wwPDB EM Validation Summary Report ⓘ

May 25, 2024 – 10:57 am BST

PDB ID	:	8QPA
EMDB ID	:	EMD-18546
Title	:	Cryo-EM Structure of Pre-B+5'ssLNG Complex (core part)
Authors	:	Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on	:	2023-10-01
Resolution	:	3.70 Å(reported)

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

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

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

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

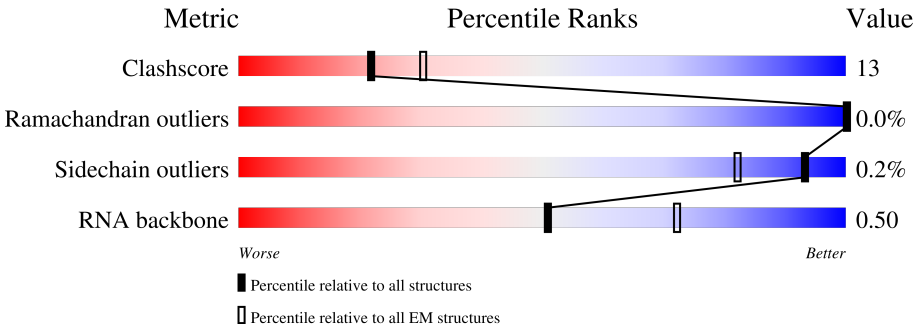
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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	B	2136	99%
2	G	820	6%, 10%, 5%, 85%
3	J	683	8%, 88%
4	L	499	25%, 51%, 24%, 25%
5	F	522	6%, 6%, 88%
6	N	941	22%, 39%, 10%, 51%
7	A	2335	8%, 58%, 27%, 16%

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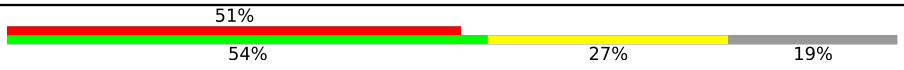
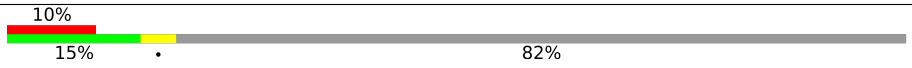
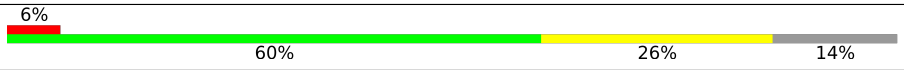
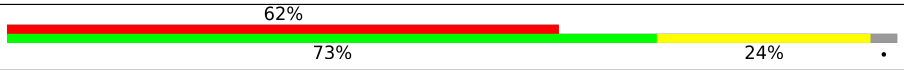
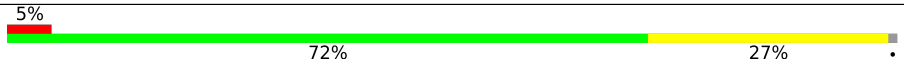
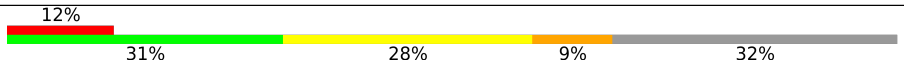
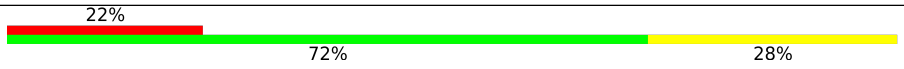
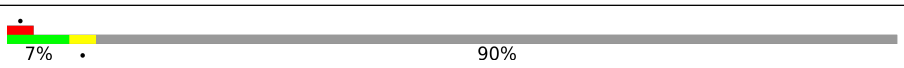
Mol	Chain	Length	Quality of chain
8	U	565	
9	S	800	
10	C	972	
11	M	128	
12	D	142	
13	5	117	
14	z	18	
15	7	793	
16	4	144	
17	6	106	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 43455 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	22	158	97	28	32	1	0	0

- Molecule 2 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	122	1077	673	205	197	2	0	0

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	85	678	416	139	120	3	0	0

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	376	2874	1788	524	550	12	0	0

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	61	488	297	97	93	1	0	0

- Molecule 6 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	457	3095	1902	591	595	7	0	0

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1971	Total	C	N	O	S	0	0
			16383	10554	2858	2901	70		

- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	456	Total	C	N	O	S	0	0
			3749	2427	635	673	14		

- Molecule 9 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	148	Total	C	N	O	S	0	0
			1167	727	216	222	2		

- Molecule 10 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	836	Total	C	N	O	S	0	0
			6592	4211	1110	1238	33		

- Molecule 11 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 12 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	141	Total	C	N	O	S	0	0
			1170	751	194	215	10		

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	79	Total	C	N	O	P	0	0
			1660	744	275	562	79		

- Molecule 14 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	z	18	Total	C	N	O	P	0	0
			384	172	69	125	18		

- Molecule 15 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	81	Total	C	N	O	S	0	0
			650	405	115	128	2		

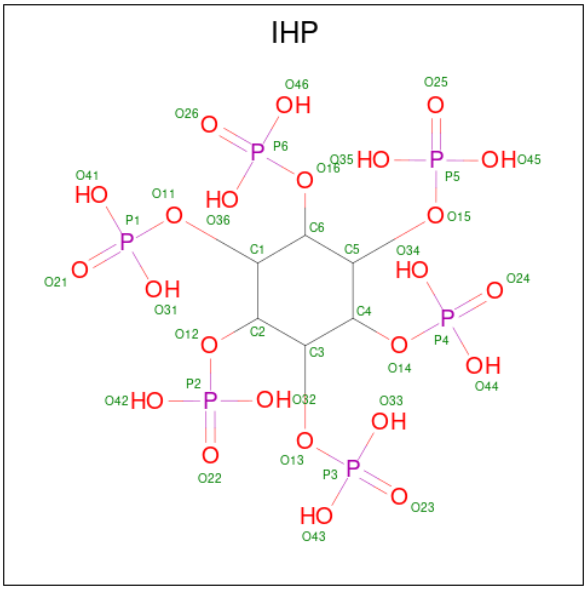
- Molecule 16 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	62	Total	C	N	O	P	0	0
			1322	590	233	437	62		

- Molecule 17 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	47	Total	C	N	O	P	0	0
			1010	453	194	317	46		

- Molecule 18 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



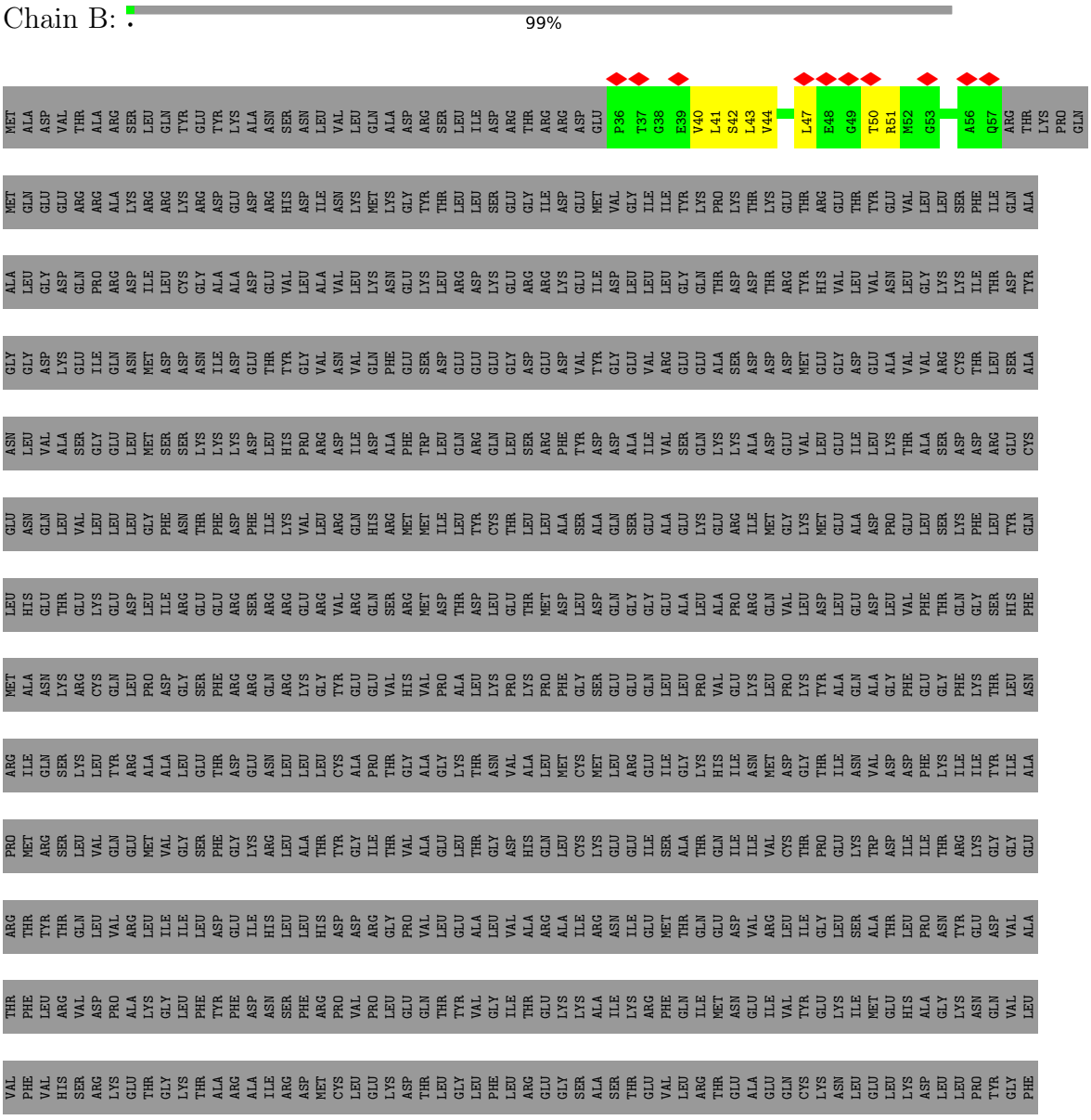
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			36	6	24	6	

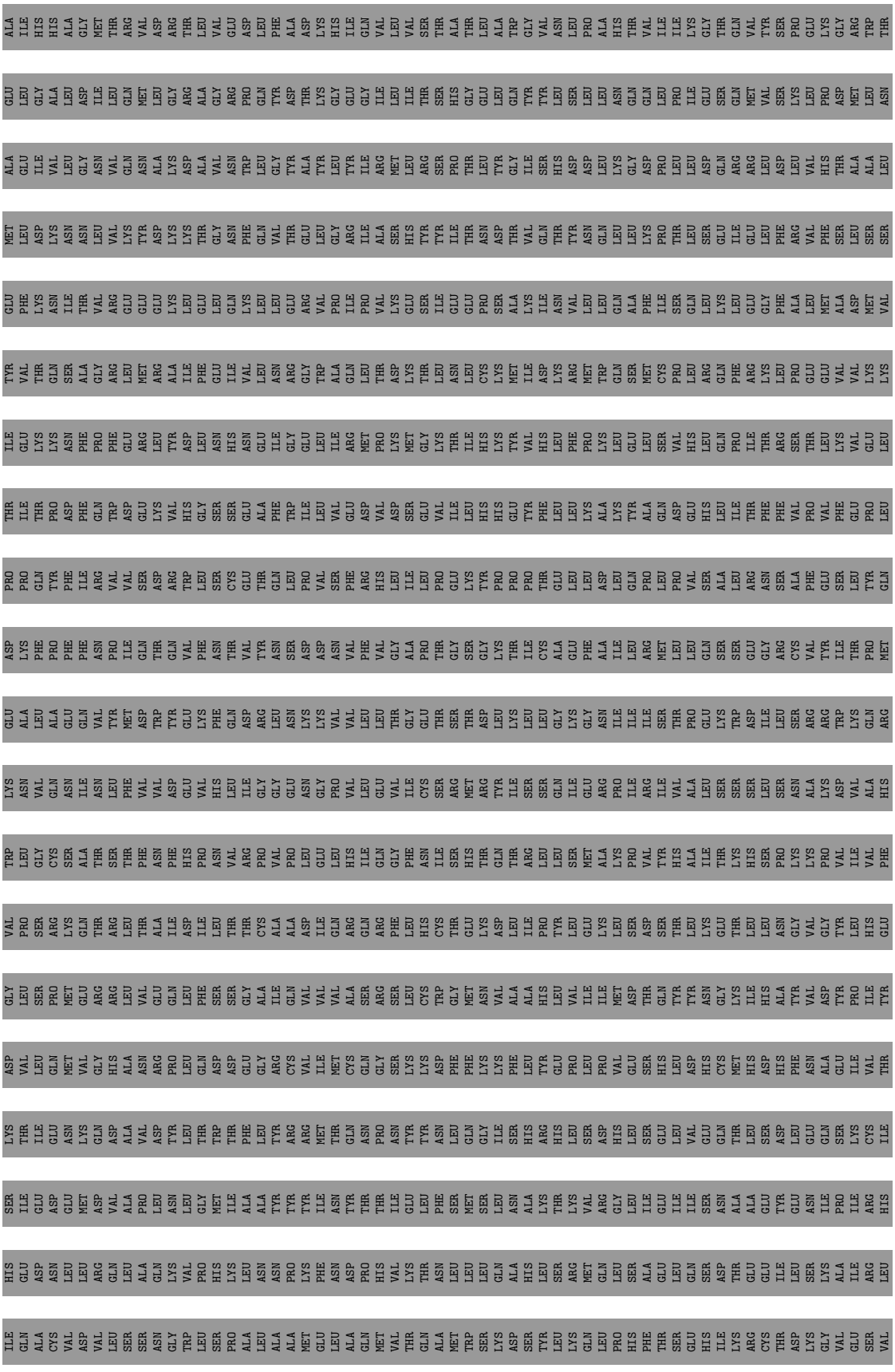
3 Residue-property plots (i)

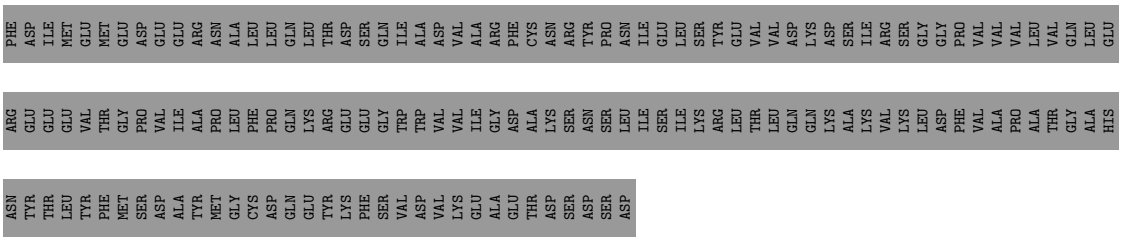
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:

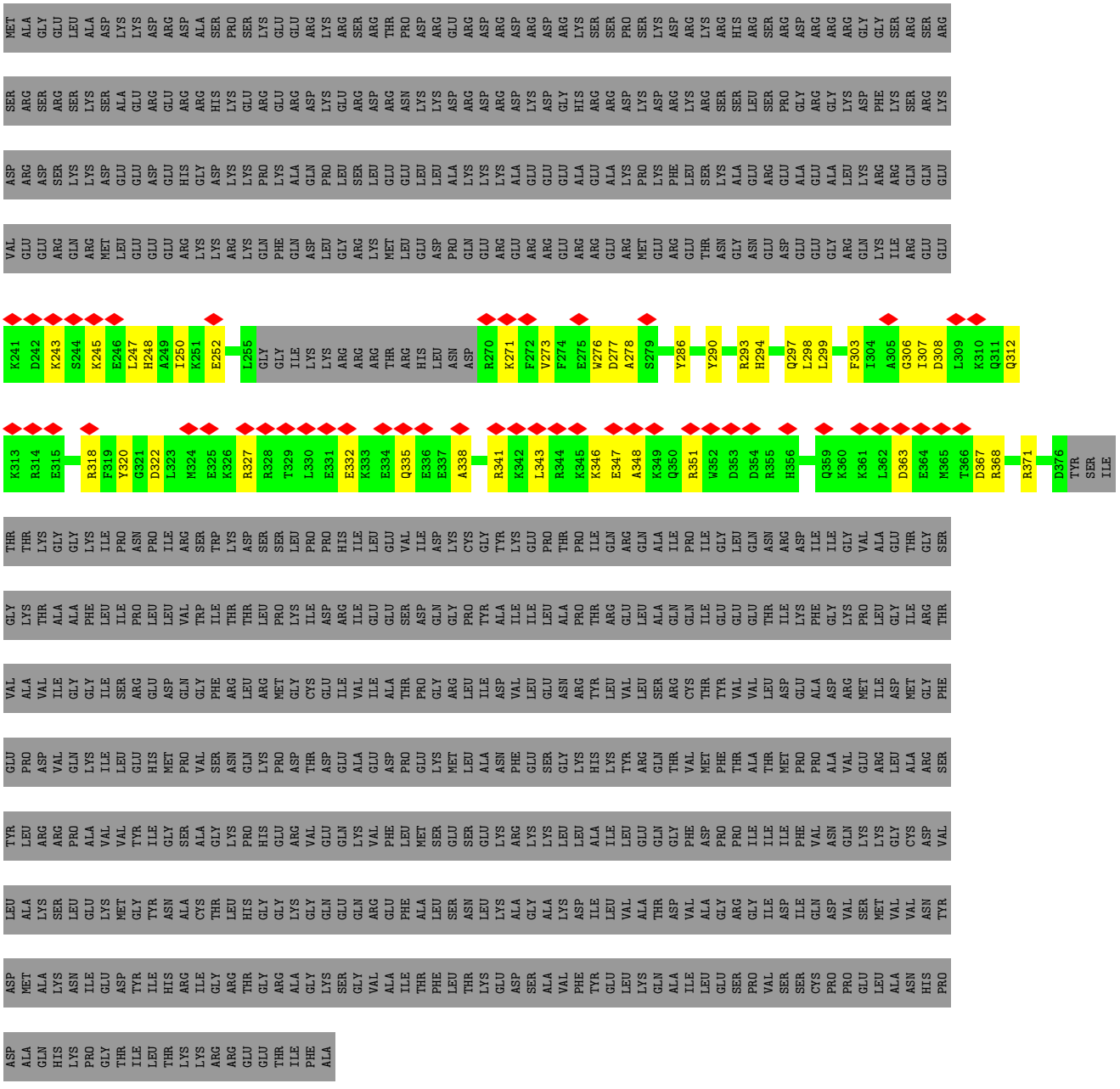






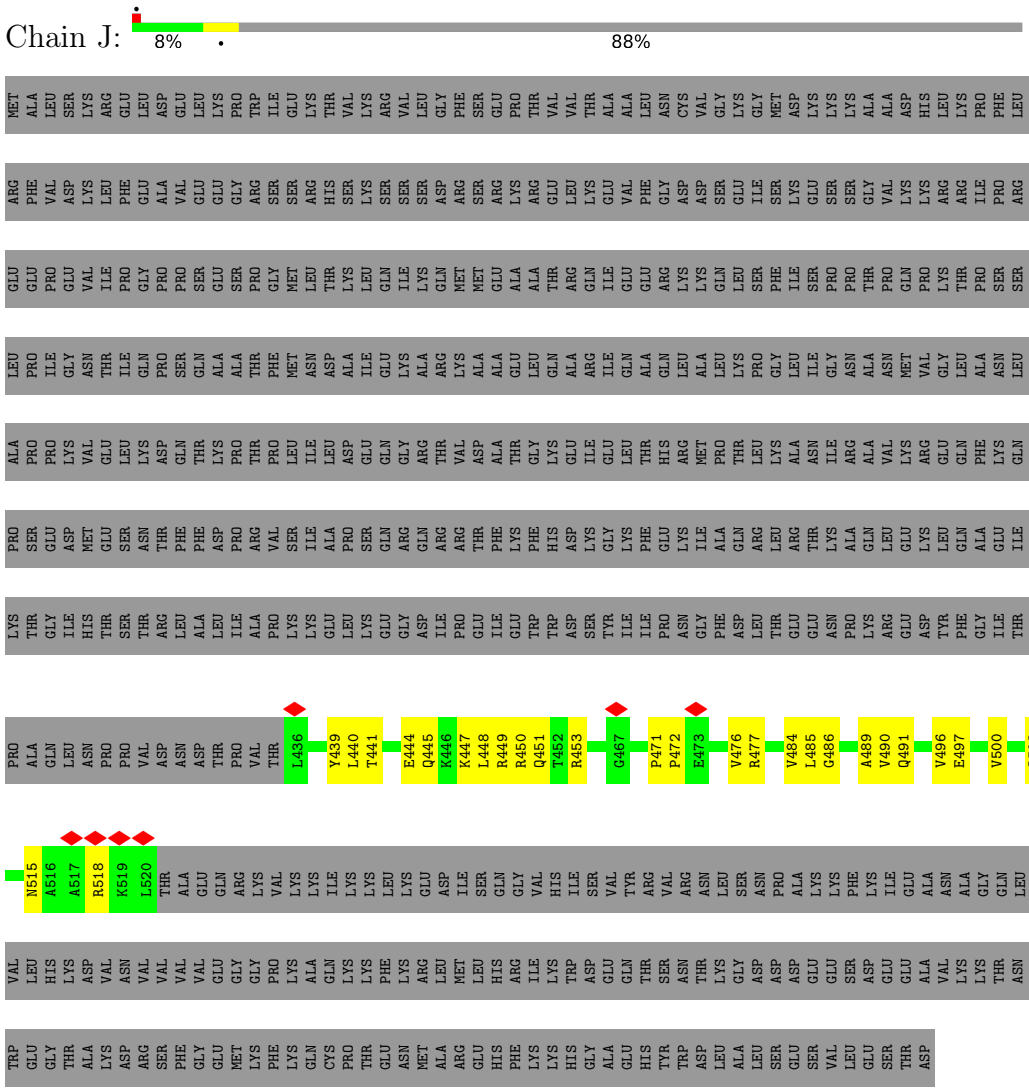
• Molecule 2: Probable ATP-dependent RNA helicase DDX23

Chain G:



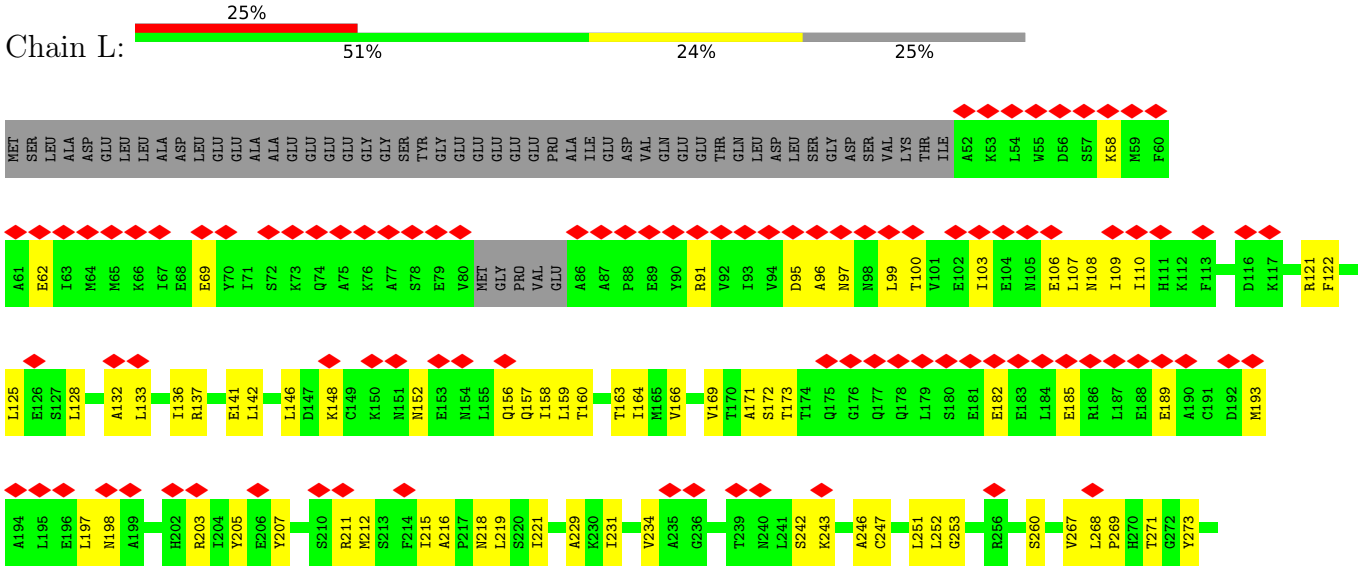
• Molecule 3: U4/U6 small nuclear ribonucleoprotein Prp3

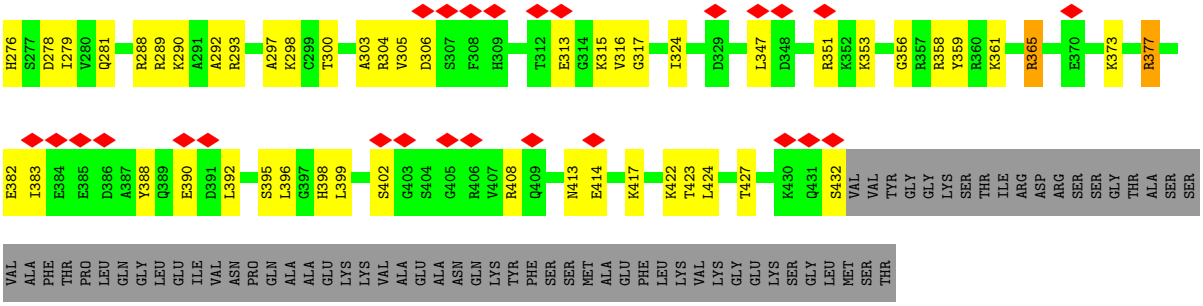
Chain J:



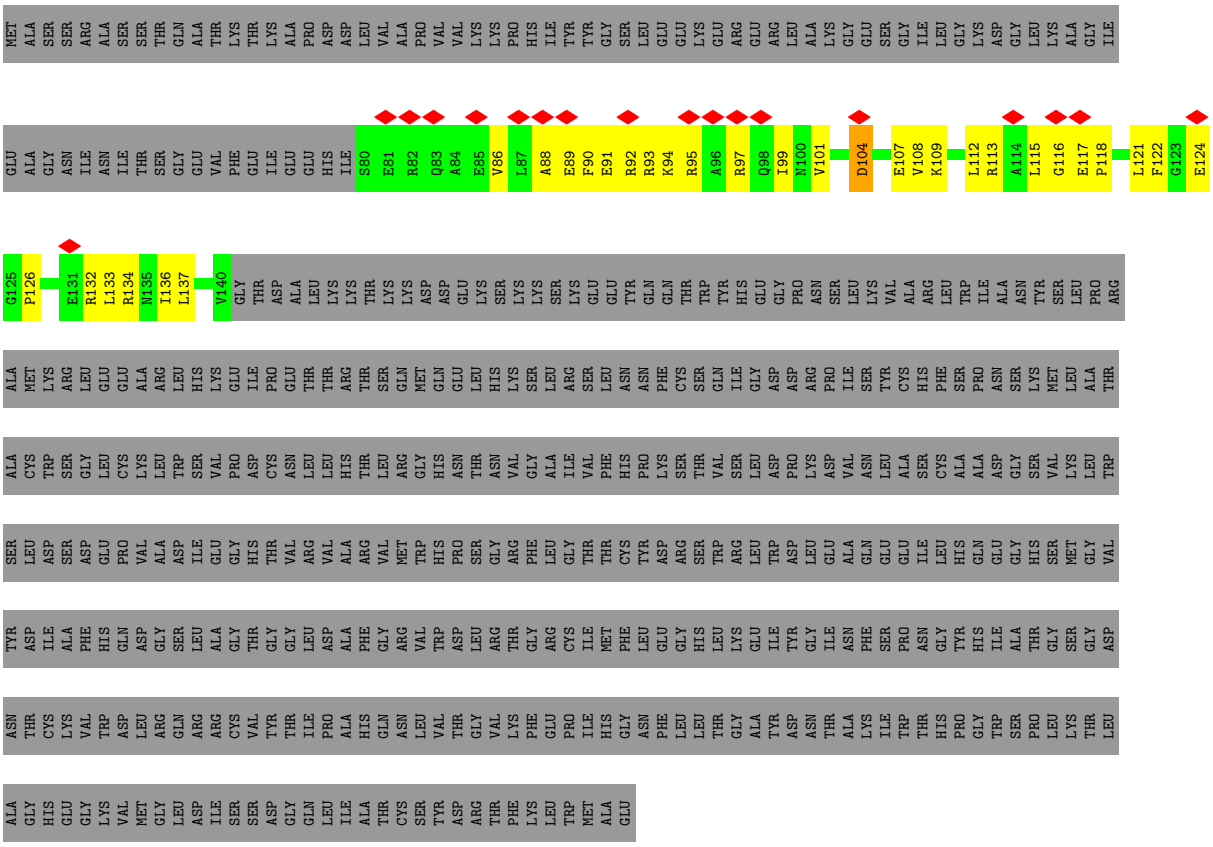
• Molecule 4: U4/U6 small nuclear ribonucleoprotein Prp31

Chain L:

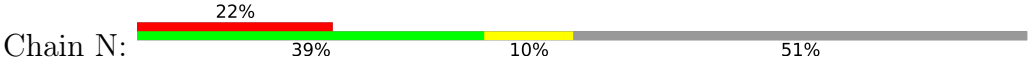


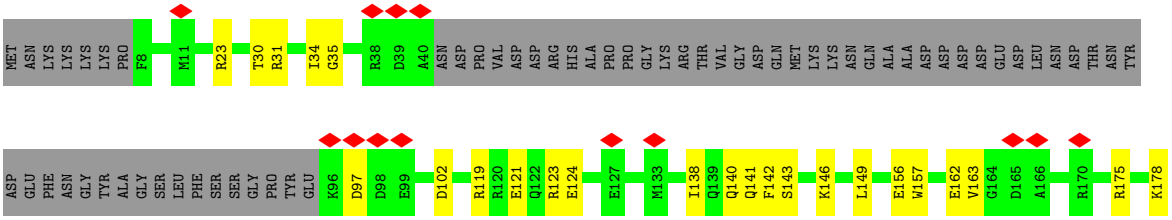


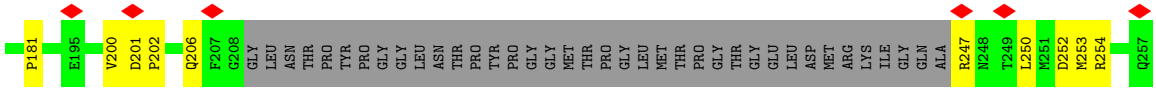
• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp4

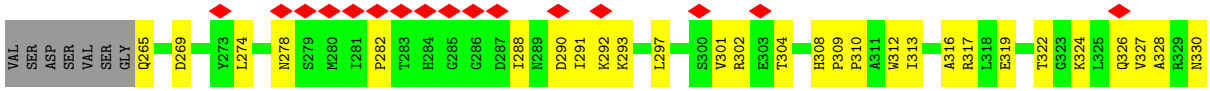


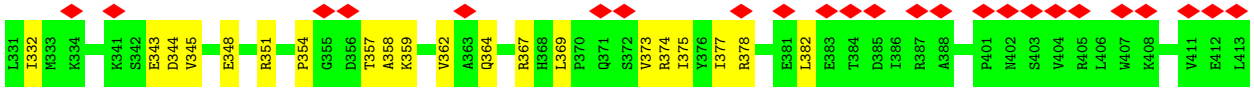
• Molecule 6: Pre-mRNA-processing factor 6

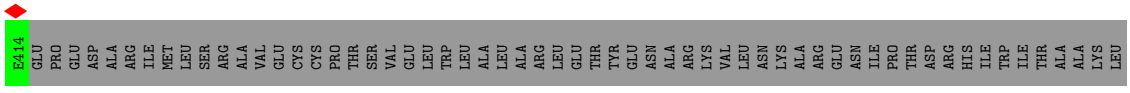


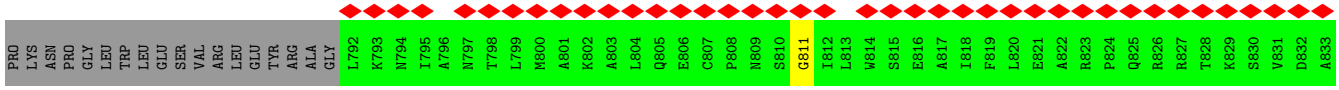


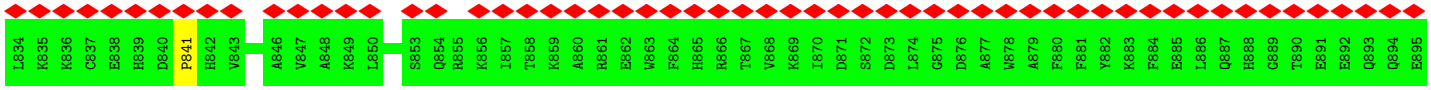


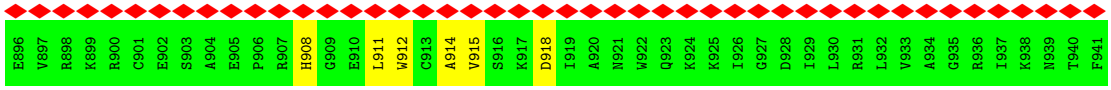






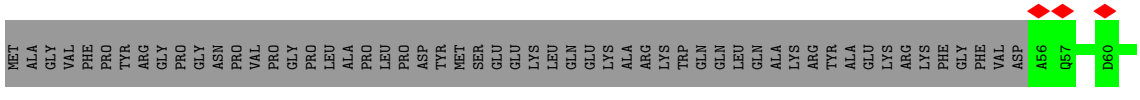


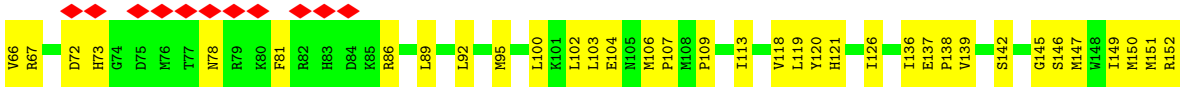


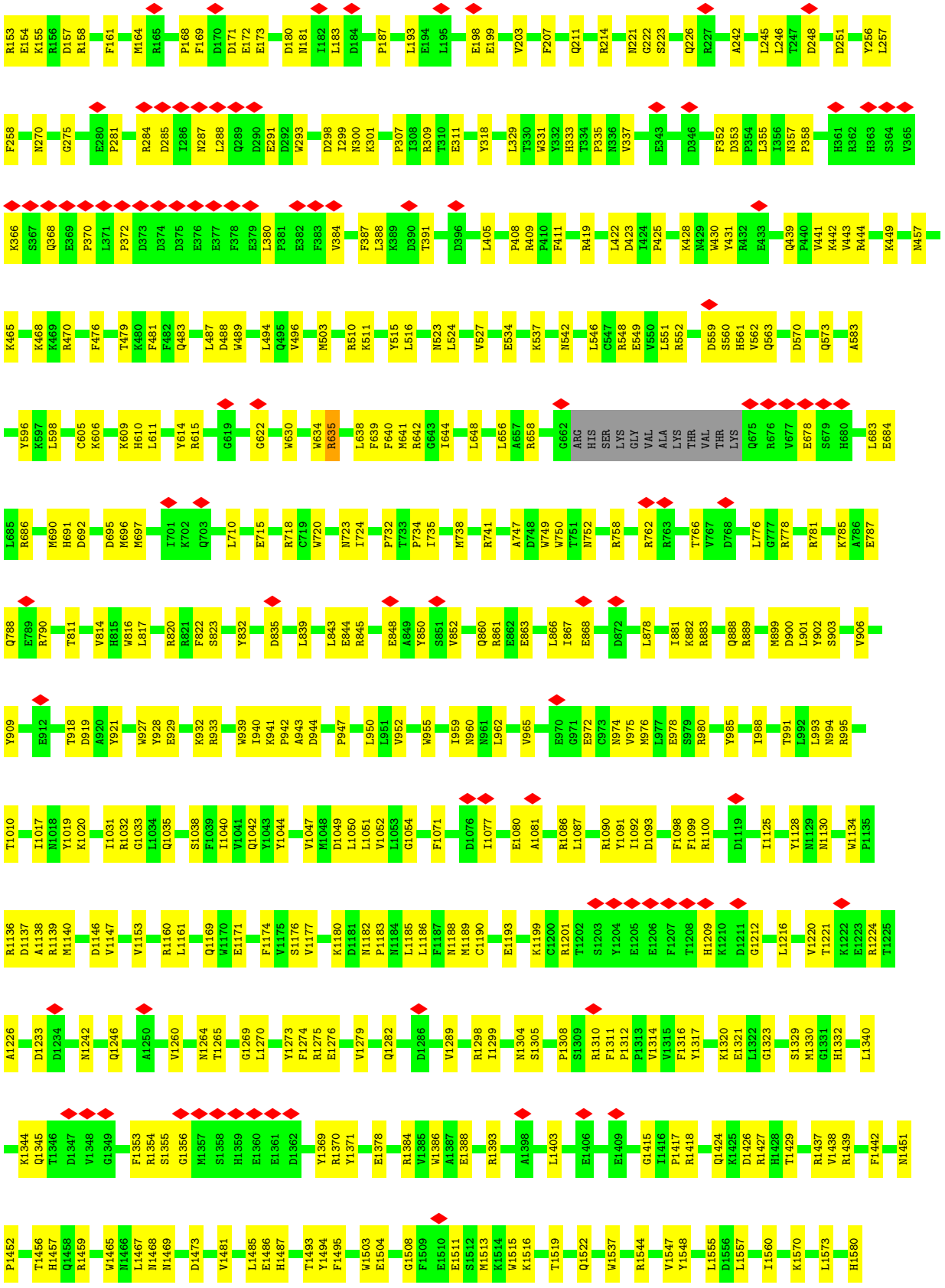


• Molecule 7: Pre-mRNA-processing-splicing factor 8

Chain A:



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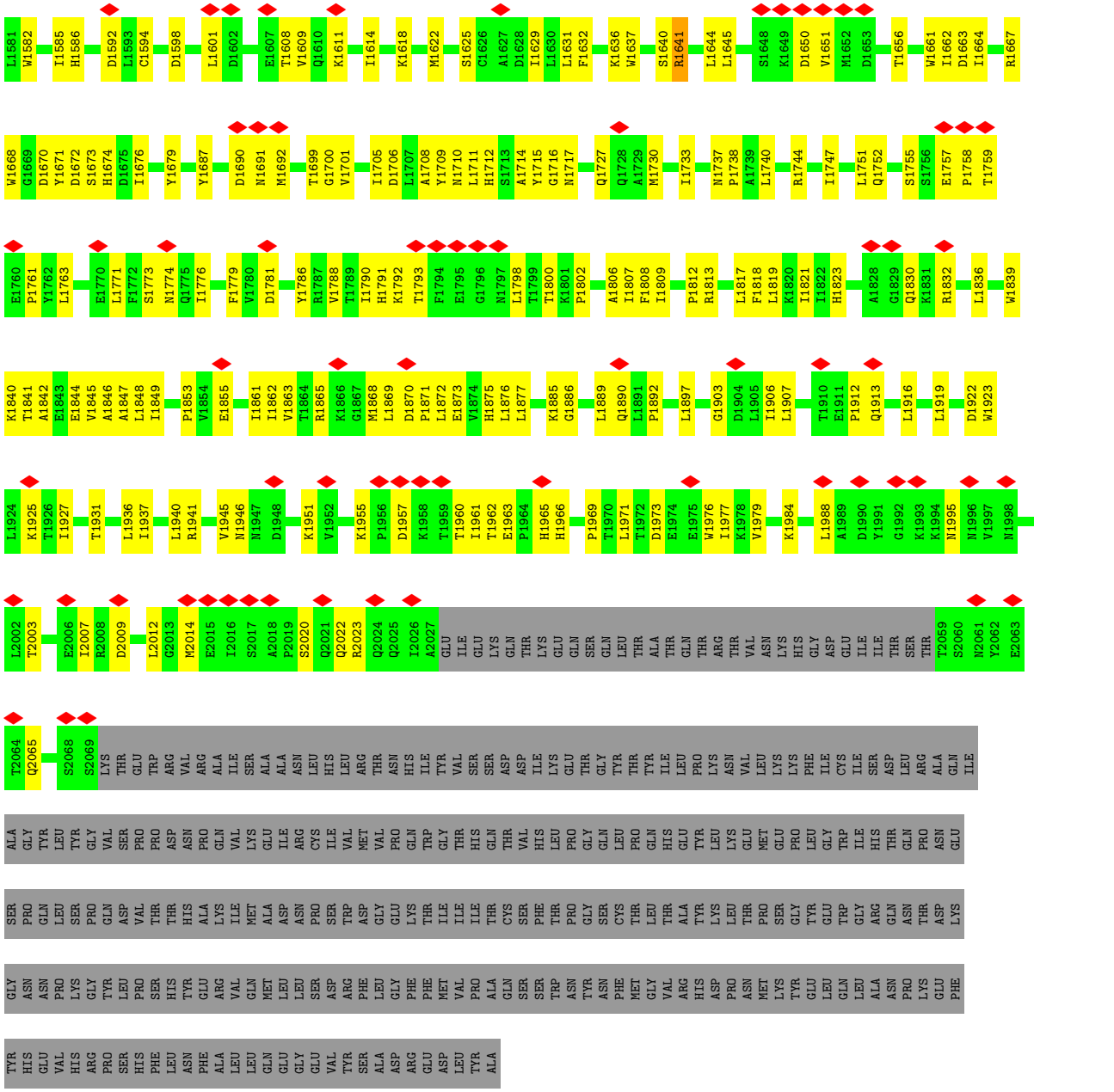
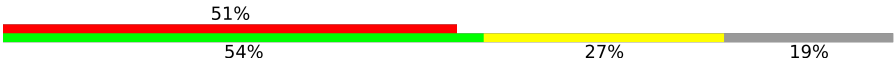
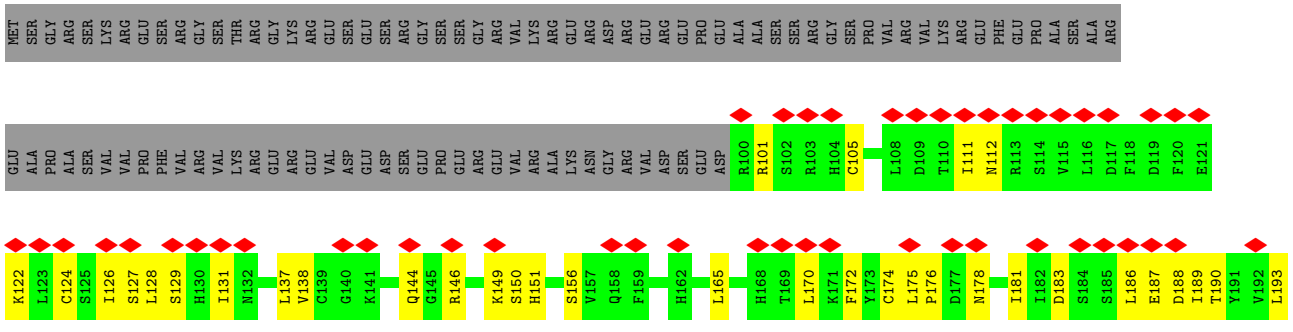
F258 N270 G275 E280 P281 R284 D285 I286 N287 L288 Q289 D290 E291 D292 W293 D298 I299 N300 K301 P307 I308 R309 T310 E311 Y318 L329 T330 W331 Y332 H333 T334 P335 N336 V337 E343 D346 F352 D353 P354 L355 I356 N357 P358 H361 R362 H363 S364 V365
K366 S367 Q368 E369 P370 L371 P372 D373 D374 D375 E376 E377 F378 E379 L380 P381 E382 F383 V384 F387 L388 K389 D390 T391 D396 L405 P408 R409 P410 F411 R419 L422 D423 I424 P425 K428 M429 W430 Y431 R432 E433 Q439 P440 V441 K442 V443 R444 K449 N457
K465 K468 K469 R470 F476 T479 K480 F481 F482 Q483 L487 D488 W489 L494 Q495 V496 M503 R510 K511 Y515 L516 N523 L524 V527 E534 K537 N542 L546 C547 R548 E549 V550 L551 R552 D559 S560 H561 V562 Q563 D570 Q573 A583
Y596 K597 L598 C605 K606 K609 H610 L611 Y614 R615 G619 G622 W630 W634 R635 L638 F639 F640 M641 R642 G643 I644 L648 L656 A657 R658 G662 ARG HIS SER LYS GLY VAL ALA LYS THR VAL THR LYS Q675 R676 V677 E678 S679 H680 L683 E684
L685 R686 M690 H691 D692 D695 M696 M697 I701 K702 Q703 L710 E715 R718 C719 W720 N723 I724 P732 T733 P734 I735 M738 R741 A747 D748 W749 W750 T751 N752 R758 R762 R763 T766 V767 D768 L776 G777 R778 R781 K785 A786 E787
Q788 E789 R790 T811 V814 H815 W816 L817 R820 R821 F822 S823 Y832 D835 L839 L843 E844 R845 E848 A849 Y850 S851 V852 Q860 R861 E862 E863 L866 I867 E868 D872 L878 I881 K882 R883 Q888 R889 M899 D900 L901 Y902 S903 V906
Y909 E912 T918 D919 A920 Y921 W927 Y928 E929 K932 R933 W939 I940 K941 P942 A943 D944 P947 L950 L951 V952 W955 I959 N960 N961 L962 V965 E970 G971 E972 Q973 N974 V975 M976 L977 E978 S979 R980 Y985 I988 T991 L992 L993 N994 R995
T1010 I1017 N1018 Y1019 K1020 I1031 R1032 G1033 L1034 Q1035 S1038 F1039 I1040 V1041 Q1042 Y1043 Y1044 V1047 M1048 D1049 L1050 L1051 V1052 L1053 G1054 F1071 D1076 I1077 E1080 A1081 R1086 L1087 R1090 Y1091 I1092 D1093 F1098 F1099 R1100 D1119 I1125 Y1128 N1129 N1130 W1134 P1135
R1136 D1137 A1138 R1139 M1140 D1146 V1147 V1153 R1160 L1161 Q1169 W1170 E1171 F1174 V1175 S1176 V1177 K1180 D1181 N1182 P1183 N1184 L1185 L1186 F1187 N1188 M1189 C1190 E1193 K1199 C1200 R1201 T1202 S1203 Y1204 E1205 E1206 F1207 T1208 H1209 K1210 D1211 G1212 L1216 V1220 T1221 K1222 E1223 R1224 T1225
A1226 D1233 D1234 N1242 Q1246 A1250 V1260 N1264 T1265 G1269 L1270 Y1273 F1274 R1275 E1276 V1279 Q1282 D1286 V1289 R1298 I1299 N1304 S1305 P1308 S1309 R1310 F1311 P1312 P1313 V1314 V1315 F1316 Y1317 K1320 E1321 L1322 G1323 S1329 M1330 G1331 H1332 L1340
K1344 Q1345 T1346 D1347 V1348 G1349 F1353 R1354 S1355 G1356 M1357 S1358 H1359 E1360 E1361 D1362 Y1369 R1370 Y1371 E1378 R1384 V1385 W1386 A1387 E1388 R1393 A1398 L1403 E1406 E1409 G1415 I1416 P1417 R1418 Q1424 K1425 D1426 R1427 H1428 T1429 R1437 V1438 R1439 F1442 N1451
P1452 T1456 H1457 Q1458 R1459 W1465 N1466 L1467 N1468 N1469 D1473 V1481 L1485 E1486 H1487 T1493 Y1494 F1495 W1503 E1504 G1508 F1509 E1510 E1511 S1512 M1513 K1514 W1515 K1516 T1519 Q1522 W1537 R1544 V1547 Y1548 L1555 D1556 L1557 I1560 K1570 L1573 H1580

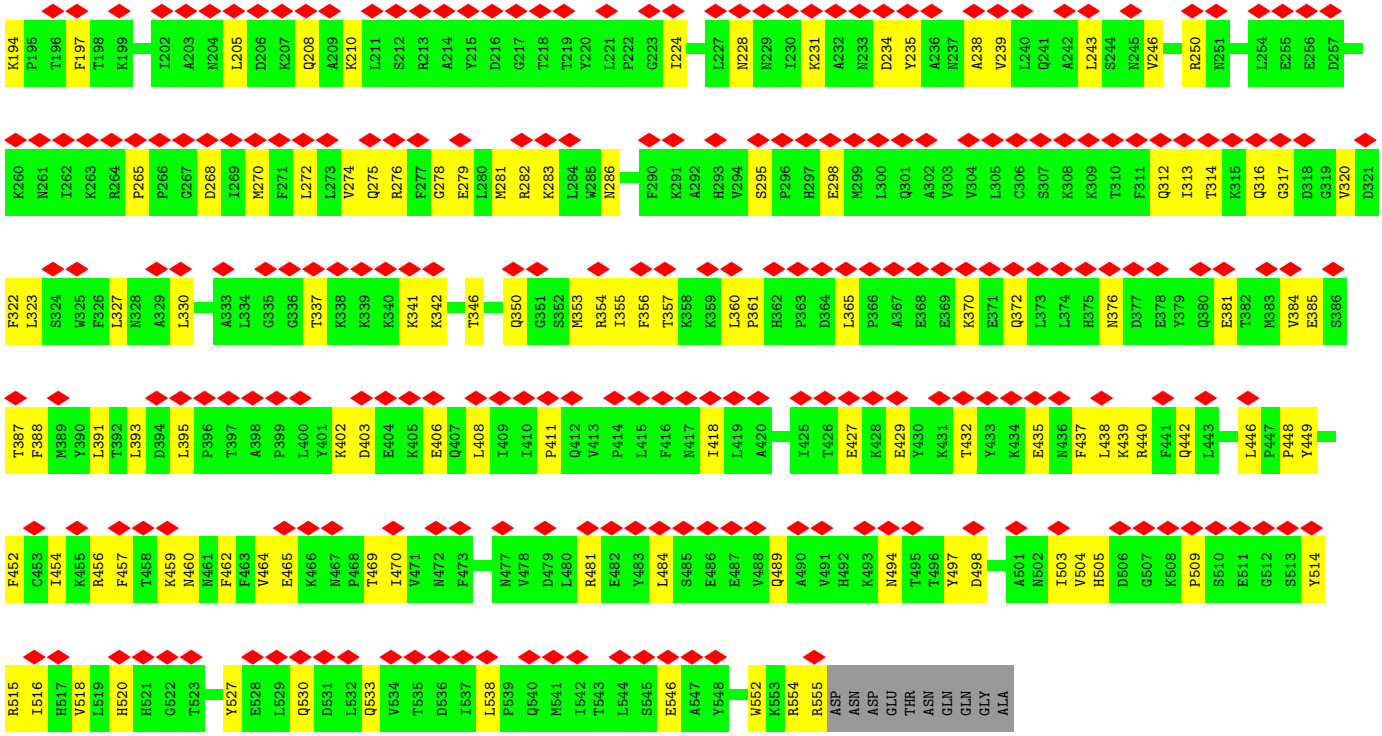


• Molecule 8: Ubiquitin carboxyl-terminal hydrolase 39

Chain U:

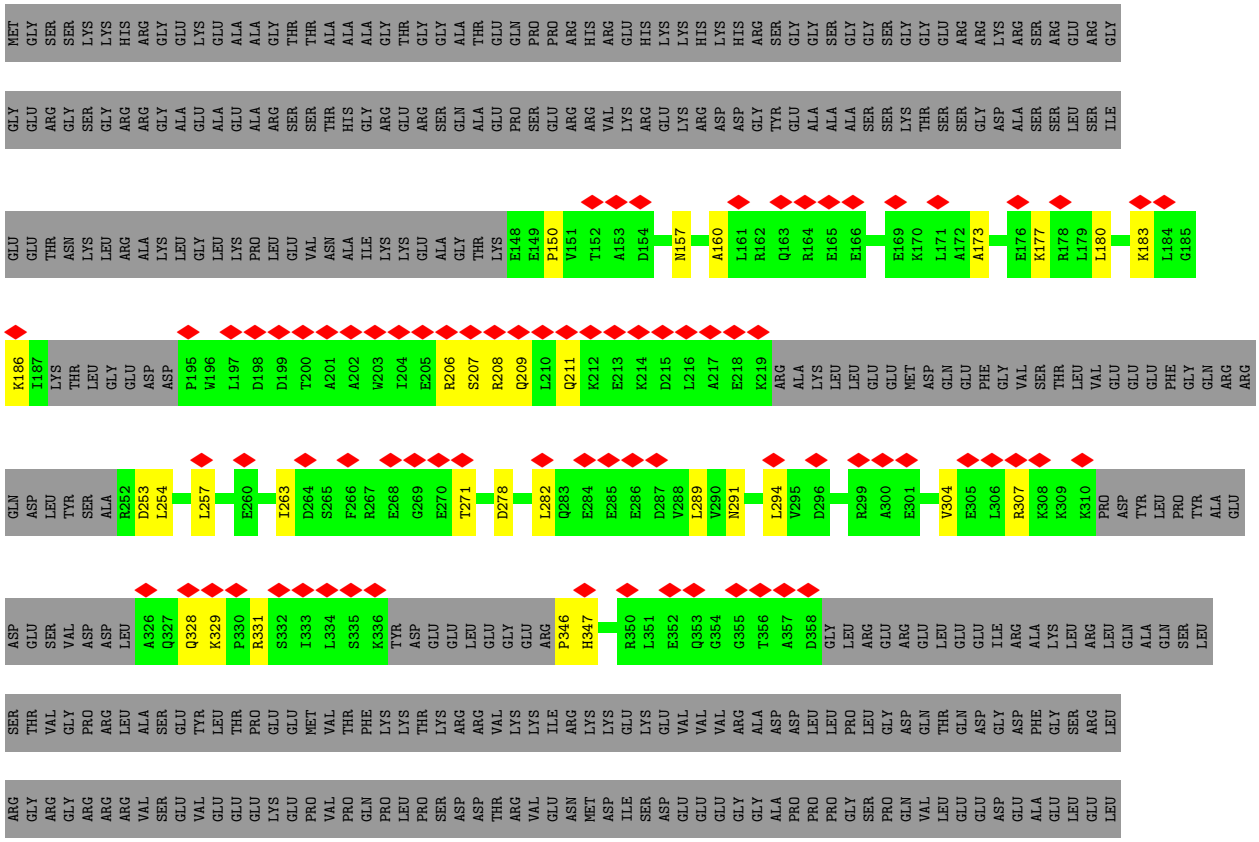


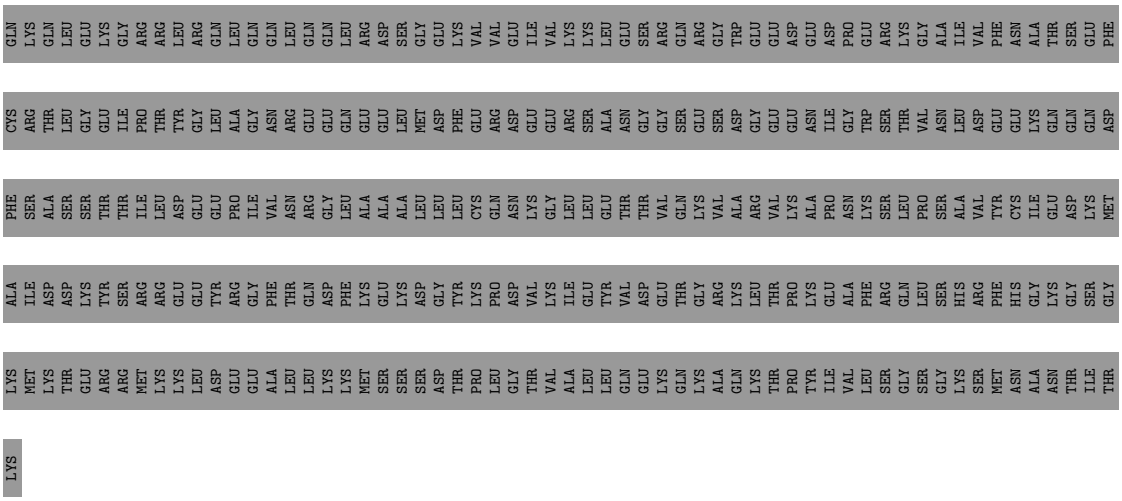




• Molecule 9: U4/U6.U5 tri-snRNP-associated protein 1

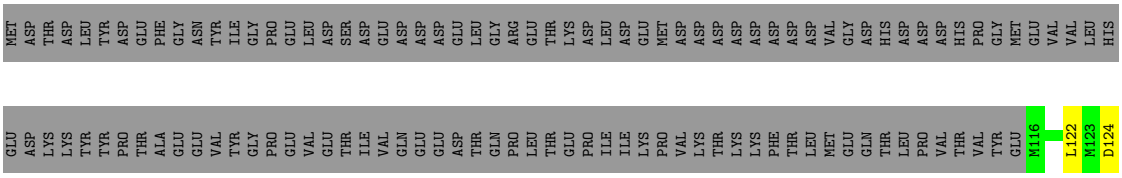
Chain S:

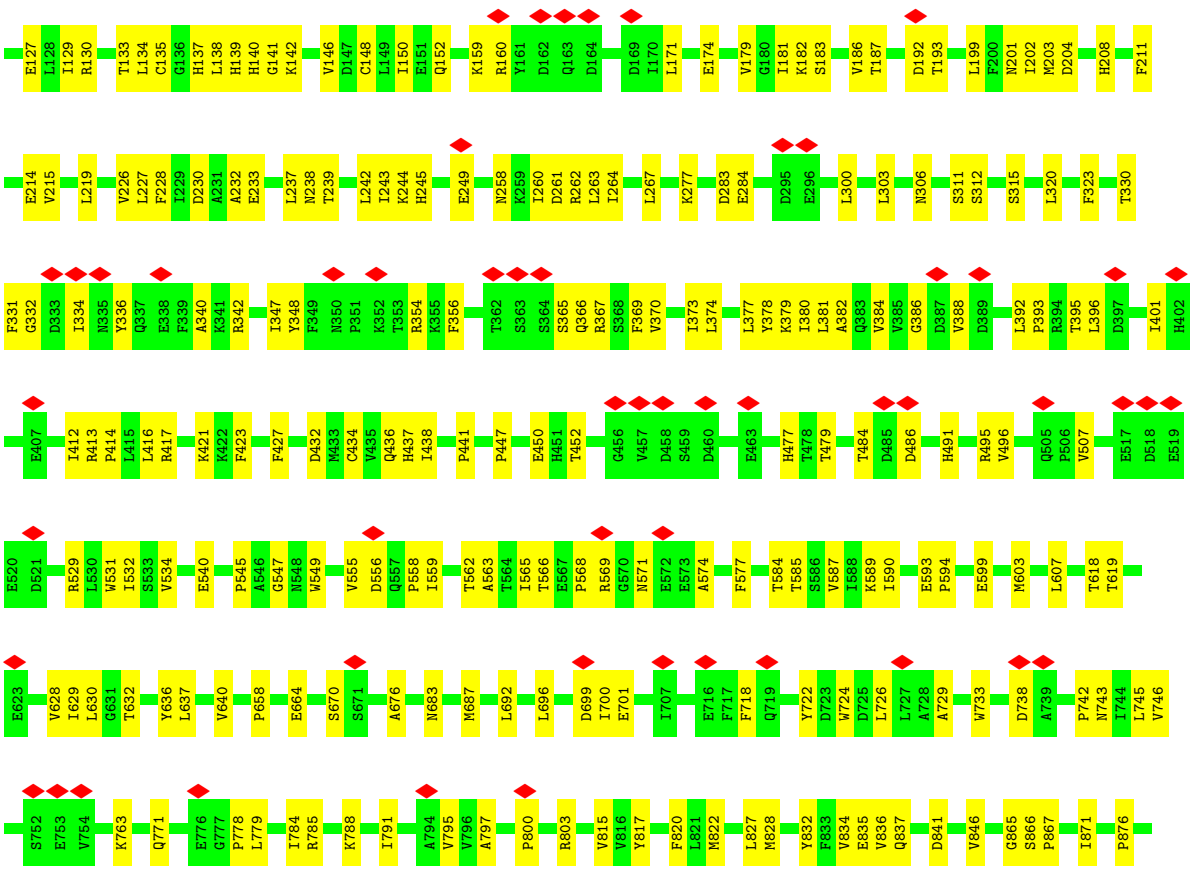


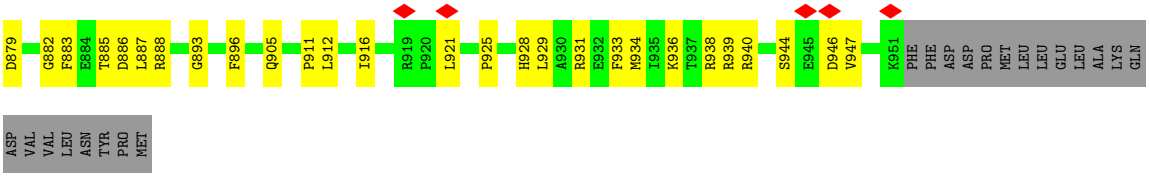


• Molecule 10: 116 kDa U5 small nuclear ribonucleoprotein component

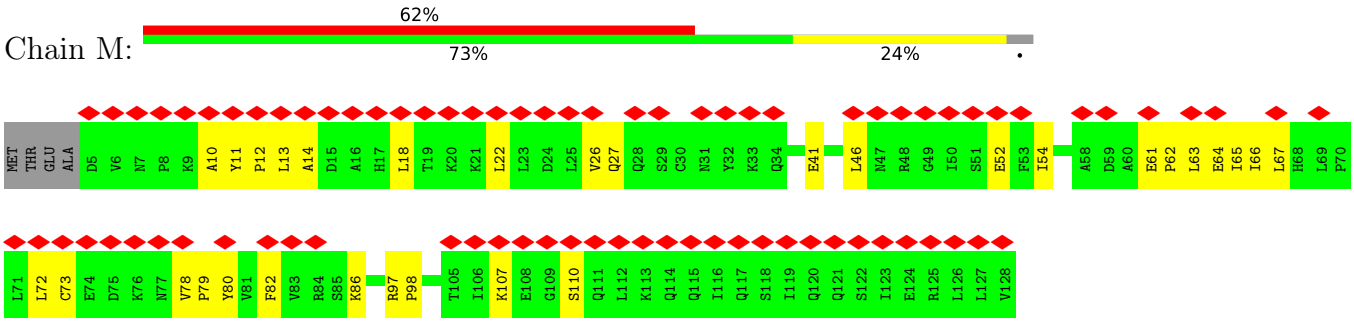
Chain C:



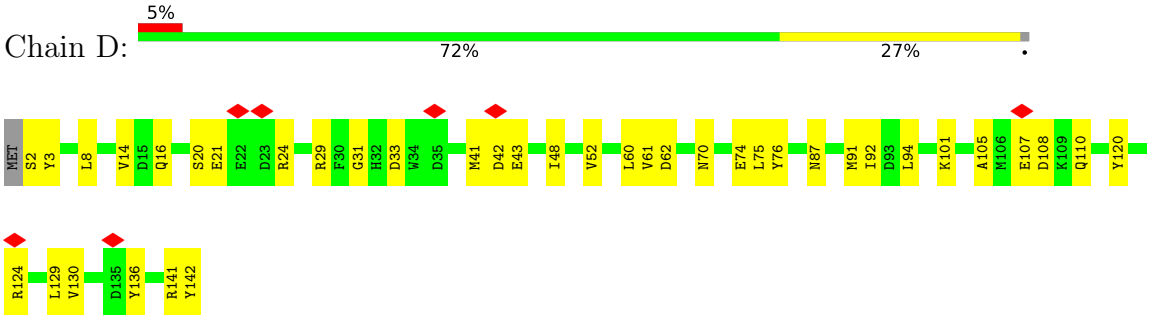




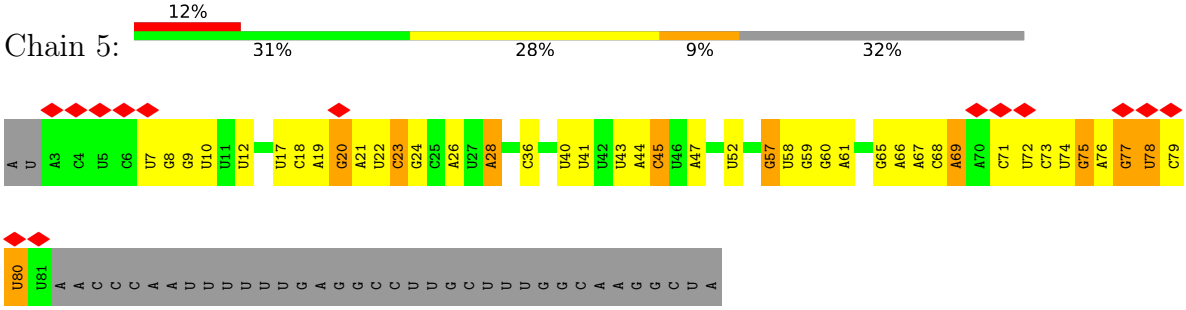
• Molecule 11: NHP2-like protein 1, N-terminally processed



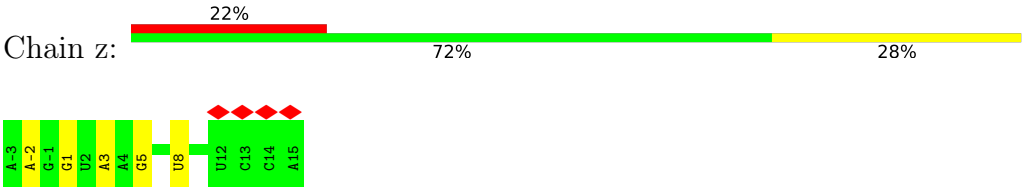
• Molecule 12: Thioredoxin-like protein 4A



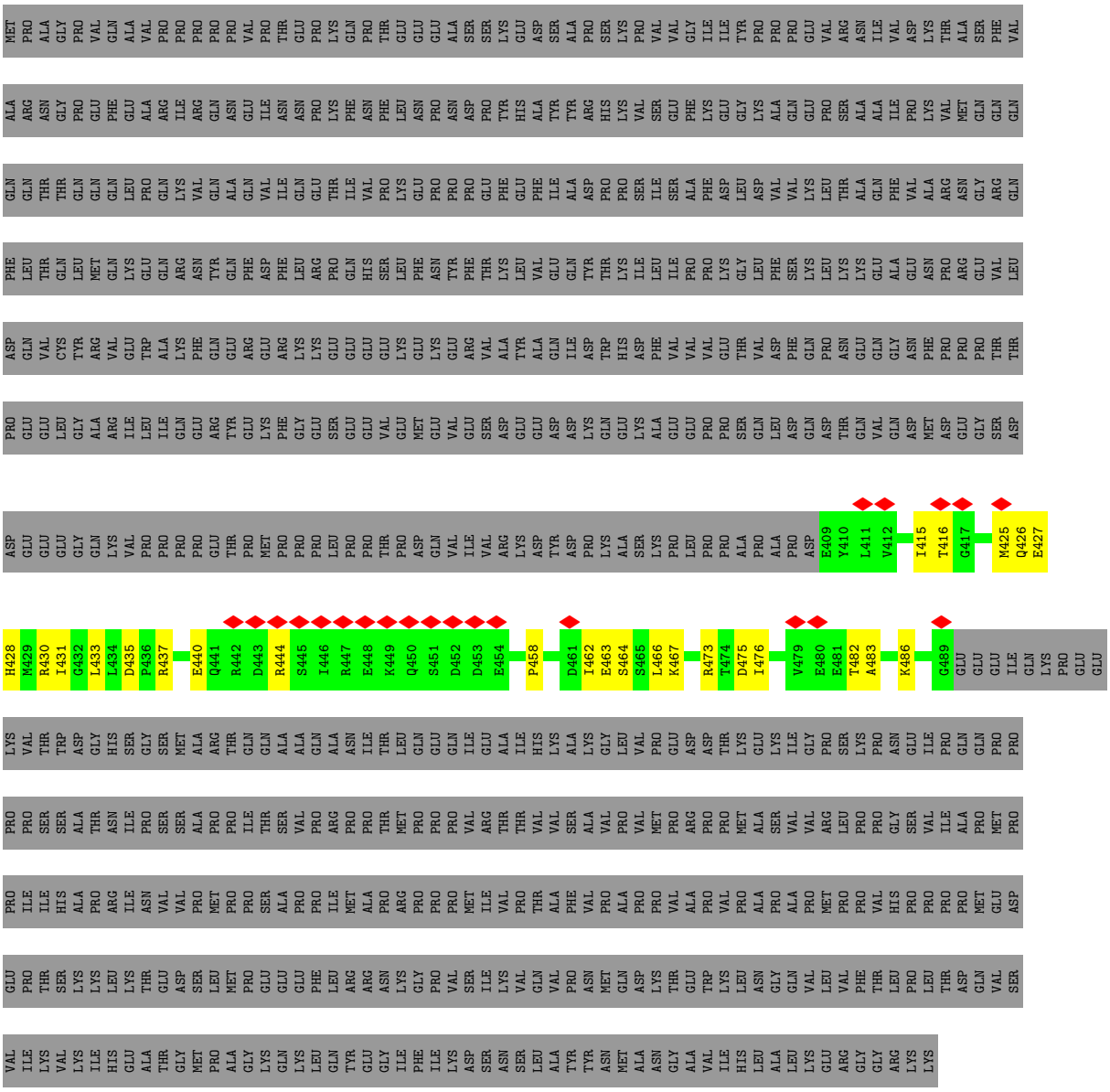
• Molecule 13: U5 snRNA



• Molecule 14: 5'ss oligo

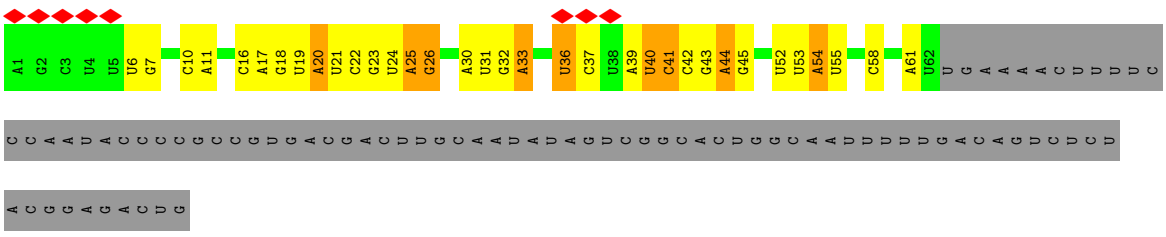


• Molecule 15: Splicing factor 3A subunit 1



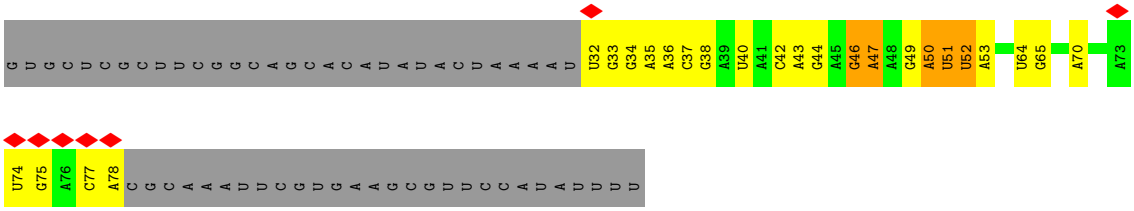
• Molecule 16: U4 snRNA

Chain 4:



• Molecule 17: U6 snRNA

Chain 6:


G U G C U C G C U U C G G C A G C A C A U A U A C U A A A A U
U32 G33 G34 A35 A36 C37 G38 A39 U40 A41 C42 A43 G44 A45 G46 A47 A48 G49 A50 U51 U52 A53 U64 G65 A70 A73
U74 G75 A76 C77 A78 C G C A A A U U C G U G A A G C G U U C C A A U A U U U

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136333	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	556.8, 556.8, 556.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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	B	0.23	0/158	0.60	0/209
2	G	0.24	0/1096	0.55	0/1455
3	J	0.26	0/685	0.57	0/911
4	L	0.25	0/2912	0.49	0/3924
5	F	0.27	0/491	0.66	0/657
6	N	0.24	0/3136	0.51	0/4273
7	A	0.26	0/16830	0.50	0/22831
8	U	0.25	0/3845	0.48	0/5208
9	S	0.23	0/1175	0.51	0/1571
10	C	0.26	0/6739	0.49	0/9151
11	M	0.24	0/974	0.50	0/1316
12	D	0.26	0/1199	0.48	0/1620
13	5	0.20	0/1850	0.77	0/2875
14	z	0.20	0/429	0.74	0/666
15	7	0.25	0/659	0.53	0/884
16	4	0.20	0/1477	0.69	0/2300
17	6	0.20	0/1133	0.71	0/1766
All	All	0.25	0/44788	0.53	0/61617

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	158	0	166	9	0
2	G	1077	0	1066	28	0
3	J	678	0	711	24	0
4	L	2874	0	2856	94	0
5	F	488	0	499	29	0
6	N	3095	0	2612	81	0
7	A	16383	0	16318	484	0
8	U	3749	0	3769	111	0
9	S	1167	0	1182	23	0
10	C	6592	0	6615	185	0
11	M	962	0	1012	29	0
12	D	1170	0	1141	28	0
13	5	1660	0	842	25	0
14	z	384	0	194	0	0
15	7	650	0	655	18	0
16	4	1322	0	666	28	0
17	6	1010	0	512	17	0
18	A	36	0	6	0	0
All	All	43455	0	40822	1060	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 13.

The worst 5 of 1060 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)
6:N:378:ARG:O	6:N:382:LEU:HB2	1.72	0.89
7:A:752:ASN:HD22	8:U:462:PHE:HB3	1.39	0.88
7:A:942:PRO:HG2	7:A:1042:GLN:HE22	1.40	0.87
8:U:460:ASN:HD21	8:U:465:GLU:HG2	1.45	0.81
17:6:42:C:H2'	17:6:43:A:C8	2.16	0.80

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	B	20/2136 (1%)	20 (100%)	0	0	100	100
2	G	118/820 (14%)	117 (99%)	1 (1%)	0	100	100
3	J	83/683 (12%)	83 (100%)	0	0	100	100
4	L	372/499 (74%)	364 (98%)	8 (2%)	0	100	100
5	F	59/522 (11%)	56 (95%)	3 (5%)	0	100	100
6	N	447/941 (48%)	433 (97%)	14 (3%)	0	100	100
7	A	1965/2335 (84%)	1899 (97%)	65 (3%)	1 (0%)	51	83
8	U	454/565 (80%)	435 (96%)	19 (4%)	0	100	100
9	S	138/800 (17%)	138 (100%)	0	0	100	100
10	C	834/972 (86%)	803 (96%)	31 (4%)	0	100	100
11	M	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
12	D	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
15	7	79/793 (10%)	78 (99%)	1 (1%)	0	100	100
All	All	4830/11336 (43%)	4675 (97%)	154 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	172	GLU

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	B	17/1908 (1%)	17 (100%)	0	100 100
2	G	113/721 (16%)	113 (100%)	0	100 100
3	J	70/599 (12%)	70 (100%)	0	100 100
4	L	299/424 (70%)	296 (99%)	3 (1%)	76 86
5	F	52/442 (12%)	51 (98%)	1 (2%)	57 76
6	N	233/792 (29%)	233 (100%)	0	100 100
7	A	1786/2108 (85%)	1783 (100%)	3 (0%)	93 97
8	U	418/511 (82%)	417 (100%)	1 (0%)	93 97
9	S	121/681 (18%)	121 (100%)	0	100 100
10	C	738/866 (85%)	738 (100%)	0	100 100
11	M	108/111 (97%)	108 (100%)	0	100 100
12	D	129/130 (99%)	129 (100%)	0	100 100
15	7	71/709 (10%)	71 (100%)	0	100 100
All	All	4155/10002 (42%)	4147 (100%)	8 (0%)	93 97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	270	MET
7	A	1641	ARG
7	A	409	ARG
5	F	104	ASP
7	A	635	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
8	U	460	ASN
10	C	238	ASN
10	C	306	ASN
9	S	291	ASN
7	A	1583	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	5	78/117 (66%)	25 (32%)	2 (2%)
14	z	17/18 (94%)	5 (29%)	0
16	4	61/144 (42%)	17 (27%)	0
17	6	46/106 (43%)	10 (21%)	3 (6%)
All	All	202/385 (52%)	57 (28%)	5 (2%)

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	5	8	G
13	5	9	G
13	5	10	U
13	5	20	G
13	5	21	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	77	G
13	5	78	U
17	6	46	G
17	6	51	U
17	6	77	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
18	IHP	A	2401	-	36,36,36	0.73	0	54,60,60	1.05	2 (3%)

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
18	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	2401	IHP	O14-C4-C5	2.20	113.88	108.69
18	A	2401	IHP	C3-C2-C1	2.03	114.86	110.41

There are no chirality outliers.

All (3) torsion outliers are listed below:

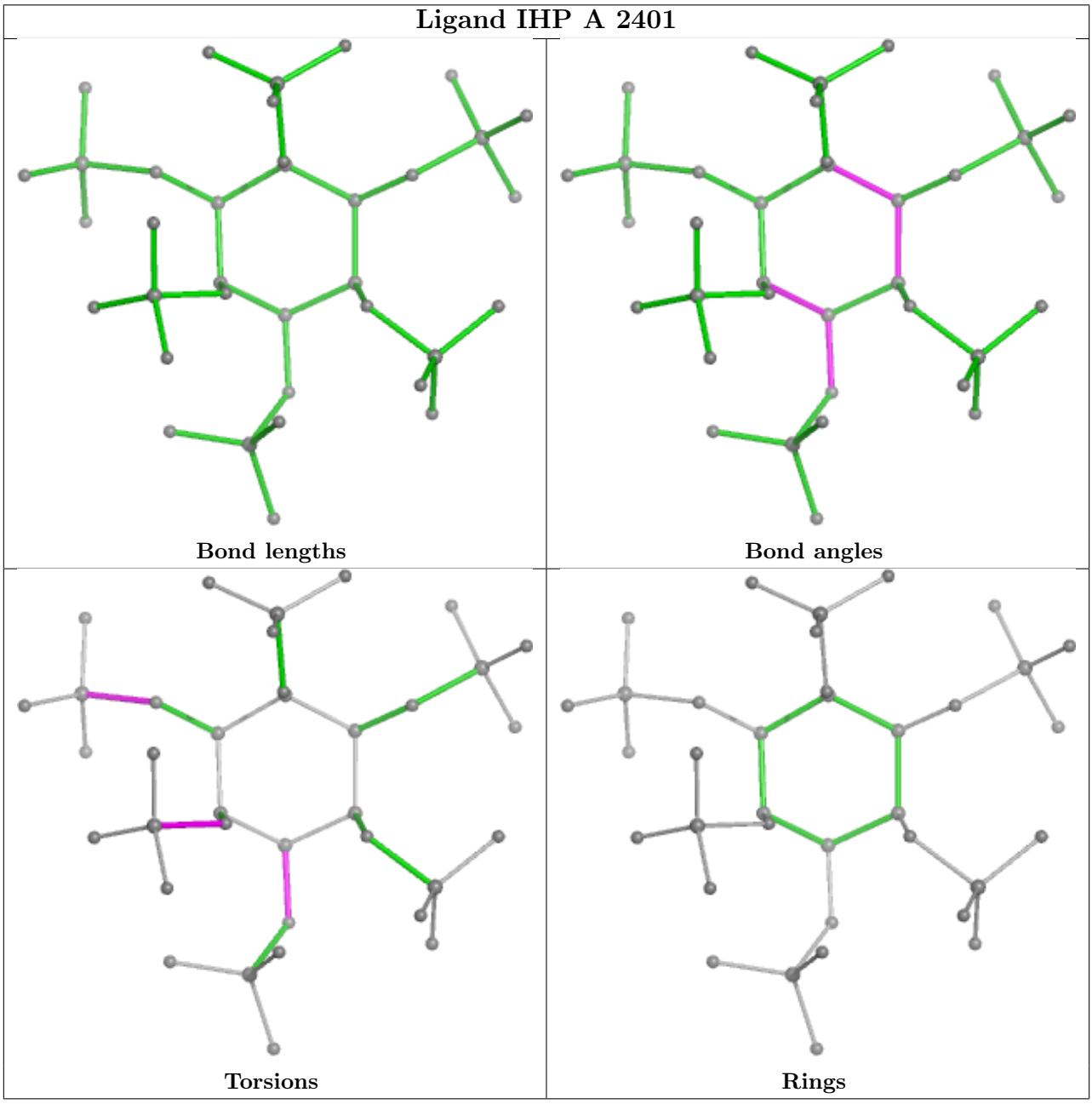
Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C5-C4-O14-P4
18	A	2401	IHP	C5-O15-P5-O25
18	A	2401	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

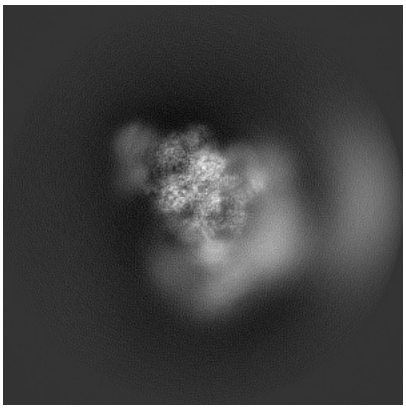
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18546. These allow visual inspection of the internal detail of the map and identification of artifacts.

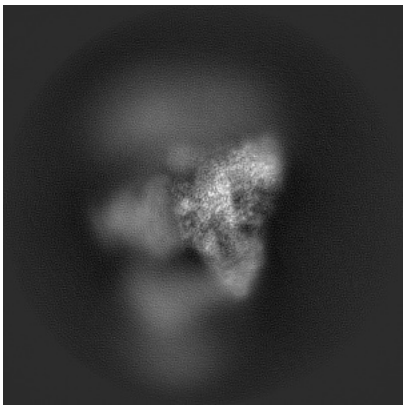
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

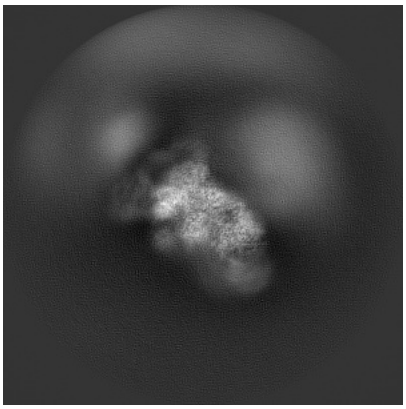
6.1.1 Primary map



X

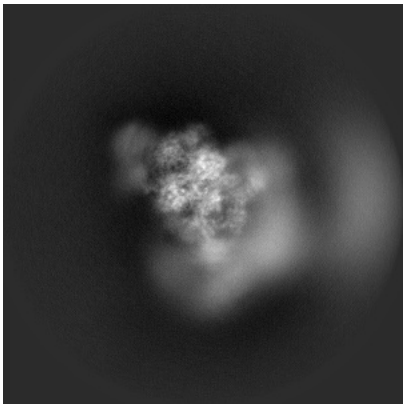


Y

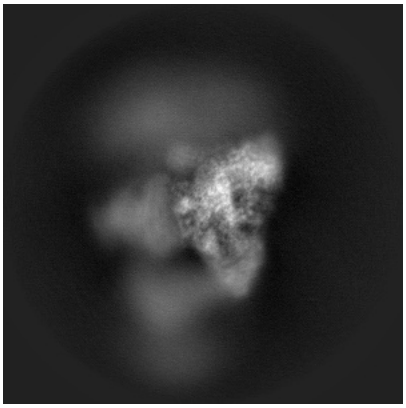


Z

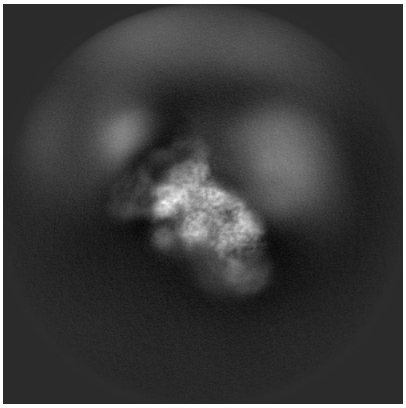
6.1.2 Raw map



X



Y

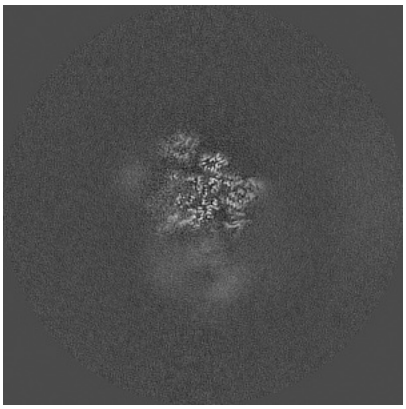


Z

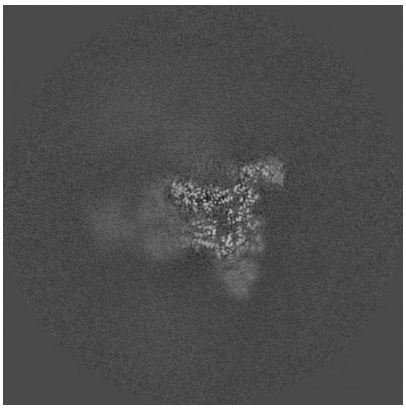
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

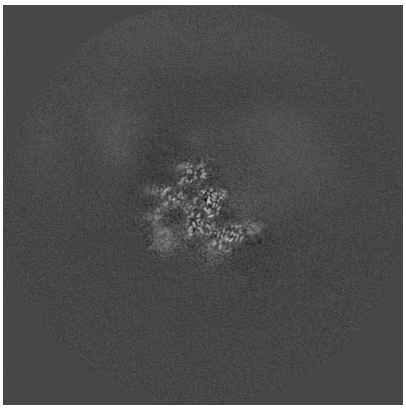
6.2.1 Primary map



X Index: 240

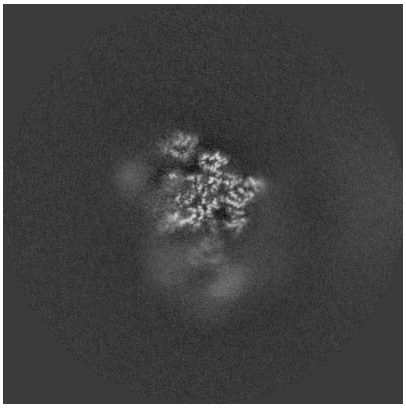


Y Index: 240

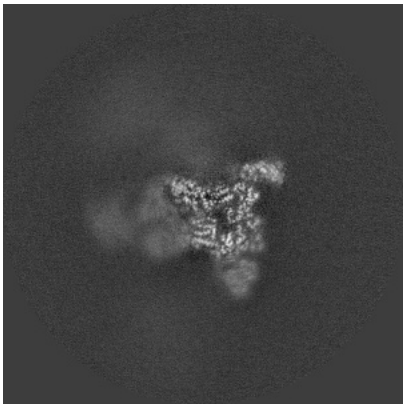


Z Index: 240

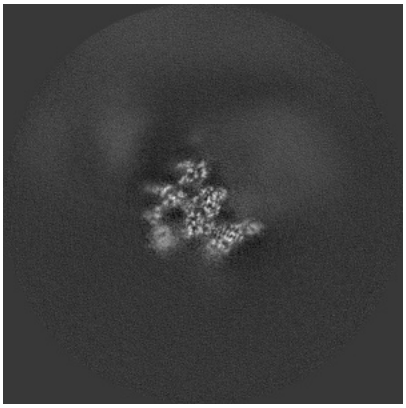
6.2.2 Raw map



X Index: 240



Y Index: 240

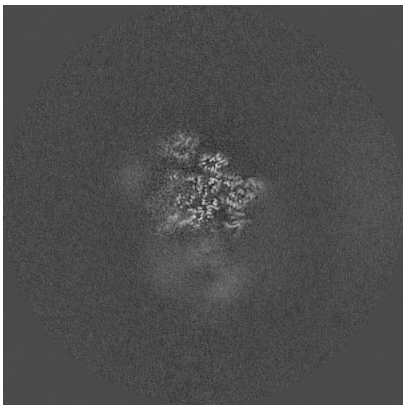


Z Index: 240

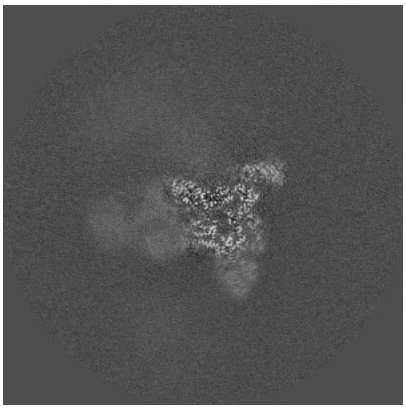
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

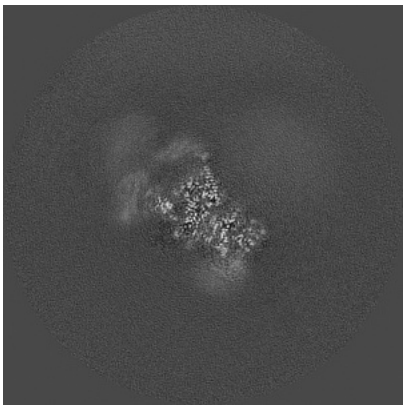
6.3.1 Primary map



X Index: 240

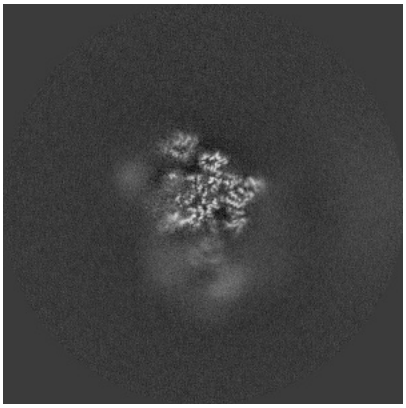


Y Index: 241

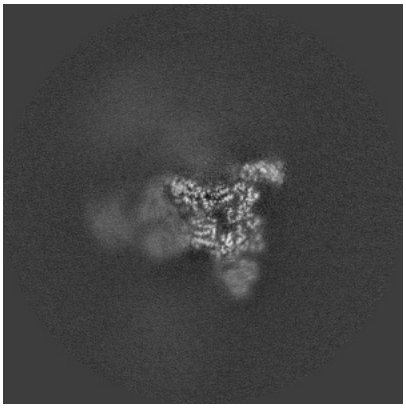


Z Index: 270

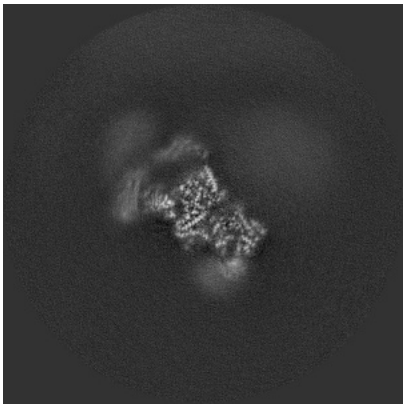
6.3.2 Raw map



X Index: 240



Y Index: 240

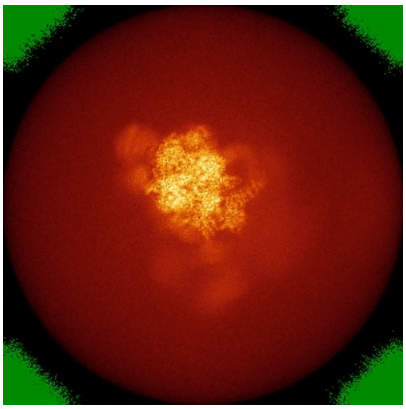


Z Index: 272

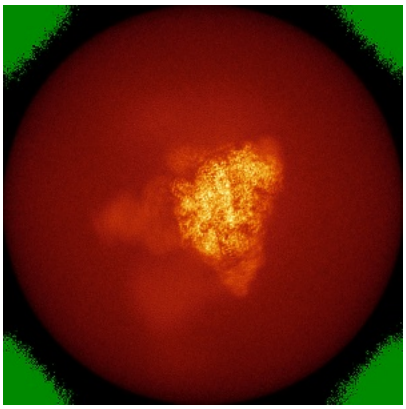
The images above show the largest variance slices of the map in three orthogonal directions.

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

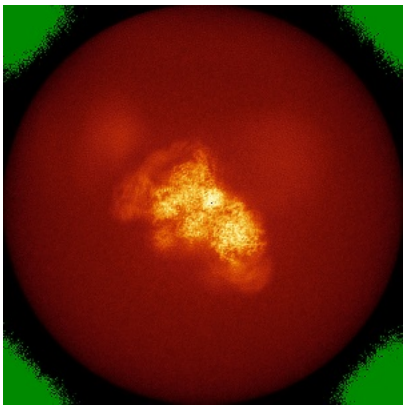
6.4.1 Primary map



X

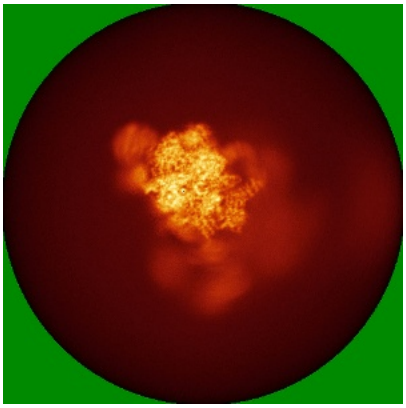


Y

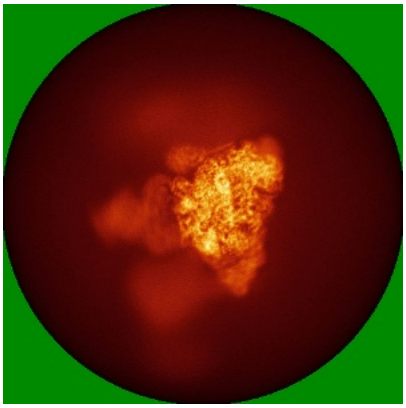


Z

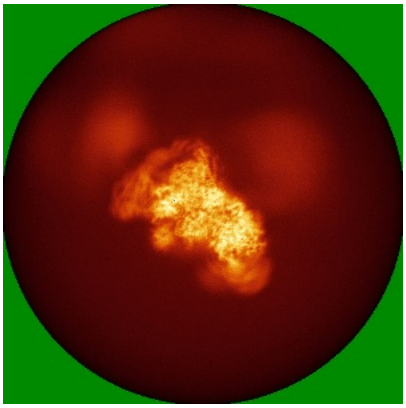
6.4.2 Raw map



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 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

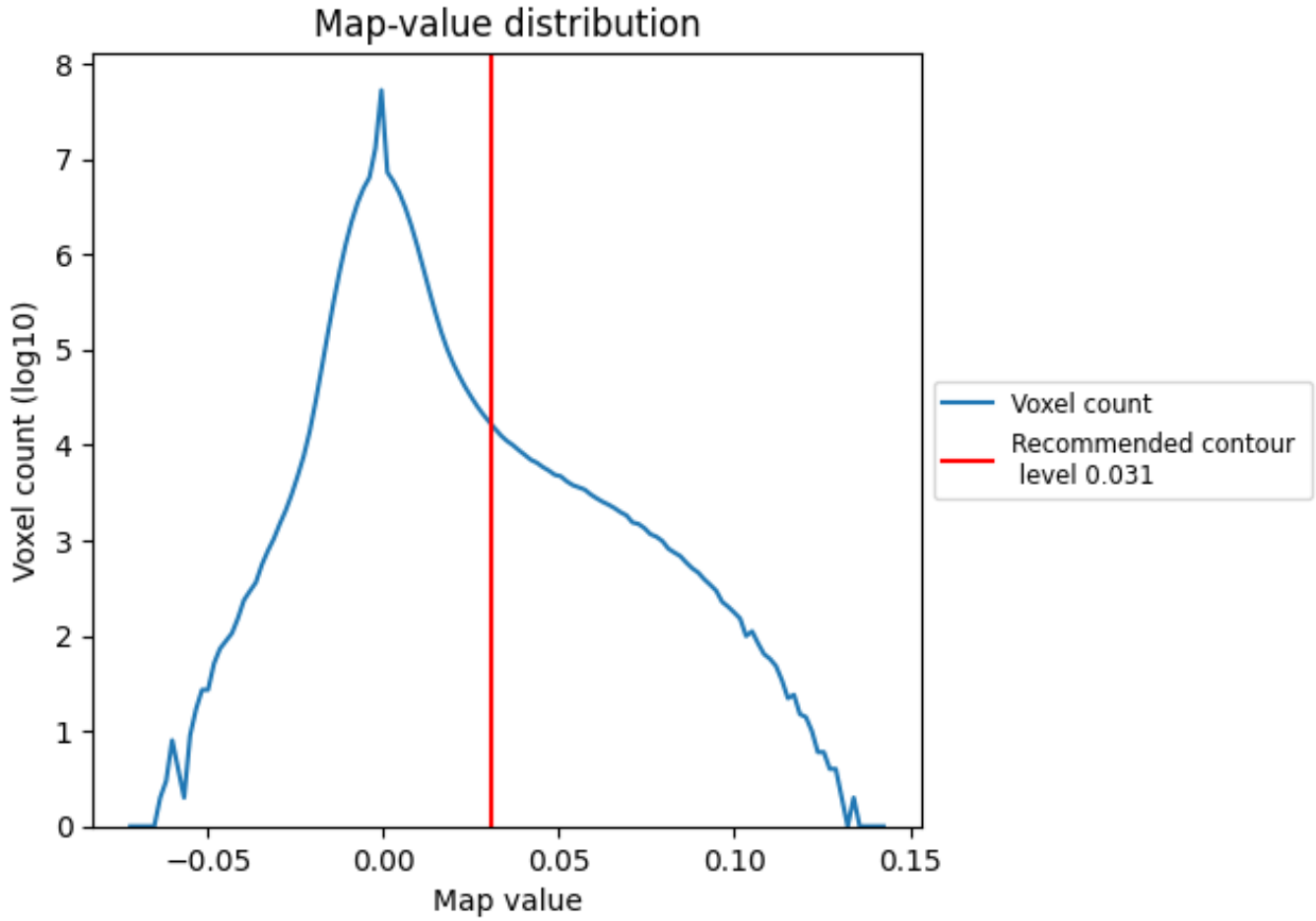
6.6 Mask visualisation (i)

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

7 Map analysis

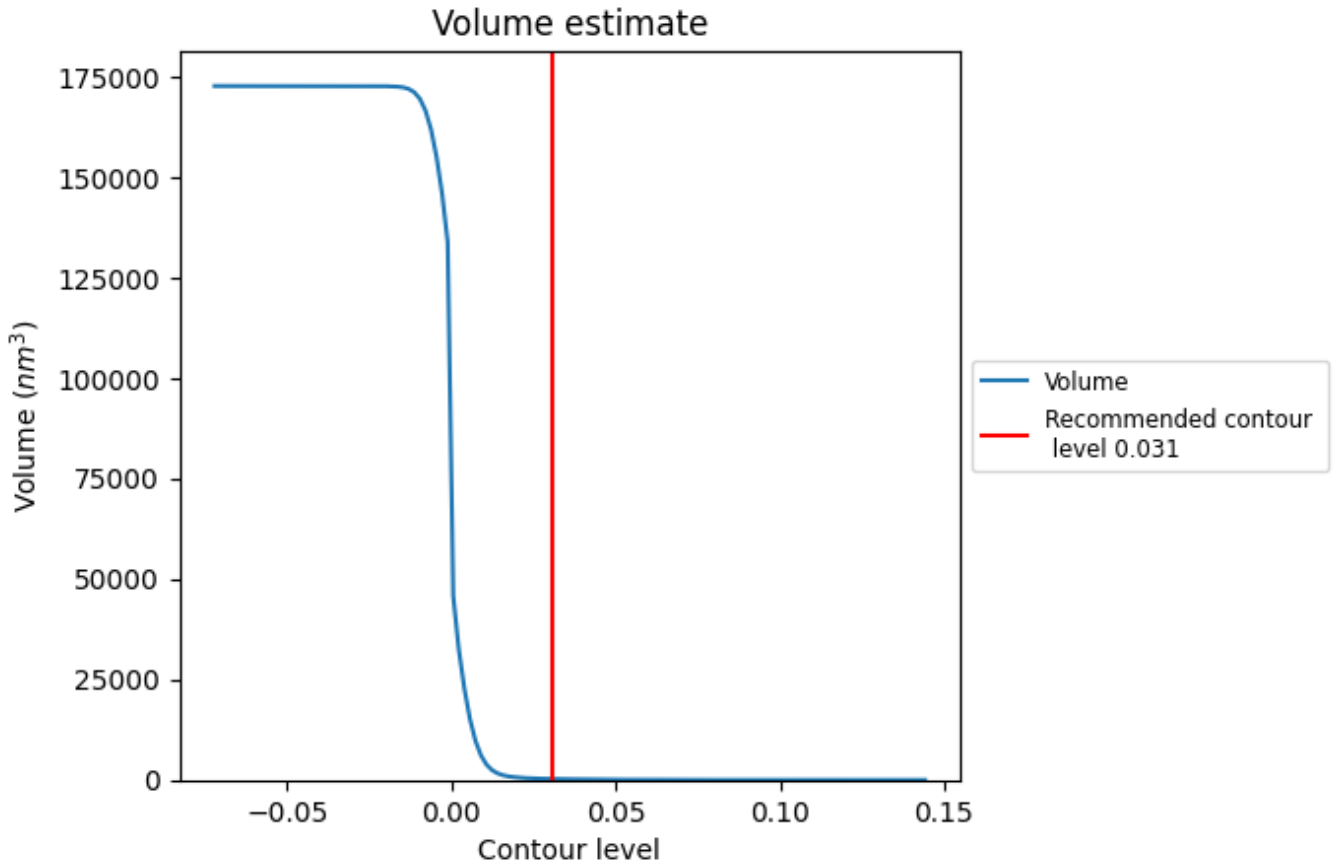
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

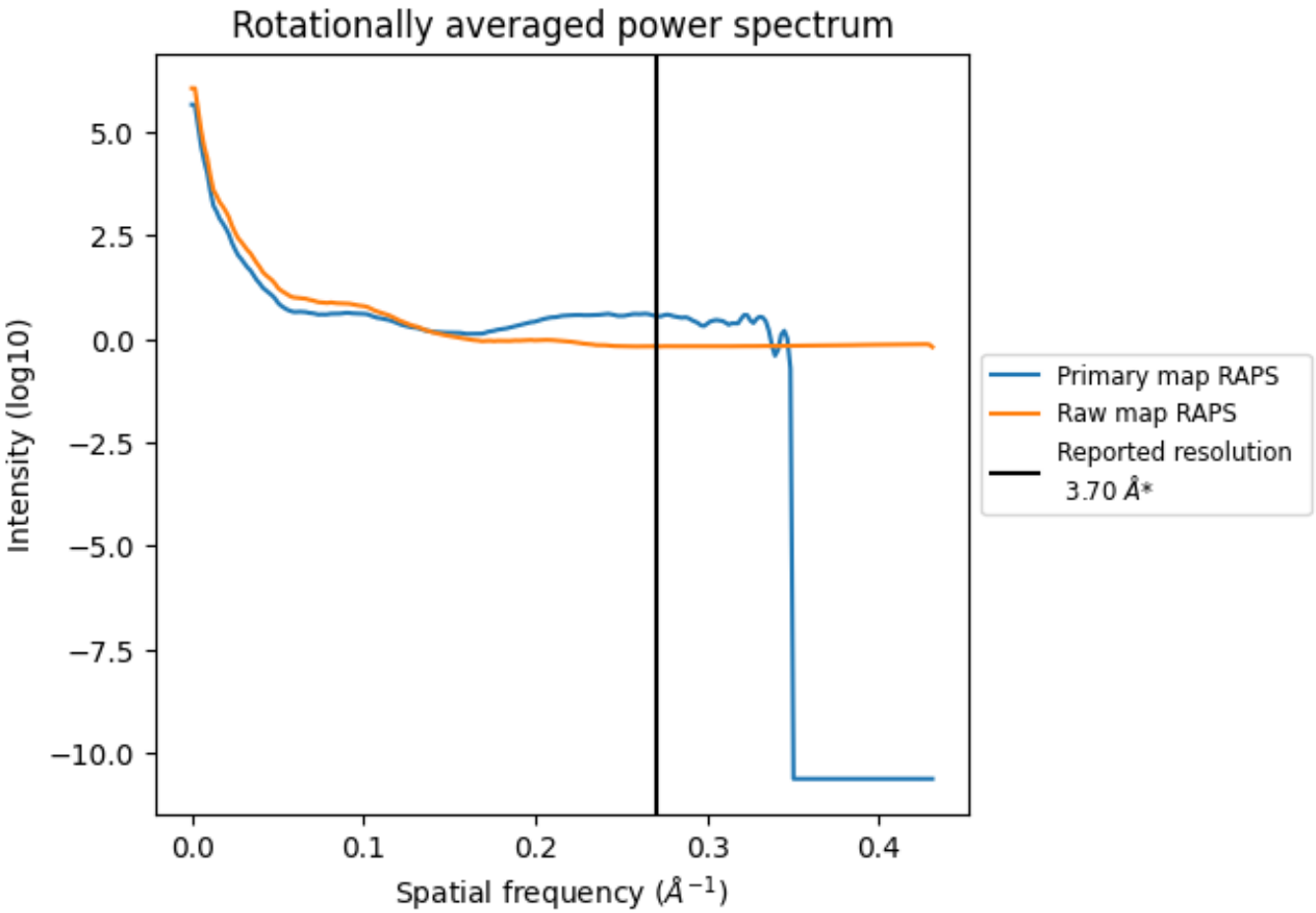
7.2 Volume estimate (i)



The volume at the recommended contour level is 238 nm^3; this corresponds to an approximate mass of 215 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)

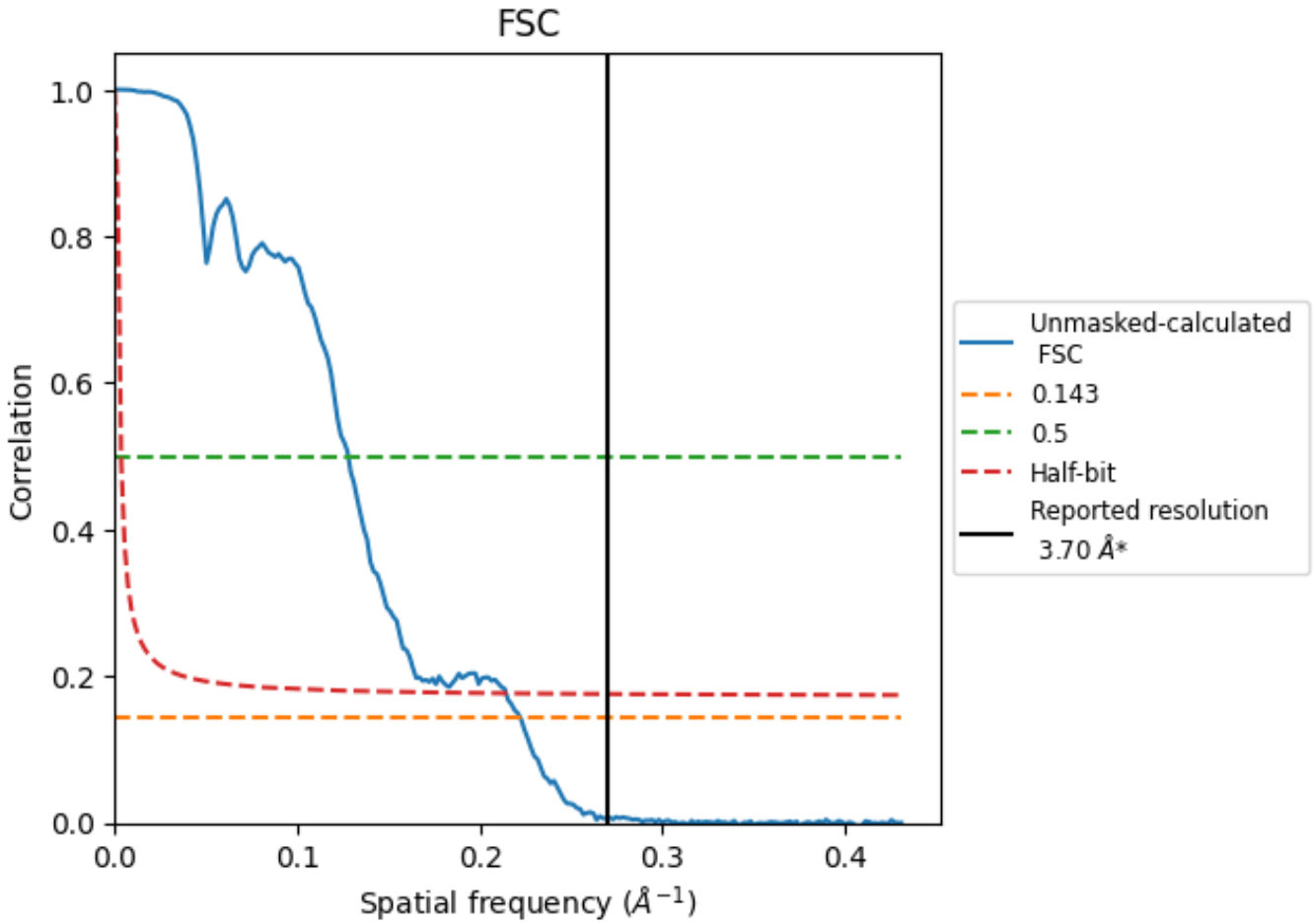


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

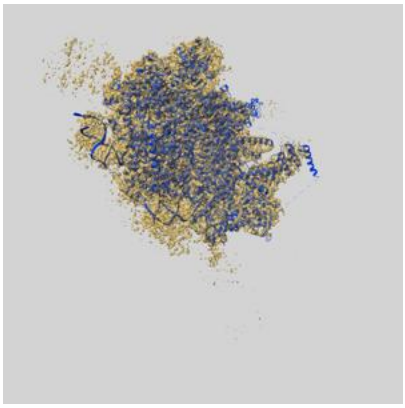
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.81	4.66

*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 4.50 differs from the reported value 3.7 by more than 10 %

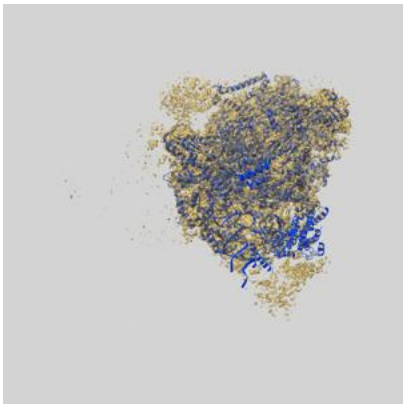
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18546 and PDB model 8QPA. Per-residue inclusion information can be found in section 3 on page 7.

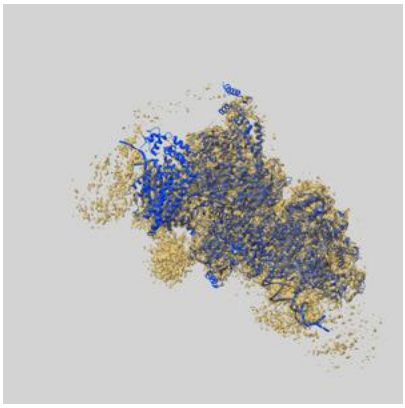
9.1 Map-model overlay



X



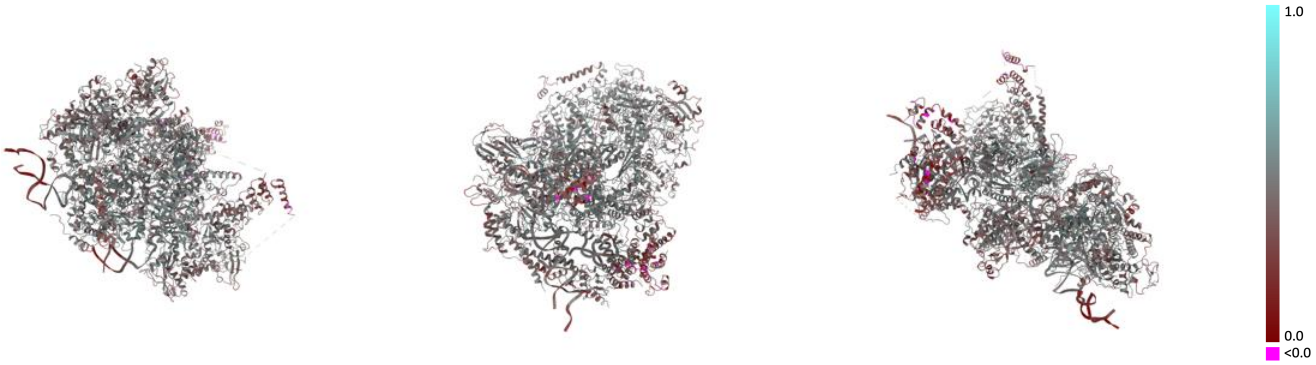
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

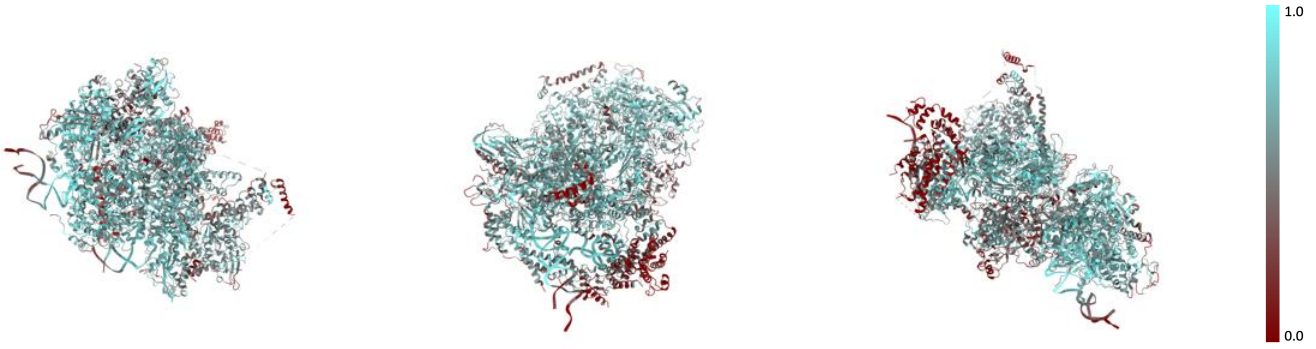
9.2 Q-score mapped to coordinate model



X Y Z

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

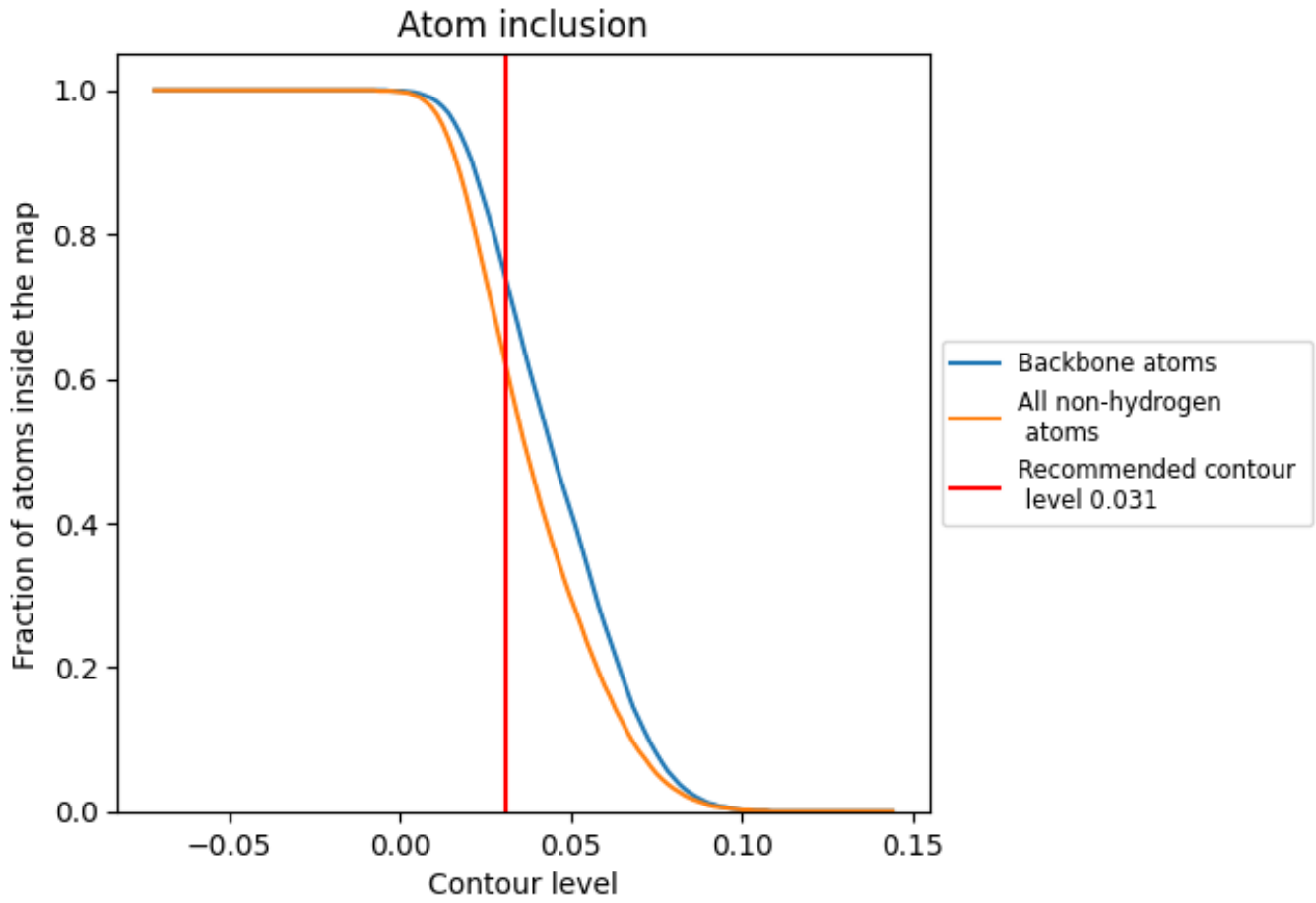
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.031).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.4390
4	0.8200	0.4640
5	0.7390	0.3960
6	0.6960	0.3970
7	0.5510	0.4130
A	0.6920	0.4740
B	0.4360	0.4480
C	0.7080	0.4540
D	0.7260	0.5050
F	0.5080	0.3480
G	0.4550	0.3950
J	0.6530	0.4490
L	0.5240	0.4130
M	0.3140	0.4010
N	0.4730	0.3870
S	0.3720	0.3700
U	0.3380	0.3960
z	0.6740	0.3540