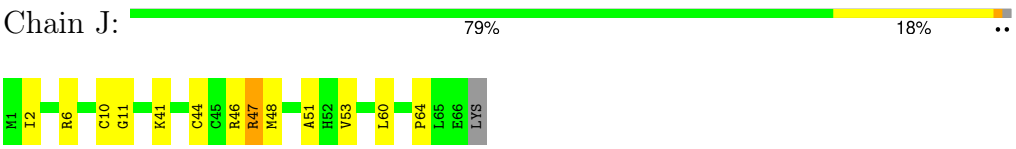
• Molecule 9: RPB9

Chain I:



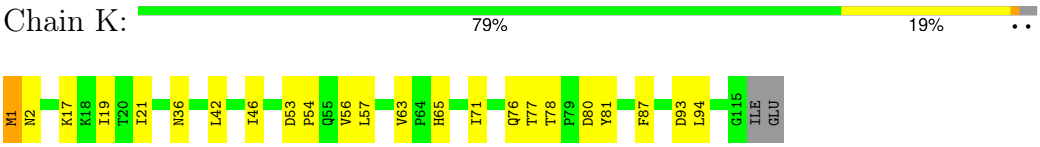
• Molecule 10: RPB10

Chain J:



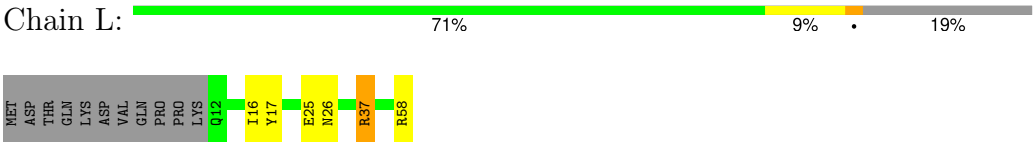
• Molecule 11: RPB11

Chain K:



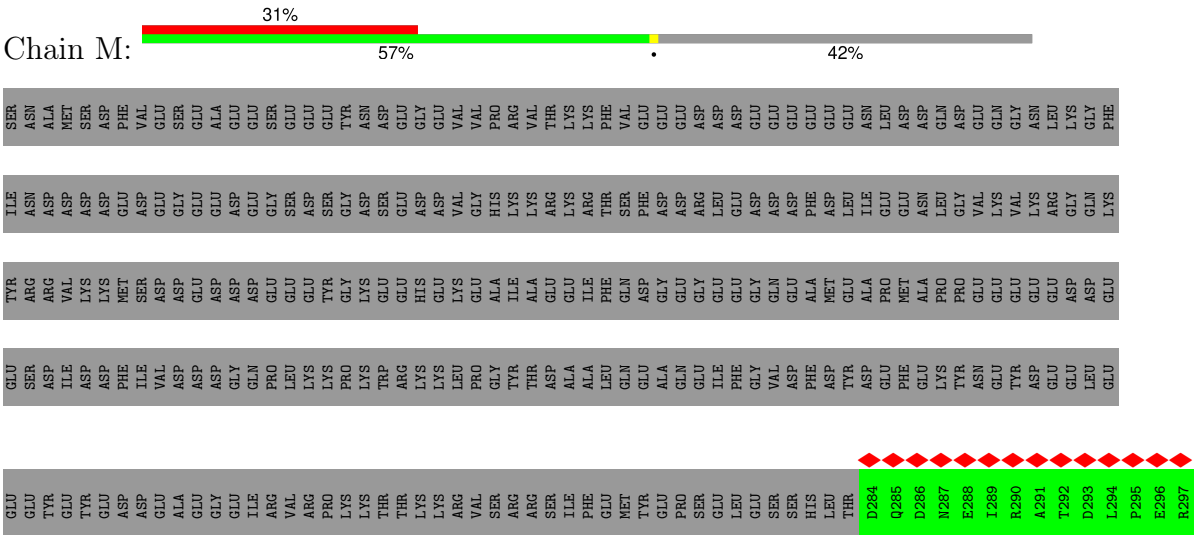
• Molecule 12: RNA polymerase II subunit K

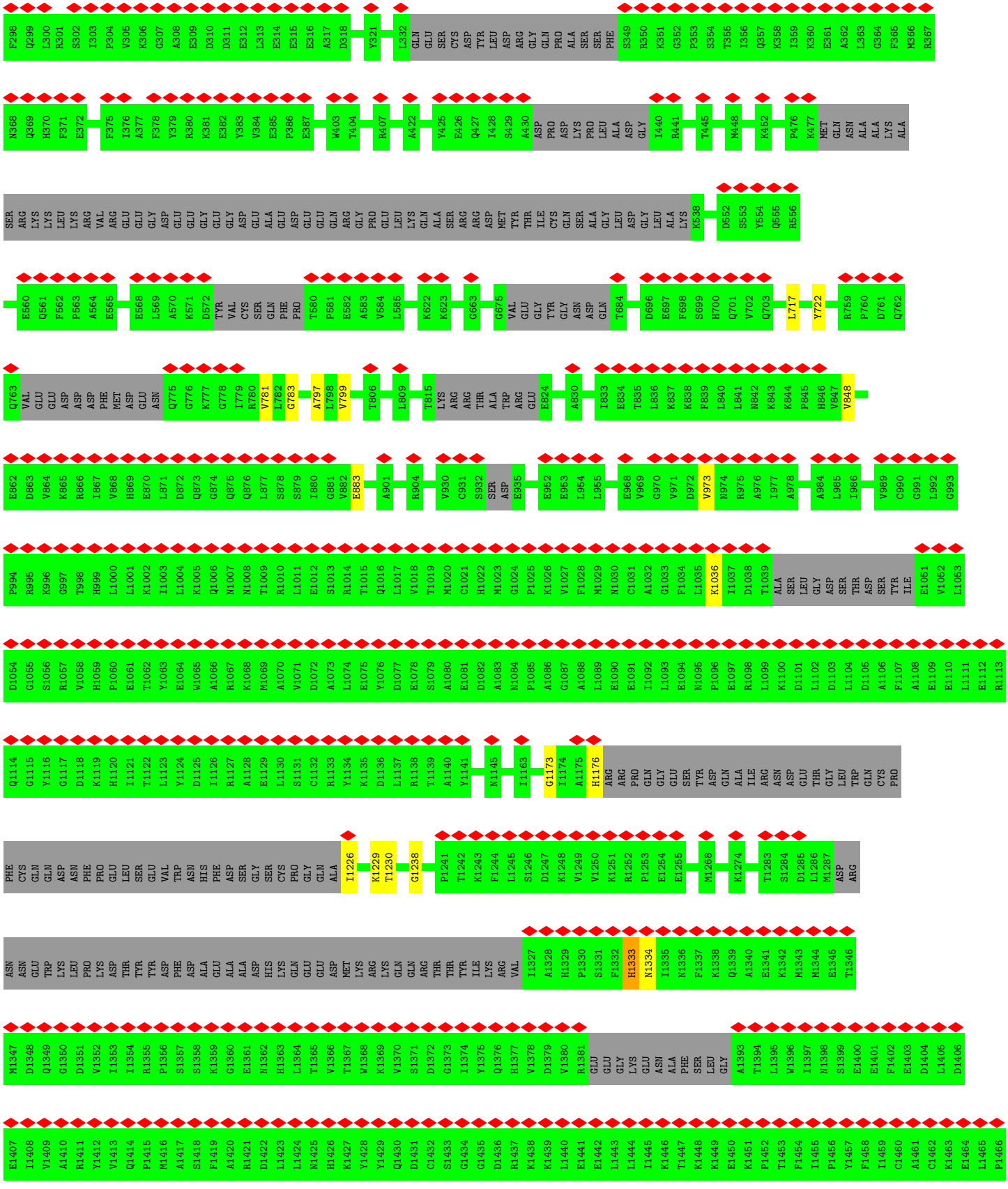
Chain L:



• Molecule 13: Transcription elongation factor SPT6

Chain M:

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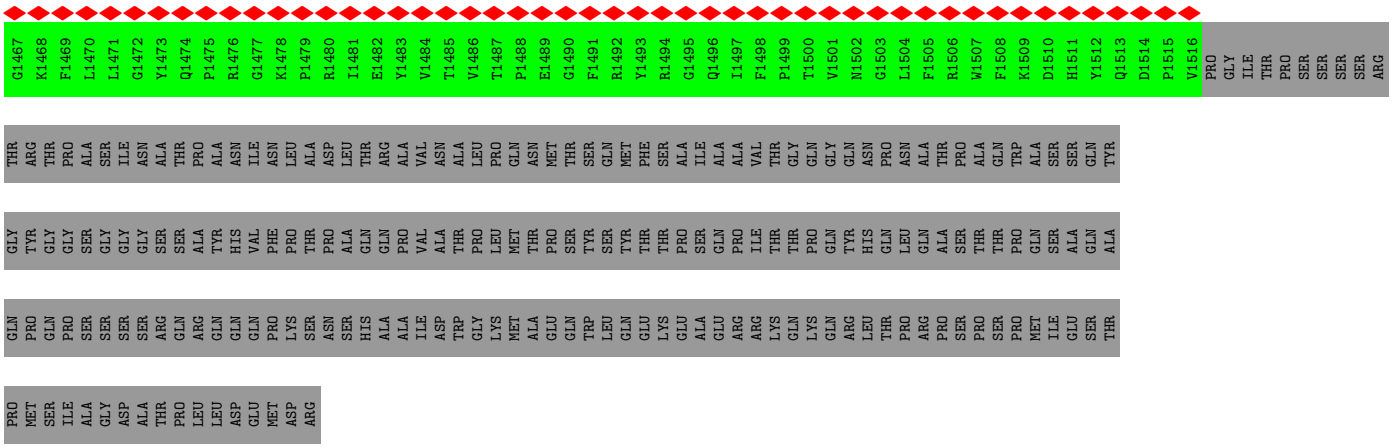
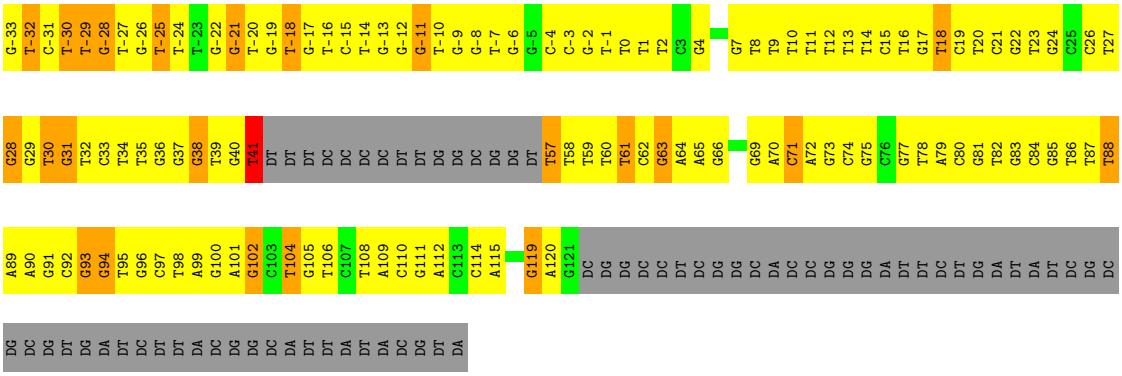
N368 Q369 H370 F371 E372 F375 I376 A377 F378 Y379 R380 K381 E382 Y383 V384 E385 P386 E387 W403 T404 R407 A422 Y425 E426 Q427 I428 S429 A430 ASP PRO ASP LYS PRO LEU ALA ASP GLY I440 R441 T445 M448 K452 P476 K477 MET GLN ASN ALA ALA LYS ALA
SER ARG LYS LYS LEU LYS ARG VAL ARG GLU GLU GLY ASP GLU GLU GLY GLU GLY ASP GLU ALA GLU ASP GLU GLU GLN ARG GLY PRO GLU LEU LYS GLN ALA SER ARG ARG ASP MET TYR THR ILE CYS GLN SER ALA GLY LEU ASP GLY LEU ALA LYS K538 D552 S553 Y554 Q555 R556
E560 Q561 F562 P563 A564 E565 E568 L569 A570 K571 D572 TYR VAL CYS SER GLN PHE PRO T580 P581 E582 A583 V584 L585 K622 K623 G663 G675 VAL GLU GLY TYR GLY ASN ASP GLN T684 D696 E697 F698 S699 H700 Q701 V702 Q703 L717 Y722 R759 P760 D761 Q762
Q763 VAL GLU GLU ASP ASP ASP PHE MET ASP GLU ASN Q775 G776 K777 G778 I779 R780 V781 L782 G783 A797 L798 V799 T806 L809 T815 LYS ARG ARG THR ALA TRP ARG GLU E824 A830 I833 E834 T835 L836 K837 K838 F839 L840 L841 N842 K843 K844 P845 H846 V847 V848
E862 D863 V864 K865 R866 I867 V868 H869 E870 L871 D872 Q873 G874 Q875 Q876 L877 S878 S879 I880 G881 V882 E883 A901 R904 V930 C931 S932 SER ASP E935 E952 E953 L954 L955 E968 V969 G970 V971 D972 V973 N974 R975 A976 I977 A978 A984 L985 I986 V989 C990 G991 L992 G993
P994 R995 K996 G997 T998 H999 L1000 L1001 K1002 I1003 L1004 K1005 Q1006 N1007 N1008 T1009 R1010 L1011 E1012 S1013 R1014 T1015 Q1016 L1017 V1018 T1019 M1020 C1021 H1022 M1023 G1024 P1025 K1026 V1027 F1028 M1029 N1030 C1031 A1032 G1033 F1034 L1035 K1036 I1037 D1038 T1039 ALA SER LEU GLY ASP SER THR ASP SER TYR ILE E1051 V1052 L1053
D1054 G1055 S1056 R1057 V1058 H1059 P1060 E1061 T1062 Y1063 E1064 W1065 A1066 R1067 K1068 M1069 A1070 V1071 D1072 A1073 L1074 E1075 Y1076 D1077 E1078 S1079 A1080 E1081 D1082 A1083 N1084 P1085 A1086 G1087 A1088 L1089 E1090 E1091 I1092 L1093 E1094 N1095 P1096 E1097 R1098 L1099 K1100 D1101 L1102 D1103 L1104 D1105 A1106 F1107 A1108 E1109 E1110 L1111 E1112 R1113
Q1114 G1115 Y1116 G1117 D1118 K1119 H1120 I1121 T1122 L1123 Y1124 D1125 I1126 R1127 A1128 E1129 L1130 S1131 C1132 R1133 Y1134 K1135 D1136 L1137 R1138 T1139 A1140 Y1141 N1145 I1163 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 K1229 T1230 G1238 P1241 T1242 K1243 F1244 L1245 S1246 D1247 K1248 V1249 V1250 K1251 R1252 P1253 E1254 E1255 M1268 K1274 T1283 S1284 D1285 L1286 M1287 ASP ARG
ASN ASN GLU TRP LYS LEU PRO LYS ASP THR TYR TYR ASP PHE ASP ALA GLU 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 I1335 N1336 F1337 K1338 Q1339 A1340 E1341 K1342 M1343 M1344 E1345 T1346
M1347 D1348 Q1349 G1350 D1351 V1352 I1353 I1354 R1355 P1356 S1357 S1358 K1359 G1360 E1361 N1362 H1363 L1364 T1365 V1366 T1367 W1368 K1369 V1370 S1371 D1372 G1373 I1374 Y1375 Q1376 H1377 V1378 D1379 V1380 R1381 GLU GLU GLY LYS GLU ASN ALA PHE SER LEU GLY A1393 T1394 L1395 W1396 I1397 N1398 S1399 E1400 E1401 F1402 E1403 D1404 L1405 D1406
E1407 I1408 V1409 A1410 R1411 Y1412 V1413 Q1414 P1415 M1416 A1417 S1418 F1419 A1420 R1421 D1422 L1423 L1424 N1425 H1426 K1427 Y1428 Y1429 Q1430 D1431 C1432 S1433 G1434 G1435 D1436 R1437 K1438 K1439 L1440 E1441 E1442 L1443 L1444 I1445 K1446 T1447 K1448 K1449 E1450 K1451 P1452 T1453 F1454 I1455 P1456 Y1457 F1458 I1459 C1460 A1461 C1462 K1463 E1464 L1465 P1466



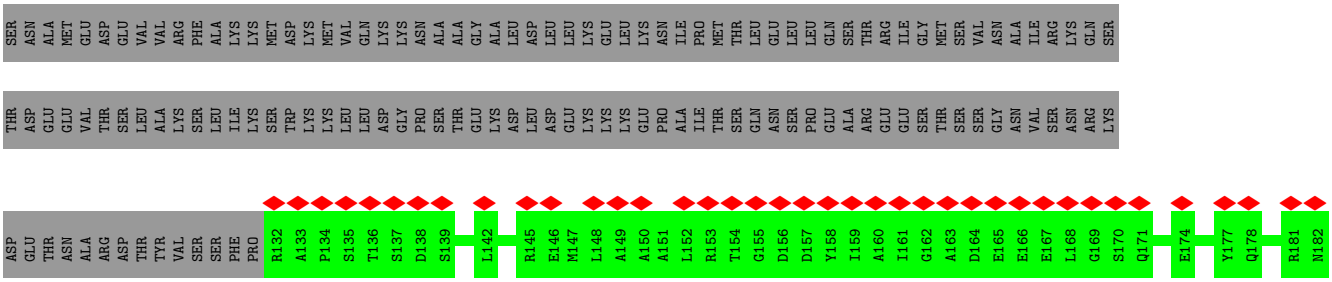
• Molecule 14: Non-template DNA

Chain N:



• Molecule 15: Transcription elongation factor A protein 1

Chain O:

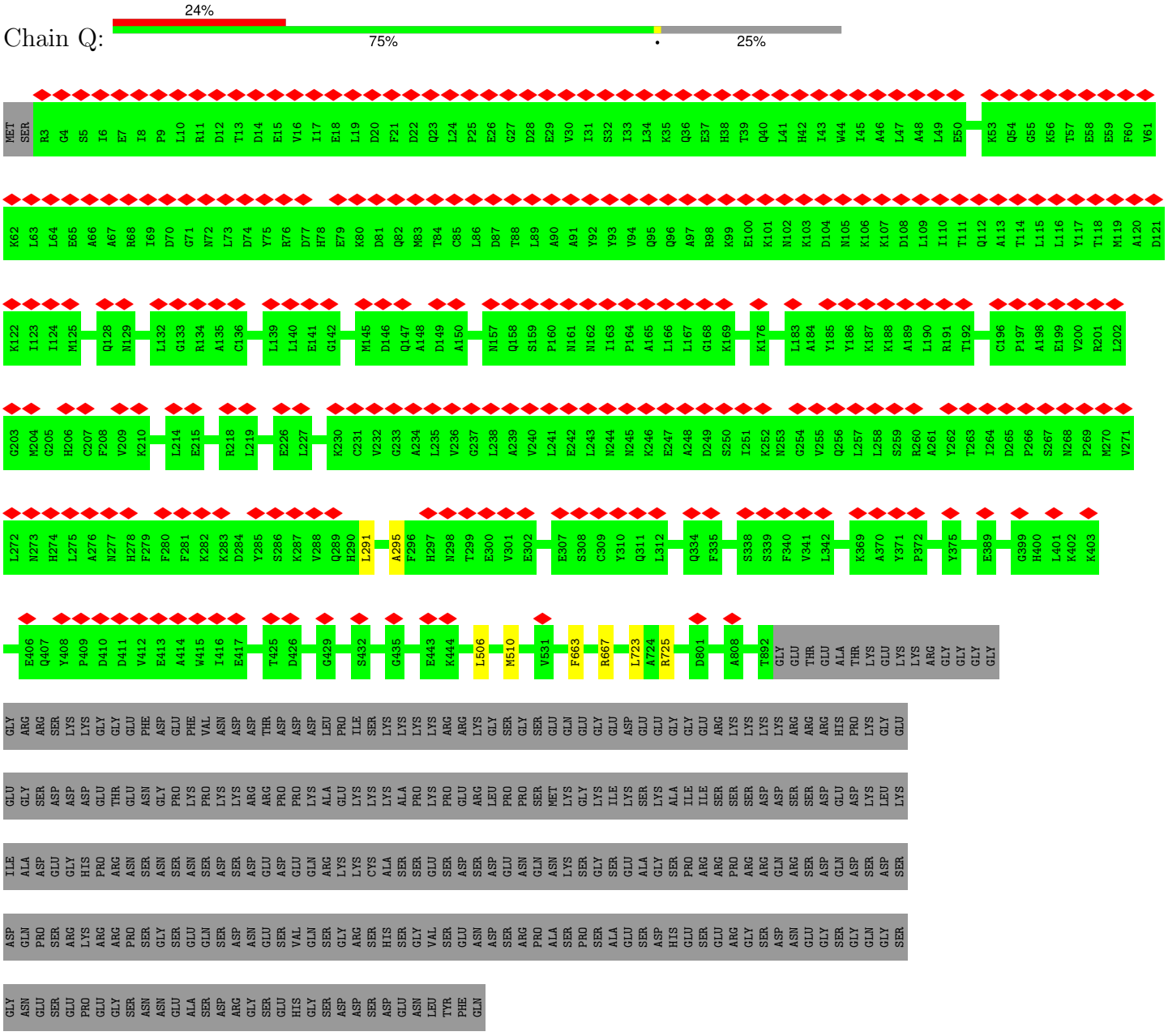


• Molecule 16: RNA

Chain P:

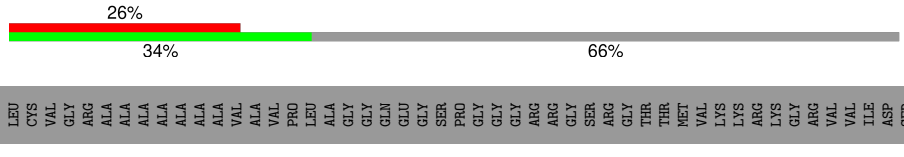
• Molecule 17: RNA polymerase-associated protein CTR9 homolog

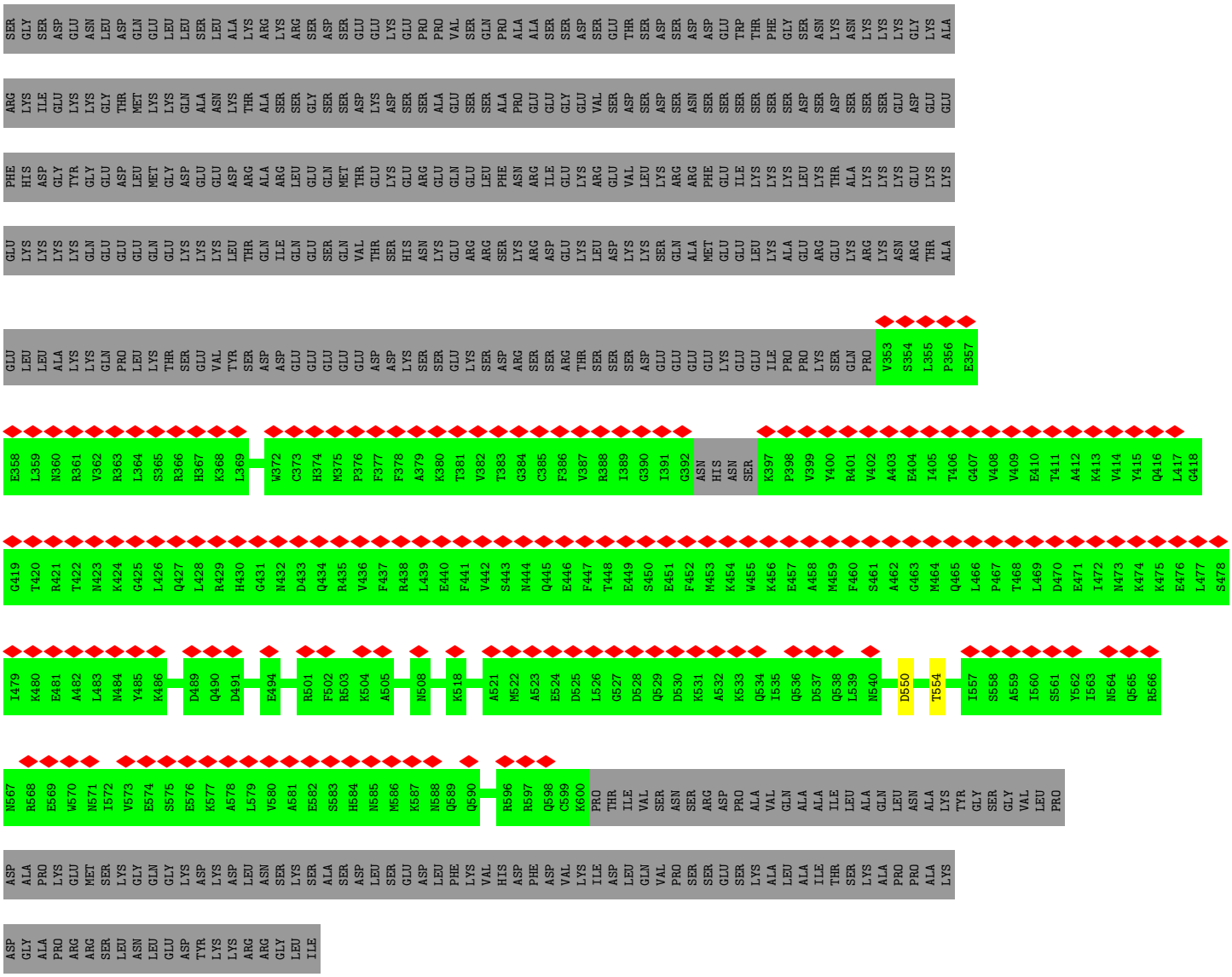
Chain Q:



• Molecule 18: RNA polymerase-associated protein RTF1 homolog

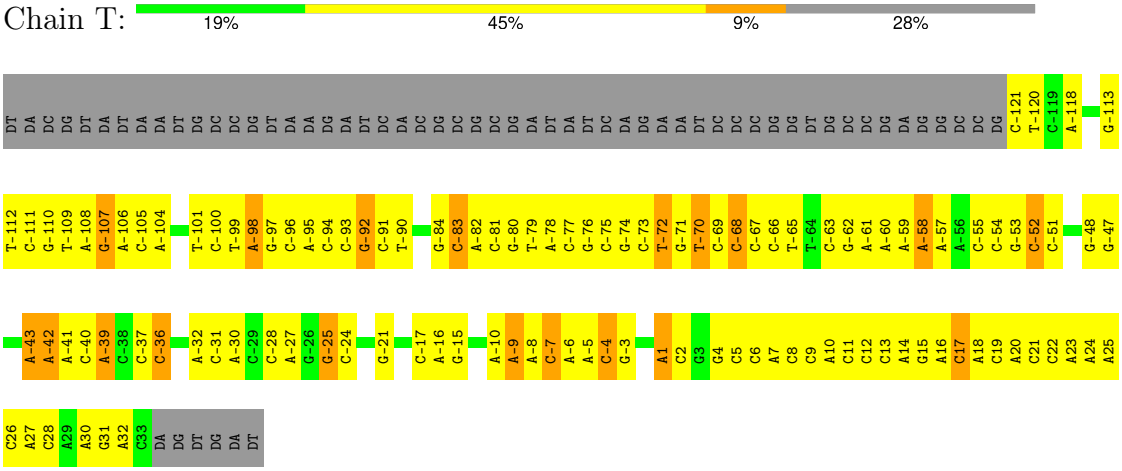
Chain R:





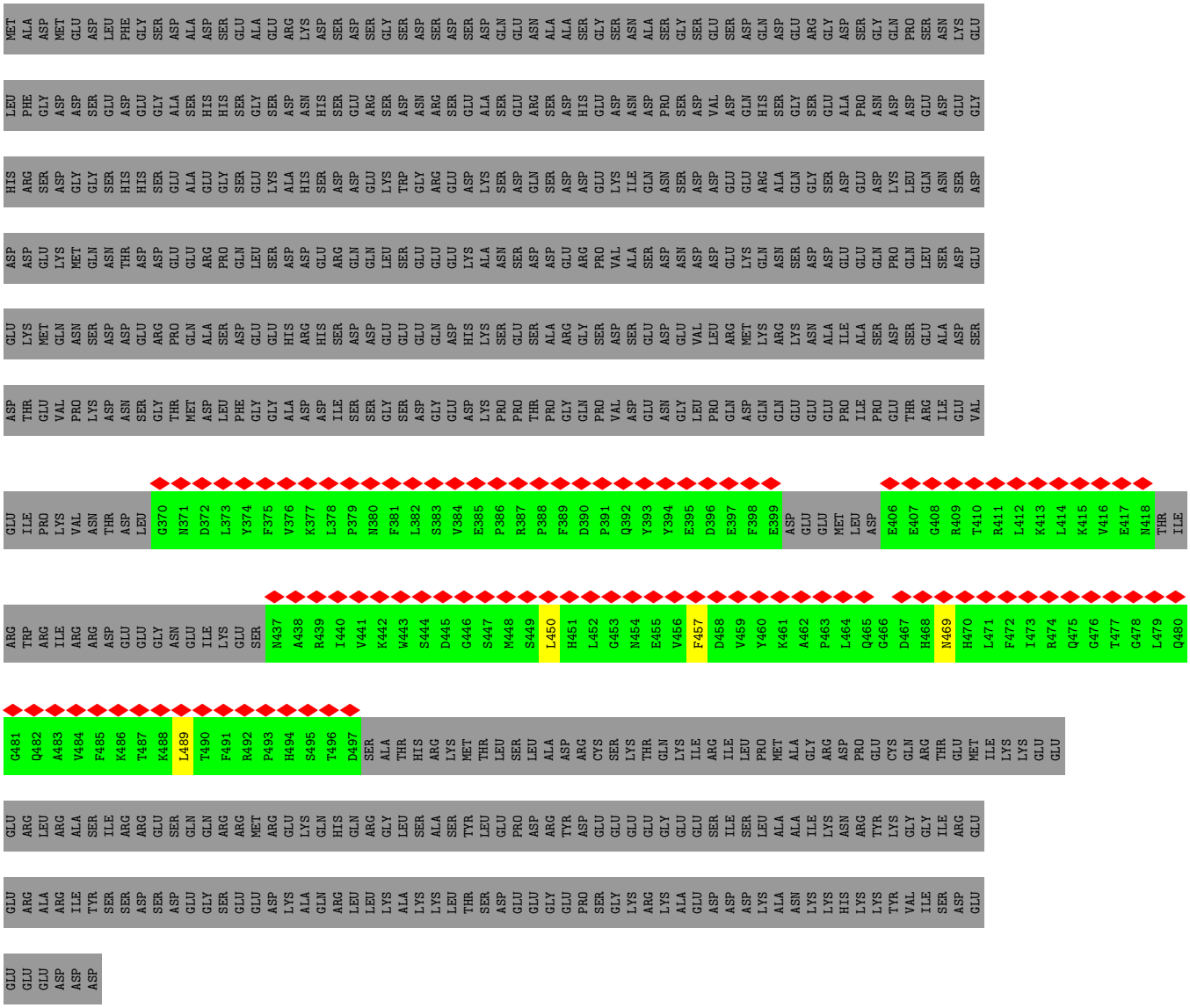
• Molecule 19: Template DNA

Chain T:



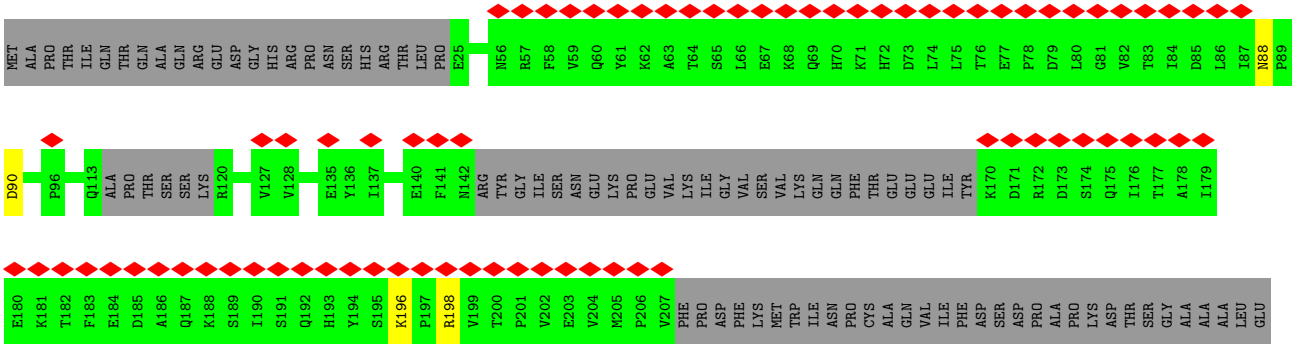
• Molecule 20: RNA polymerase-associated protein LEO1

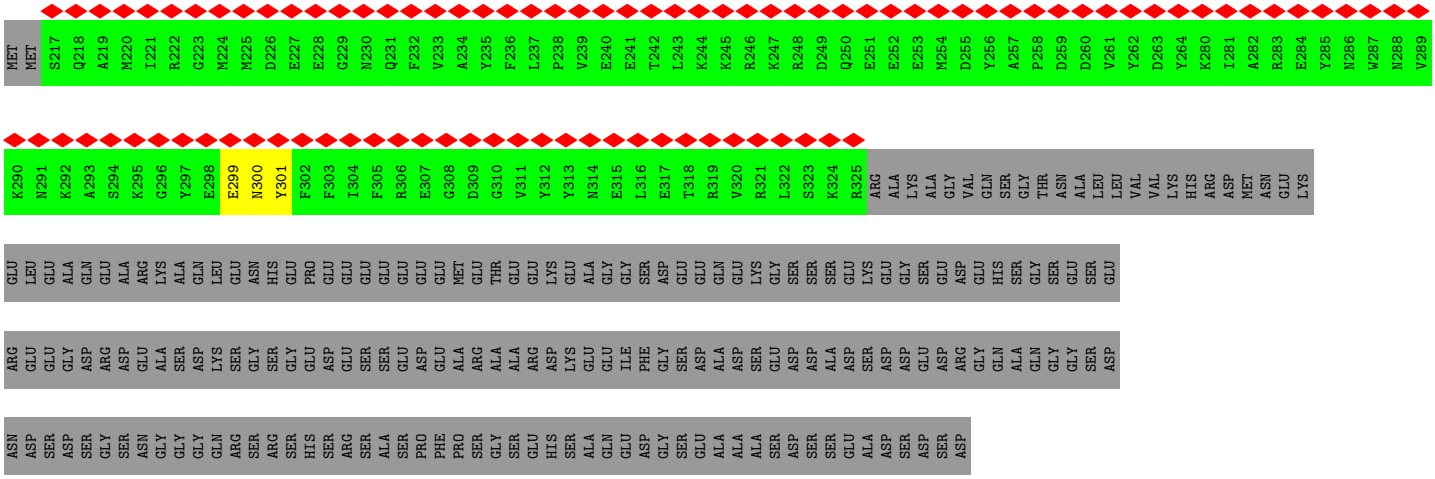
Chain U:



• Molecule 21: RNA polymerase II-associated factor 1 homolog

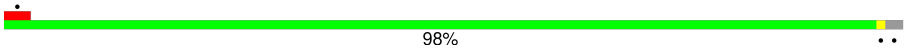
Chain V:

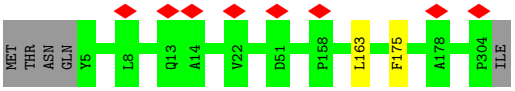




- Molecule 22: WDR61

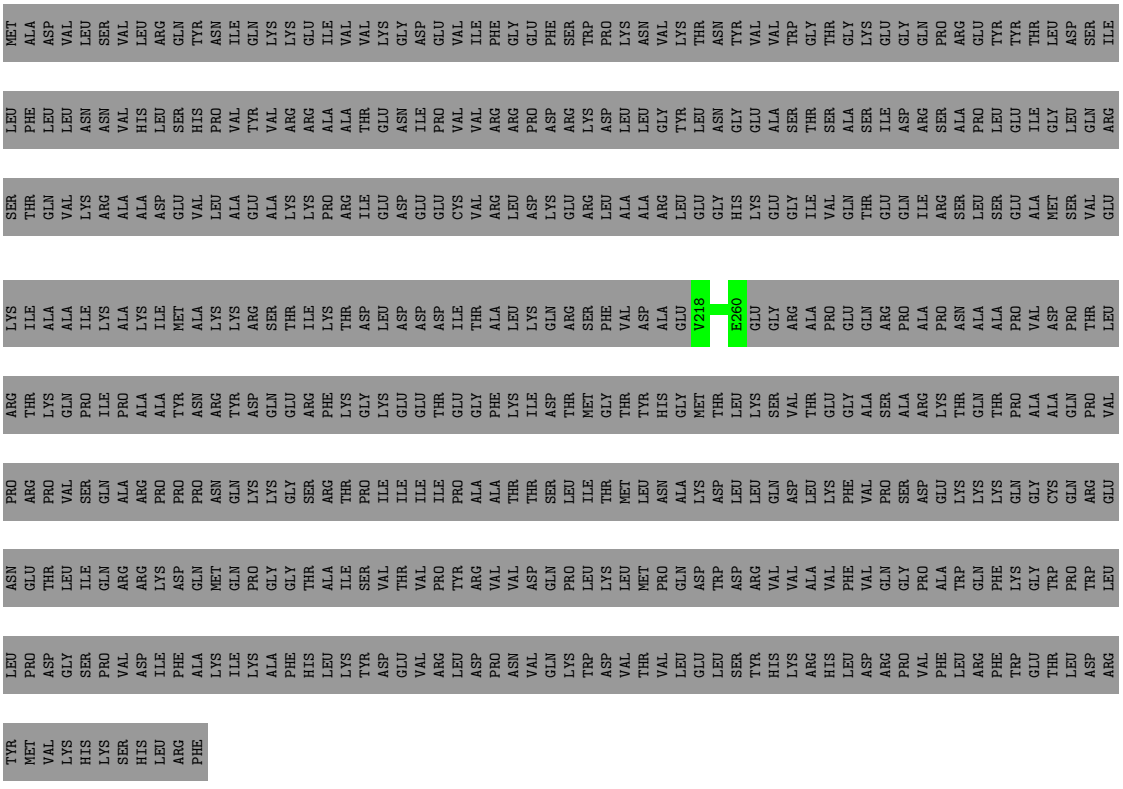
Chain W:





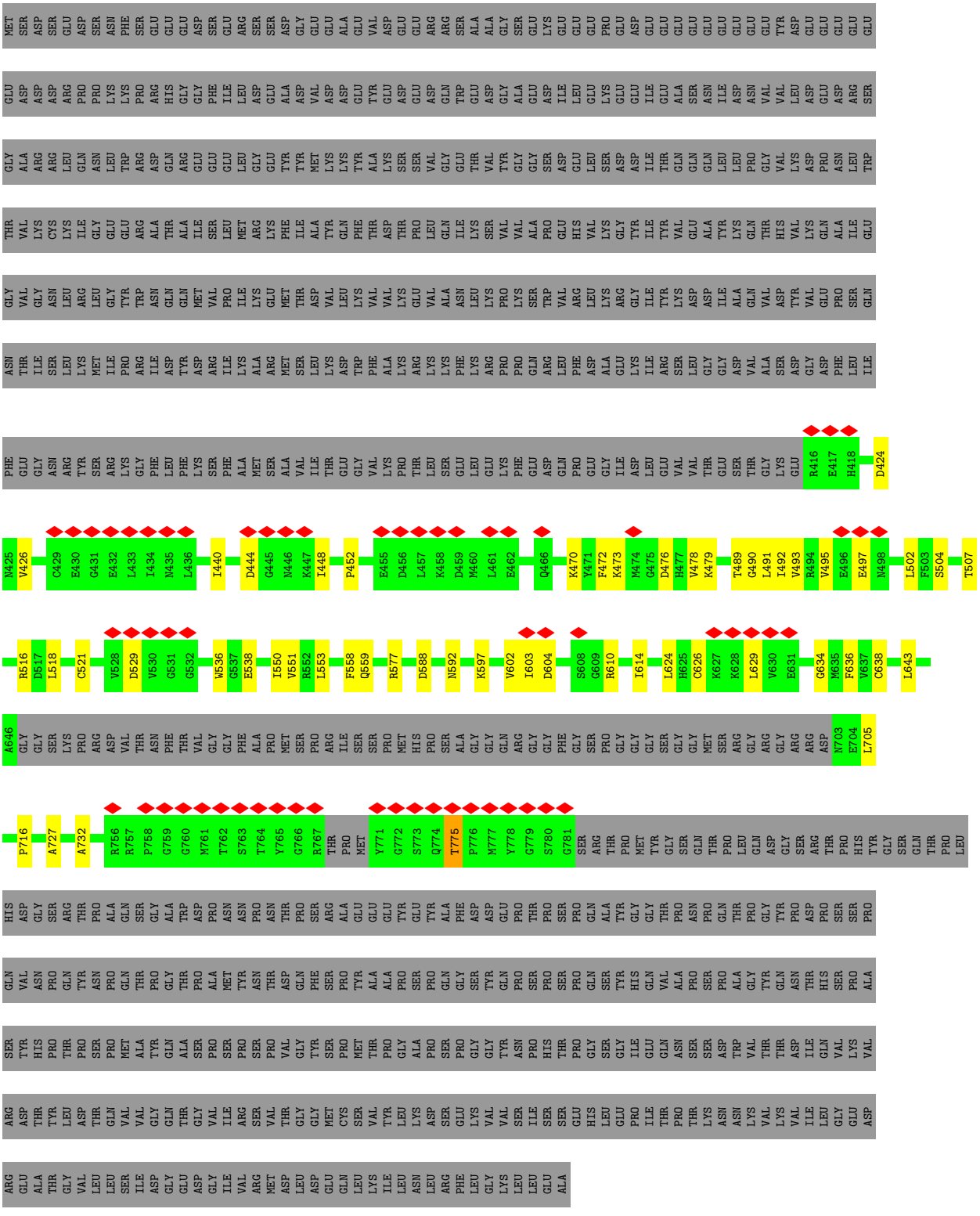
- Molecule 23: Parafibromin

Chain X:



- Molecule 24: Transcription elongation factor SPT5

Chain Z:

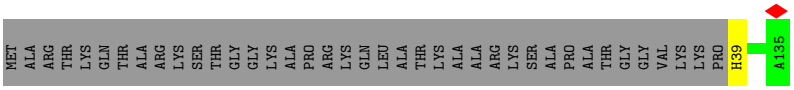


• Molecule 25: Histone H3.2

Chain a:

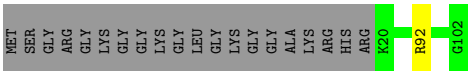
• Molecule 25: Histone H3.2

Chain e:



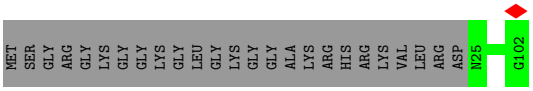
• Molecule 26: Histone H4

Chain b:



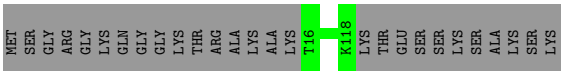
• Molecule 26: Histone H4

Chain f:



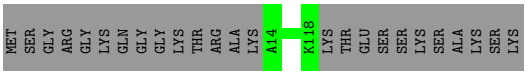
• Molecule 27: Histone H2A

Chain c:



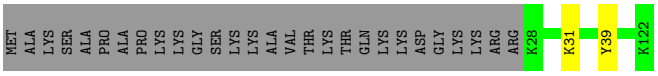
• Molecule 27: Histone H2A

Chain g:



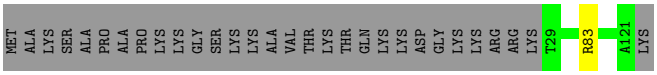
• Molecule 28: Histone H2B 1.1

Chain d:



• Molecule 28: Histone H2B 1.1

Chain h:


MET
ALA
LYS
SER
ALA
PRO
ALA
PRO
LYS
LYS
GLY
SER
LYS
LYS
ALA
VAL
THR
LYS
THR
GLN
LYS
LYS
ASP
GLY
LYS
LYS
ARG
ARG
LYS
T29
R83
A121
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105420	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-0.485	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/11437	0.61	2/15433 (0.0%)
2	B	0.42	0/9124	0.58	0/12313
3	C	0.42	0/2115	0.54	0/2873
4	D	0.26	0/1017	0.48	0/1368
5	E	0.33	0/1751	0.57	0/2366
6	F	0.45	0/636	0.57	0/859
7	G	0.29	0/1364	0.51	0/1853
8	H	0.38	0/1219	0.55	0/1644
9	I	0.33	0/964	0.54	0/1305
10	J	0.51	0/533	0.57	0/719
11	K	0.41	0/939	0.54	0/1271
12	L	0.41	0/403	0.66	0/536
13	M	0.26	0/3995	0.50	1/4971 (0.0%)
14	N	0.77	1/3226 (0.0%)	1.33	29/4986 (0.6%)
15	O	0.36	0/643	0.62	0/799
16	P	0.63	0/367	1.13	2/568 (0.4%)
17	Q	0.23	0/3559	0.47	0/4447
18	R	0.23	0/974	0.48	0/1214
19	T	0.80	1/3564 (0.0%)	1.19	22/5487 (0.4%)
20	U	0.25	0/413	0.48	0/511
21	V	0.27	0/972	0.53	0/1208
22	W	0.24	0/1199	0.55	0/1497
23	X	0.24	0/171	0.46	0/212
24	Z	0.26	0/2414	0.53	0/3250
25	a	0.30	0/814	0.62	0/1092
25	e	0.28	0/812	0.57	0/1088
26	b	0.33	0/669	0.60	0/894
26	f	0.32	0/626	0.59	0/837
27	c	0.28	0/805	0.56	0/1088
27	g	0.29	0/819	0.56	0/1106
28	d	0.29	0/756	0.50	0/1015
28	h	0.32	0/737	0.50	0/993

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.42	2/59037 (0.0%)	0.70	56/79803 (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
7	G	0	1
10	J	0	1
13	M	0	1
14	N	0	1
21	V	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	41	DT	C4'-O4'	5.26	1.50	1.45
19	T	-51	DC	C3'-O3'	-5.19	1.37	1.44

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	581	LYS	C-N-CD	-28.87	57.08	120.60
19	T	-42	DA	O4'-C1'-N9	10.77	115.54	108.00
14	N	28	DG	O4'-C1'-N9	10.03	115.02	108.00
14	N	38	DG	O4'-C1'-N9	9.74	114.82	108.00
19	T	1	DA	O4'-C1'-N9	9.66	114.76	108.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ARG	Sidechain
1	A	430	ARG	Sidechain
2	B	491	ARG	Sidechain
2	B	743	ARG	Sidechain
2	B	859	ARG	Sidechain

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	11255	11388	11374	221	0
2	B	8947	9002	8994	118	0
3	C	2072	2024	2019	21	0
4	D	1004	981	980	4	0
5	E	1720	1738	1737	29	0
6	F	626	658	657	8	0
7	G	1333	1321	1321	17	0
8	H	1197	1157	1156	9	0
9	I	942	880	872	17	0
10	J	524	544	540	11	0
11	K	920	942	942	17	0
12	L	397	406	405	4	0
13	M	4008	1259	1035	8	0
14	N	2886	1594	1596	160	0
15	O	645	0	171	30	0
16	P	332	170	169	3	0
17	Q	3560	1796	940	4	0
18	R	976	491	255	1	0
19	T	3166	1719	1720	133	0
20	U	416	210	111	2	0
21	V	976	481	240	2	0
22	W	1200	617	341	1	0
23	X	172	87	44	0	0
24	Z	2388	2363	2360	43	0
25	a	802	841	841	0	0
25	e	801	839	838	0	0
26	b	662	710	709	0	0
26	f	619	660	659	0	0
27	c	795	847	846	0	0
27	g	809	865	864	0	0
28	d	745	774	773	0	0
28	h	726	748	747	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	R	1	0	0	0	0
30	A	1	0	0	0	0
All	All	57630	48112	46256	753	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 8.

The worst 5 of 753 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:PRO:CG	15:O:249:GLN:O	1.79	1.27
1:A:1314:THR:C	15:O:295:GLY:HA3	1.56	1.23
1:A:729:PRO:HB3	15:O:247:GLU:O	1.38	1.21
1:A:203:LYS:NZ	19:T:-67:DC:OP1	1.75	1.20
1:A:729:PRO:CB	15:O:247:GLU:O	1.90	1.17

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1408/1984 (71%)	1297 (92%)	109 (8%)	2 (0%)	48 81
2	B	1107/1251 (88%)	1022 (92%)	85 (8%)	0	100 100
3	C	254/275 (92%)	241 (95%)	13 (5%)	0	100 100
4	D	124/184 (67%)	118 (95%)	6 (5%)	0	100 100
5	E	207/210 (99%)	199 (96%)	8 (4%)	0	100 100
6	F	76/127 (60%)	71 (93%)	5 (7%)	0	100 100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100 100
8	H	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	114/125 (91%)	100 (88%)	14 (12%)	0	100	100
10	J	64/67 (96%)	60 (94%)	3 (5%)	1 (2%)	8	34
11	K	113/117 (97%)	106 (94%)	7 (6%)	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%)	48	81
15	O	157/304 (52%)	154 (98%)	3 (2%)	0	100	100
17	Q	888/1179 (75%)	832 (94%)	56 (6%)	0	100	100
18	R	240/713 (34%)	227 (95%)	13 (5%)	0	100	100
20	U	98/666 (15%)	87 (89%)	11 (11%)	0	100	100
21	V	236/531 (44%)	200 (85%)	34 (14%)	2 (1%)	16	51
22	W	298/305 (98%)	271 (91%)	27 (9%)	0	100	100
23	X	41/531 (8%)	38 (93%)	3 (7%)	0	100	100
24	Z	300/1087 (28%)	274 (91%)	25 (8%)	1 (0%)	37	70
25	a	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
25	e	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
26	b	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
26	f	76/103 (74%)	72 (95%)	4 (5%)	0	100	100
27	c	101/130 (78%)	97 (96%)	4 (4%)	0	100	100
27	g	103/130 (79%)	99 (96%)	4 (4%)	0	100	100
28	d	93/123 (76%)	88 (95%)	5 (5%)	0	100	100
28	h	91/123 (74%)	87 (96%)	4 (4%)	0	100	100
All	All	7797/12749 (61%)	7242 (93%)	547 (7%)	8 (0%)	50	81

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	PRO
13	M	1334	ASN
21	V	300	ASN
8	H	77	PRO
1	A	478	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1245/1761 (71%)	1226 (98%)	19 (2%)	60	83
2	B	983/1084 (91%)	968 (98%)	15 (2%)	60	83
3	C	235/252 (93%)	231 (98%)	4 (2%)	56	81
4	D	109/160 (68%)	108 (99%)	1 (1%)	75	89
5	E	191/192 (100%)	188 (98%)	3 (2%)	58	82
6	F	68/111 (61%)	66 (97%)	2 (3%)	37	70
7	G	146/153 (95%)	143 (98%)	3 (2%)	48	77
8	H	130/131 (99%)	128 (98%)	2 (2%)	60	83
9	I	104/112 (93%)	102 (98%)	2 (2%)	52	79
10	J	55/56 (98%)	54 (98%)	1 (2%)	54	80
11	K	104/106 (98%)	103 (99%)	1 (1%)	73	88
12	L	44/55 (80%)	42 (96%)	2 (4%)	23	57
24	Z	257/939 (27%)	256 (100%)	1 (0%)	89	95
25	a	85/111 (77%)	85 (100%)	0	100	100
25	e	84/111 (76%)	83 (99%)	1 (1%)	67	86
26	b	68/79 (86%)	67 (98%)	1 (2%)	60	83
26	f	63/79 (80%)	63 (100%)	0	100	100
27	c	82/102 (80%)	82 (100%)	0	100	100
27	g	83/102 (81%)	83 (100%)	0	100	100
28	d	81/103 (79%)	79 (98%)	2 (2%)	42	73
28	h	79/103 (77%)	78 (99%)	1 (1%)	65	85
All	All	4296/5902 (73%)	4235 (99%)	61 (1%)	62	83

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	808	SER
24	Z	624	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	63	PHE
12	L	58	ARG
25	e	39	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1040	GLN
24	Z	642	HIS
3	C	260	GLN
26	f	64	ASN
11	K	2	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	4 (26%)	2 (13%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	41	U
16	P	42	U
16	P	44	U
16	P	46	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	43	U
16	P	45	C

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

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	$\#\|Z\| > 2$
1	SEP	A	1547	1	8,9,10	1.62	1 (12%)	7,12,14	1.35	1 (14%)
1	TPO	A	1525	1	8,10,11	1.64	1 (12%)	10,14,16	2.08	1 (10%)
24	TPO	Z	775	24	8,10,11	1.66	1 (12%)	10,14,16	1.70	1 (10%)

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
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	2/9/11/13	-
24	TPO	Z	775	24	-	4/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.54	1.61	1.50
24	Z	775	TPO	P-O1P	3.53	1.61	1.50
1	A	1525	TPO	P-O1P	3.51	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1525	TPO	P-OG1-CB	-5.80	107.56	123.33
24	Z	775	TPO	P-OG1-CB	-4.44	111.27	123.33
1	A	1547	SEP	OG-CB-CA	2.94	111.00	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	CB-OG1-P-O2P
1	A	1525	TPO	N-CA-CB-CG2
24	Z	775	TPO	CB-OG1-P-O1P
24	Z	775	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

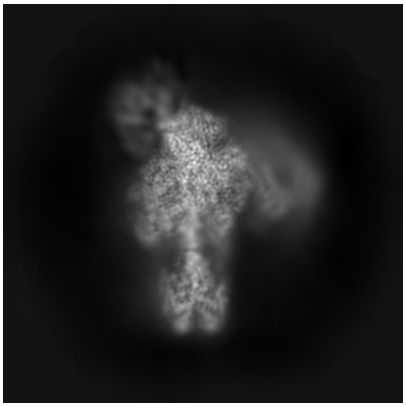
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26620. These allow visual inspection of the internal detail of the map and identification of artifacts.

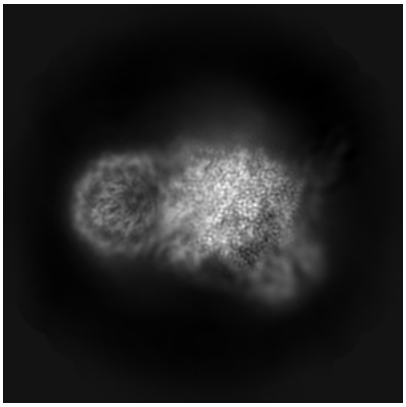
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

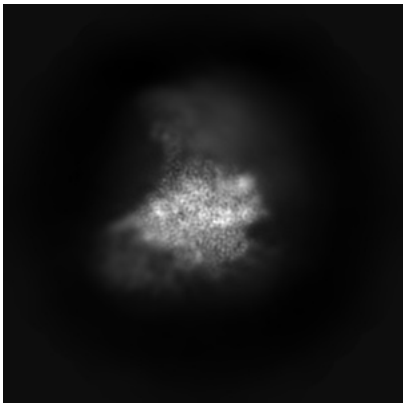
6.1.1 Primary map



X



Y

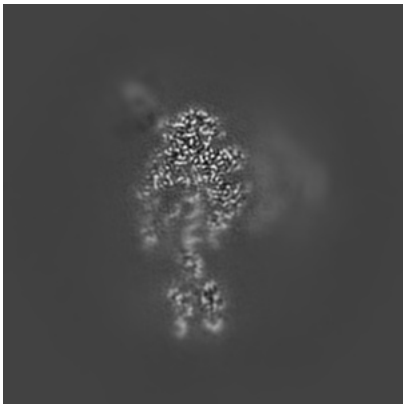


Z

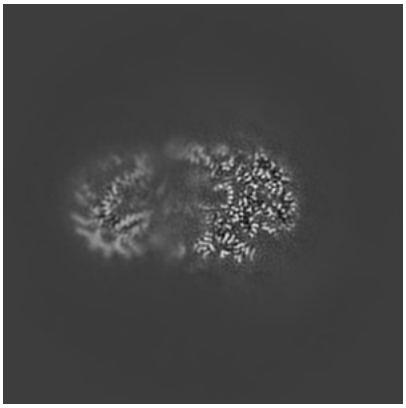
The images above show the map projected in three orthogonal directions.

6.2 Central slices

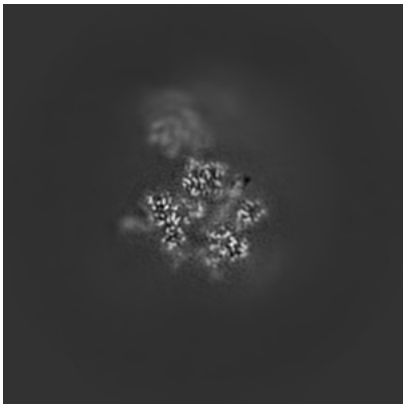
6.2.1 Primary map



X Index: 225



Y Index: 225

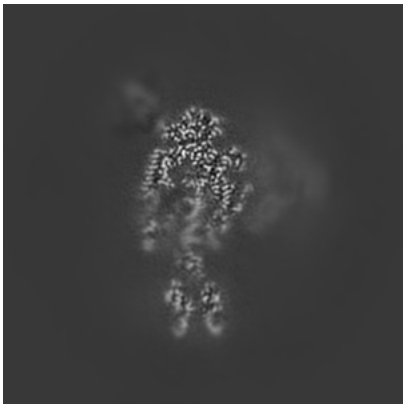


Z Index: 225

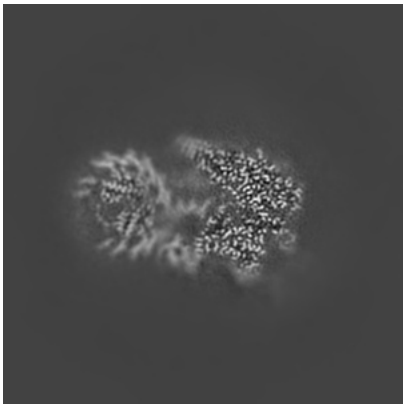
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

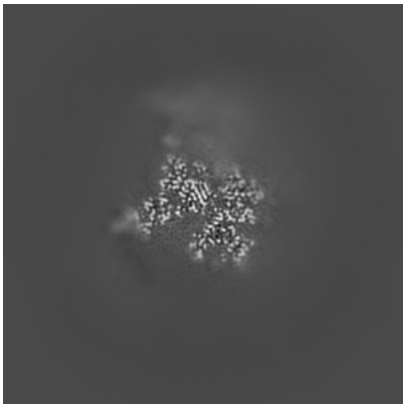
6.3.1 Primary map



X Index: 222



Y Index: 214

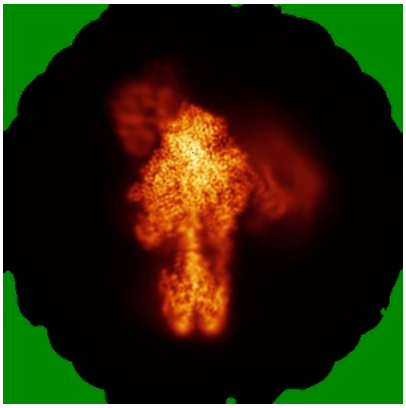


Z Index: 266

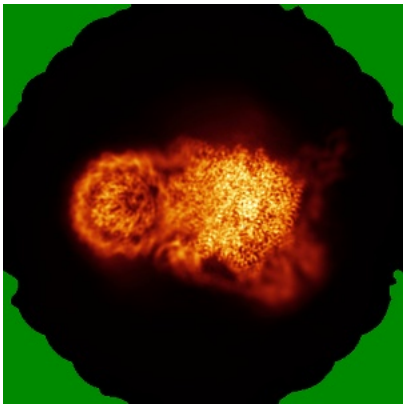
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

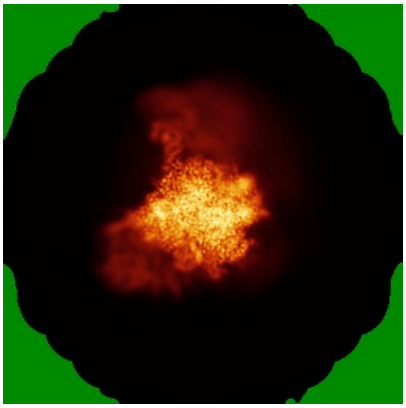
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

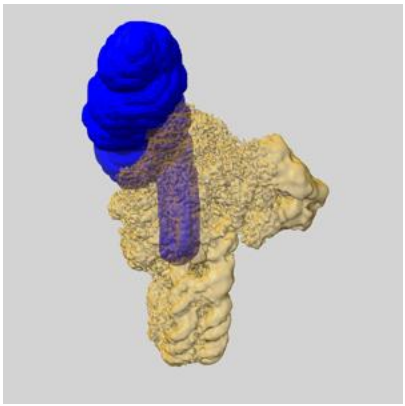
6.6 Mask visualisation

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

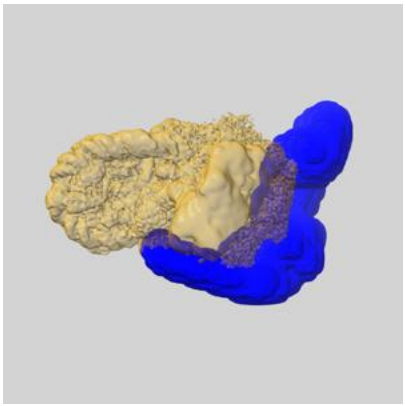
A mask typically either:

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

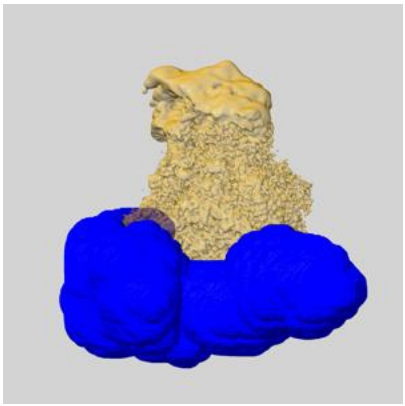
6.6.1 emd_26620_msk_1.map



X

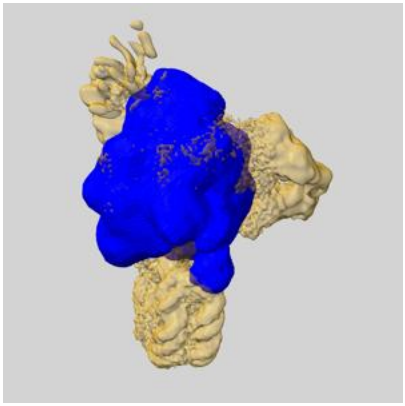


Y

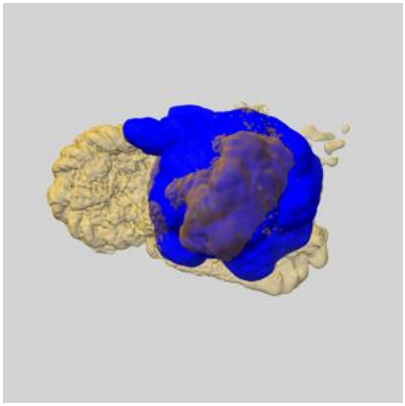


Z

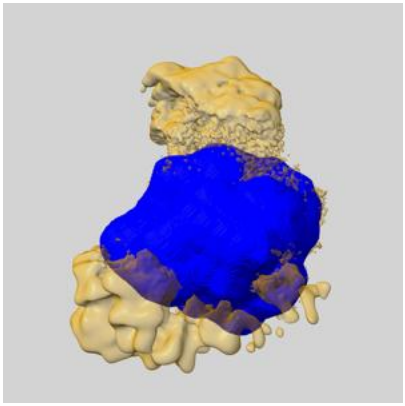
6.6.2 emd_26620_msk_2.map



X

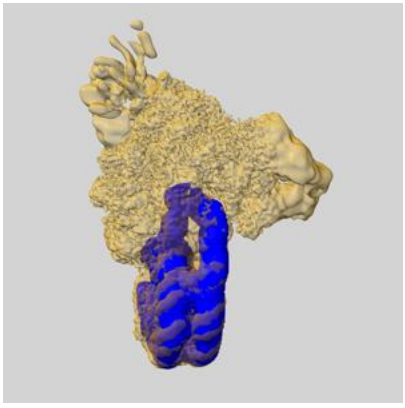


Y

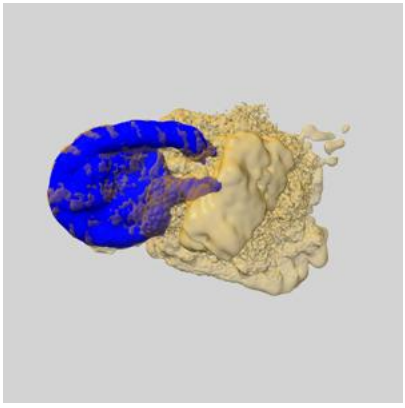


Z

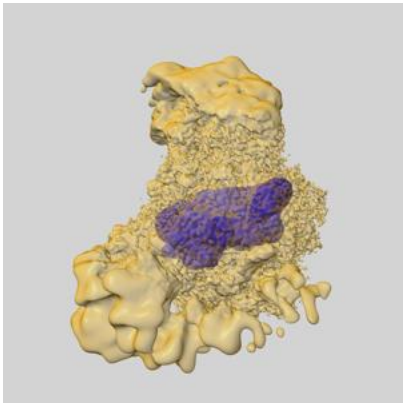
6.6.3 emd_26620_msk_3.map ⓘ



X



Y

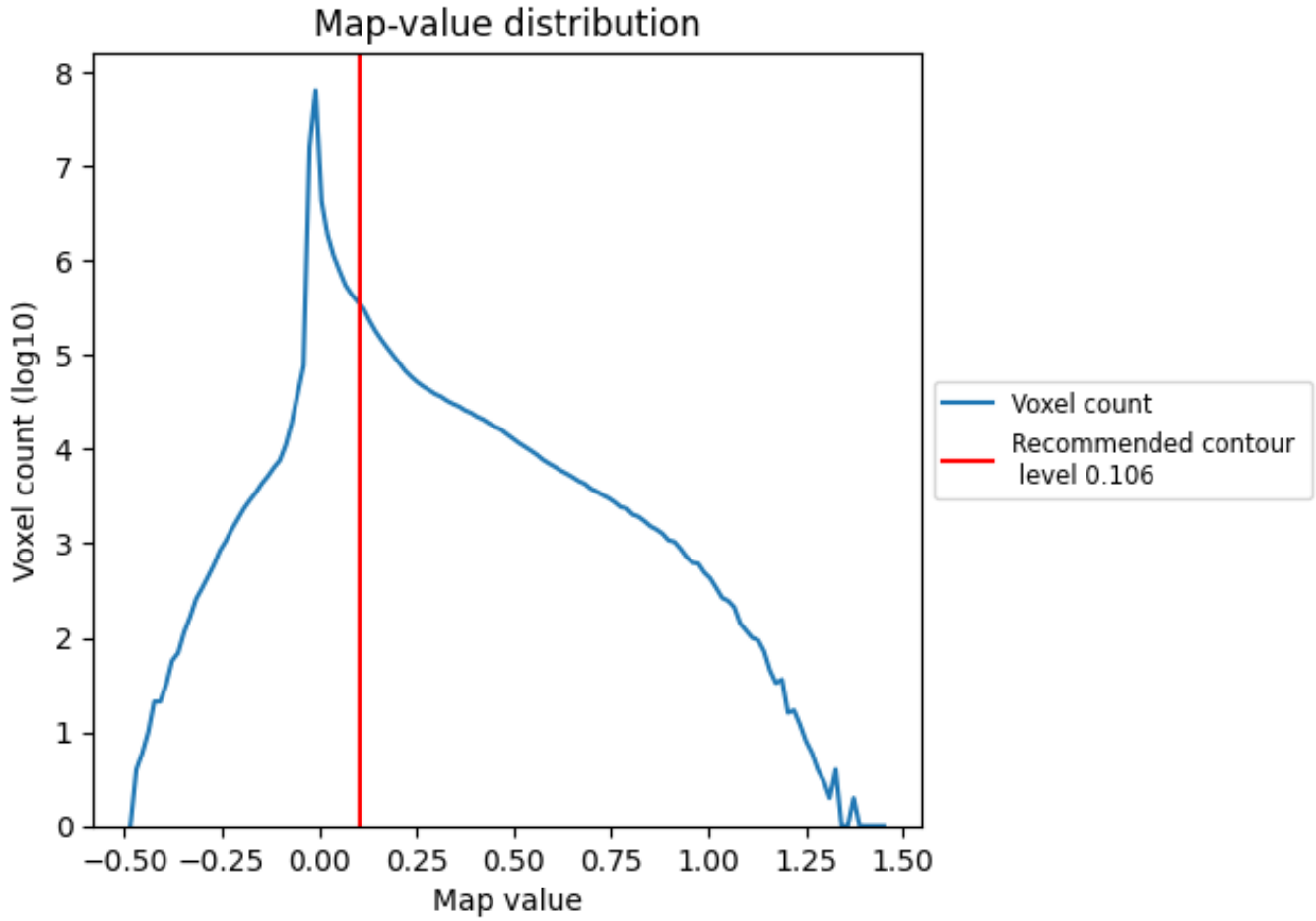


Z

7 Map analysis

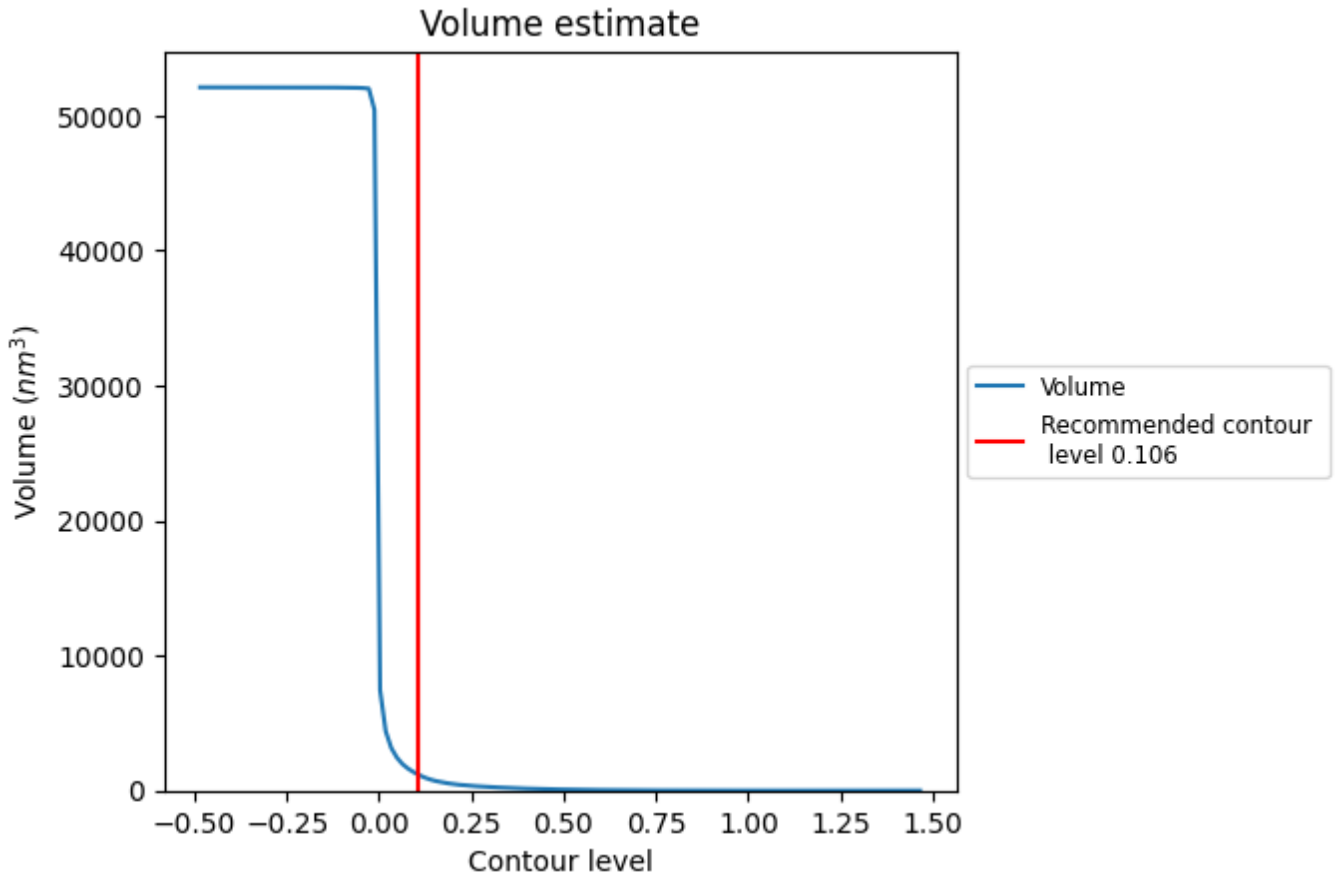
This section contains the results of statistical analysis of the map.

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.

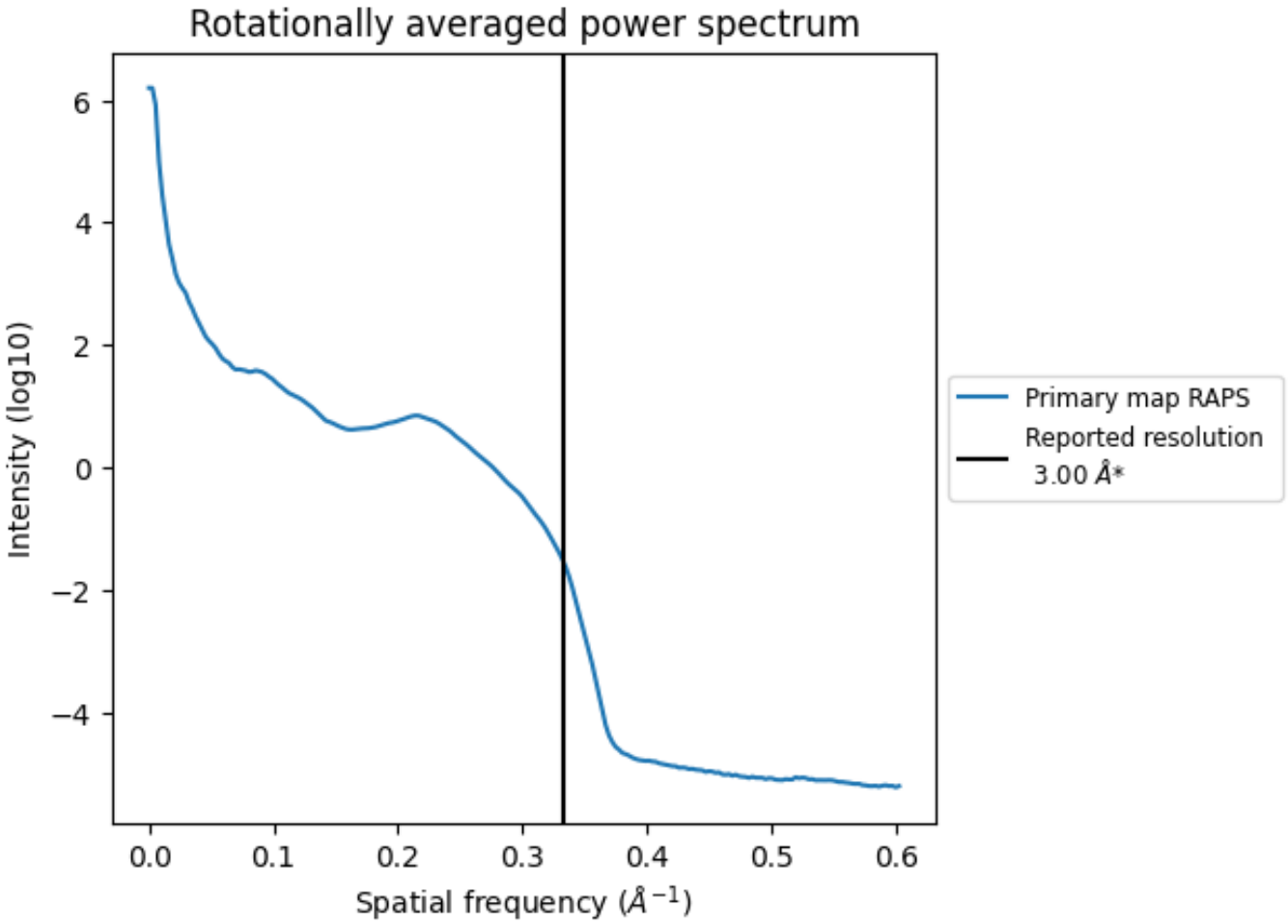
7.2 Volume estimate (i)



The volume at the recommended contour level is 1190 nm^3; this corresponds to an approximate mass of 1075 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

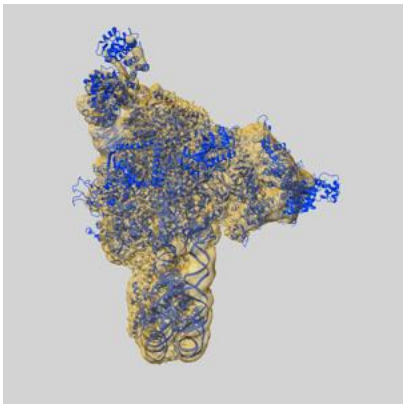
8 Fourier-Shell correlation (i)

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

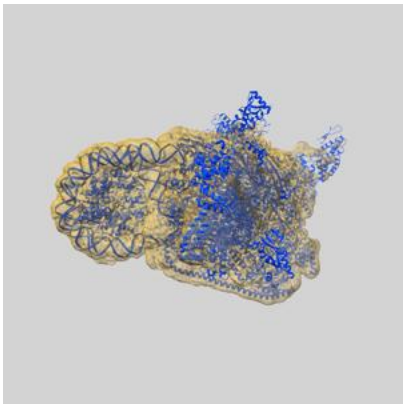
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26620 and PDB model 7UNC. Per-residue inclusion information can be found in section 3 on page 10.

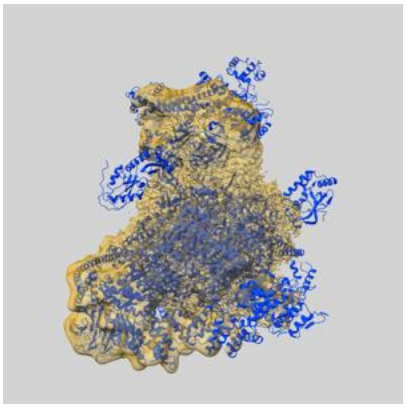
9.1 Map-model overlay



X



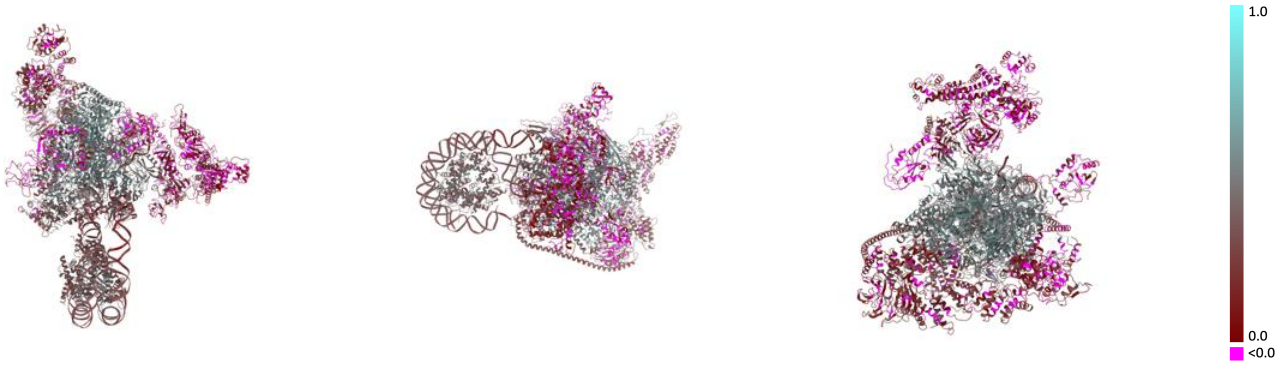
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

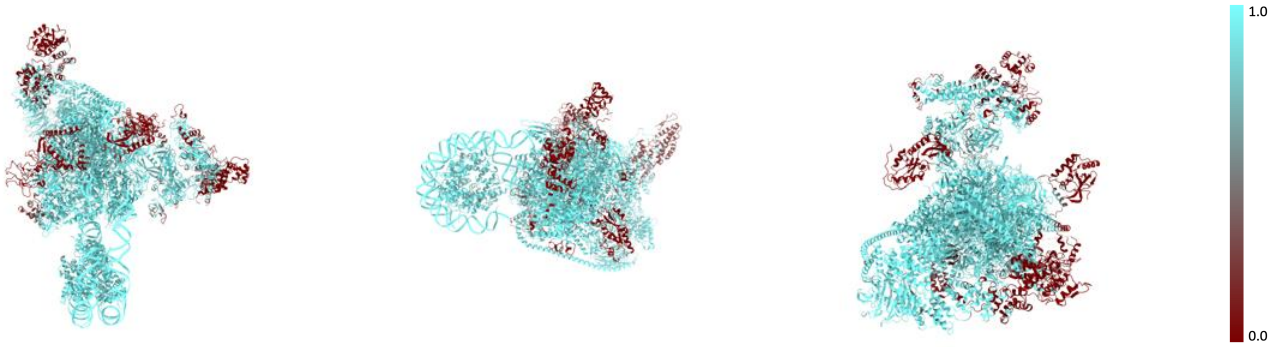
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

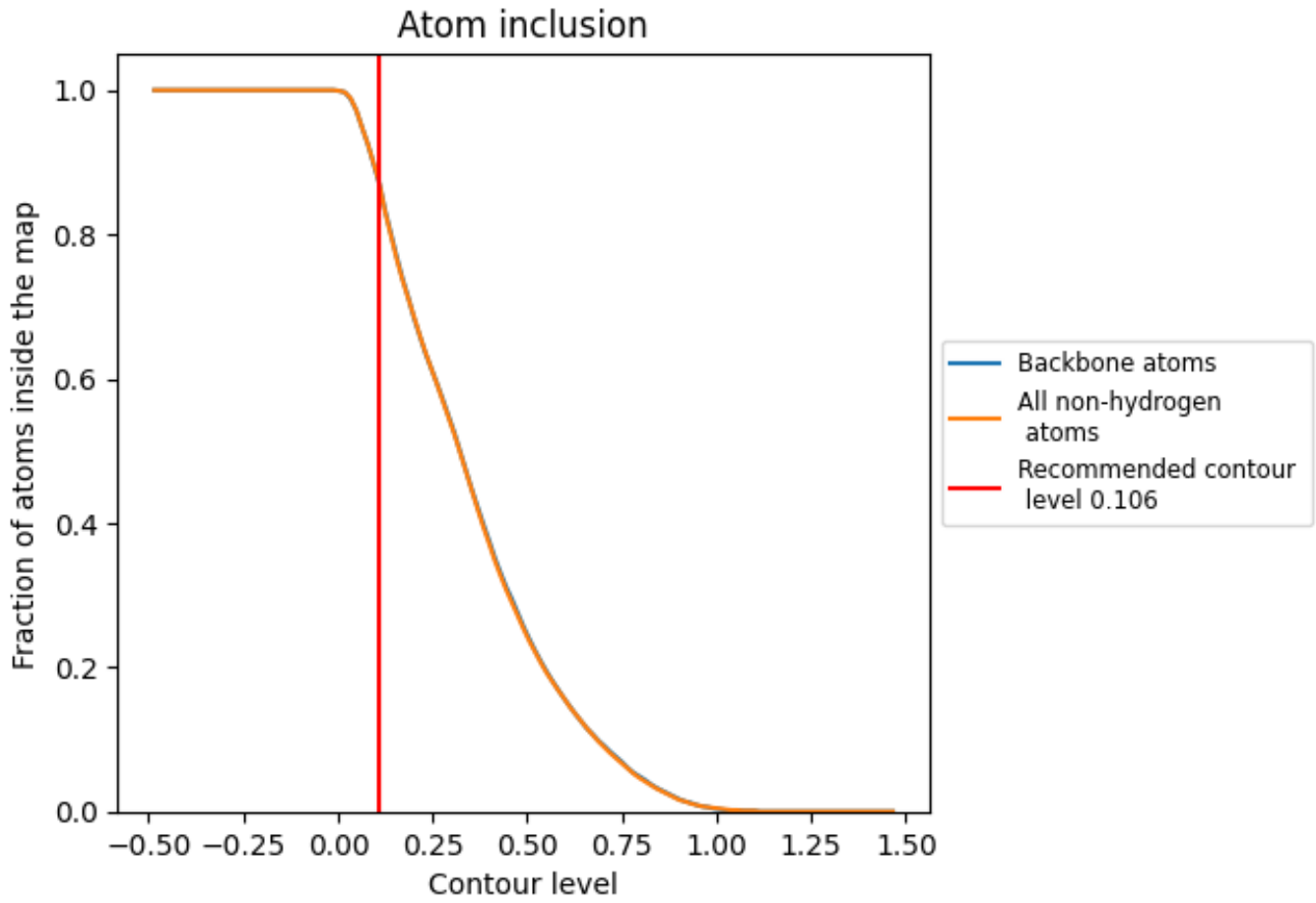
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.106).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.3440
A	0.9760	0.4790
B	0.9910	0.4950
C	0.9950	0.5280
D	0.9570	0.1580
E	0.9910	0.3560
F	0.9920	0.5280
G	0.9770	0.2300
H	0.9830	0.4160
I	0.9970	0.3840
J	0.9820	0.5340
K	0.9920	0.5250
L	0.9760	0.4380
M	0.4380	0.0470
N	0.9980	0.2890
O	0.2820	0.1330
P	1.0000	0.4100
Q	0.6660	0.1610
R	0.1910	0.0900
T	1.0000	0.3130
U	0.0050	0.0230
V	0.2770	0.1000
W	0.9510	0.1380
X	0.9830	0.2460
Z	0.7620	0.1280
a	0.9870	0.3510
b	0.9890	0.3960
c	0.9700	0.3650
d	0.9740	0.3460
e	0.9730	0.3290
f	0.9830	0.3670
g	0.9750	0.3930
h	0.9890	0.3890