wwPDB EM Validation Summary Report

Nov 3, 2024 – 12:43 am GMT

PDB ID	:	6QX9
EMDB ID	:	EMD-4665
Title	:	Structure of a human fully-assembled precatalytic spliceosome (pre-B complex).
Authors	:	Charenton, C.; Wilkinson, M.E.; Nagai, K.
Deposited on	:	2019-03-07
Resolution	:	3.28 Å(reported)

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

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

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

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

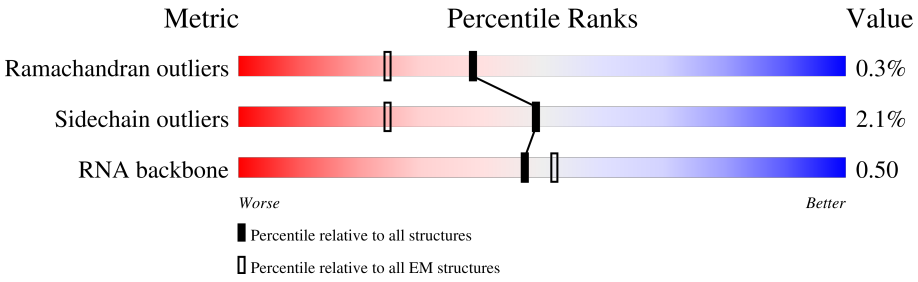
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.28 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)
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	1	164	100% 66% 30%
2	6	106	17% 36% 12% 50%
3	5O	357	75% 85% 14%
4	B4	424	18% 18% 82%
5	13	126	64% 56% 6% 36%
5	23	126	66% 66% 34%
5	43	126	53% 65% 34%
5	53	126	67% 33%

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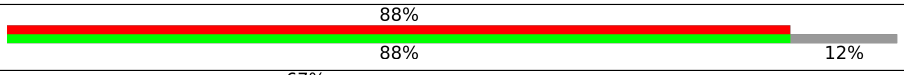
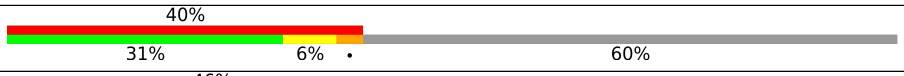
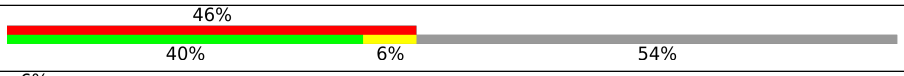
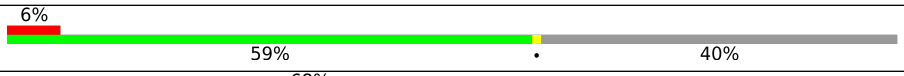
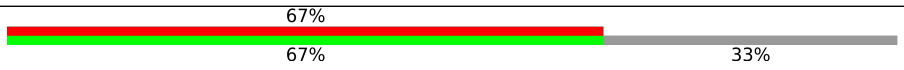
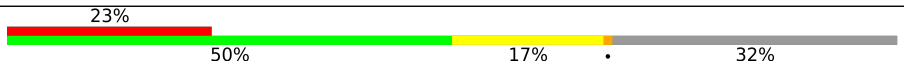
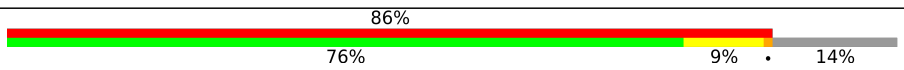
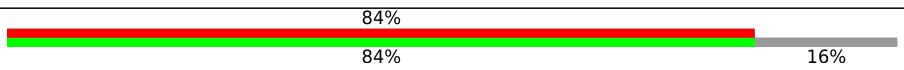
Mol	Chain	Length	Quality of chain
6	4B	522	
7	1e	92	
7	2e	92	
7	4e	92	
7	5e	92	
8	I	62	
9	1K	437	
10	4C	499	
11	11	119	
11	21	119	
11	41	119	
11	51	119	
12	R	480	
13	1f	86	
13	2f	86	
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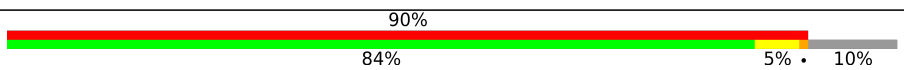
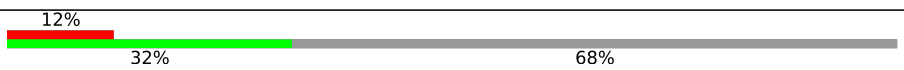
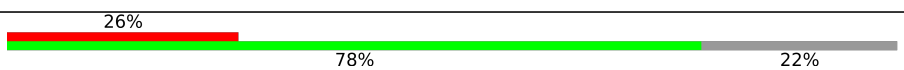
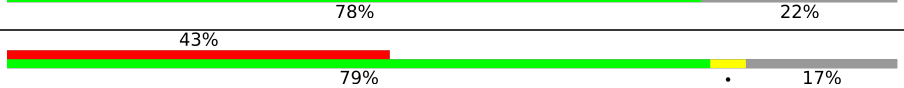
13	5f	86	
14	66	80	
15	X	155	
16	12	118	
16	22	118	
16	42	118	
16	52	118	
17	5	117	
18	67	103	

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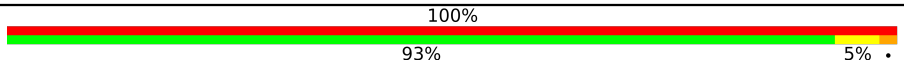
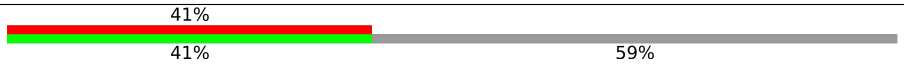
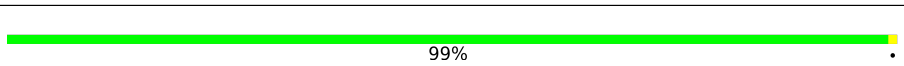
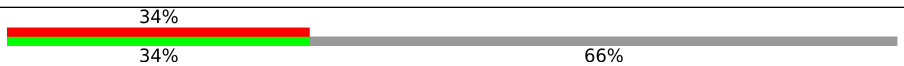
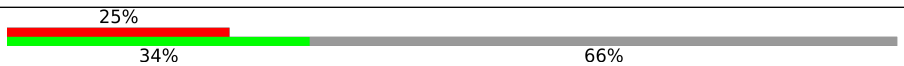
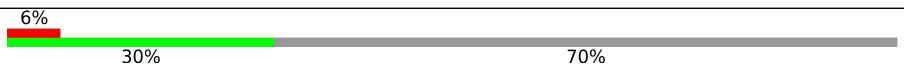
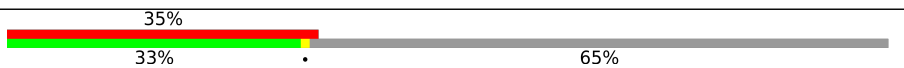
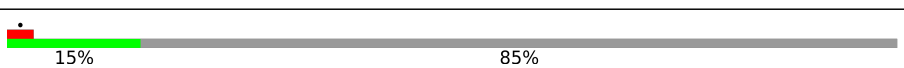
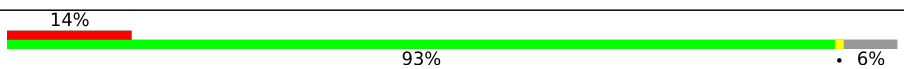
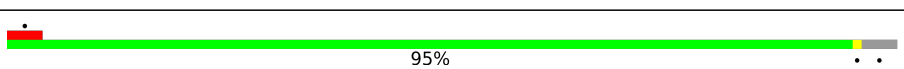
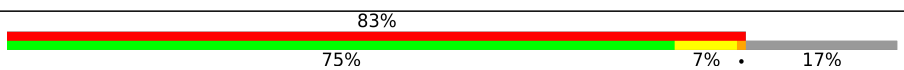
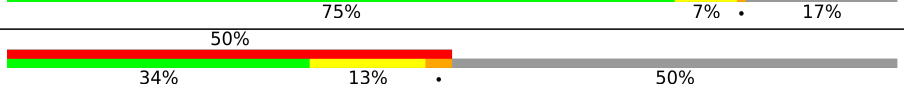
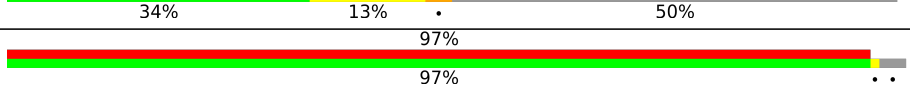
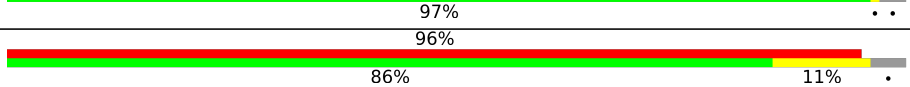
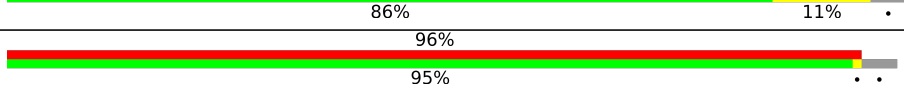
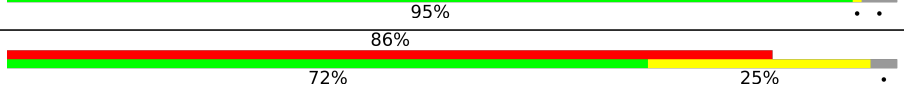
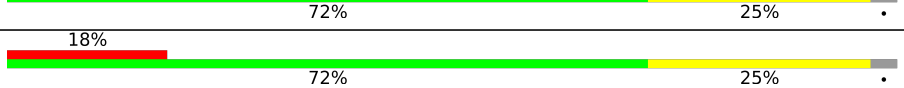
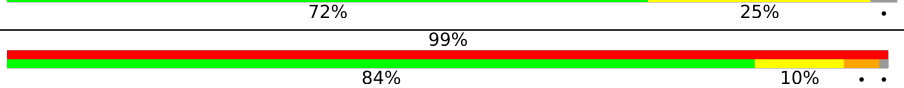
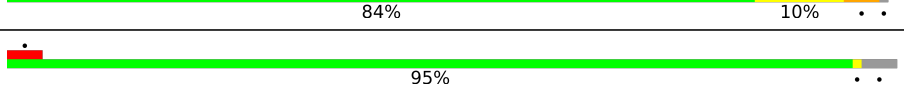
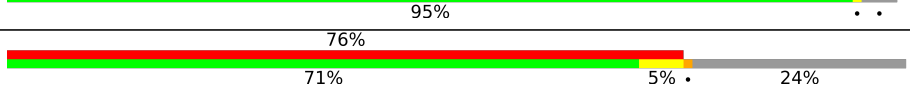
Mol	Chain	Length	Quality of chain
19	62	95	
20	2B	225	
21	A2	209	
22	B2	895	
23	5C	854	
24	5X	820	
25	1b	240	
25	2b	240	
25	4b	240	
25	5b	240	
26	B5	86	
27	1A	282	
28	S	800	
29	5J	850	
30	4D	128	
31	63	102	
32	2	188	
33	B3	1217	
34	1g	76	
34	2g	76	
34	4g	76	
34	5g	76	
35	68	96	
36	5A	2311	
37	A3	501	

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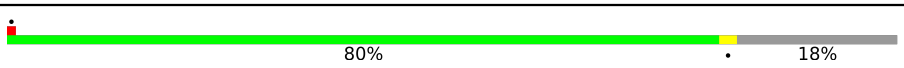
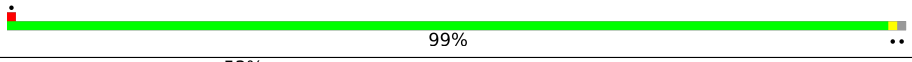
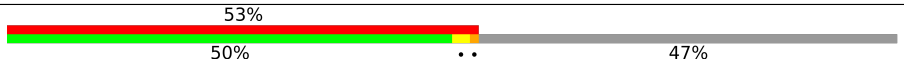
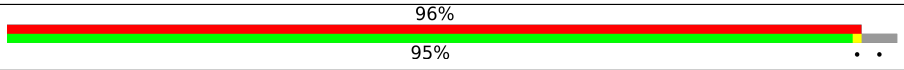
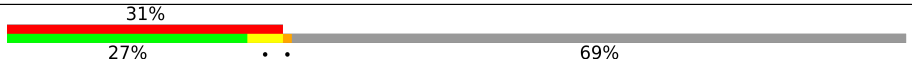
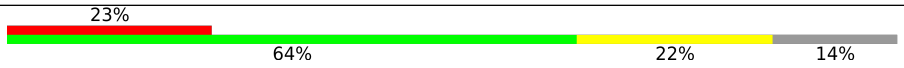
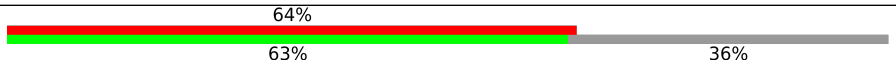
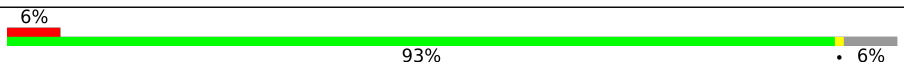
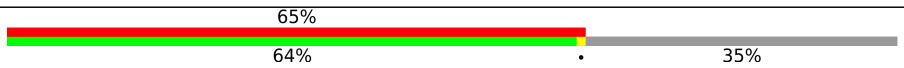
Mol	Chain	Length	Quality of chain
38	U	555	
39	5D	142	
40	64	139	
41	BP	104	
42	1C	159	
43	K	1007	
44	4A	683	
45	4	146	
46	2A	255	
47	A1	647	
48	65	91	
49	5B	2136	
50	B1	1304	

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 137494 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 RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	164	Total	C	N	O	P	0	0
			3485	1555	607	1159	164		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	53	Total	C	N	O	P	0	0
			1133	506	203	371	53		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5O	306	Total	C	N	O	S	0	0
			2394	1501	422	457	14		

- Molecule 4 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B4	78	Total	C	N	O	S	0	0
			618	399	101	115	3		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	13	81	Total	C	N	O	S	0	0
			637	400	112	119	6		
5	53	84	Total	C	N	O	S	0	0
			657	412	116	123	6		
5	23	83	Total	C	N	O	S	0	0
			652	409	115	122	6		
5	43	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4B	359	Total	C	N	O	S	0	0
			2842	1793	509	521	19		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		
7	4e	76	Total	C	N	O	S	0	0
			631	400	112	114	5		
7	1e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		
7	2e	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 8 is a RNA chain called AdML pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	25	Total	C	N	O	P	0	0
			530	237	92	177	24		

- Molecule 9 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1K	201	Total	C	N	O	S	0	0
			1649	1036	317	291	5		

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4C	301	Total	C	N	O	S	0	0
			2375	1486	418	456	15		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	41	81	Total	C	N	O	S	0	0
			641	408	112	118	3		
11	11	81	Total	C	N	O	S	0	0
			641	408	112	118	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	51	81	Total 641	C 408	N 112	O 118	S 3	0	0
11	21	80	Total 634	C 404	N 111	O 115	S 4	0	0

- Molecule 12 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	106	Total 874	C 553	N 160	O 157	S 4	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1f	74	Total 576	C 373	N 95	O 103	S 5	0	0
13	2f	72	Total 562	C 364	N 93	O 100	S 5	0	0
13	5f	73	Total 567	C 367	N 94	O 101	S 5	0	0
13	4f	72	Total 562	C 364	N 93	O 100	S 5	0	0

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	66	72	Total 567	C 360	N 97	O 108	S 2	0	0

- Molecule 15 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	49	Total 394	C 247	N 74	O 69	S 4	0	0

- Molecule 16 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	22	95	Total 774	C 486	N 141	O 142	S 5	0	0
16	42	92	Total 737	C 463	N 138	O 131	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	52	98	Total	C	N	O	S	0	0
			796	498	144	148	6		
16	12	95	Total	C	N	O	S	0	0
			777	486	141	144	6		

- Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	67	77	Total	C	N	O	S	0	0
			604	383	102	116	3		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	62	95	Total	C	N	O	S	0	0
			761	486	126	145	4		

- Molecule 20 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2B	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 21 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A2	144	Total	C	N	O	S	0	0
			1221	782	219	214	6		

- Molecule 22 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B2	208	Total	C	N	O	S	0	0
			1699	1093	302	295	9		

- Molecule 23 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5C	852	Total	C	N	O	S	0	0
			6727	4300	1127	1266	34		

- Molecule 24 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5X	583	Total	C	N	O	S	7	0
			4780	3014	855	893	18		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1b	86	Total	C	N	O	S	0	0
			692	435	126	124	7		
25	2b	82	Total	C	N	O	S	0	0
			664	419	121	117	7		
25	5b	73	Total	C	N	O	S	0	0
			594	376	108	103	7		
25	4b	82	Total	C	N	O	S	0	0
			669	423	122	117	7		

- Molecule 26 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B5	69	Total	C	N	O	S	0	0
			567	360	99	103	5		

- Molecule 27 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1A	98	Total	C	N	O	S	0	0
			787	506	134	143	4		

- Molecule 28 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	120	Total	C	N	O	S	0	0
			917	576	168	168	5		

- Molecule 29 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5J	803	Total	C	N	O	S	0	0
			6316	3963	1155	1170	28		

- Molecule 30 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4D	123	Total	C	N	O	S	0	0
			955	604	170	176	5		

- Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	63	85	Total	C	N	O	S	0	0
			699	440	120	136	3		

- Molecule 32 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2	94	Total	C	N	O	P	0	0
			1984	887	331	672	94		

- Molecule 33 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B3	1186	Total	C	N	O	S	0	0
			9296	5898	1580	1773	45		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
34	2g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
34	5g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
34	4g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		

- Molecule 35 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	68	95	Total	C	N	O	S	0	0
			722	446	124	151	1		

- Molecule 36 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5A	2212	Total	C	N	O	S	0	0
			18366	11840	3193	3253	80		

- Molecule 37 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A3	383	Total	C	N	O	S	0	0
			3227	2029	566	618	14		

- Molecule 38 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	U	456	Total	C	N	O	S	0	0
			3750	2427	635	674	14		

- Molecule 39 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5D	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 40 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	64	73	Total	C	N	O	S	0	0
			596	376	105	109	6		

- Molecule 41 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	100	Total	C	N	O	S	0	0
			766	473	135	145	13		

- Molecule 42 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1C	50	Total	C	N	O	S	0	0
			425	266	73	82	4		

- Molecule 43 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	322	Total	C	N	O	S	0	0
			2626	1682	462	467	15		

- Molecule 44 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	4A	239	Total	C	N	O	S	0	0
			1946	1237	360	342	7		

- Molecule 45 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4	126	Total	C	N	O	P	0	0
			2690	1202	474	888	126		

- Molecule 46 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2A	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 47 is a protein called Splicing factor 3A subunit 1,Splicing factor 3A subunit 1,Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	A1	168	Total	C	N	O	S	0	0
			1339	855	237	245	2		

- Molecule 48 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	65	76	Total	C	N	O	S	0	0
			587	373	96	114	4		

- Molecule 49 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5B	2001	Total	C	N	O	S	0	0
			16077	10235	2767	2991	84		

- Molecule 50 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B1	848	Total	C	N	O	S	0	0
			6749	4330	1160	1220	39		

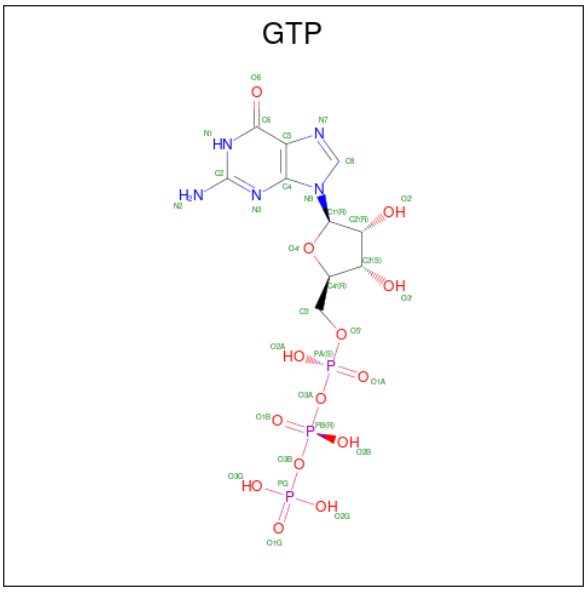
- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	A2	1	Total	Zn	0
			1	1	
51	U	1	Total	Zn	0
			1	1	
51	BP	3	Total	Zn	0
			3	3	
51	1C	1	Total	Zn	0
			1	1	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

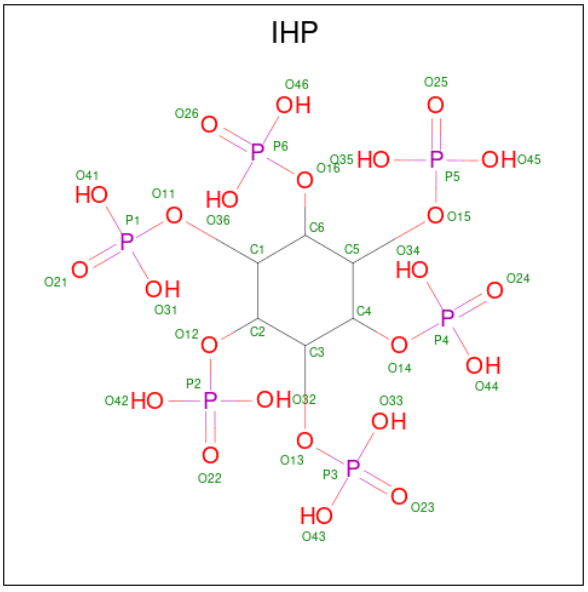
Mol	Chain	Residues	Atoms		AltConf
52	5C	1	Total	Mg	0
			1	1	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
53	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 54 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



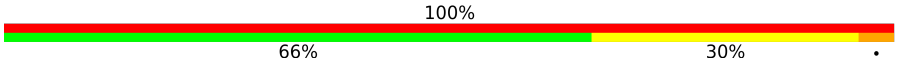
Mol	Chain	Residues	Atoms				AltConf
54	5A	1	Total	C	O	P	0
			36	6	24	6	

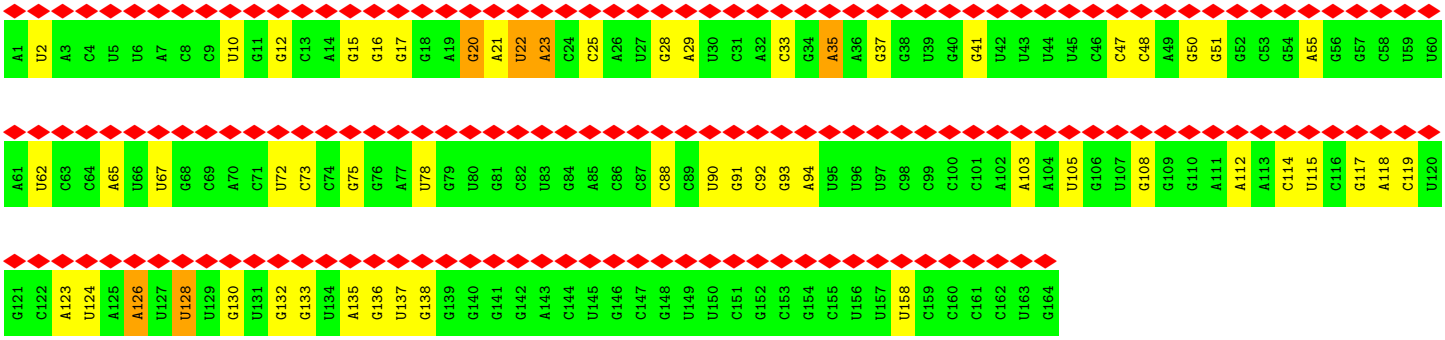
3 Residue-property plots (i)

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: U1 snRNA

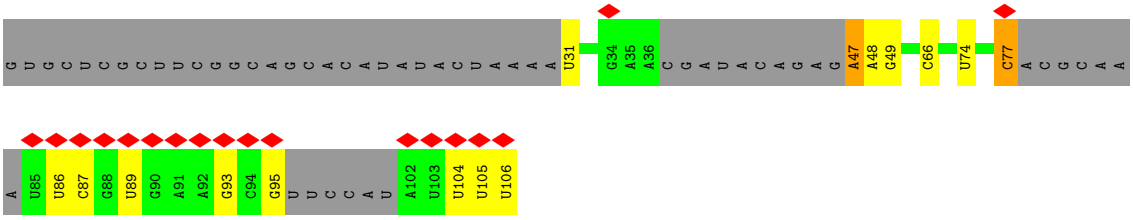
Chain 1:





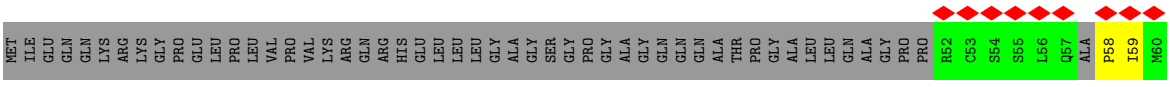
• Molecule 2: U6 snRNA

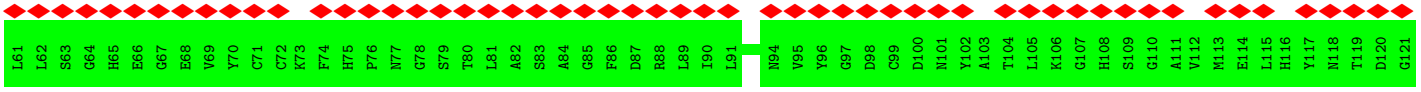
Chain 6:

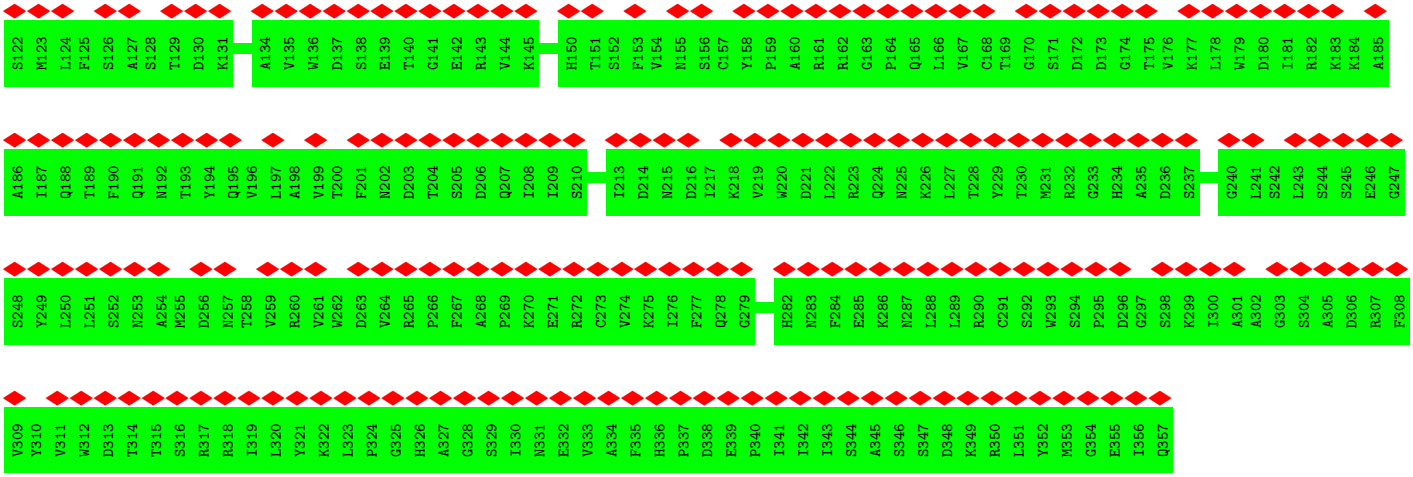


• Molecule 3: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain 5O:

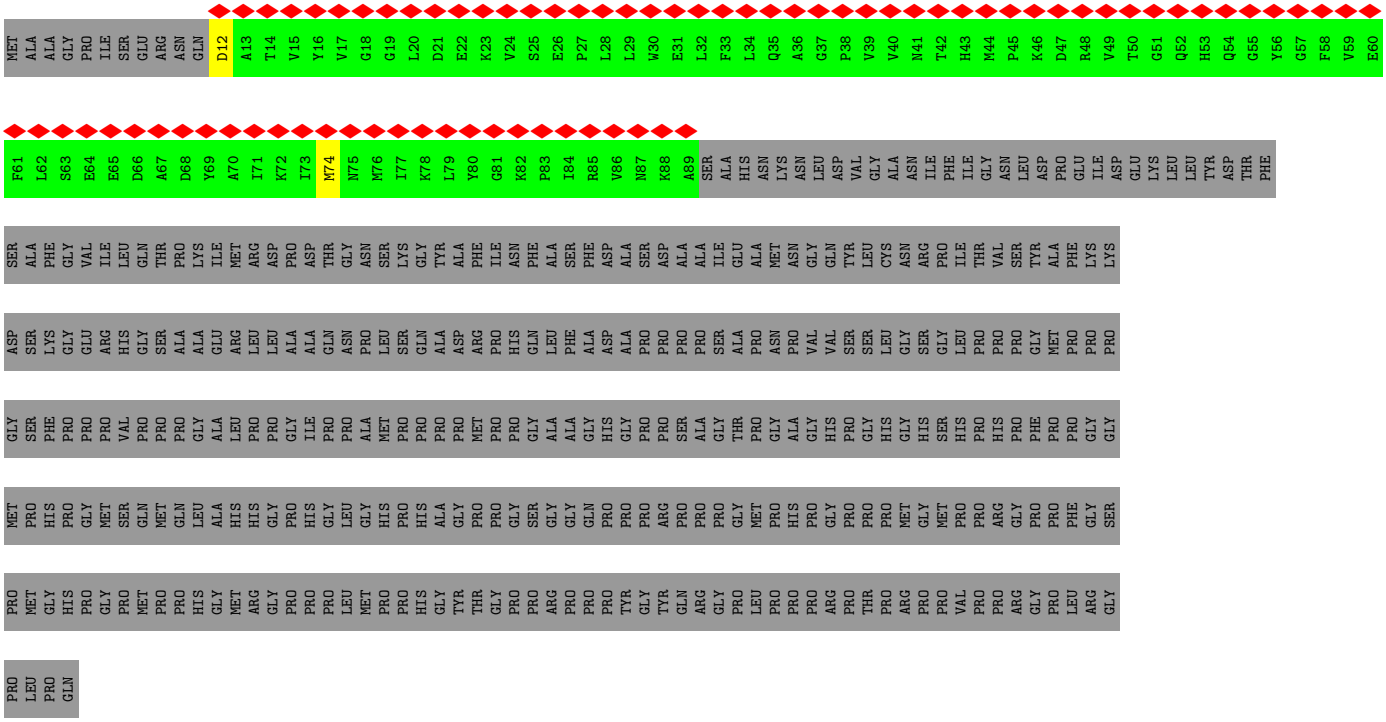






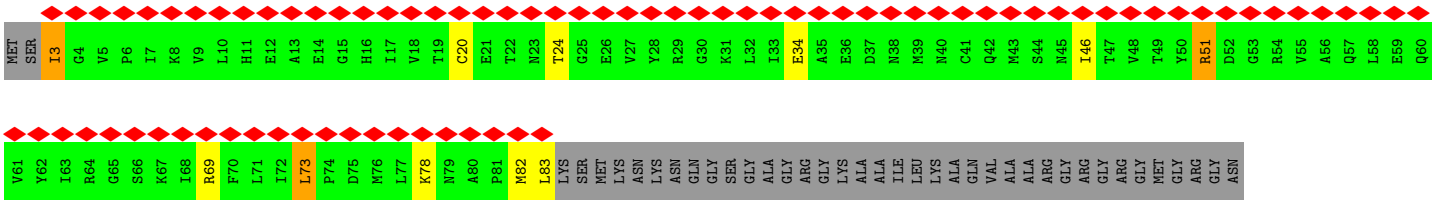
• Molecule 4: Splicing factor 3B subunit 4

Chain B4:



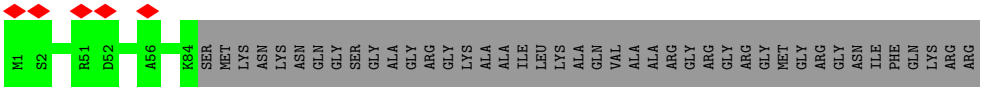
• Molecule 5: Small nuclear ribonucleoprotein Sm D3

Chain 13:



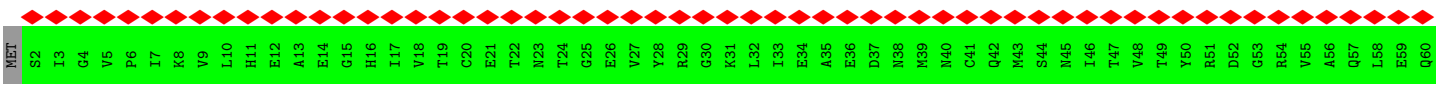
• Molecule 5: Small nuclear ribonucleoprotein Sm D3

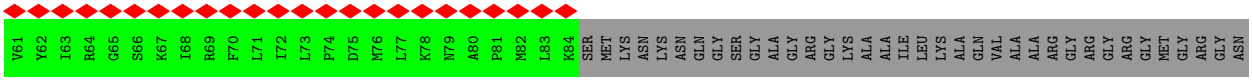
Chain 53:



• Molecule 5: Small nuclear ribonucleoprotein Sm D3

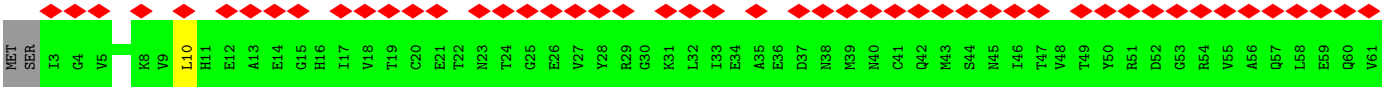
Chain 23:

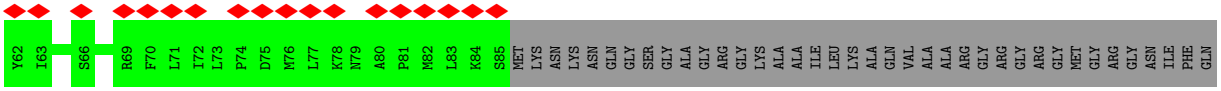




• Molecule 5: Small nuclear ribonucleoprotein Sm D3

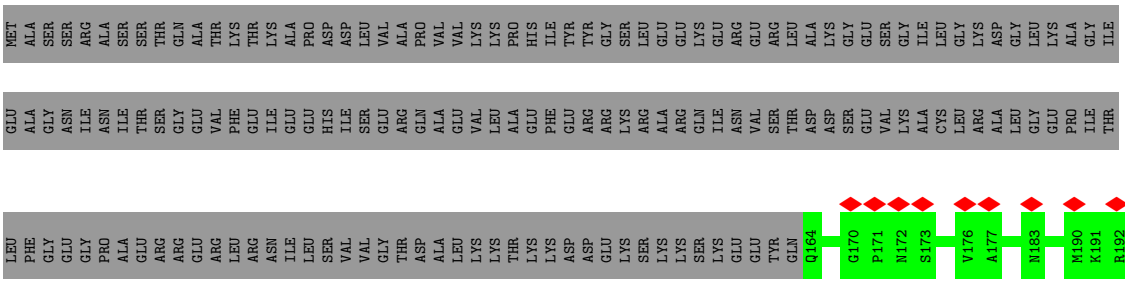
Chain 43:

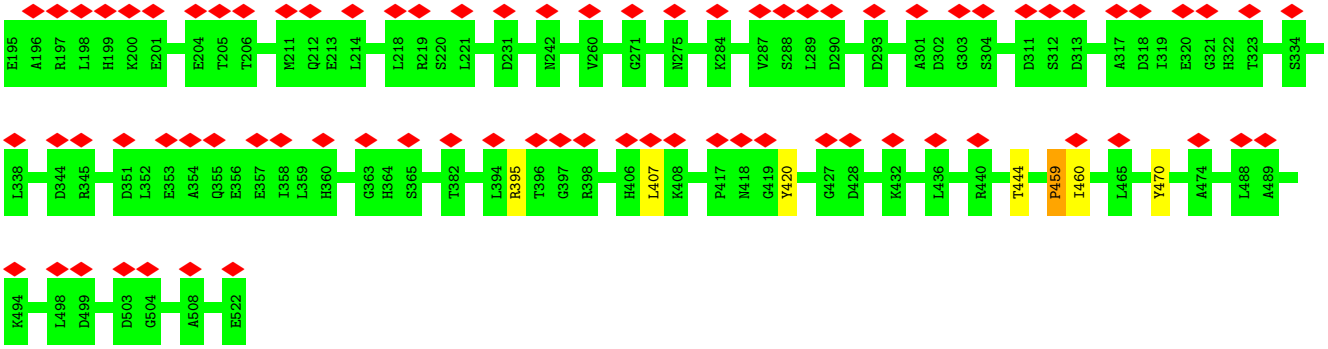




• Molecule 6: U4/U6 small nuclear ribonucleoprotein Prp4

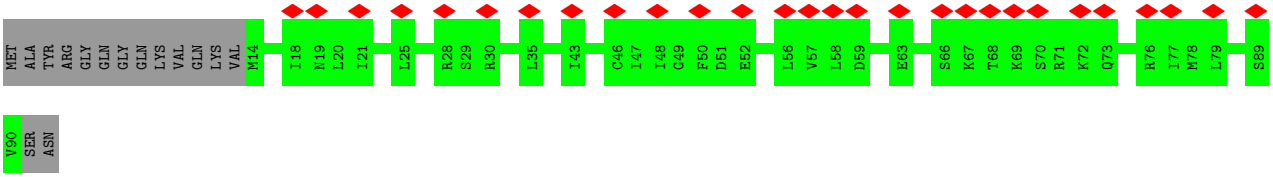
Chain 4B:





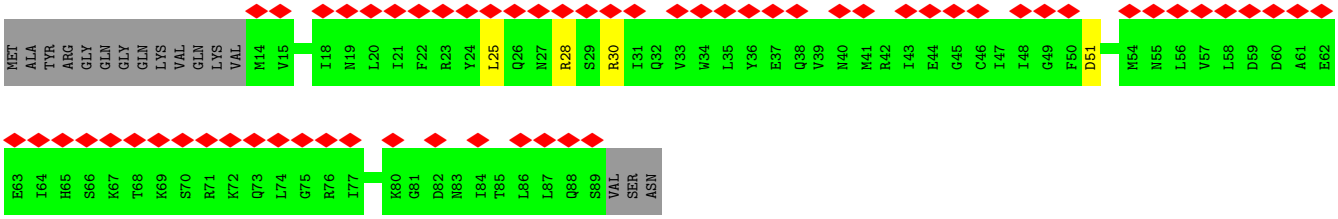
• Molecule 7: Small nuclear ribonucleoprotein E

Chain 5e:



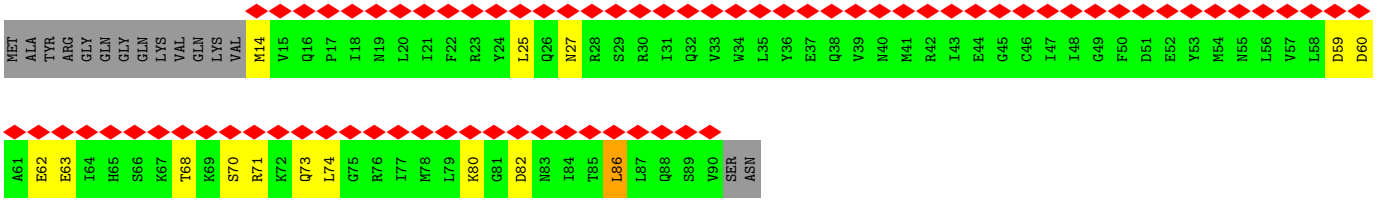
• Molecule 7: Small nuclear ribonucleoprotein E

Chain 4e:



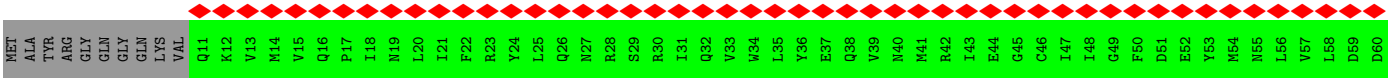
• Molecule 7: Small nuclear ribonucleoprotein E

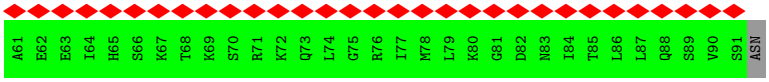
Chain 1e:



• Molecule 7: Small nuclear ribonucleoprotein E

Chain 2e:



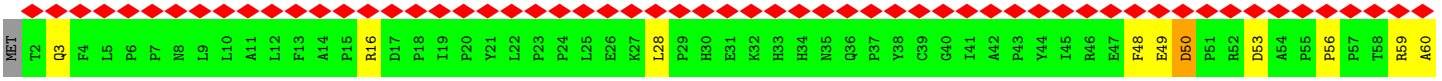


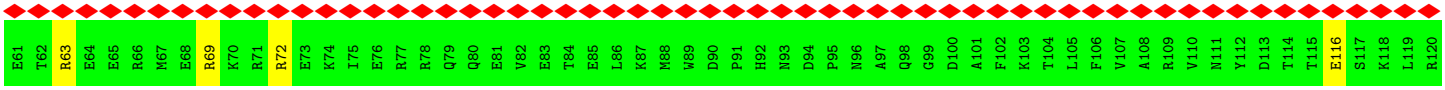
• Molecule 8: AdML pre-mRNA

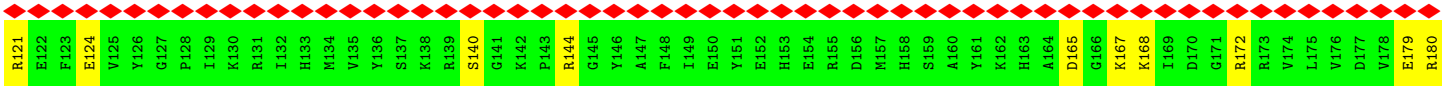
Chain I:

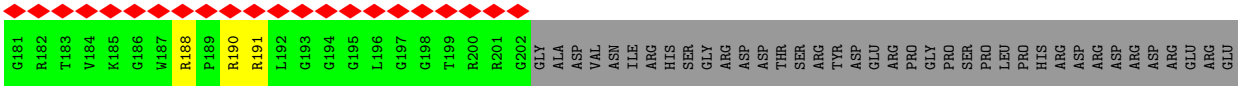
• Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

Chain 1K:



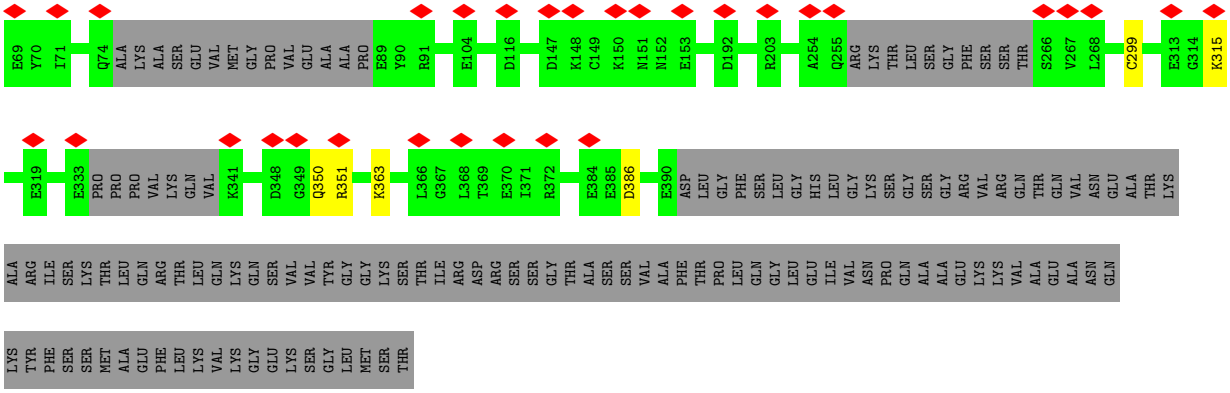




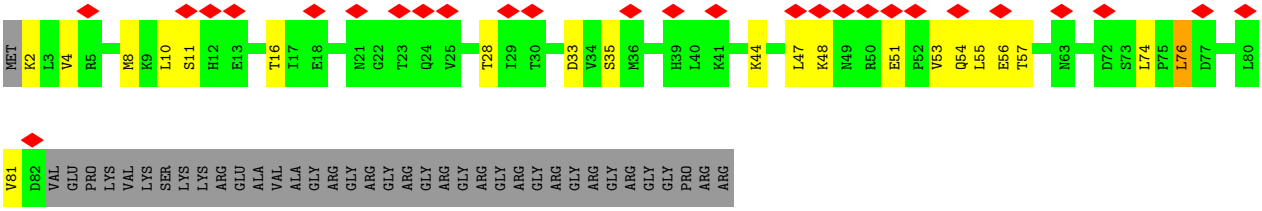


• Molecule 10: U4/U6 small nuclear ribonucleoprotein Prp31

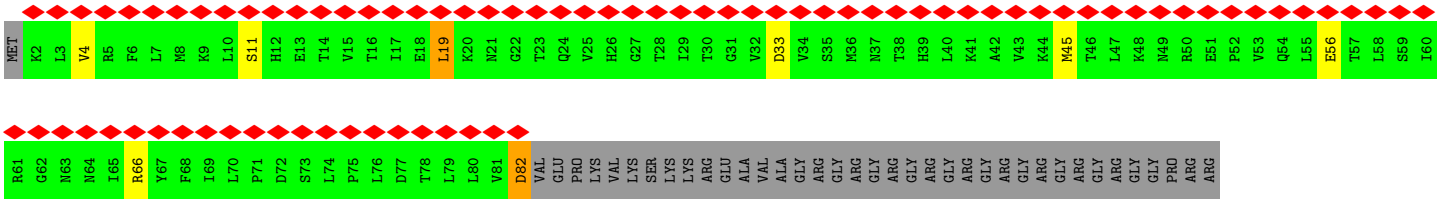
Chain 4C:



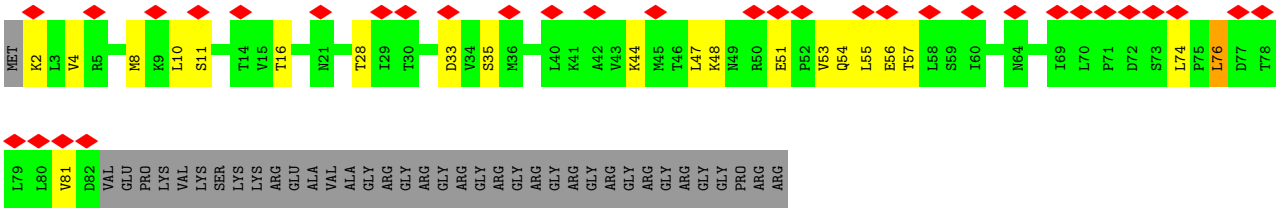
• Molecule 11: Small nuclear ribonucleoprotein Sm D1



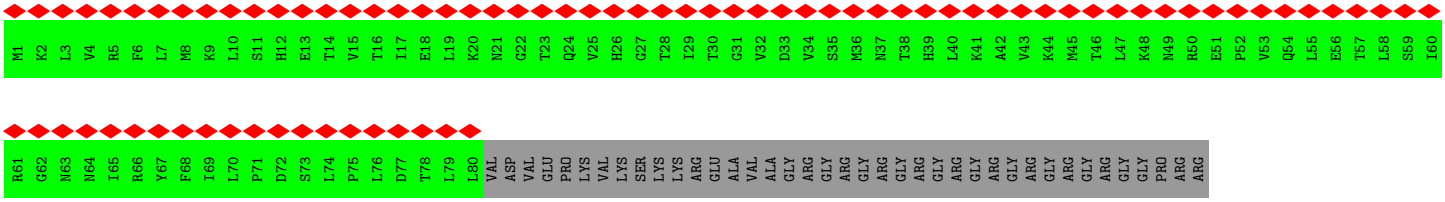
• Molecule 11: Small nuclear ribonucleoprotein Sm D1



• Molecule 11: Small nuclear ribonucleoprotein Sm D1

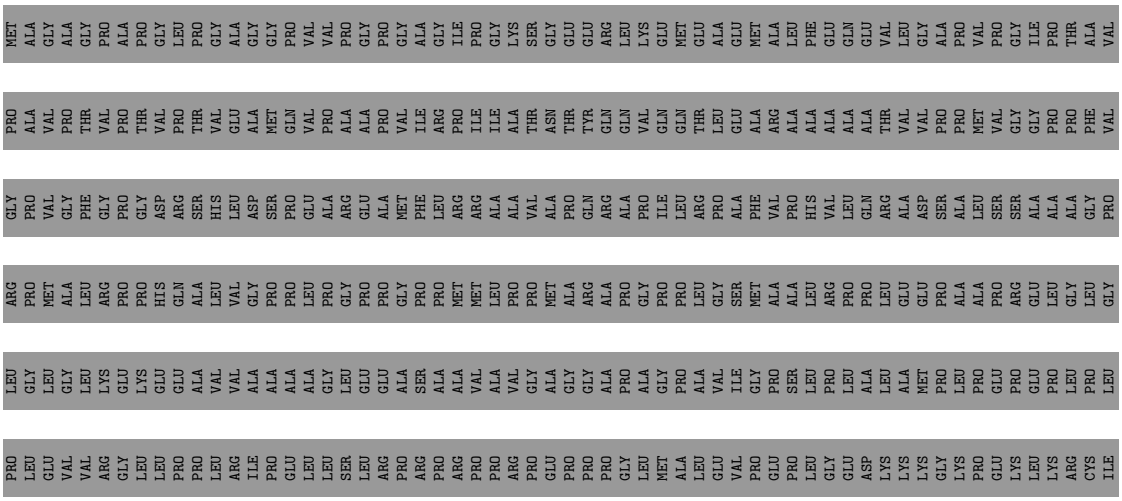


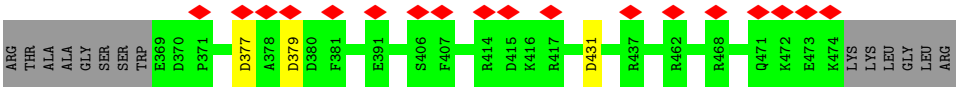
• Molecule 11: Small nuclear ribonucleoprotein Sm D1



• Molecule 12: RNA-binding protein 42

Chain R:



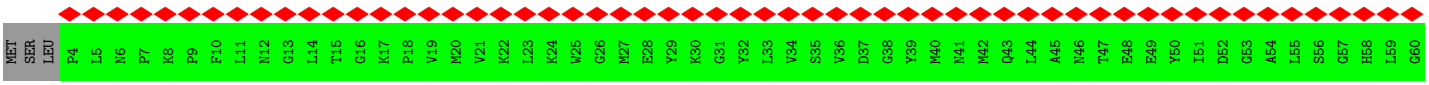


• Molecule 13: Small nuclear ribonucleoprotein F

Chain 1f:

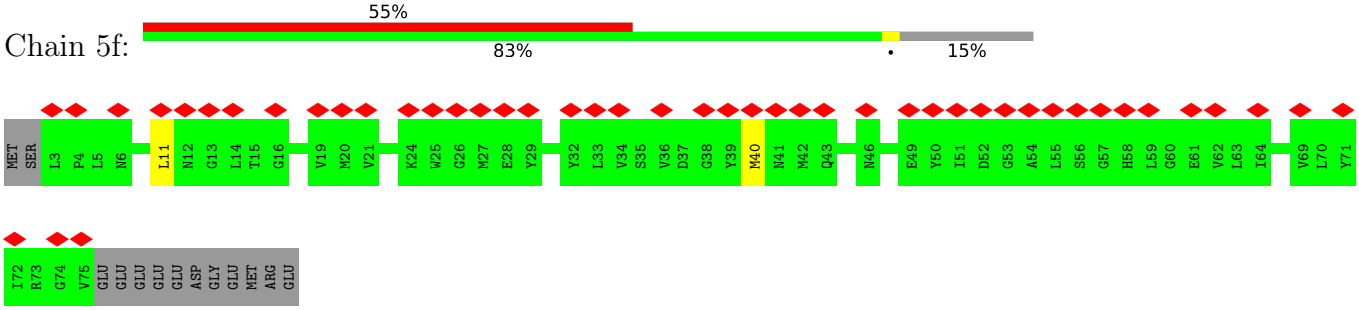
• Molecule 13: Small nuclear ribonucleoprotein F

Chain 2f:



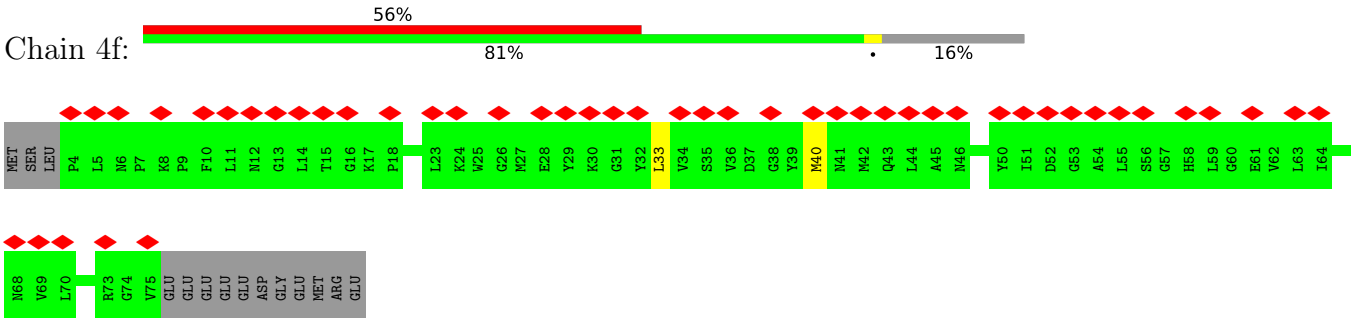
• Molecule 13: Small nuclear ribonucleoprotein F

Chain 5f:



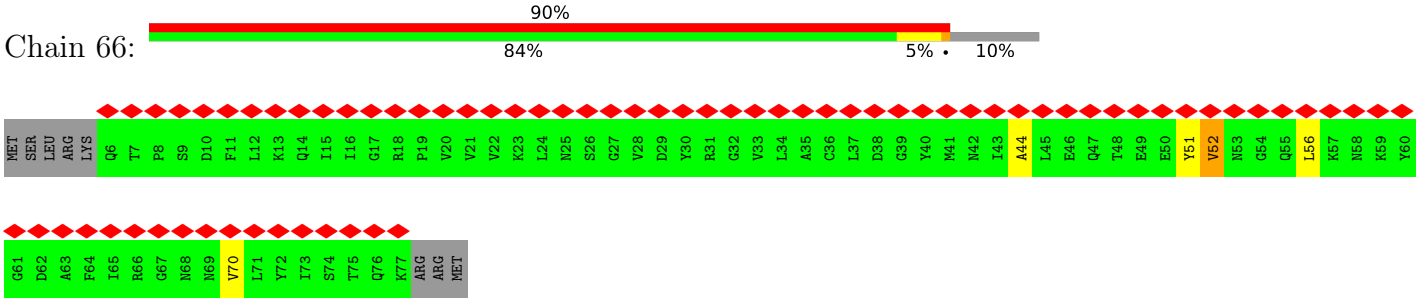
• Molecule 13: Small nuclear ribonucleoprotein F

Chain 4f:



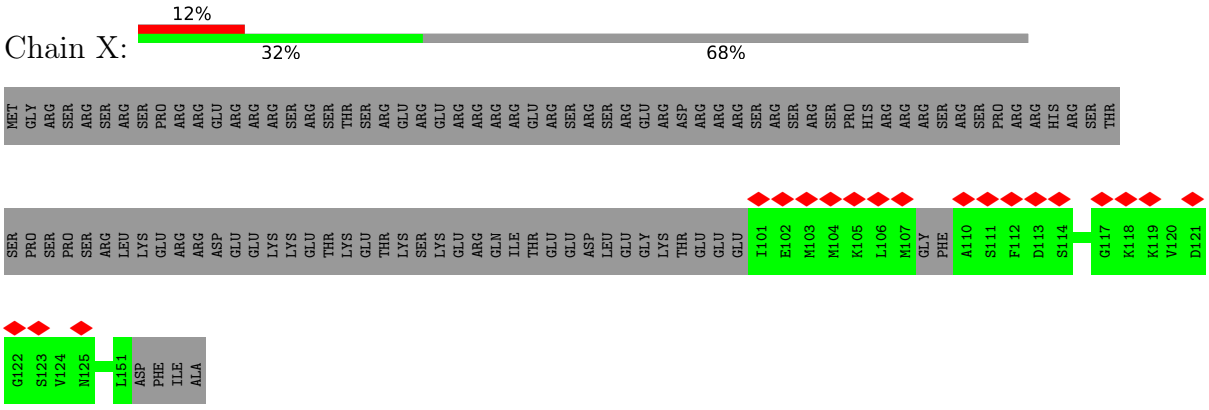
• Molecule 14: U6 snRNA-associated Sm-like protein LSm6

Chain 66:



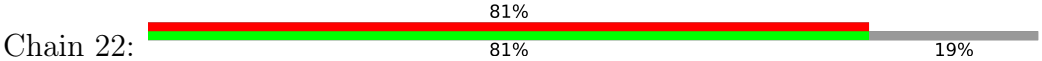
• Molecule 15: U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein

Chain X:



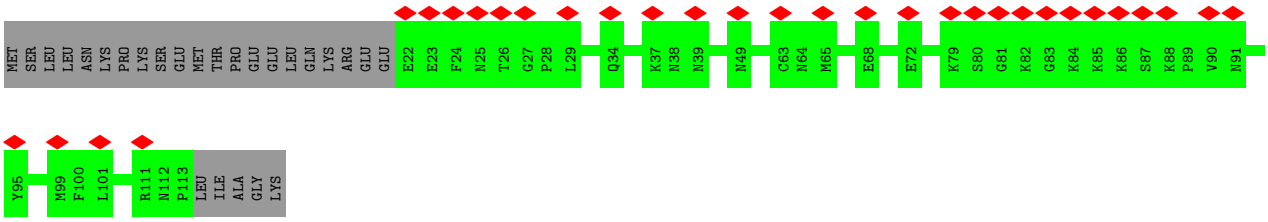
• Molecule 16: Small nuclear ribonucleoprotein Sm D2

Chain 22:



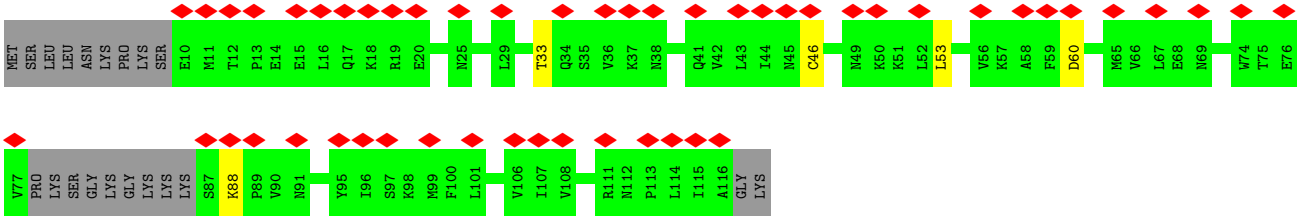
• Molecule 16: Small nuclear ribonucleoprotein Sm D2

Chain 42:



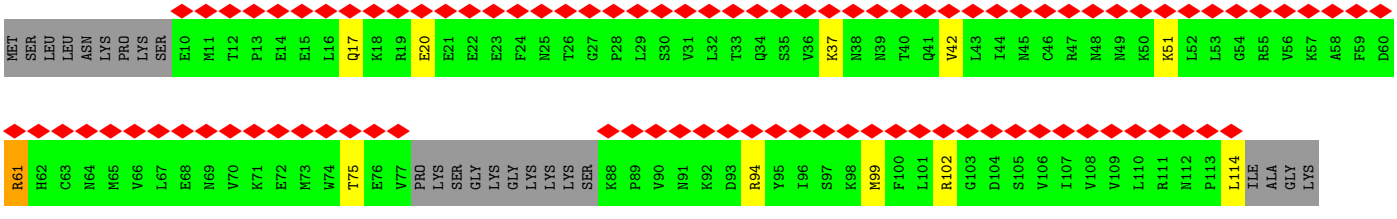
• Molecule 16: Small nuclear ribonucleoprotein Sm D2

Chain 52:



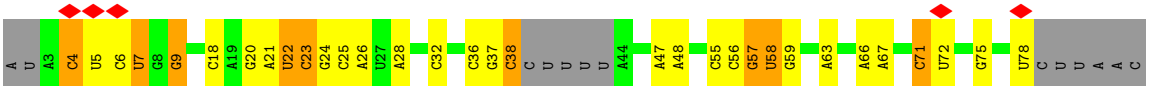
• Molecule 16: Small nuclear ribonucleoprotein Sm D2

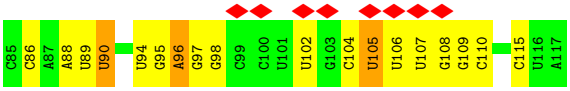
Chain 12:



• Molecule 17: U5 snRNA

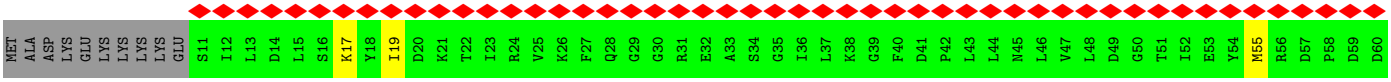
Chain 5:

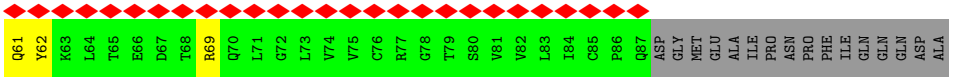




• Molecule 18: U6 snRNA-associated Sm-like protein LSm7

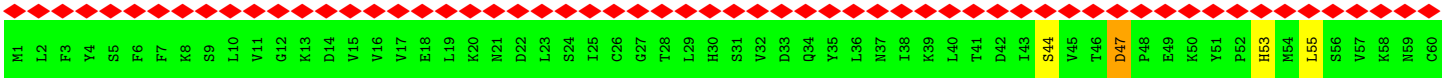
Chain 67:





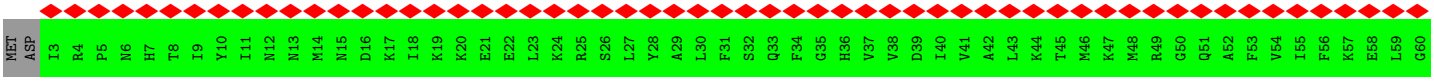
• Molecule 19: U6 snRNA-associated Sm-like protein LSm2

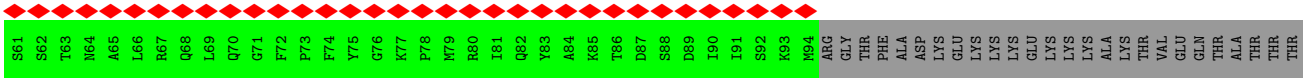
Chain 62:



• Molecule 20: U2 small nuclear ribonucleoprotein B”

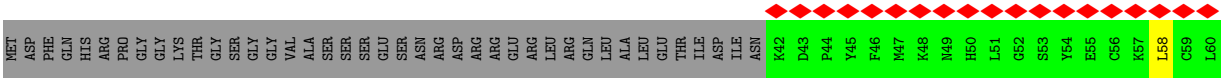
Chain 2B:

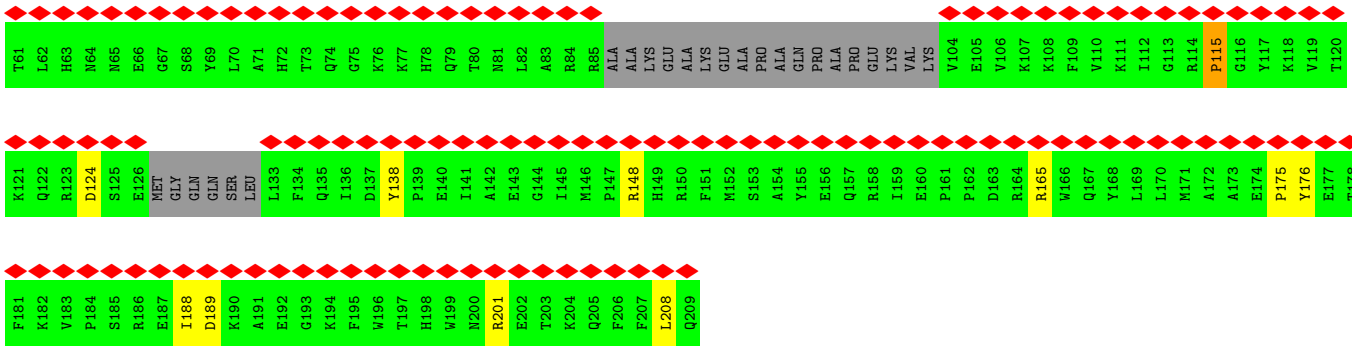




• Molecule 21: Splicing factor 3A subunit 2

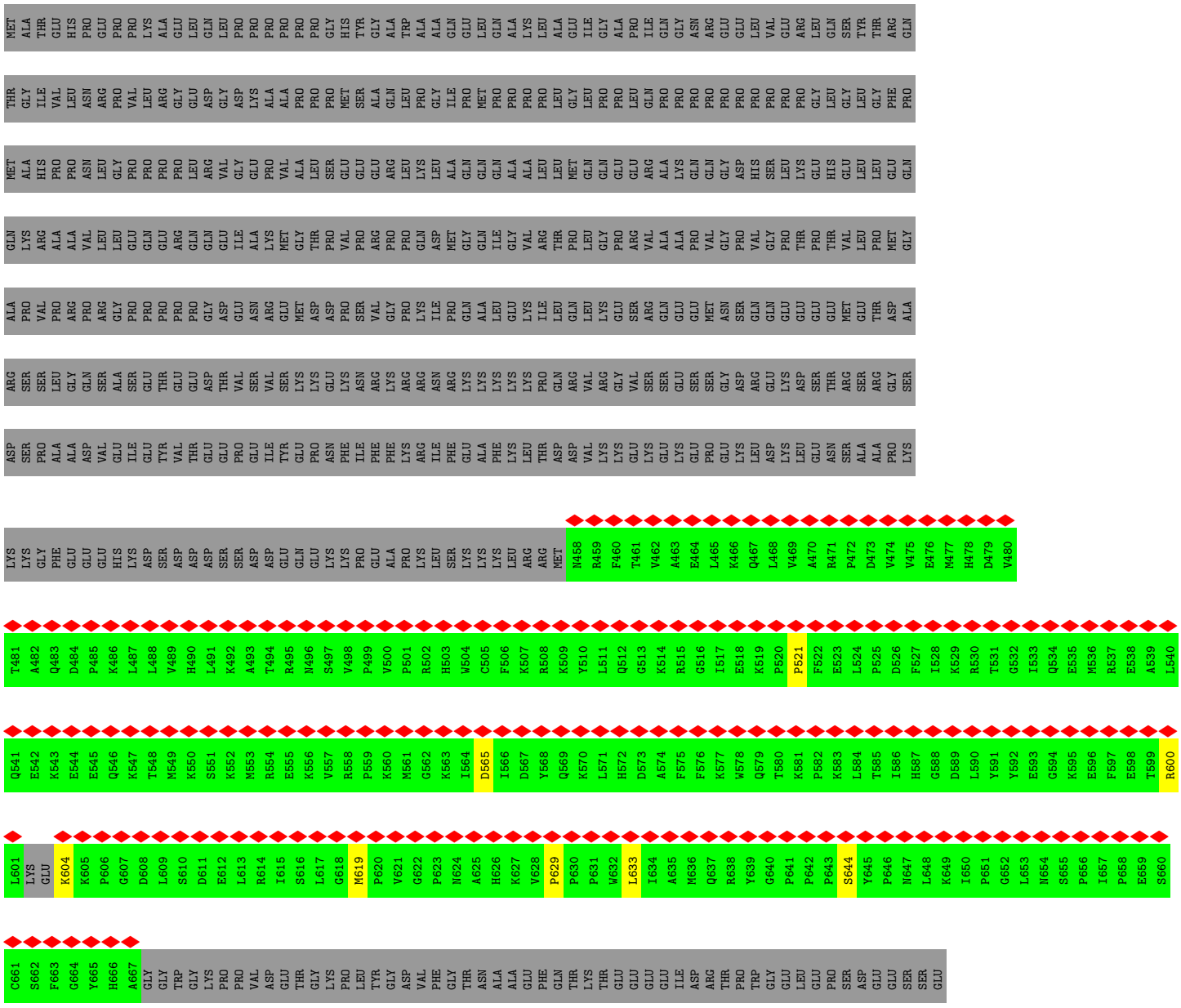
Chain A2:

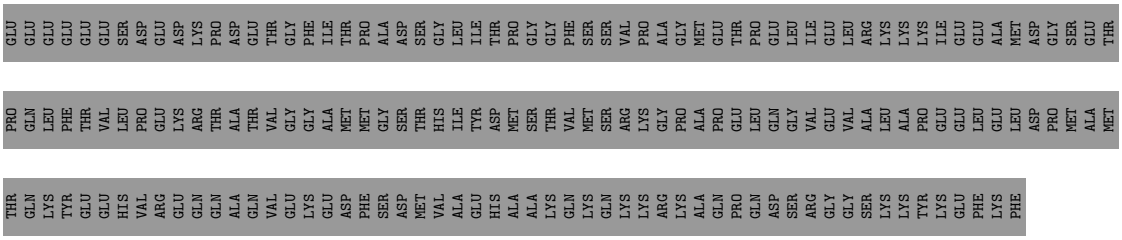




• Molecule 22: Splicing factor 3B subunit 2

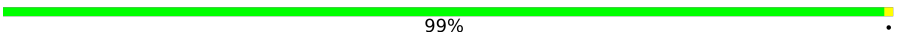
Chain B2:

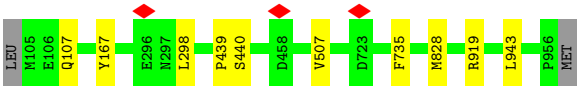




• Molecule 23: 116 kDa U5 small nuclear ribonucleoprotein component

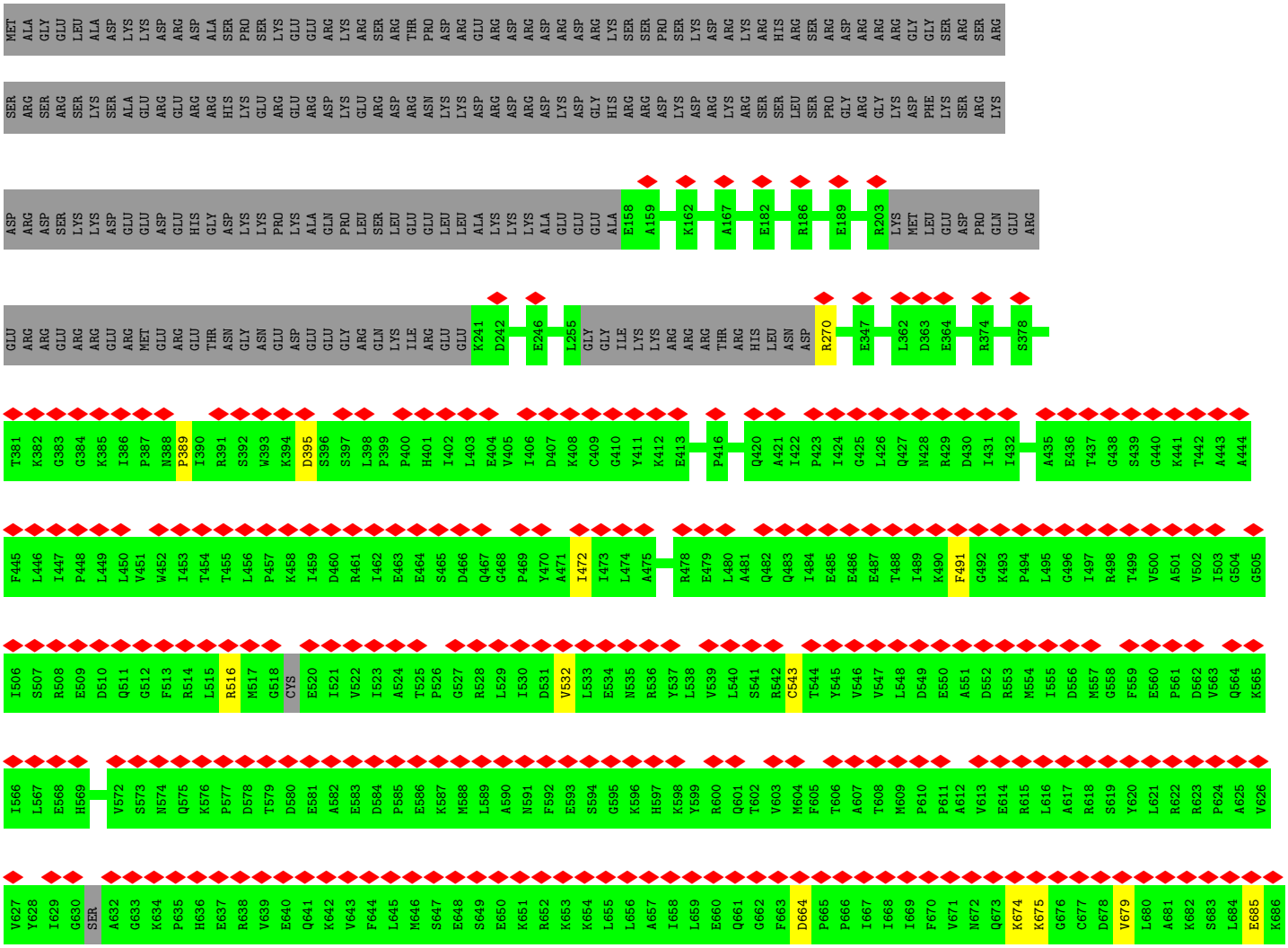
Chain 5C:

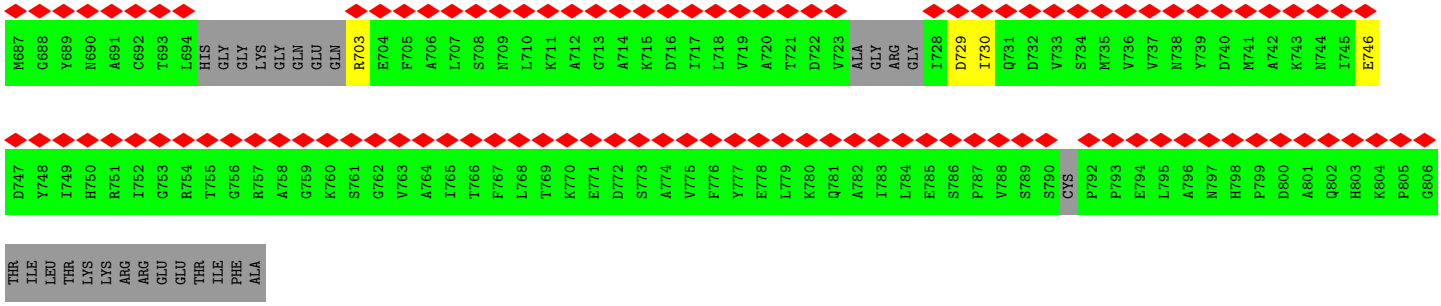




• Molecule 24: Probable ATP-dependent RNA helicase DDX23

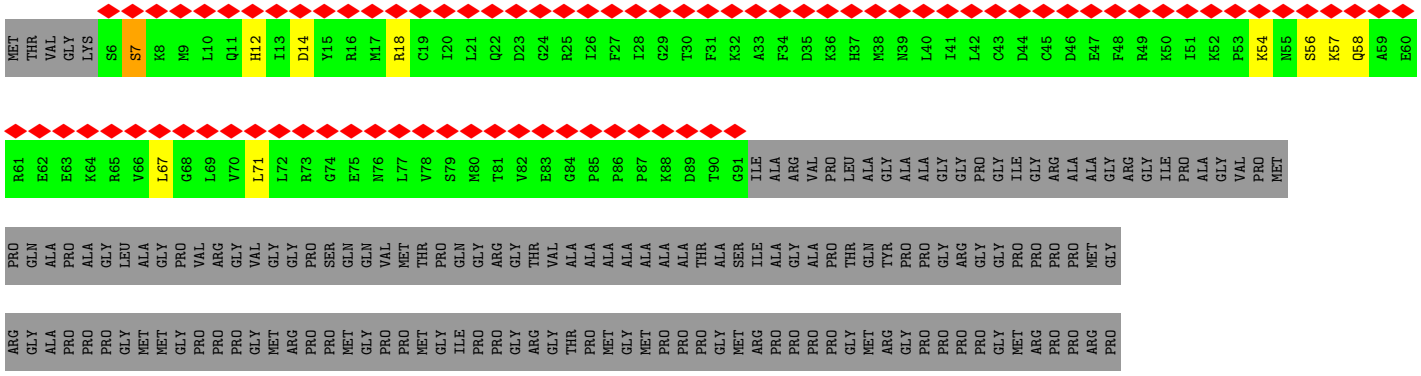
Chain 5X:





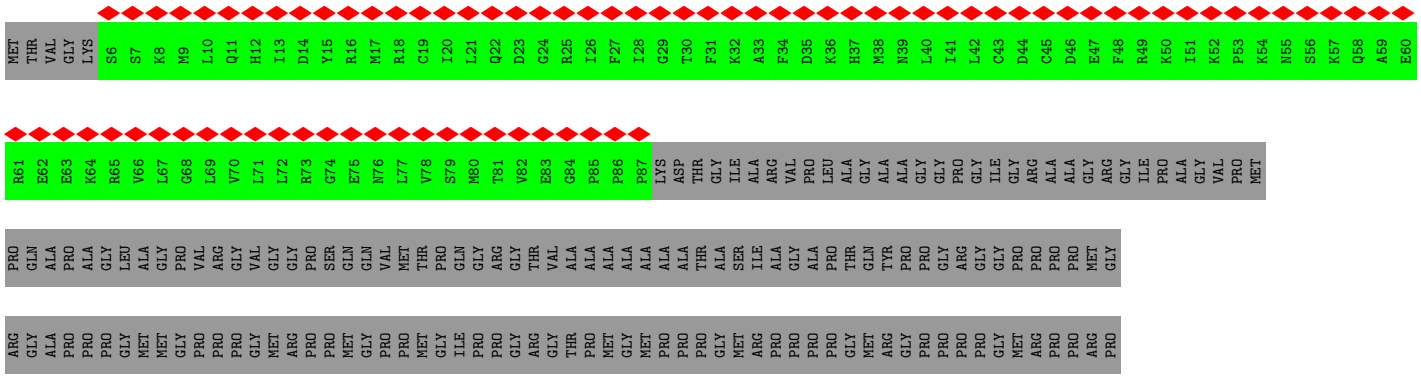
• Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 1b:



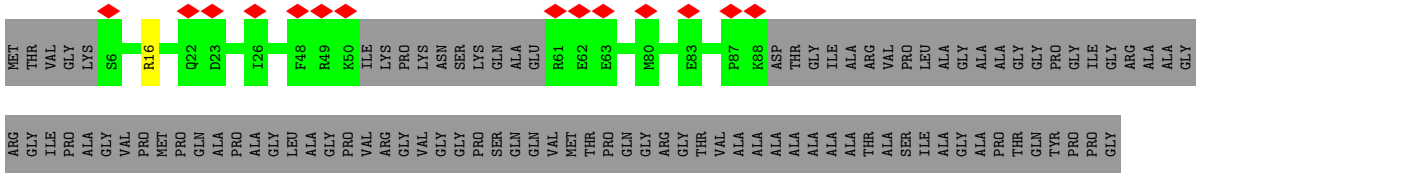
• Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

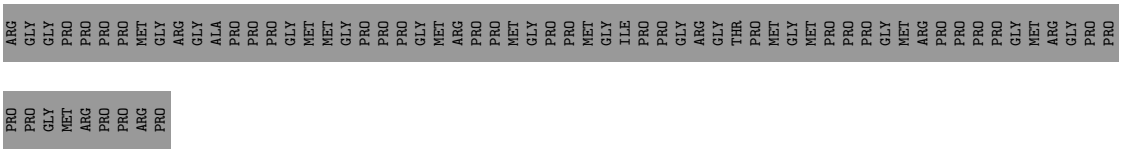
Chain 2b:



• Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

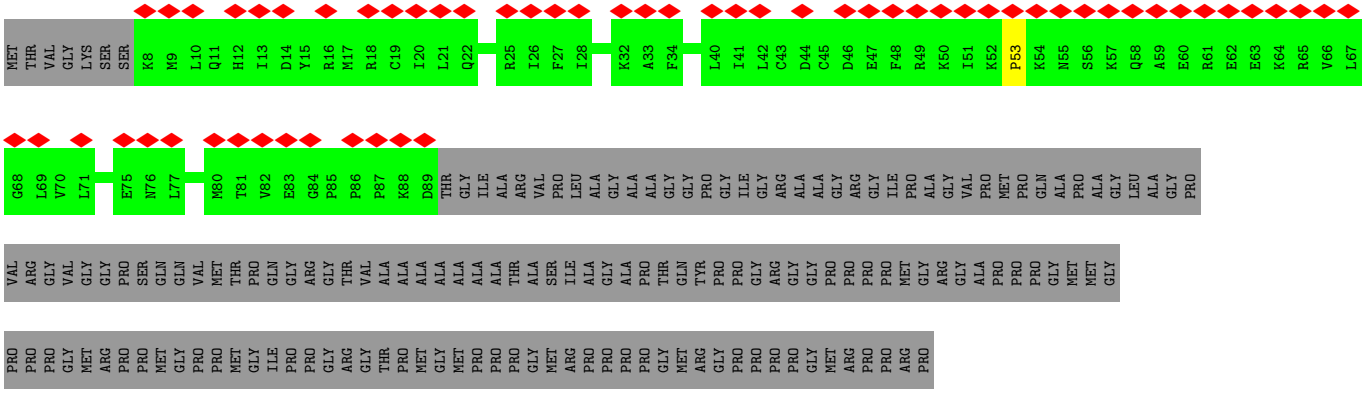
Chain 5b:





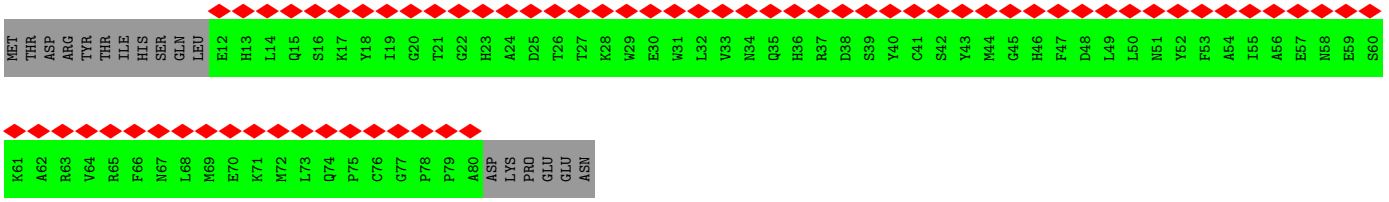
• Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 4b:



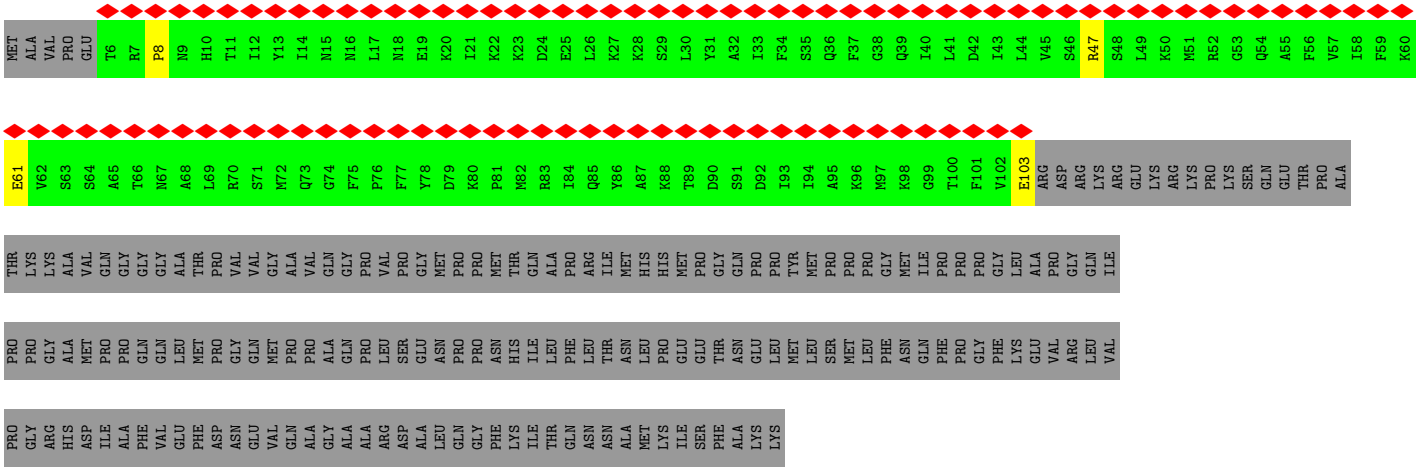
• Molecule 26: Splicing factor 3B subunit 5

Chain B5:



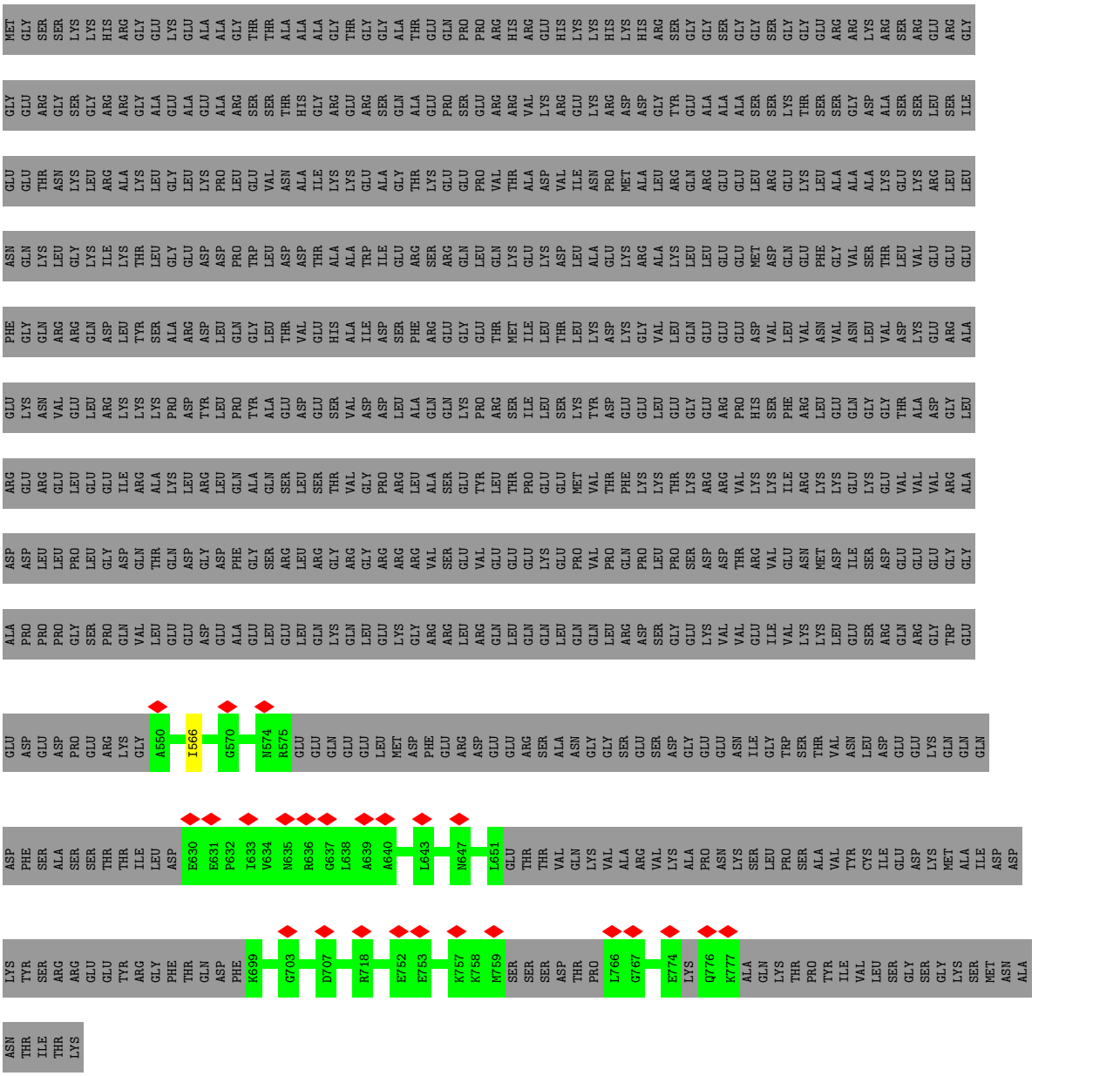
• Molecule 27: U1 small nuclear ribonucleoprotein A

Chain 1A:



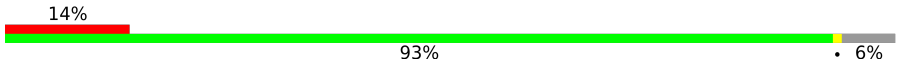
• Molecule 28: U4/U6.U5 tri-snRNP-associated protein 1

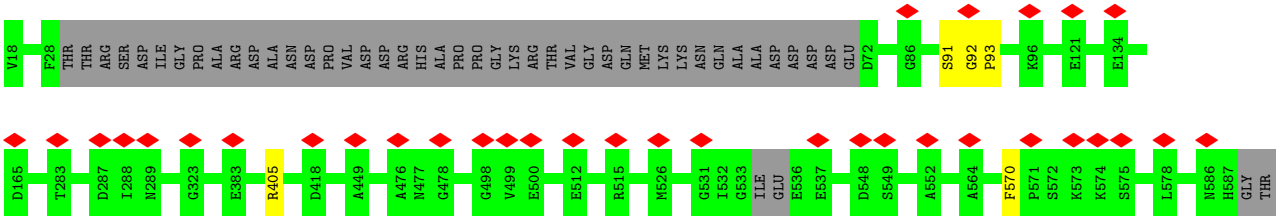
Chain S:

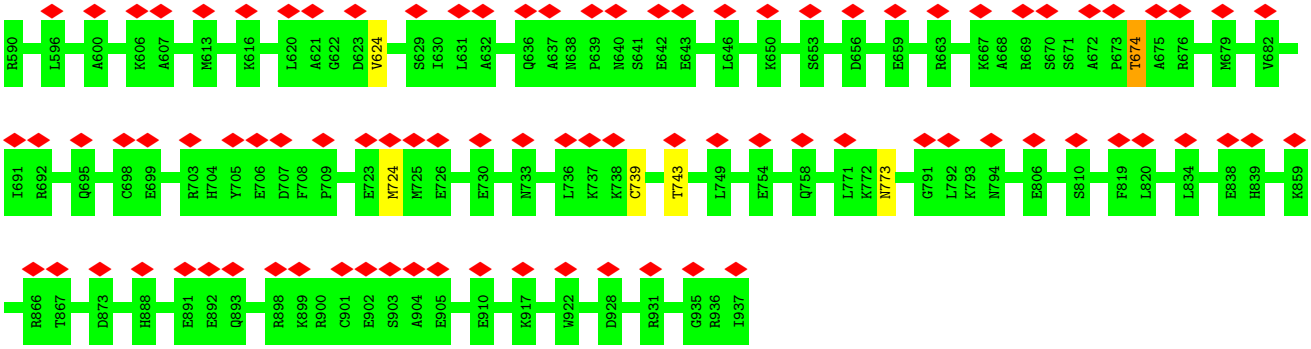


• Molecule 29: Pre-mRNA-processing factor 6

Chain 5J:

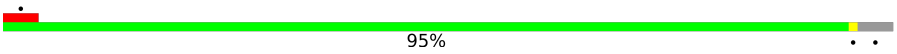


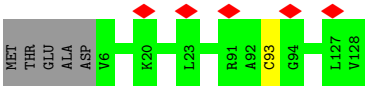




• Molecule 30: NHP2-like protein 1

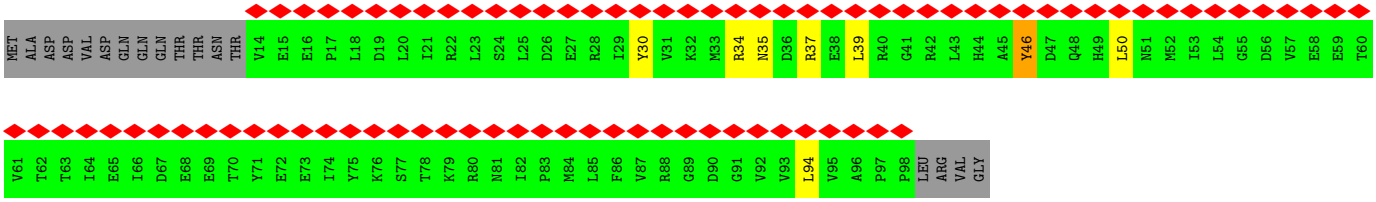
Chain 4D:





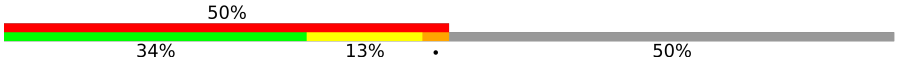
• Molecule 31: U6 snRNA-associated Sm-like protein LSm3

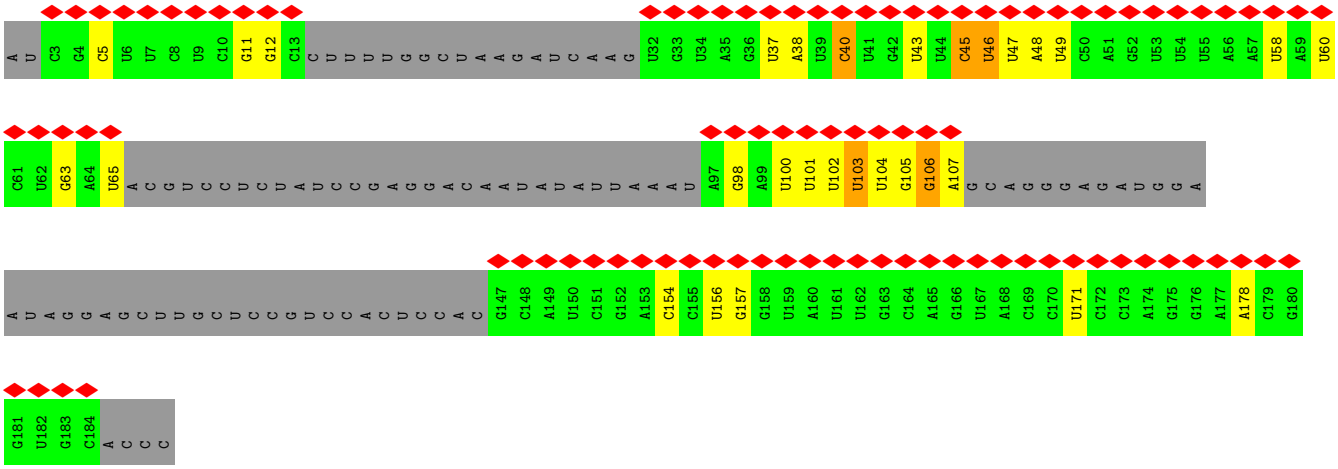
Chain 63:



• Molecule 32: U2 snRNA

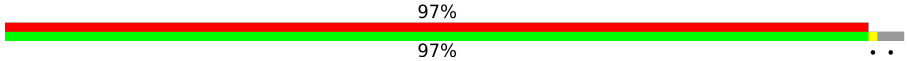
Chain 2:

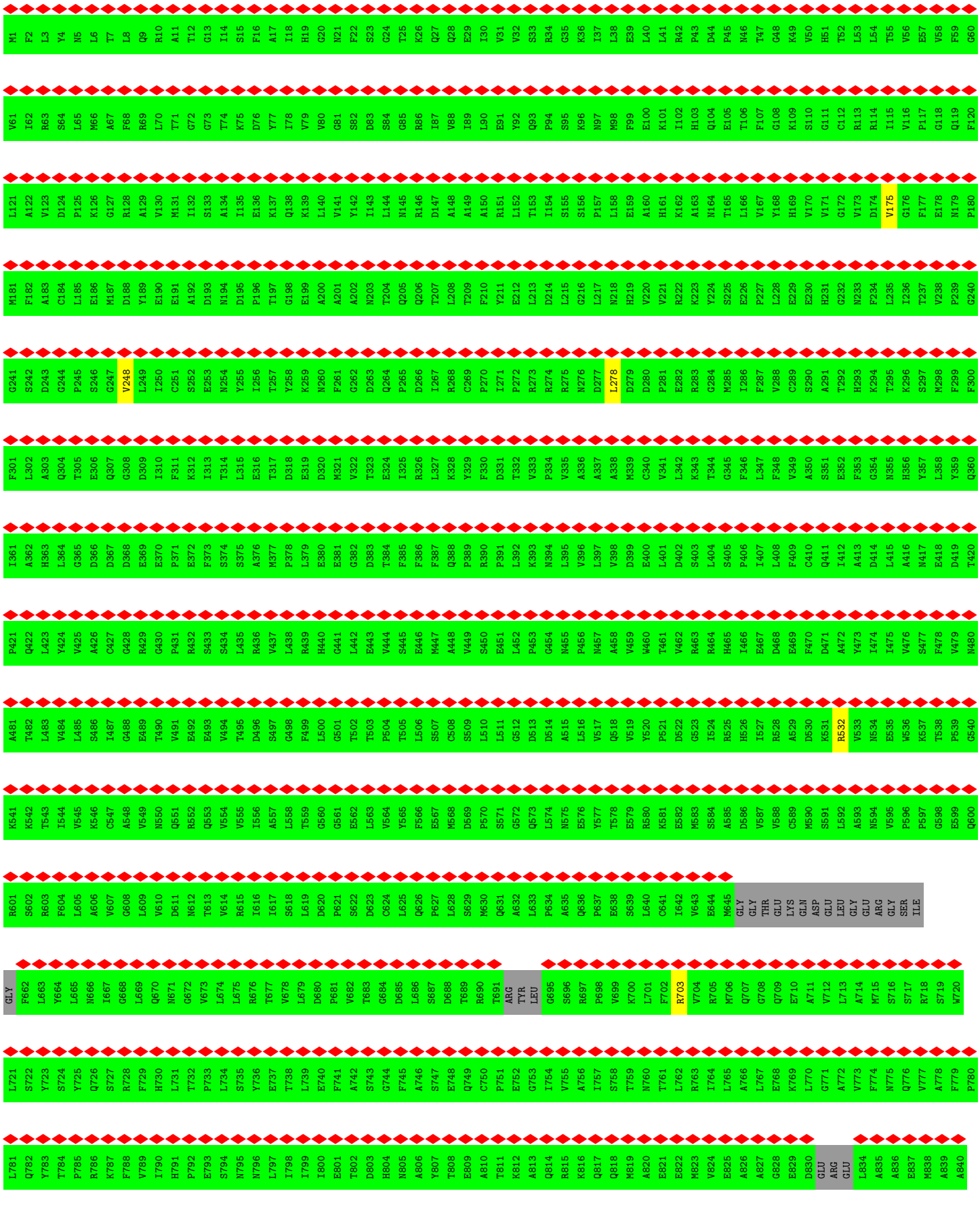




• Molecule 33: Splicing factor 3B subunit 3

Chain B3:




M1 F2 L3 Y4 N5 L6 T7 L8 Q9 R10 A11 T12 G13 I14 S15 F16 A17 I18 H19 G20 N21 F22 S23 G24 T25 K26 Q27 Q28 E29 I30 V31 V32 S33 R34 G35 K36 I37 L38 E39 L40 L41 R42 P43 D44 P45 N46 T47 G48 K49 V50 H51 T52 L53 L54 T55 V56 E57 V58 F59 G60
V61 I62 R63 S64 L65 M66 A67 F68 R69 L70 T71 G72 G73 T74 K75 D76 Y77 I78 V79 V80 G81 S82 D83 S84 G85 R86 I87 V88 I89 L90 E91 Y92 Q93 P94 S95 K96 N97 M98 F99 E100 K101 I102 H103 Q104 E105 T106 F107 G108 K109 S110 G111 C112 R113 R114 I115 V116 P117 G118 Q119 F120
L121 A122 V123 D124 P125 K126 G127 R128 A129 V130 M131 I132 S133 A134 I135 E136 K137 Q138 K139 L140 V141 Y142 I143 L144 N145 R146 D147 A148 A149 A150 R151 L152 T153 I154 S155 S156 P157 L158 E159 A160 H161 K162 A163 N164 T165 L166 V167 Y168 H169 V170 V171 G172 V173 D174 V175 G176 F177 E178 N179 P180
M181 F182 A183 C184 L185 E186 M187 D188 Y189 E190 E191 A192 D193 N194 D195 P196 T197 G198 E199 A200 A201 A202 N203 T204 Q205 Q206 T207 L208 T209 F210 Y211 E212 L213 D214 L215 G216 L217 N218 H219 V220 V221 R222 K223 Y224 S225 E226 P227 L228 E229 E230 H231 G232 N233 F234 L235 I236 T237 V238 P239 G240
G241 S242 D243 G244 P245 S246 G247 Y248 L249 I250 C251 S252 E253 N254 Y255 I256 T257 Y258 K259 N260 F261 G262 D263 Q264 P265 D266 I267 R268 C269 P270 I271 P272 R273 R274 R275 N276 D277 L278 D279 D280 P281 E282 R283 G284 M285 I286 F287 V288 C289 S290 A291 T292 H293 K294 T295 K296 S297 M298 F299 F300
F301 L302 A303 Q304 T305 E306 Q307 G308 D309 I310 F311 K312 I313 T314 L315 E316 T317 D318 E319 D320 M321 V322 T323 E324 I325 R326 L327 K328 Y329 F330 D331 T332 V333 P334 V335 A336 A337 A338 M339 C340 V341 L342 K343 T344 G345 F346 L347 F348 V349 A350 S351 E352 F353 G354 N355 H356 Y357 L358 Y359 Q360
I361 A362 H363 L364 G365 D366 D367 D368 E369 E370 P371 E372 F373 S374 S375 A376 M377 P378 L379 E380 E381 G382 D383 T384 F385 P386 F387 Q388 P389 R390 P391 L392 K393 N394 L395 V396 L397 V398 D399 E400 L401 D402 S403 L404 S405 P406 I407 L408 F409 C410 Q411 I412 A413 D414 L415 A416 N417 E418 D419 T420
P421 Q422 L423 Y424 V425 A426 C427 G428 R429 G430 P431 R432 S433 S434 L435 R436 V437 L438 R439 H440 G441 L442 E443 V444 S445 E446 M447 A448 V449 S450 E451 L452 P453 G454 N455 P456 M457 A458 V459 W460 T461 V462 R463 R464 H465 I466 E467 D468 E469 F470 D471 A472 Y473 I474 I475 V476 S477 F478 V479 N480
A481 T482 L483 V484 L485 S486 I487 G488 E489 T490 V491 E492 E493 V494 T495 D496 S497 G498 F499 L500 G501 T502 T503 P504 T505 L506 S507 C508 S509 L510 L511 G512 D513 D514 A515 L516 V517 Q518 V519 Y520 P521 D522 G523 I524 R525 H526 I527 R528 A529 D530 K531 R532 V533 N534 E535 W536 K537 T538 P539 G540
K541 K542 T543 I544 V545 K546 C547 A548 V549 N550 Q551 R552 Q553 V554 V555 I556 A557 L558 T559 G560 G561 E562 L563 V564 Y565 F566 E567 M568 D569 P570 S571 G572 Q573 L574 N575 E576 Y577 T578 E579 R580 K581 E582 M583 S584 A585 D586 V587 V588 C589 M590 S591 L592 A593 N594 V595 P596 P597 G598 E599 Q600
R601 S602 R603 F604 V605 A606 V607 G608 L609 V610 D611 N612 T613 V614 R615 I616 I617 S618 L619 D620 P621 S622 D623 C624 L625 Q626 P627 L628 S629 M630 Q631 A632 L633 P634 A635 Q636 P637 E638 S639 L640 C641 I642 V643 E644 M645 GLY GLY THR GLU LYS GLN ASP GLU LEU GLY GLU ARG GLY SER ILE
GLY F662 L663 Y664 L665 N666 I667 G668 L669 Q670 M671 G672 V673 L674 L675 R676 T677 V678 L679 D680 P681 V682 T683 G684 D685 L686 S687 D688 T689 R690 T691 ARG TYR LEU G695 S696 R697 P698 V699 K700 L701 F702 R703 V704 R705 M706 Q707 G708 Q709 E710 A711 V712 L713 A714 M715 S716 S717 R718 S719 W720
L721 S722 Y723 S724 Y725 Q726 S727 R728 F729 H730 L731 T732 P733 L734 S735 Y736 E737 T738 L739 E740 F741 A742 S743 G744 F745 A746 S747 E748 Q749 C750 P751 E752 G753 I754 V755 A756 I757 S758 T759 N760 T761 L762 R763 I764 L765 A766 L767 E768 K769 L770 G771 A772 V773 F774 N775 Q776 V777 A778 F779 P780
L781 Q782 Y783 T784 P785 R786 K787 F788 V789 I790 H791 P792 E793 S794 N795 N796 L797 I798 I799 I800 E801 T802 D803 H804 N805 A806 Y807 T808 E809 A810 T811 K812 A813 Q814 R815 K816 Q817 Q818 M819 A820 E821 E822 M823 V824 E825 A826 A827 G828 E829 D830 GLU ARG GLU L834 A835 A836 E837 M838 A839 A840

A841 F842 L843 N844 E845 N846 L847 P848 E849 S850 I851 F852 G853 A854 P855 K856 A857 G858 N859 G860 Q861 W862 A863 S864 V865 I866 R867 V868 M869 N870 P871 I872 Q873 G874 N875 T876 L877 D878 L879 V880 Q881 L882 E883 Q884 N885 E886 A887 A888 F889 S890 V891 A892 V893 C894 R895 F896 S897 N898 T899 G900

E901 D902 W903 Y904 V905 L906 V907 G908 V909 A910 K911 D912 L913 I914 L915 N916 P917 R918 S919 V920 A921 G922 G923 F924 V925 Y926 T927 Y928 K929 L930 V931 N932 N933 G934 E935 K936 L937 E938 F939 L940 H941 K942 T943 P944 V945 E946 E947 V948 P949 A950 A951 I952 A953 P954 F955 Q956 G957 R958 V959 L960

I961 G962 V963 G964 K965 L966 L967 R968 V969 Y970 D971 L972 G973 K974 K975 K976 L977 L978 R979 K980 C981 E982 N983 K984 H985 I986 A987 N988 Y989 I990 S991 G992 I993 Q994 T995 I996 G997 H998 R999 V1000 I1001 V1002 S1003 D1004 V1005 Q1006 E1007 S1008 F1009 I1010 W1011 V1012 R1013 Y1014 K1015 R1016 N1017 E1018 N1019 Q1020

L1021 I1022 I1023 F1024 A1025 D1026 D1027 T1028 Y1029 P1030 R1031 W1032 V1033 T1034 T1035 A1036 S1037 L1038 L1039 D1040 Y1041 D1042 T1043 V1044 A1045 G1046 A1047 D1048 K1049 F1050 G1051 N1052 I1053 C1054 V1055 V1056 R1057 L1058 P1059 P1060 N1061 T1062 N1063 D1064 E1065 V1066 D1067 E1068 ASP PRO THR GLY ASN LYS ALA LEU TRP D1078 R1079 G1080

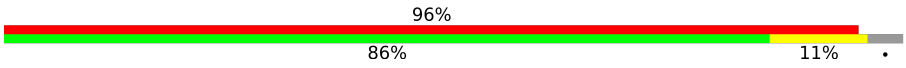
L1081 L1082 N1083 G1084 A1085 S1086 Q1087 K1088 A1089 E1090 V1091 I1092 M1093 N1094 Y1095 H1096 V1097 G1098 E1099 T1100 V1101 L1102 S1103 L1104 Q1105 K1106 T1107 T1108 L1109 I1110 P1111 G1112 G1113 S1114 E1115 S1116 L1117 V1118 Y1119 T1120 T1121 L1122 S1123 G1124 G1125 I1126 G1127 I1128 L1129 V1130 P1131 F1132 T1133 S1134 H1135 E1136 D1137 H1138 D1139 F1140

F1141 Q1142 H1143 V1144 E1145 M1146 H1147 L1148 R1149 S1150 E1151 H1152 P1153 P1154 L1155 C1156 G1157 R1158 D1159 H1160 L1161 S1162 F1163 R1164 S1165 Y1166 Y1167 F1168 P1169 V1170 K1171 N1172 V1173 I1174 D1175 G1176 D1177 L1178 C1179 E1180 Q1181 F1182 N1183 S1184 M1185 E1186 P1187 N1188 K1189 Q1190 K1191 N1192 V1193 S1194 E1195 E1196 L1197 D1198 R1199 T1200

P1201 P1202 E1203 V1204 S1205 K1206 K1207 L1208 E1209 D1210 I1211 R1212 T1213 R1214 Y1215 A1216 F1217

• Molecule 34: Small nuclear ribonucleoprotein G

Chain 1g:

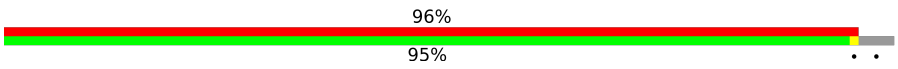


MET SER LYS A4 H5 P6 P7 E8 L9 K10 K11 F12 M13 D14 K15 K16 L17 S18 L19 K20 L21 N22 G23 G24 R25 H26 V27 Q28 G29 I30 L31 R32 G33 F34 D35 P36 F37 M38 N39 L40 V41 I42 D43 E44 C45 V46 E47 M48 A49 T50 S51 G52 Q53 Q54 N55 N56 I57 G58 M59 V60

V61 I62 R63 G64 N65 S66 I67 I68 M69 L70 E71 A72 L73 E74 R75 V76

• Molecule 34: Small nuclear ribonucleoprotein G

Chain 2g:

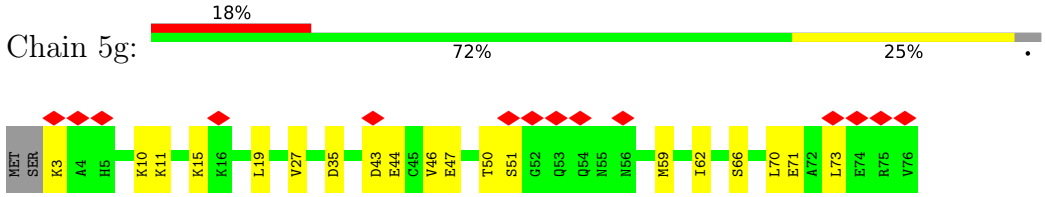


MET SER LYS A4 H5 P6 P7 E8 L9 K10 K11 F12 M13 D14 K15 K16 L17 S18 L19 K20 L21 N22 G23 G24 R25 H26 V27 Q28 G29 I30 L31 R32 G33 F34 D35 P36 F37 M38 N39 L40 V41 I42 D43 E44 C45 V46 E47 M48 A49 T50 S51 G52 Q53 Q54 N55 N56 I57 G58 M59 V60

V61 I62 R63 G64 N65 S66 I67 I68 M69 L70 E71 A72 L73 E74 R75 V76

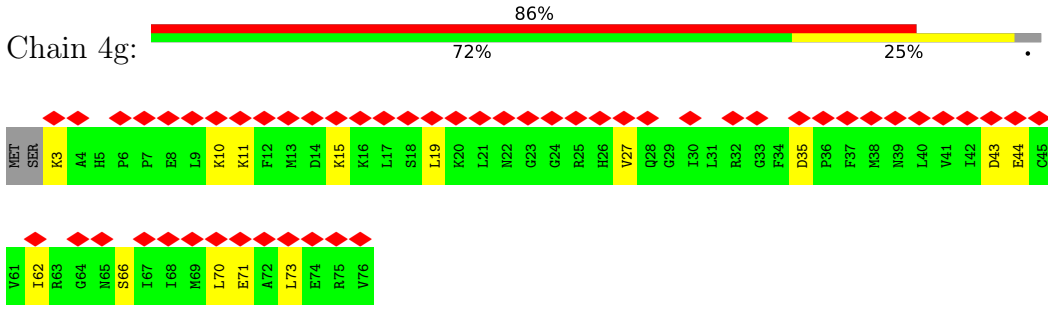
• Molecule 34: Small nuclear ribonucleoprotein G

Chain 5g:



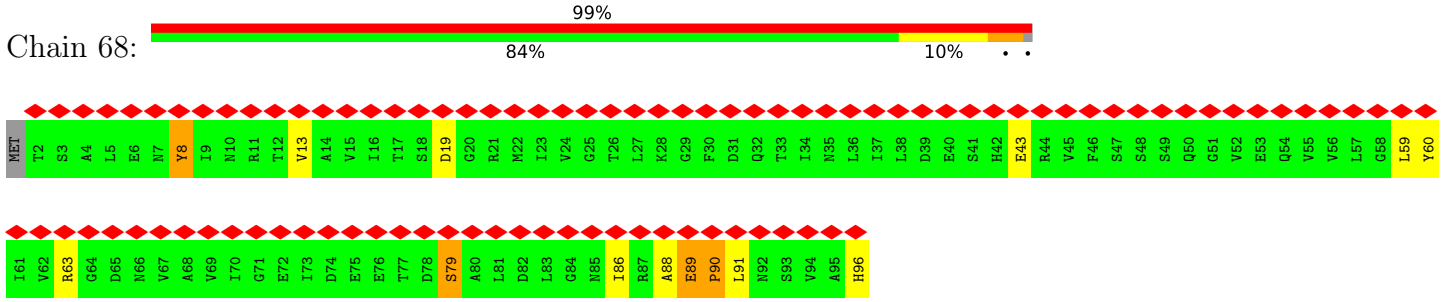
• Molecule 34: Small nuclear ribonucleoprotein G

Chain 4g:



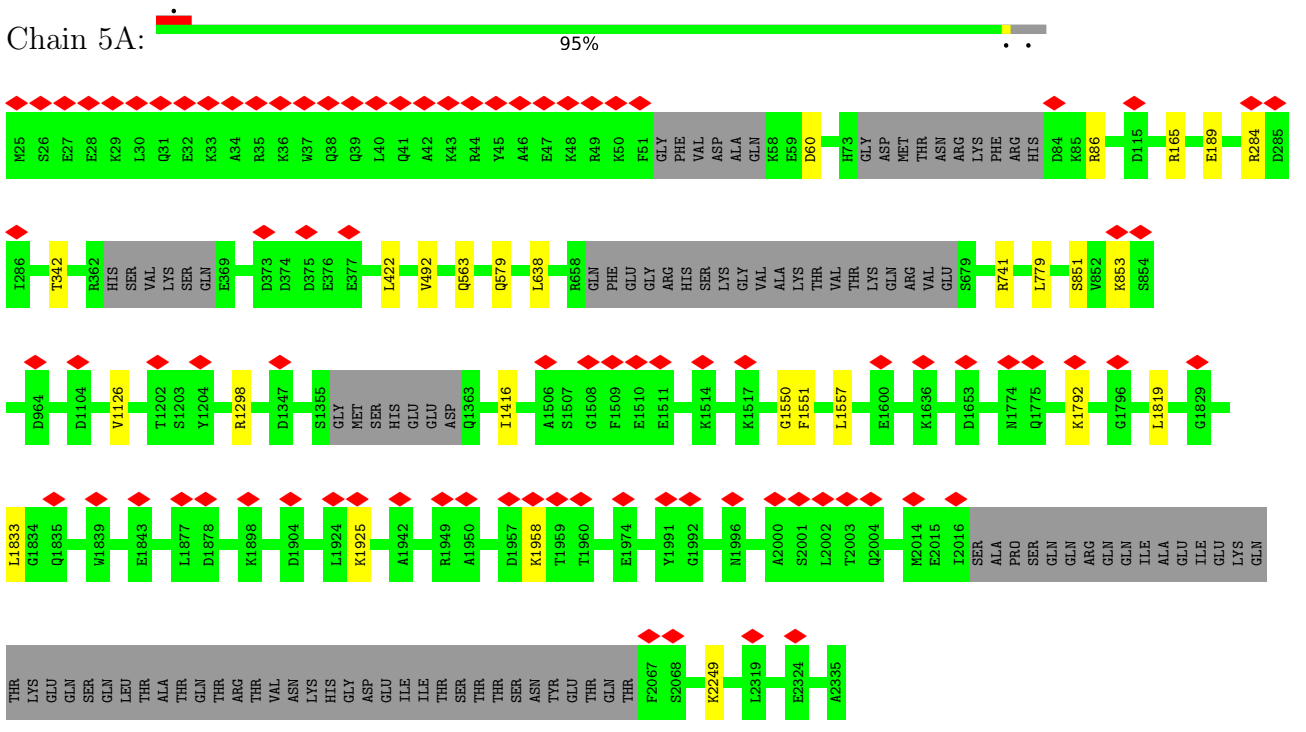
• Molecule 35: U6 snRNA-associated Sm-like protein LSm8

Chain 68:



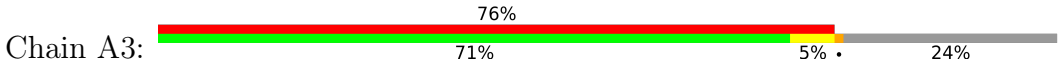
• Molecule 36: Pre-mRNA-processing-splicing factor 8

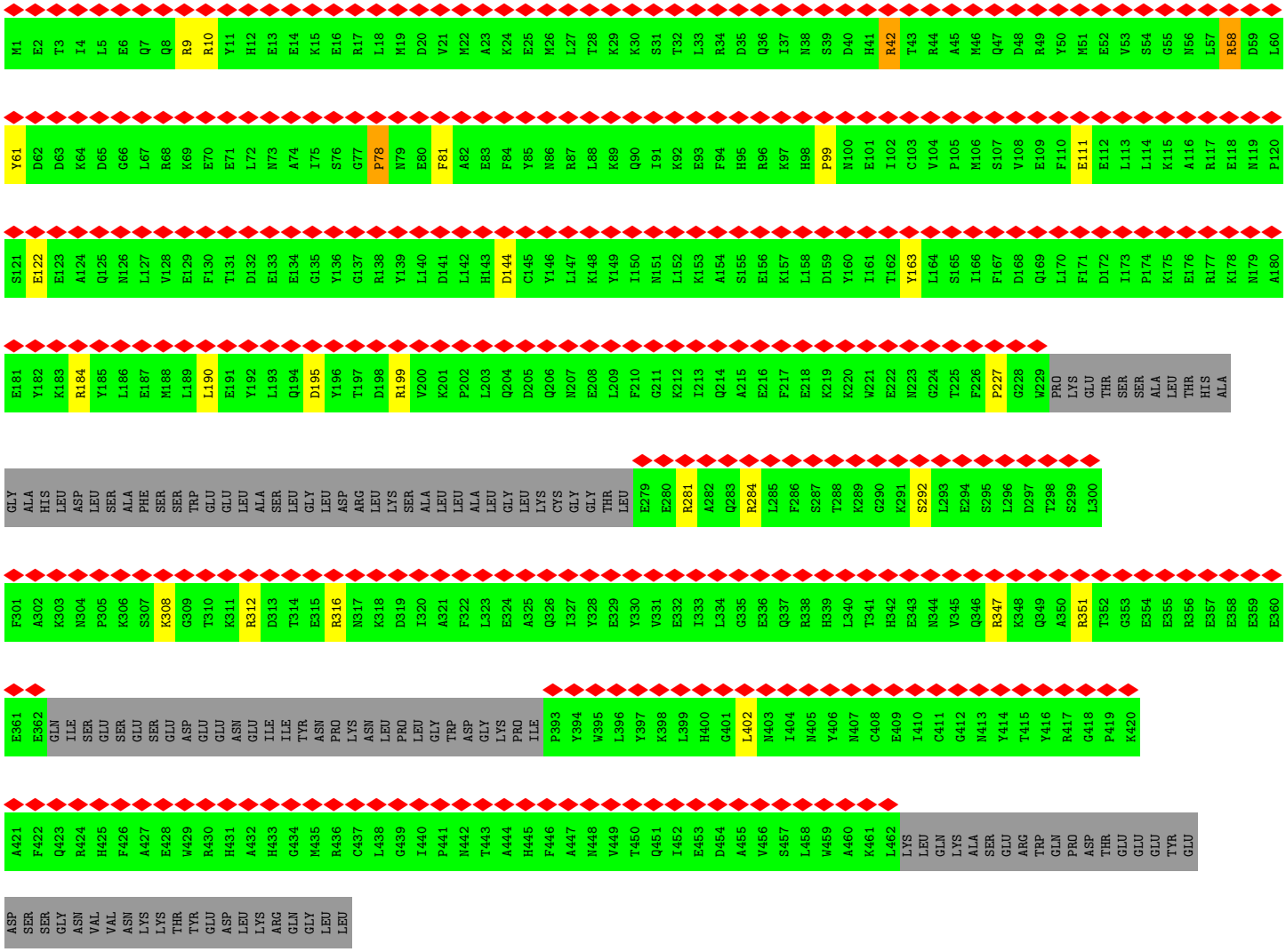
Chain 5A:



• Molecule 37: Splicing factor 3A subunit 3

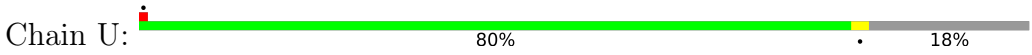
Chain A3:

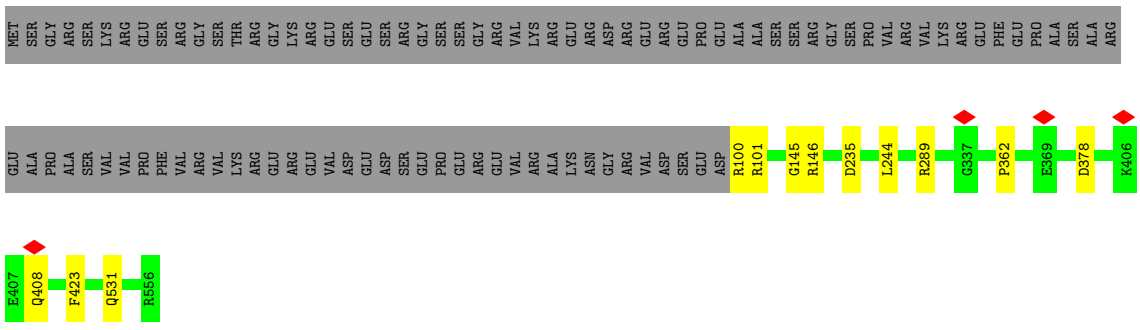




• Molecule 38: U4/U6.U5 tri-snRNP-associated protein 2

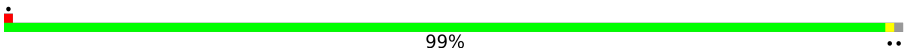
Chain U:

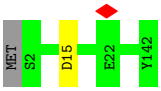




• Molecule 39: Thioredoxin-like protein 4A

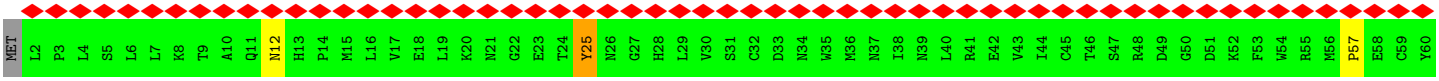
Chain 5D:





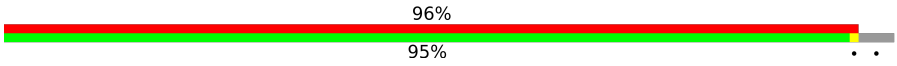
• Molecule 40: U6 snRNA-associated Sm-like protein LSm4

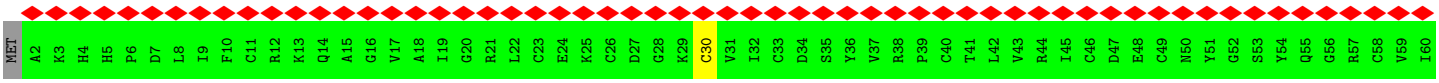
Chain 64:

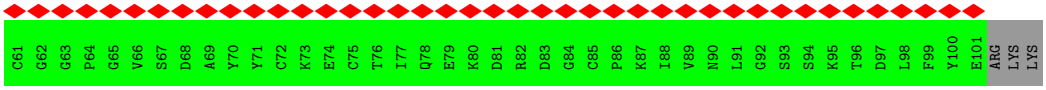


• Molecule 41: PHD finger-like domain-containing protein 5A

Chain BP:

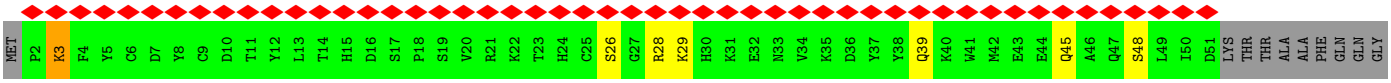


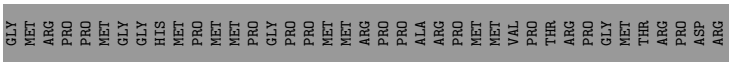




• Molecule 42: U1 small nuclear ribonucleoprotein C

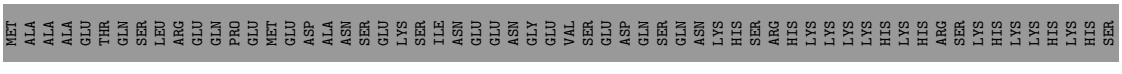
Chain 1C:

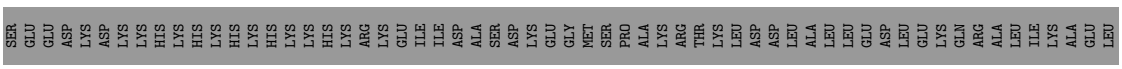


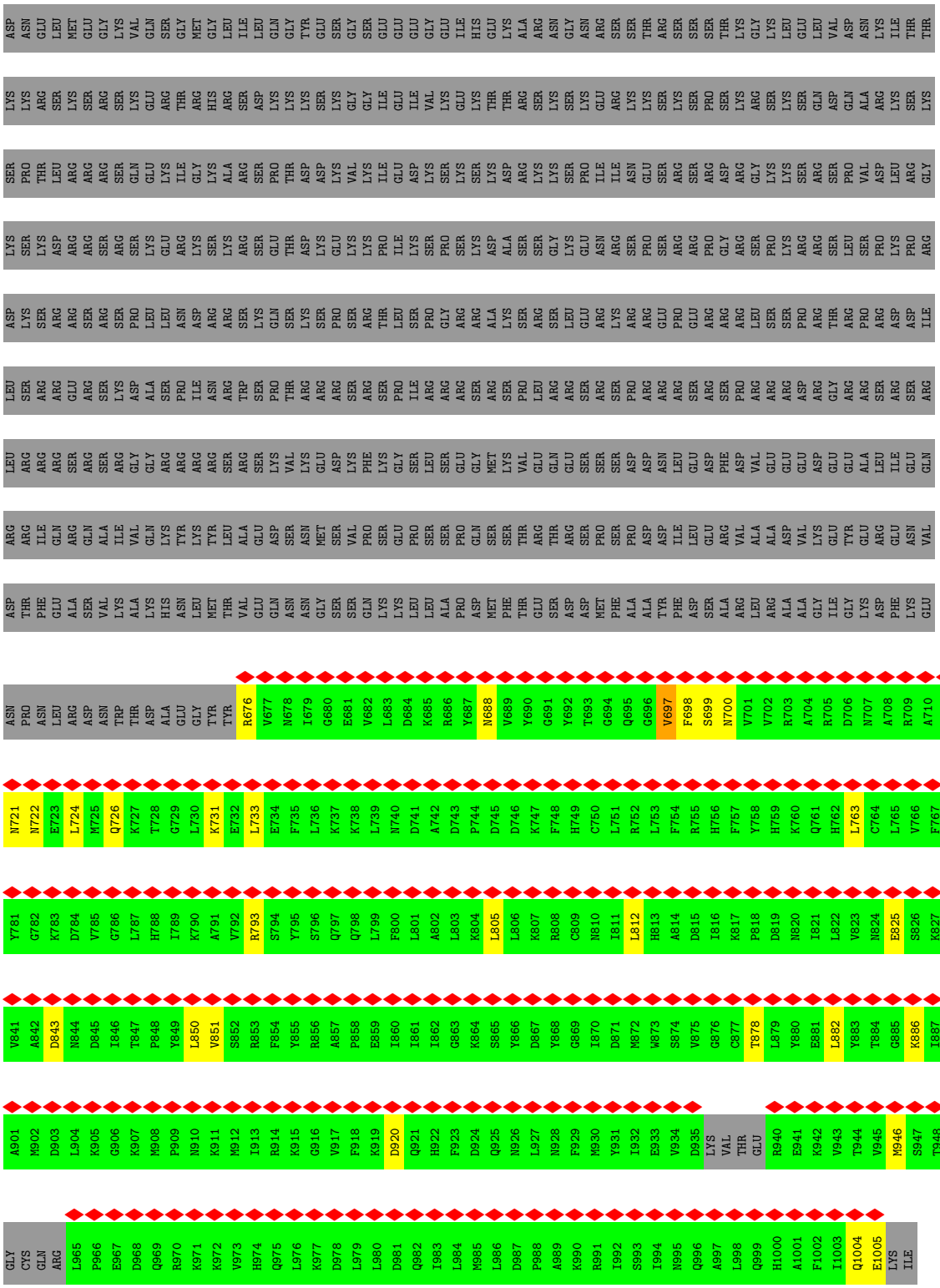


• Molecule 43: Serine/threonine-protein kinase PRP4 homolog

Chain K:

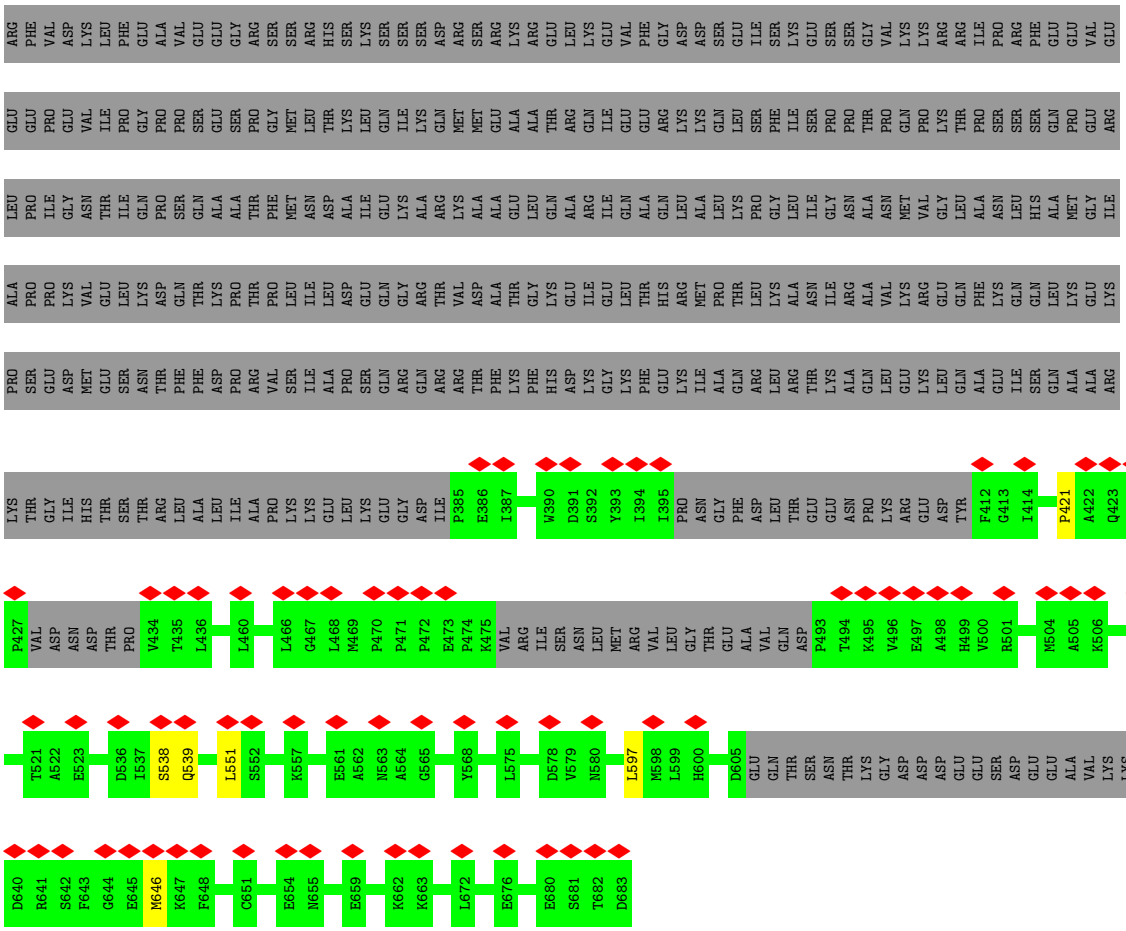






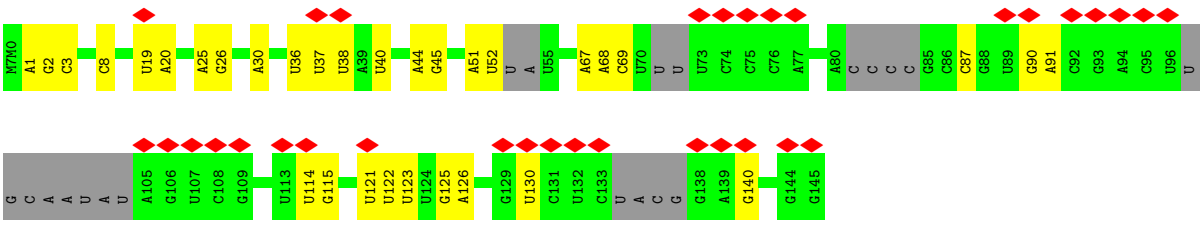
• Molecule 44: U4/U6 small nuclear ribonucleoprotein Prp3

Chain 4A:



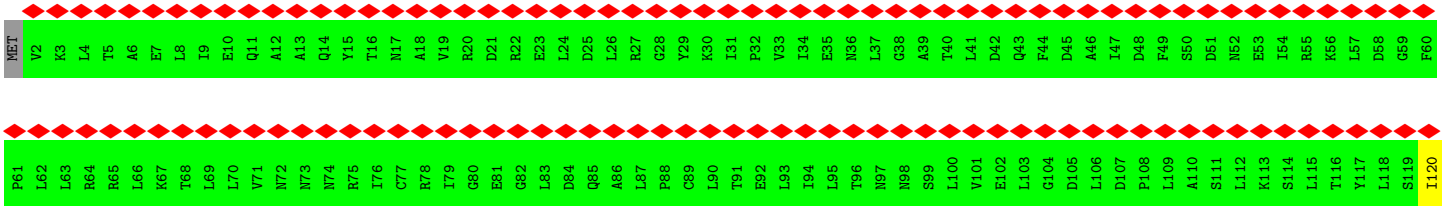
• Molecule 45: U4 snRNA

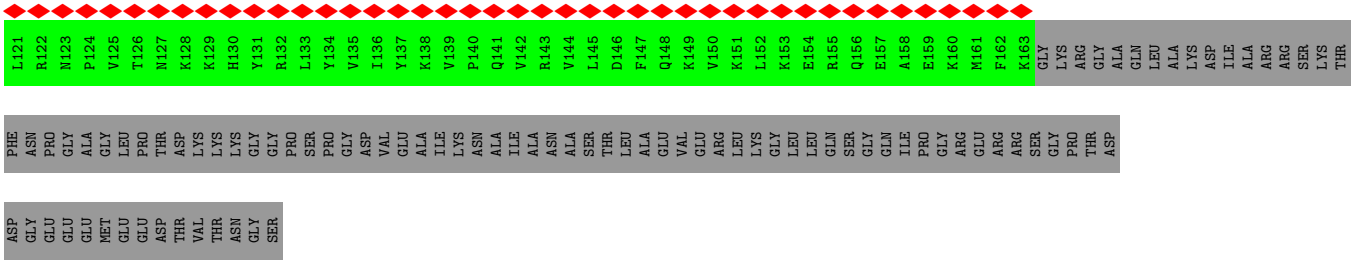
Chain 4:



• Molecule 46: U2 small nuclear ribonucleoprotein A'

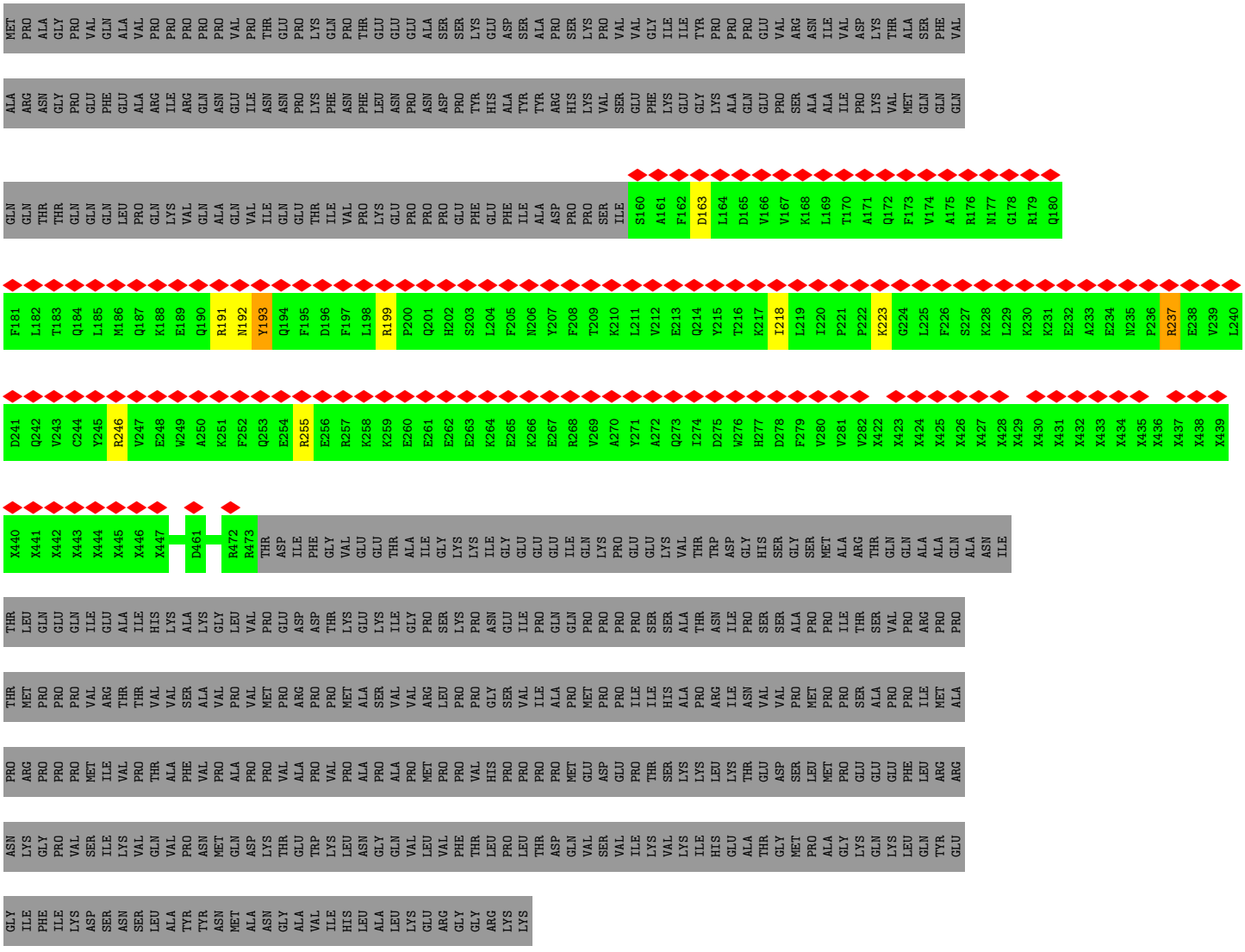
Chain 2A:





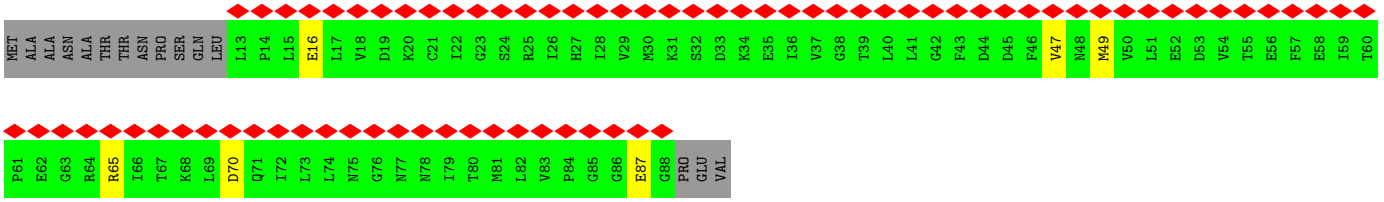
• Molecule 47: Splicing factor 3A subunit 1,Splicing factor 3A subunit 1,Splicing factor 3A subunit 1

Chain A1:



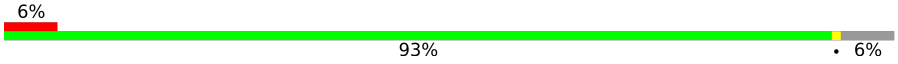
• Molecule 48: U6 snRNA-associated Sm-like protein LSm5

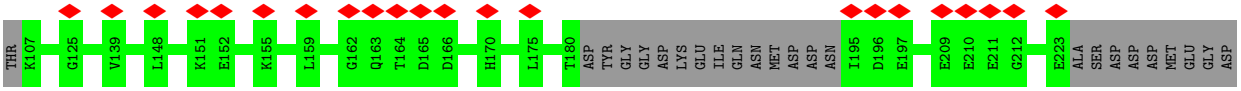
Chain 65:

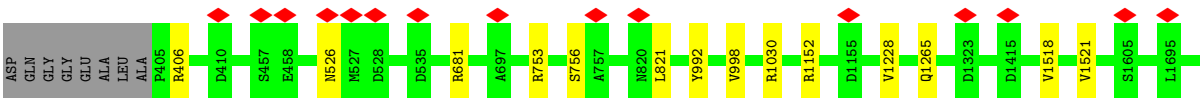


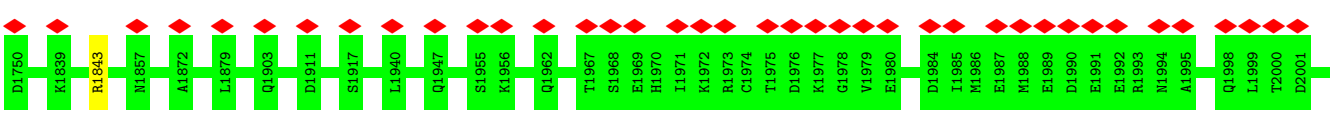
• Molecule 49: U5 small nuclear ribonucleoprotein 200 kDa helicase

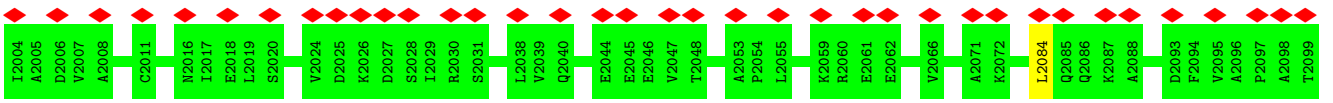
Chain 5B:





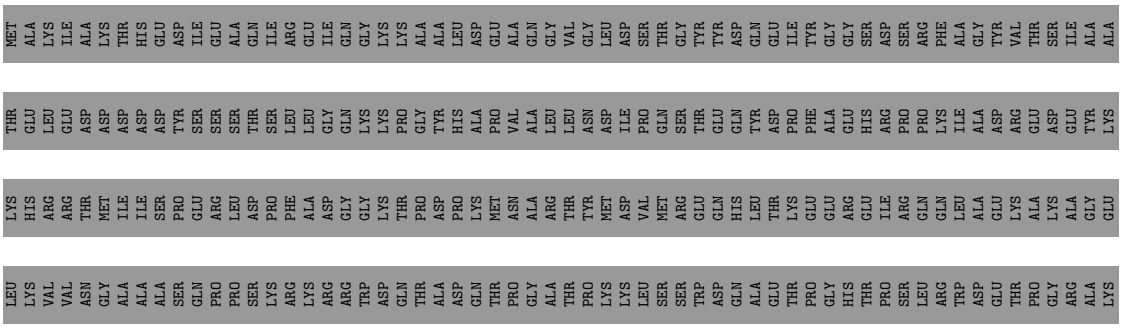


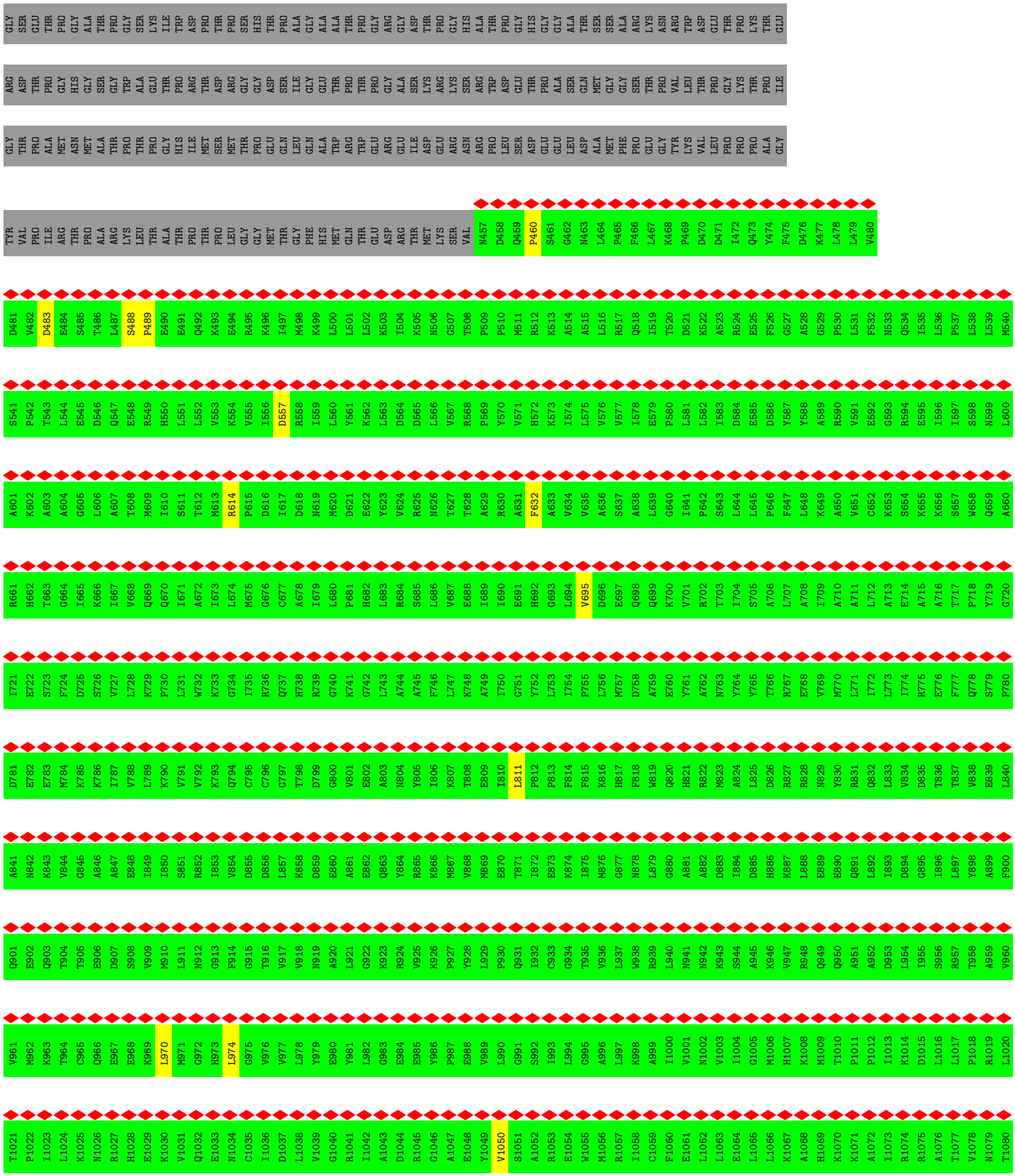




• Molecule 50: Splicing factor 3B subunit 1

Chain B1:




GLY SER GLU THR PRO GLY ALA THR PRO GLY SER LYS ILE TRP ASP PRO THR PRO SER HIS THR PRO ALA GLY ALA ALA THR PRO GLY ARG GLY ASP THR PRO GLY GLY HIS ALA THR PRO GLY GLY ALA THR SER SER ALA ARG LYS ASN ARG TRP ASP GLU THR PRO GLY LYS THR THR GLU
ARG ASP THR PRO GLY HIS GLY SER GLY TRP ALA GLU THR PRO ARG THR ASP ARG GLY GLY ASP SER HIS ILE GLY GLU THR PRO THR PRO GLY ALA SER LYS ARG LYS SER ARG TRP ASP GLU THR PRO GLY LYS THR PRO ILE
GLY THR PRO ALA MET ASN MET ALA THR PRO THR PRO GLY HIS ILE MET SER MET THR PRO GLY GLN LEU GLN ALA THR TRP ARG TRP GLU GLU ILE ASP GLU ARG ASN ARG PRO LEU SER ASP GLU THR PRO ALA MET PHE PRO GLU GLY GLY TYR LYS VAL LEU THR PRO GLY LYS THR PRO ALA GLY
TYR VAL PRO ILE ARG THR PRO ALA ARG LYS LEU THR ALA THR PRO THR PRO LEU GLY GLY MET THR GLY PHE HIS MET GLN THR GLU ASP ARG THR MET LYS SER VAL N457 D458 Q459 P460 S461 G462 N463 L464 P465 F466 L467 K468 P469 D470 D471 I472 Q473 Y474 F475 D476 K477 L478 L479 V480
D481 V482 D483 E484 S485 T486 L487 S488 P489 E490 E491 Q492 K493 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 N506 G507 T508 P509 P510 M511 R512 K513 A514 A515 L516 R517 Q518 I519 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 F532 N533 Q534 I535 L536 P537 L538 L539 M540
S541 P542 T543 L544 E545 D546 Q547 E548 R549 H550 L551 L552 V553 K554 V555 I556 D557 R558 I559 L560 Y561 K562 L563 D564 D565 L566 V567 R568 P569 Y570 V571 H572 K573 I574 L575 V576 V577 I578 E579 P580 L581 L582 I583 D584 E585 D586 Y587 Y588 A589 R590 V591 E592 G593 R594 E595 I596 I597 S598 N599 L600
A601 K602 A603 A604 G605 L606 A607 T608 M609 I610 S611 T612 M613 R614 P615 D616 I617 D618 N619 M620 D621 E622 Y623 V624 R625 N626 T627 T628 A629 R630 A631 F632 A633 V634 V635 A636 S637 A638 L639 G640 I641 P642 S643 L644 L645 P646 F647 L648 K649 A650 V651 C652 K653 S654 K655 K656 S657 W658 Q659 A660
R661 H662 T663 G664 I665 K666 I667 V668 Q669 Q670 I671 A672 I673 L674 M675 G676 C677 A678 I679 L680 P681 H682 L683 R684 S685 L686 V687 E688 I689 I690 E691 H692 G693 L694 V695 D696 E697 Q698 Q699 K700 V701 R702 T703 I704 S705 A706 L707 A708 I709 A710 A711 L712 A713 E714 A715 A716 T717 P718 Y719 G720
I721 E722 S723 F724 D725 S726 V727 L728 K729 P730 L731 W732 K733 G734 I735 R736 Q737 H738 R739 G740 K741 G742 L743 A744 A745 F746 L747 K748 A749 I750 G751 Y752 L753 I754 F755 L756 M757 D758 A759 E760 Y761 A762 N763 Y764 Y765 T766 R767 E768 V769 M770 L771 I772 L773 I774 R775 E776 F777 Q778 S779 P780
D781 E782 E783 M784 K785 K786 I787 V788 L789 K790 V791 V792 K793 Q794 C795 C796 G797 T798 D799 G800 V801 E802 A803 N804 Y805 I806 K807 T808 E809 I810 L811 P812 P813 F814 F815 K816 H817 F818 W819 Q820 H821 R822 M823 A824 L825 D826 R827 R828 N829 Y830 R831 Q832 L833 V834 D835 T836 T837 V838 E839 L840
A841 N842 K843 V844 G845 A846 A847 E848 I849 I850 S851 R852 I853 V854 D855 D856 L857 K858 D859 E860 A861 E862 Q863 Y864 R865 K866 M867 V868 M869 E870 T871 I872 E873 K874 I875 M876 G877 N878 L879 G880 A881 A882 D883 I884 D885 H886 K887 L888 E889 E890 Q891 L892 I893 D894 G895 I896 L897 Y898 A899 F900
Q901 E902 Q903 T904 T905 E906 D907 S908 V909 M910 L911 N912 G913 F914 G915 T916 V917 V918 N919 A920 L921 G922 K923 R924 V925 K926 P927 Y928 L929 P930 Q931 I932 C933 G934 T935 V936 L937 W938 R939 L940 N941 N942 K943 S944 A945 K946 V947 R948 Q949 Q950 A951 A952 D953 L954 I955 S956 R957 T958 A959 V960
V961 M962 K963 T964 C965 Q966 E967 E968 K969 L970 M971 G972 H973 L974 G975 V976 V977 L978 Y979 E980 Y981 L982 G983 E984 E985 Y986 P987 E988 V989 L990 G991 S992 I993 L994 G995 A996 L997 K998 A999 I1000 V1001 N1002 V1003 I1004 G1005 M1006 H1007 K1008 M1009 T1010 P1011 P1012 I1013 K1014 D1015 L1016 L1017 P1018 R1019 L1020
T1021 P1022 I1023 L1024 K1025 N1026 R1027 H1028 E1029 K1030 V1031 Q1032 E1033 N1034 C1035 I1036 D1037 L1038 V1039 G1040 R1041 I1042 A1043 D1044 R1045 G1046 A1047 E1048 Y1049 V1050 S1051 A1052 R1053 E1054 W1055 M1056 R1057 I1058 C1059 F1060 E1061 L1062 L1063 E1064 L1065 L1066 K1067 A1068 H1069 K1070 K1071 A1072 I1073 R1074 R1075 A1076 T1077 V1078 N1079 T1080

F1081 G1082 Y1083 I1084 A1085 K1086 A1087 I1088 G1089 P1090 H1091 D1092 V1093 L1094 A1095 T1096 L1097 L1098 N1099 N1100 L1101 K1102 V1103 Q1104 E1105 R1106 Q1107 N1108 R1109 V1110 C1111 T1112 T1113 V1114 A1115 I1116 A1117 I1118 V1119 A1120 E1121 T1122 C1123 S1124 P1125 F1126 T1127 V1128 L1129 P1130 A1131 L1132 M1133 N1134 E1135 Y1136 R1137 V1138 P1139 E1140

L1141 N1142 V1143 Q1144 N1145 G1146 V1147 L1148 K1149 S1150 L1151 S1152 F1153 L1154 F1155 E1156 Y1157 I1158 G1159 E1160 M1161 G1162 K1163 D1164 Y1165 I1166 Y1167 A1168 V1169 T1170 P1171 L1172 L1173 E1174 D1175 A1176 L1177 M1178 D1179 R1180 D1181 L1182 V1183 H1184 R1185 Q1186 T1187 A1188 S1189 A1190 V1191 V1192 Q1193 H1194 M1195 S1196 L1197 G1198 V1199 Y1200

G1201 F1202 G1203 C1204 E1205 D1206 S1207 L1208 N1209 H1210 L1211 L1212 N1213 Y1214 V1215 W1216 P1217 N1218 V1219 F1220 E1221 T1222 S1223 P1224 H1225 V1226 I1227 Q1228 A1229 V1230 M1231 G1232 A1233 L1234 E1235 G1236 L1237 R1238 V1239 A1240 I1241 G1242 P1243 C1244 R1245 M1246 L1247 Q1248 Y1249 C1250 L1251 Q1252 G1253 L1254 F1255 H1256 P1257 A1258 R1259 K1260

V1261 R1262 D1263 V1264 Y1265 W1266 K1267 I1268 Y1269 N1270 S1271 I1272 Y1273 I1274 G1275 S1276 Q1277 D1278 A1279 L1280 I1281 A1282 H1283 Y1284 P1285 R1286 I1287 Y1288 N1289 D1290 D1291 K1292 N1293 T1294 Y1295 I1296 R1297 Y1298 E1299 L1300 D1301 Y1302 I1303 L1304

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86146	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	429.24, 429.24, 429.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.022, 1.022, 1.022	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IHP, GTP, MG, M7M

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	1	0.75	8/3891 (0.2%)	0.87	9/6061 (0.1%)
2	6	0.72	5/1264 (0.4%)	1.19	8/1961 (0.4%)
3	5O	0.31	0/2448	0.58	0/3316
4	B4	0.72	0/632	1.02	2/855 (0.2%)
5	13	0.53	0/645	1.19	6/870 (0.7%)
5	23	0.48	0/660	0.61	0/889
5	43	0.34	0/660	0.67	1/889 (0.1%)
5	53	0.44	0/665	0.56	0/896
6	4B	0.48	0/2921	0.65	0/3966
7	1e	0.62	0/646	1.27	5/867 (0.6%)
7	2e	0.48	0/677	0.60	0/908
7	4e	0.37	0/639	0.78	1/857 (0.1%)
7	5e	0.37	0/646	0.70	0/867
8	I	0.86	0/590	1.30	8/916 (0.9%)
9	1K	1.13	2/1695 (0.1%)	1.19	15/2288 (0.7%)
10	4C	0.34	0/2406	0.56	0/3232
11	11	0.68	0/649	1.24	7/878 (0.8%)
11	21	0.40	0/642	0.56	0/867
11	41	0.40	0/649	0.73	1/878 (0.1%)
11	51	0.40	0/649	0.73	1/878 (0.1%)
12	R	0.39	0/891	0.77	0/1188
13	1f	0.66	1/588 (0.2%)	1.18	4/795 (0.5%)
13	2f	0.49	0/574	0.59	0/775
13	4f	0.42	0/574	0.74	1/775 (0.1%)
13	5f	0.41	0/579	0.78	0/783
14	66	0.83	1/575 (0.2%)	1.25	3/776 (0.4%)
15	X	0.42	0/398	0.59	0/524
16	12	0.69	0/786	1.15	3/1055 (0.3%)
16	22	0.43	0/784	0.56	0/1053
16	42	0.43	0/747	0.66	0/1000
16	52	0.40	0/805	0.74	1/1081 (0.1%)
17	5	0.63	0/2444	1.47	59/3798 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
18	67	0.81	1/611 (0.2%)	1.29	3/824 (0.4%)
19	62	0.79	0/773	1.21	4/1043 (0.4%)
20	2B	0.38	0/759	0.50	0/1016
21	A2	0.65	0/1254	0.93	4/1682 (0.2%)
22	B2	0.67	3/1747 (0.2%)	0.88	7/2356 (0.3%)
23	5C	0.54	0/6879	0.61	3/9344 (0.0%)
24	5X	0.52	1/4859 (0.0%)	0.61	0/6522
25	1b	0.64	0/702	1.16	3/936 (0.3%)
25	2b	0.45	0/674	0.55	0/899
25	4b	0.33	0/679	0.62	0/905
25	5b	0.38	0/602	0.57	0/801
26	B5	0.60	0/584	0.59	0/789
27	1A	1.04	0/801	1.02	2/1074 (0.2%)
28	S	0.39	0/925	0.66	0/1229
29	5J	0.35	0/6430	0.62	6/8681 (0.1%)
30	4D	0.51	1/967 (0.1%)	0.56	0/1305
31	63	0.80	0/709	1.22	3/959 (0.3%)
32	2	0.72	3/2209 (0.1%)	1.15	14/3429 (0.4%)
33	B3	0.48	0/9485	0.61	0/12870
34	1g	0.58	0/575	1.17	4/768 (0.5%)
34	2g	0.48	0/575	0.62	0/768
34	4g	0.41	0/584	0.71	1/779 (0.1%)
34	5g	0.41	0/584	0.72	1/779 (0.1%)
35	68	0.80	0/728	1.30	7/987 (0.7%)
36	5A	0.48	1/18874 (0.0%)	0.59	10/25606 (0.0%)
37	A3	0.70	0/3294	1.07	12/4423 (0.3%)
38	U	0.54	0/3846	0.63	2/5208 (0.0%)
39	5D	0.39	0/1198	0.58	1/1620 (0.1%)
40	64	0.82	0/609	1.25	2/824 (0.2%)
41	BP	0.65	0/779	0.56	0/1047
42	1C	0.56	0/437	1.16	4/587 (0.7%)
43	K	0.37	0/2673	0.54	0/3593
44	4A	0.42	0/1983	0.59	2/2657 (0.1%)
45	4	0.59	2/2967 (0.1%)	1.00	7/4610 (0.2%)
46	2A	0.32	0/1299	0.62	0/1761
47	A1	0.71	0/1234	1.03	4/1657 (0.2%)
48	65	0.83	0/593	1.25	3/800 (0.4%)
49	5B	0.44	0/16393	0.59	3/22174 (0.0%)
50	B1	0.53	0/6878	0.65	3/9315 (0.0%)
All	All	0.54	29/141171 (0.0%)	0.77	250/193369 (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
6	4B	0	3
7	4e	0	1
9	1K	0	1
10	4C	0	2
13	4f	0	1
13	5f	0	1
14	66	0	1
16	12	0	1
16	52	0	3
18	67	0	1
19	62	0	1
21	A2	0	4
23	5C	0	2
25	4b	0	1
29	5J	0	2
31	63	0	2
33	B3	0	1
35	68	0	3
36	5A	0	2
37	A3	0	6
38	U	0	3
40	64	0	1
44	4A	0	2
45	4	0	1
47	A1	0	4
49	5B	0	2
50	B1	0	4
All	All	0	56

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	78	U	O3'-P	-19.56	1.37	1.61
1	1	2	U	O3'-P	-18.25	1.39	1.61
45	4	87	C	O3'-P	11.52	1.75	1.61
1	1	35	A	O3'-P	-7.25	1.52	1.61
22	B2	629	PRO	N-CD	-7.23	1.37	1.47

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5J	92	GLY	C-N-CD	-13.53	90.84	120.60
17	5	57	G	O4'-C1'-N9	12.51	118.20	108.20
1	1	78	U	P-O3'-C3'	12.36	134.54	119.70
42	1C	28	ARG	NE-CZ-NH1	12.33	126.47	120.30
17	5	58	U	O5'-P-OP2	-10.23	96.50	105.70

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	1K	56	PRO	Peptide
6	4B	420	TYR	Peptide
6	4B	459	PRO	Peptide
6	4B	470	TYR	Peptide
10	4C	350	GLN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
3	5O	304/357 (85%)	283 (93%)	19 (6%)	2 (1%)	19 49
4	B4	76/424 (18%)	76 (100%)	0	0	100 100
5	13	79/126 (63%)	75 (95%)	4 (5%)	0	100 100
5	23	81/126 (64%)	76 (94%)	5 (6%)	0	100 100
5	43	81/126 (64%)	76 (94%)	5 (6%)	0	100 100
5	53	82/126 (65%)	77 (94%)	5 (6%)	0	100 100
6	4B	357/522 (68%)	330 (92%)	25 (7%)	2 (1%)	22 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1e	75/92 (82%)	70 (93%)	5 (7%)	0	100	100
7	2e	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
7	4e	74/92 (80%)	71 (96%)	3 (4%)	0	100	100
7	5e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
9	1K	199/437 (46%)	184 (92%)	12 (6%)	3 (2%)	8	33
10	4C	293/499 (59%)	275 (94%)	18 (6%)	0	100	100
11	11	79/119 (66%)	77 (98%)	2 (2%)	0	100	100
11	21	78/119 (66%)	75 (96%)	3 (4%)	0	100	100
11	41	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
11	51	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
12	R	104/480 (22%)	91 (88%)	13 (12%)	0	100	100
13	1f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
13	2f	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
13	4f	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
13	5f	71/86 (83%)	64 (90%)	7 (10%)	0	100	100
14	66	70/80 (88%)	69 (99%)	0	1 (1%)	9	34
15	X	45/155 (29%)	39 (87%)	6 (13%)	0	100	100
16	12	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
16	22	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
16	42	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
16	52	94/118 (80%)	87 (93%)	7 (7%)	0	100	100
18	67	75/103 (73%)	72 (96%)	2 (3%)	1 (1%)	10	36
19	62	93/95 (98%)	84 (90%)	6 (6%)	3 (3%)	3	19
20	2B	90/225 (40%)	88 (98%)	2 (2%)	0	100	100
21	A2	138/209 (66%)	123 (89%)	11 (8%)	4 (3%)	3	21
22	B2	204/895 (23%)	181 (89%)	22 (11%)	1 (0%)	25	56
23	5C	850/854 (100%)	817 (96%)	31 (4%)	2 (0%)	44	72
24	5X	574/820 (70%)	561 (98%)	13 (2%)	0	100	100
25	1b	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
25	2b	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
25	4b	80/240 (33%)	71 (89%)	9 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	5b	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
26	B5	67/86 (78%)	61 (91%)	6 (9%)	0	100	100
27	1A	96/282 (34%)	94 (98%)	2 (2%)	0	100	100
28	S	110/800 (14%)	101 (92%)	8 (7%)	1 (1%)	14	44
29	5J	793/850 (93%)	748 (94%)	44 (6%)	1 (0%)	48	77
30	4D	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
31	63	83/102 (81%)	79 (95%)	3 (4%)	1 (1%)	11	38
33	B3	1176/1217 (97%)	1082 (92%)	92 (8%)	2 (0%)	44	72
34	1g	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
34	2g	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
34	4g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
34	5g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
35	68	93/96 (97%)	81 (87%)	6 (6%)	6 (6%)	1	7
36	5A	2198/2311 (95%)	2094 (95%)	102 (5%)	2 (0%)	48	77
37	A3	377/501 (75%)	346 (92%)	26 (7%)	5 (1%)	10	36
38	U	454/555 (82%)	424 (93%)	27 (6%)	3 (1%)	19	49
39	5D	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
40	64	71/139 (51%)	66 (93%)	3 (4%)	2 (3%)	4	22
41	BP	98/104 (94%)	92 (94%)	6 (6%)	0	100	100
42	1C	48/159 (30%)	47 (98%)	1 (2%)	0	100	100
43	K	316/1007 (31%)	294 (93%)	18 (6%)	4 (1%)	10	36
44	4A	229/683 (34%)	210 (92%)	18 (8%)	1 (0%)	30	61
46	2A	160/255 (63%)	147 (92%)	13 (8%)	0	100	100
47	A1	138/647 (21%)	129 (94%)	7 (5%)	2 (1%)	9	34
48	65	74/91 (81%)	70 (95%)	2 (3%)	2 (3%)	4	22
49	5B	1989/2136 (93%)	1885 (95%)	103 (5%)	1 (0%)	48	77
50	B1	846/1304 (65%)	792 (94%)	53 (6%)	1 (0%)	48	77
All	All	15337/23178 (66%)	14438 (94%)	846 (6%)	53 (0%)	38	67

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	5O	59	ILE

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Mol	Chain	Res	Type
9	1K	59	ARG
9	1K	63	ARG
19	62	47	ASP
19	62	53	HIS

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
3	5O	263/300 (88%)	263 (100%)	0	100 100
4	B4	66/336 (20%)	66 (100%)	0	100 100
5	13	71/101 (70%)	61 (86%)	10 (14%)	3 13
5	23	73/101 (72%)	73 (100%)	0	100 100
5	43	73/101 (72%)	73 (100%)	0	100 100
5	53	73/101 (72%)	73 (100%)	0	100 100
6	4B	306/442 (69%)	303 (99%)	3 (1%)	73 84
7	1e	72/84 (86%)	61 (85%)	11 (15%)	2 10
7	2e	76/84 (90%)	76 (100%)	0	100 100
7	4e	71/84 (84%)	69 (97%)	2 (3%)	38 63
7	5e	72/84 (86%)	72 (100%)	0	100 100
9	1K	170/373 (46%)	161 (95%)	9 (5%)	19 46
10	4C	255/424 (60%)	251 (98%)	4 (2%)	58 75
11	11	76/101 (75%)	72 (95%)	4 (5%)	19 46
11	21	75/101 (74%)	75 (100%)	0	100 100
11	41	76/101 (75%)	55 (72%)	21 (28%)	0 1
11	51	76/101 (75%)	55 (72%)	21 (28%)	0 1
12	R	94/369 (26%)	91 (97%)	3 (3%)	34 60
13	1f	63/74 (85%)	56 (89%)	7 (11%)	5 20
13	2f	61/74 (82%)	61 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	4f	61/74 (82%)	61 (100%)	0	100 100
13	5f	61/74 (82%)	60 (98%)	1 (2%)	58 75
14	66	62/70 (89%)	62 (100%)	0	100 100
15	X	42/144 (29%)	42 (100%)	0	100 100
16	12	91/110 (83%)	83 (91%)	8 (9%)	8 28
16	22	91/110 (83%)	91 (100%)	0	100 100
16	42	86/110 (78%)	86 (100%)	0	100 100
16	52	93/110 (84%)	92 (99%)	1 (1%)	70 82
18	67	69/91 (76%)	68 (99%)	1 (1%)	62 78
19	62	88/88 (100%)	86 (98%)	2 (2%)	45 68
20	2B	81/195 (42%)	81 (100%)	0	100 100
21	A2	129/180 (72%)	128 (99%)	1 (1%)	79 87
22	B2	187/776 (24%)	185 (99%)	2 (1%)	70 82
23	5C	754/756 (100%)	751 (100%)	3 (0%)	89 93
24	5X	517/721 (72%)	501 (97%)	16 (3%)	35 61
25	1b	78/177 (44%)	70 (90%)	8 (10%)	6 22
25	2b	75/177 (42%)	75 (100%)	0	100 100
25	4b	75/177 (42%)	75 (100%)	0	100 100
25	5b	67/177 (38%)	66 (98%)	1 (2%)	60 77
26	B5	60/77 (78%)	60 (100%)	0	100 100
27	1A	85/240 (35%)	82 (96%)	3 (4%)	31 57
28	S	91/681 (13%)	91 (100%)	0	100 100
29	5J	636/715 (89%)	631 (99%)	5 (1%)	79 87
30	4D	107/111 (96%)	107 (100%)	0	100 100
31	63	79/94 (84%)	76 (96%)	3 (4%)	28 55
33	B3	1027/1051 (98%)	1021 (99%)	6 (1%)	84 90
34	1g	63/66 (96%)	57 (90%)	6 (10%)	7 25
34	2g	63/66 (96%)	62 (98%)	1 (2%)	58 75
34	4g	64/66 (97%)	46 (72%)	18 (28%)	0 1
34	5g	64/66 (97%)	46 (72%)	18 (28%)	0 1
35	68	81/82 (99%)	77 (95%)	4 (5%)	21 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	5A	2002/2090 (96%)	1990 (99%)	12 (1%)	84 90
37	A3	345/446 (77%)	339 (98%)	6 (2%)	56 74
38	U	418/503 (83%)	414 (99%)	4 (1%)	73 84
39	5D	129/130 (99%)	129 (100%)	0	100 100
40	64	68/111 (61%)	68 (100%)	0	100 100
41	BP	86/90 (96%)	85 (99%)	1 (1%)	67 81
42	1C	48/135 (36%)	42 (88%)	6 (12%)	3 16
43	K	291/919 (32%)	259 (89%)	32 (11%)	5 20
44	4A	210/599 (35%)	208 (99%)	2 (1%)	73 84
46	2A	139/218 (64%)	138 (99%)	1 (1%)	81 88
47	A1	130/550 (24%)	127 (98%)	3 (2%)	45 68
48	65	68/80 (85%)	67 (98%)	1 (2%)	60 77
49	5B	1779/1908 (93%)	1766 (99%)	13 (1%)	81 88
50	B1	733/1104 (66%)	729 (100%)	4 (0%)	86 91
All	All	13735/20051 (68%)	13447 (98%)	288 (2%)	49 70

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	K	830	LEU
50	B1	695	VAL
43	K	892	LYS
34	4g	59	MET
27	1A	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
34	5g	26	HIS
49	5B	785	HIS
43	K	722	ASN
44	4A	524	GLN
49	5B	1209	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	163/164 (99%)	49 (30%)	6 (3%)
17	5	101/117 (86%)	42 (41%)	4 (3%)
2	6	50/106 (47%)	5 (10%)	2 (4%)
32	2	90/188 (47%)	23 (25%)	4 (4%)
45	4	120/146 (82%)	25 (20%)	3 (2%)
8	I	23/62 (37%)	5 (21%)	0
All	All	547/783 (69%)	149 (27%)	19 (3%)

5 of 149 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	U
1	1	12	G
1	1	15	G
1	1	16	G
1	1	17	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	2	103	U
45	4	68	A
45	4	114	U
45	4	1	A
17	5	57	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	IHP	5A	2401	-	36,36,36	0.71	0	54,60,60	0.58	0
53	GTP	5C	1002	52	26,34,34	1.36	3 (11%)	32,54,54	1.61	7 (21%)

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
54	IHP	5A	2401	-	-	8/30/54/54	0/1/1/1
53	GTP	5C	1002	52	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	5C	1002	GTP	C5-C6	-4.45	1.38	1.47
53	5C	1002	GTP	C5-C4	-2.15	1.37	1.43
53	5C	1002	GTP	O4'-C4'	-2.11	1.40	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	5C	1002	GTP	PB-O3B-PG	-3.54	120.68	132.83
53	5C	1002	GTP	C5-C6-N1	3.51	120.14	113.95
53	5C	1002	GTP	C8-N7-C5	3.05	108.80	102.99
53	5C	1002	GTP	C2-N1-C6	-3.00	119.58	125.10
53	5C	1002	GTP	PA-O3A-PB	-2.50	124.26	132.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

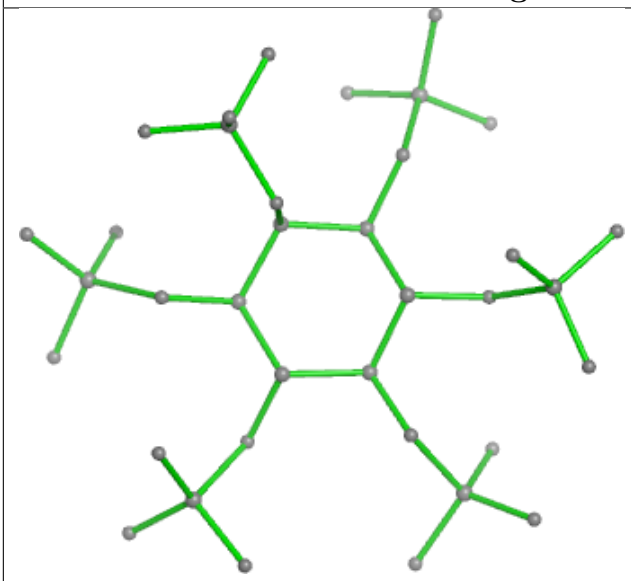
Mol	Chain	Res	Type	Atoms
54	5A	2401	IHP	C1-O11-P1-O41
54	5A	2401	IHP	C3-O13-P3-O23
53	5C	1002	GTP	O4'-C4'-C5'-O5'
53	5C	1002	GTP	PB-O3A-PA-O2A
53	5C	1002	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

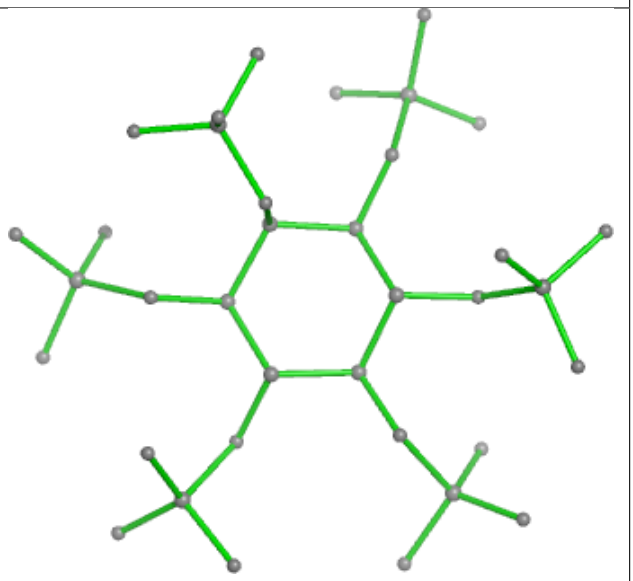
No monomer is involved in short contacts.

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.

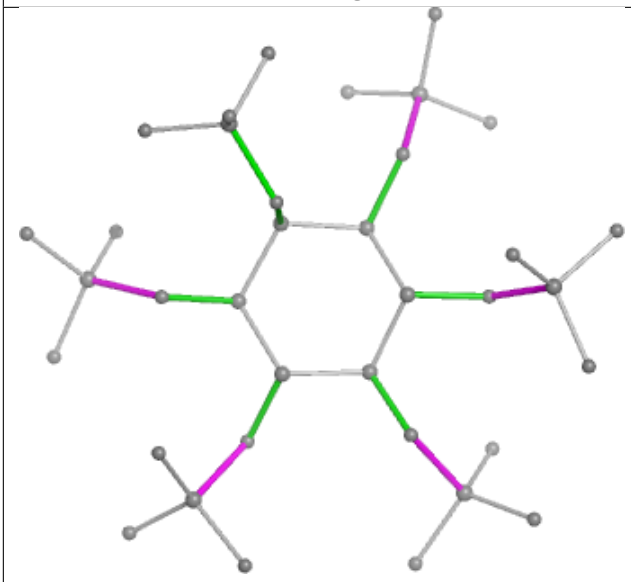
Ligand IHP 5A 2401



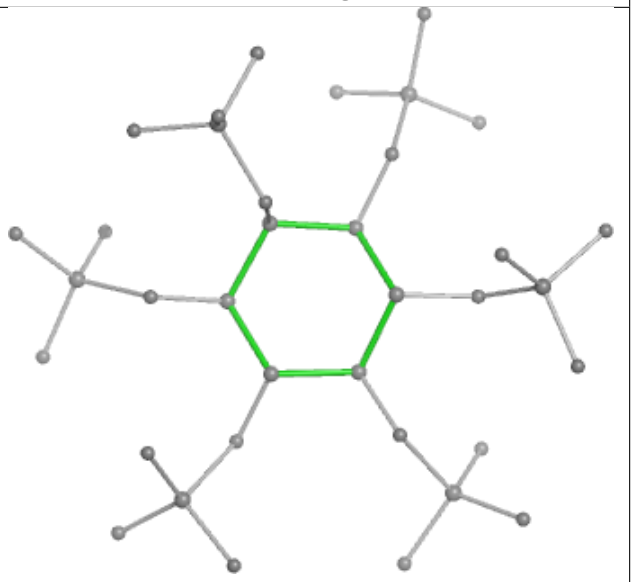
Bond lengths



Bond angles

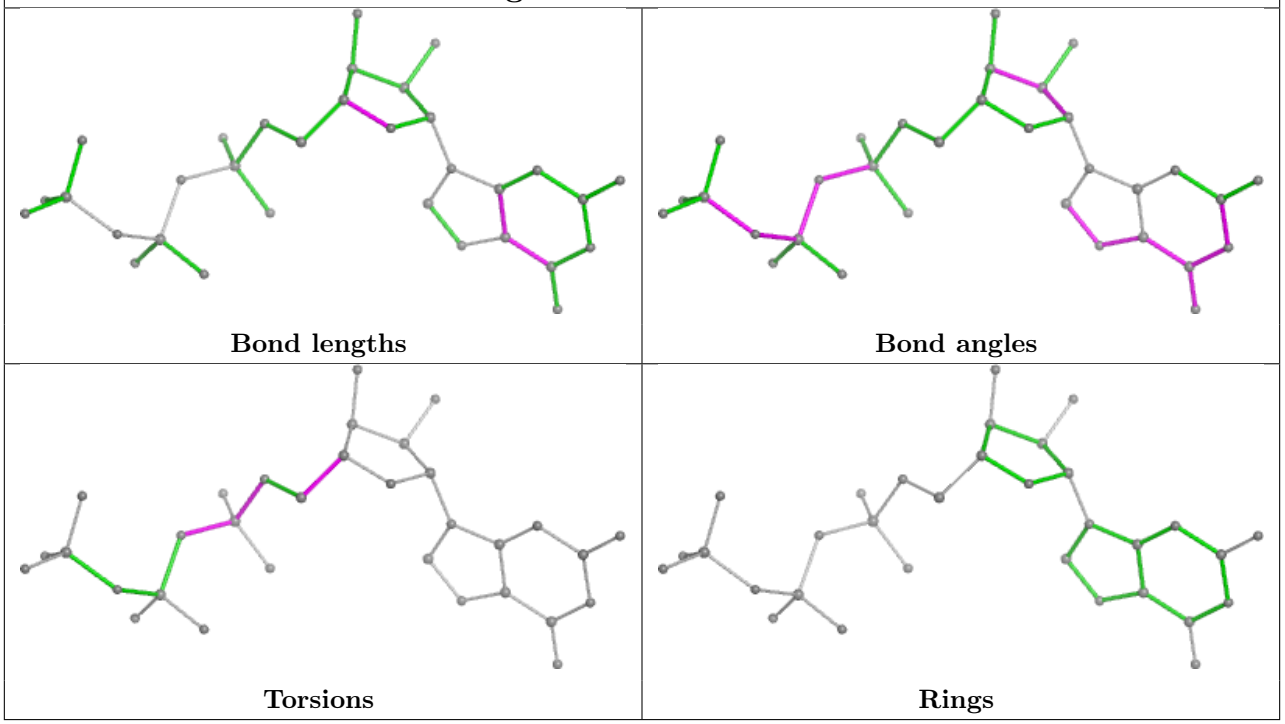


Torsions



Rings

Ligand GTP 5C 1002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	A1	2
1	1	2
29	5J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	282:VAL	C	422:UNK	N	108.26
1	5J	165:ASP	C	236:GLY	N	34.19
1	A1	447:UNK	C	455:VAL	N	4.52
1	1	2:U	O3'	3:A	P	1.39
1	1	78:U	O3'	79:G	P	1.37

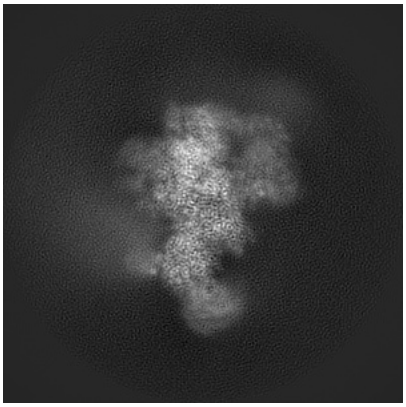
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4665. These allow visual inspection of the internal detail of the map and identification of artifacts.

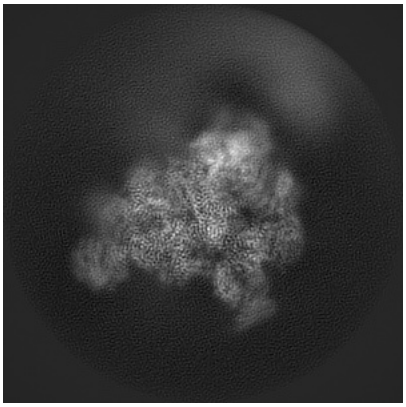
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

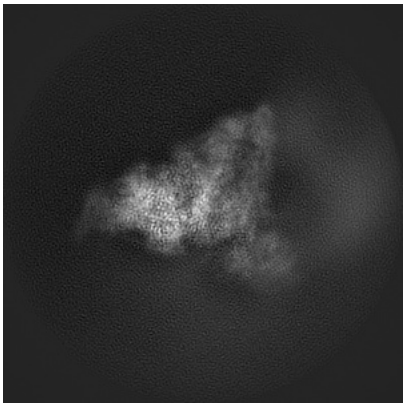
6.1.1 Primary map



X



Y

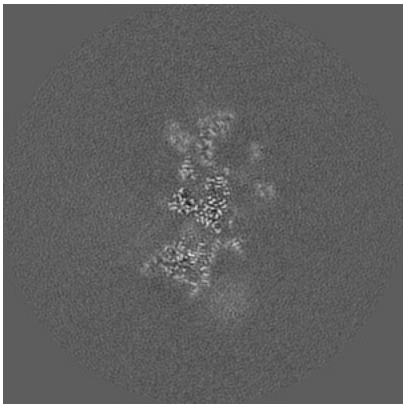


Z

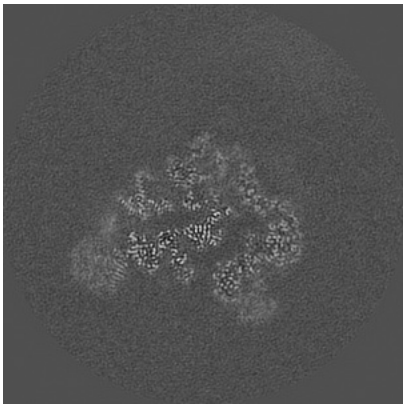
The images above show the map projected in three orthogonal directions.

6.2 Central slices

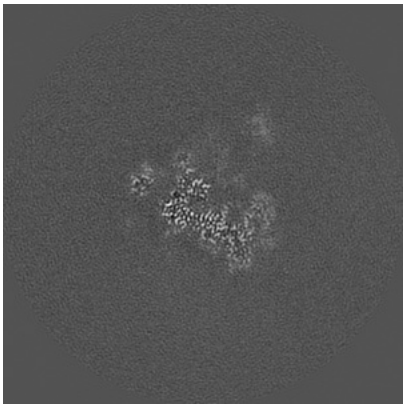
6.2.1 Primary map



X Index: 210



Y Index: 210

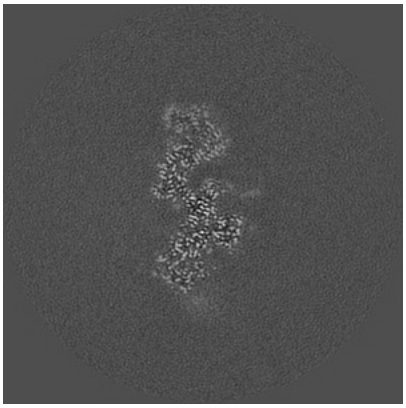


Z Index: 210

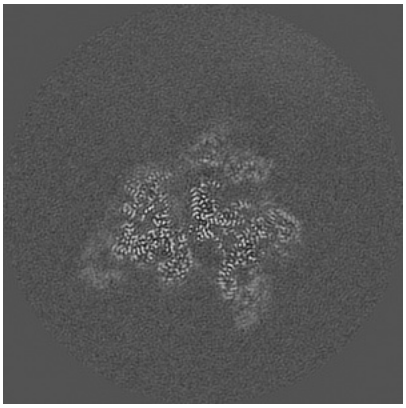
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

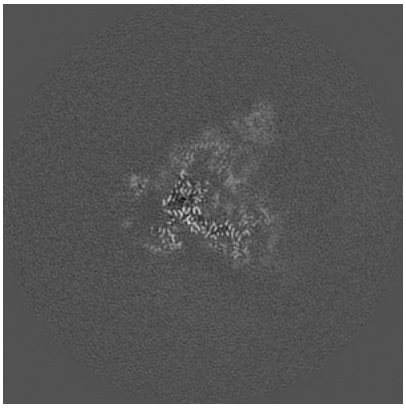
6.3.1 Primary map



X Index: 177



Y Index: 193

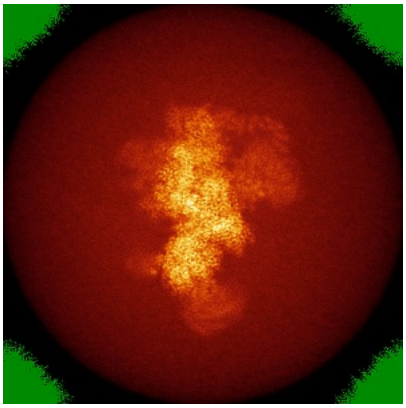


Z Index: 218

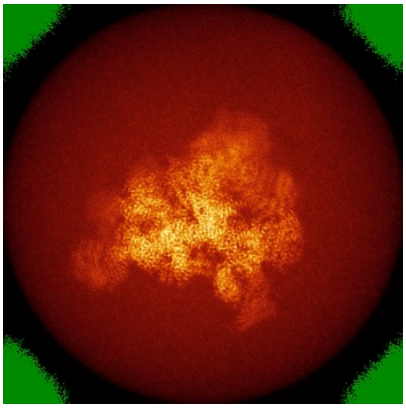
The images above show the largest variance slices of the map in three orthogonal directions.

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

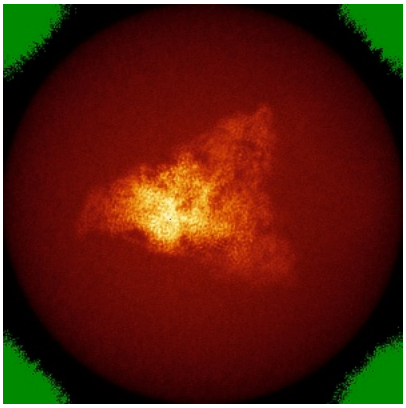
6.4.1 Primary map



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

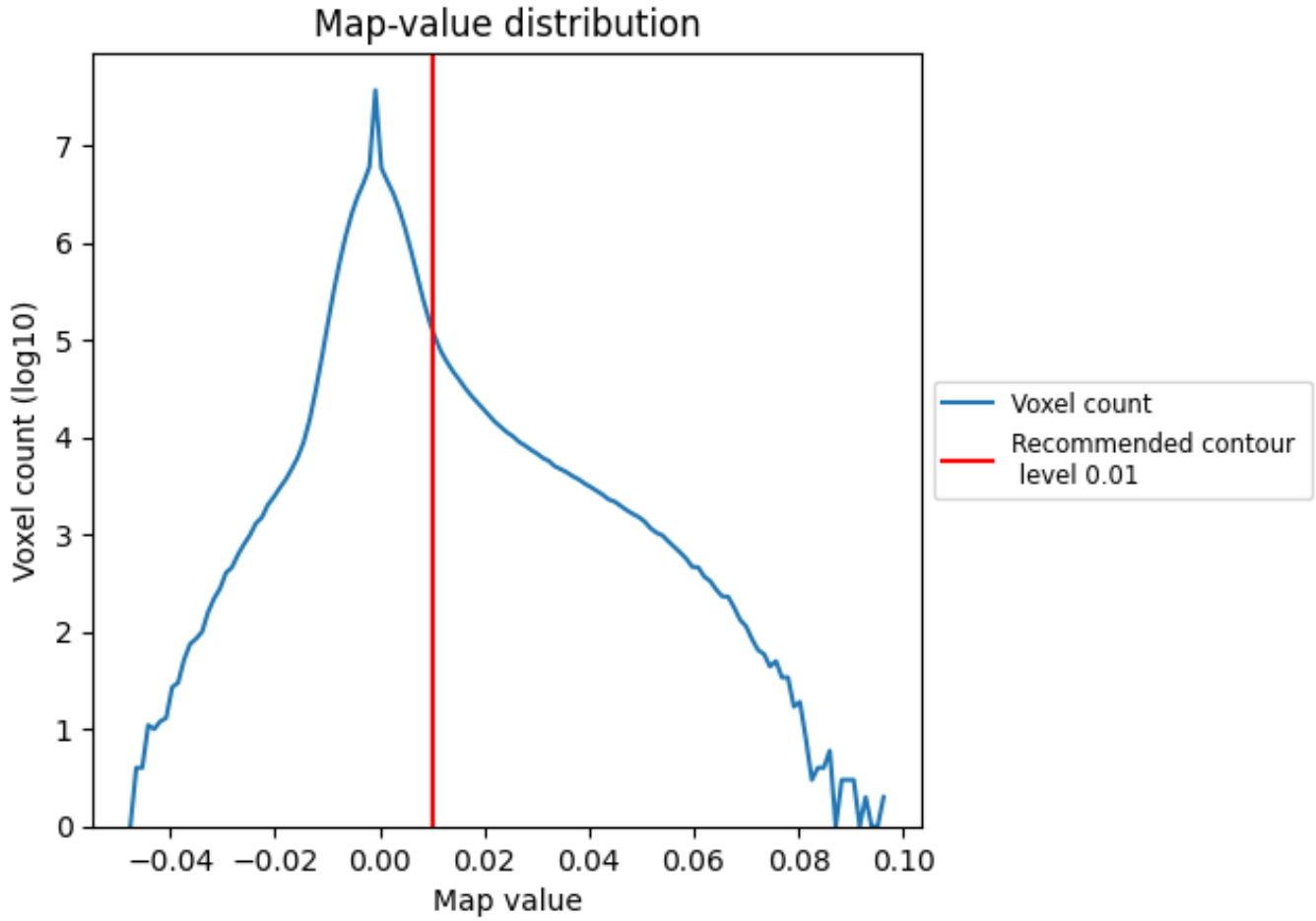
6.6 Mask visualisation (i)

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

7 Map analysis

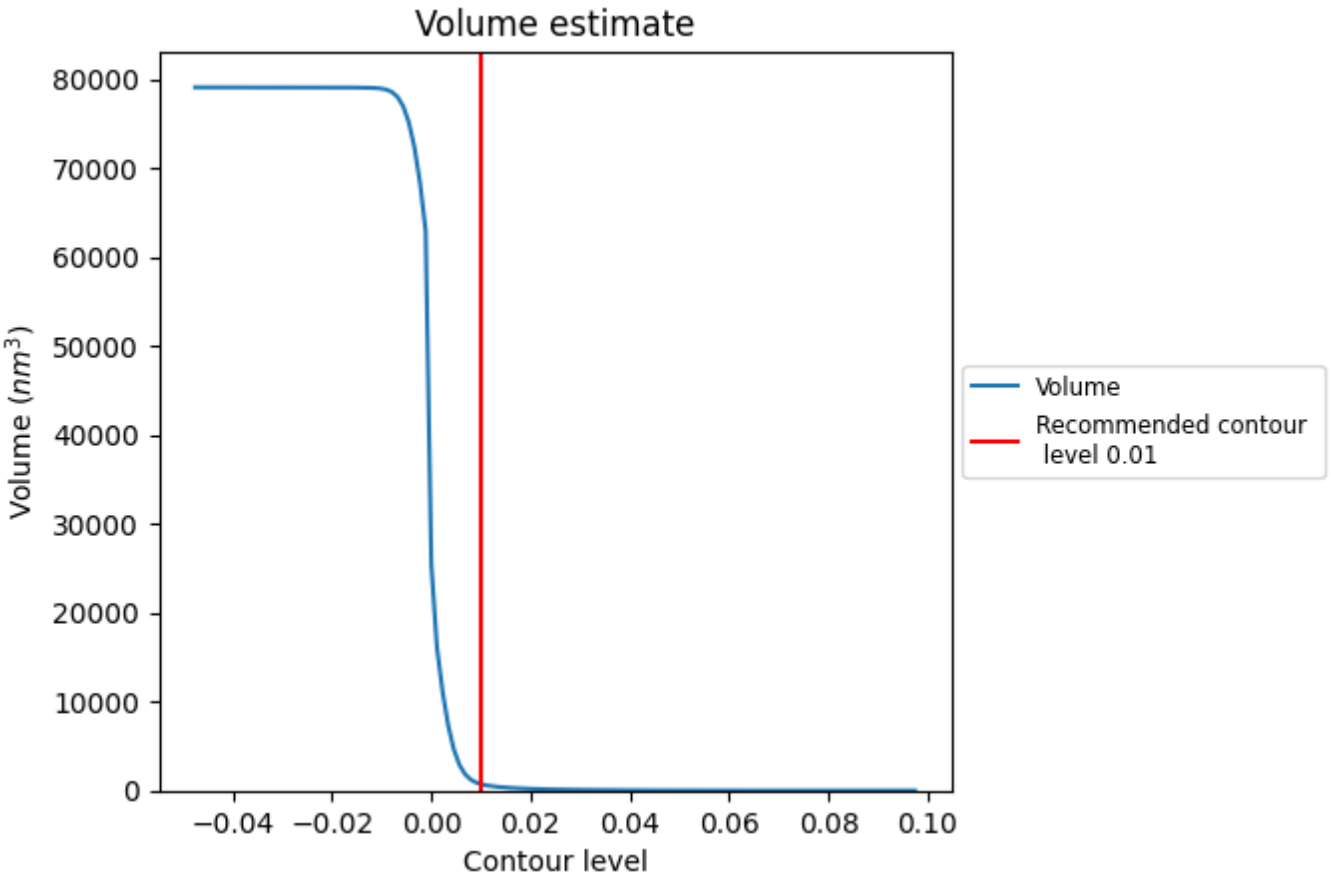
This section contains the results of statistical analysis of the map.

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.

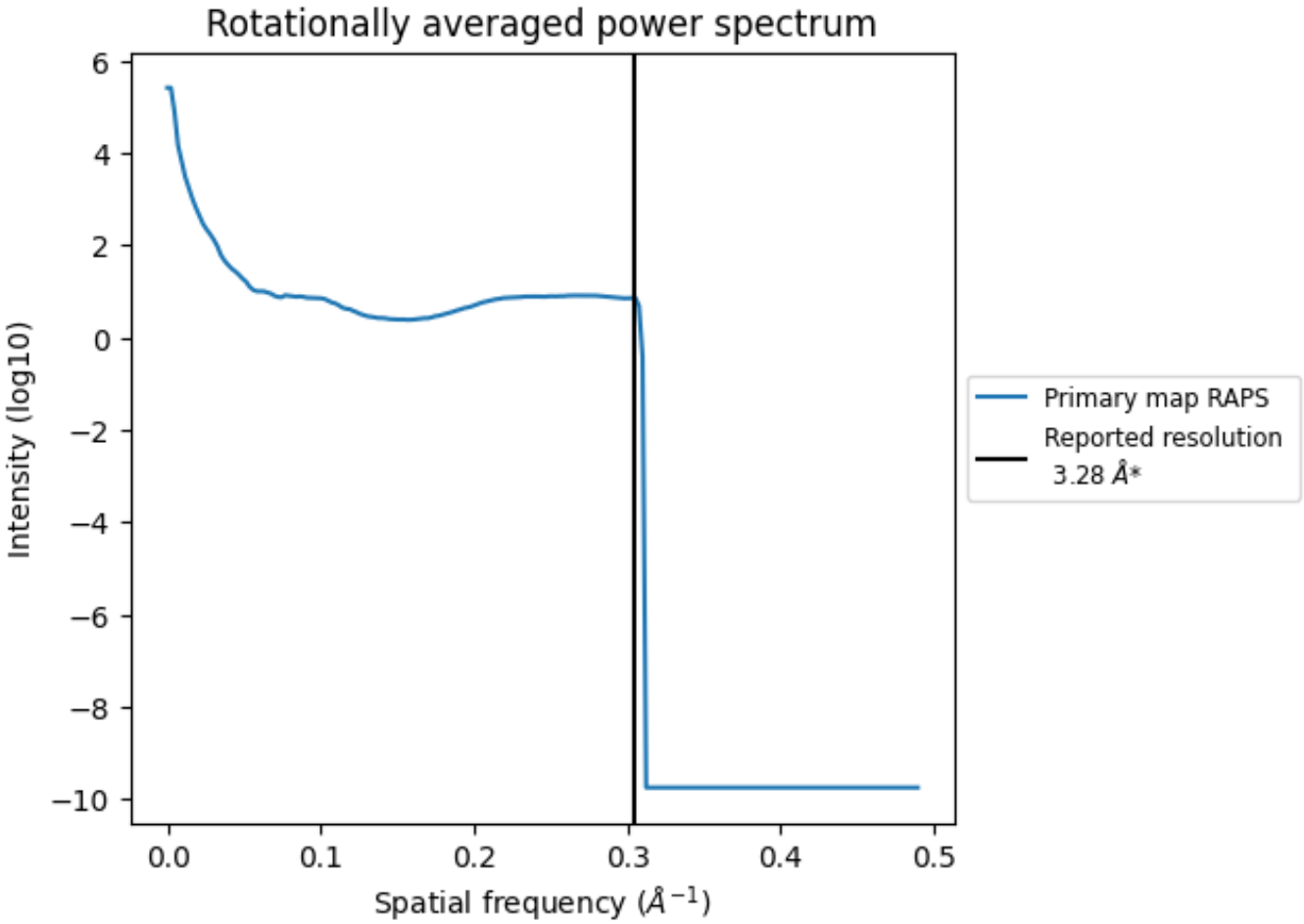
7.2 Volume estimate (i)



The volume at the recommended contour level is 726 nm^3; this corresponds to an approximate mass of 656 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)

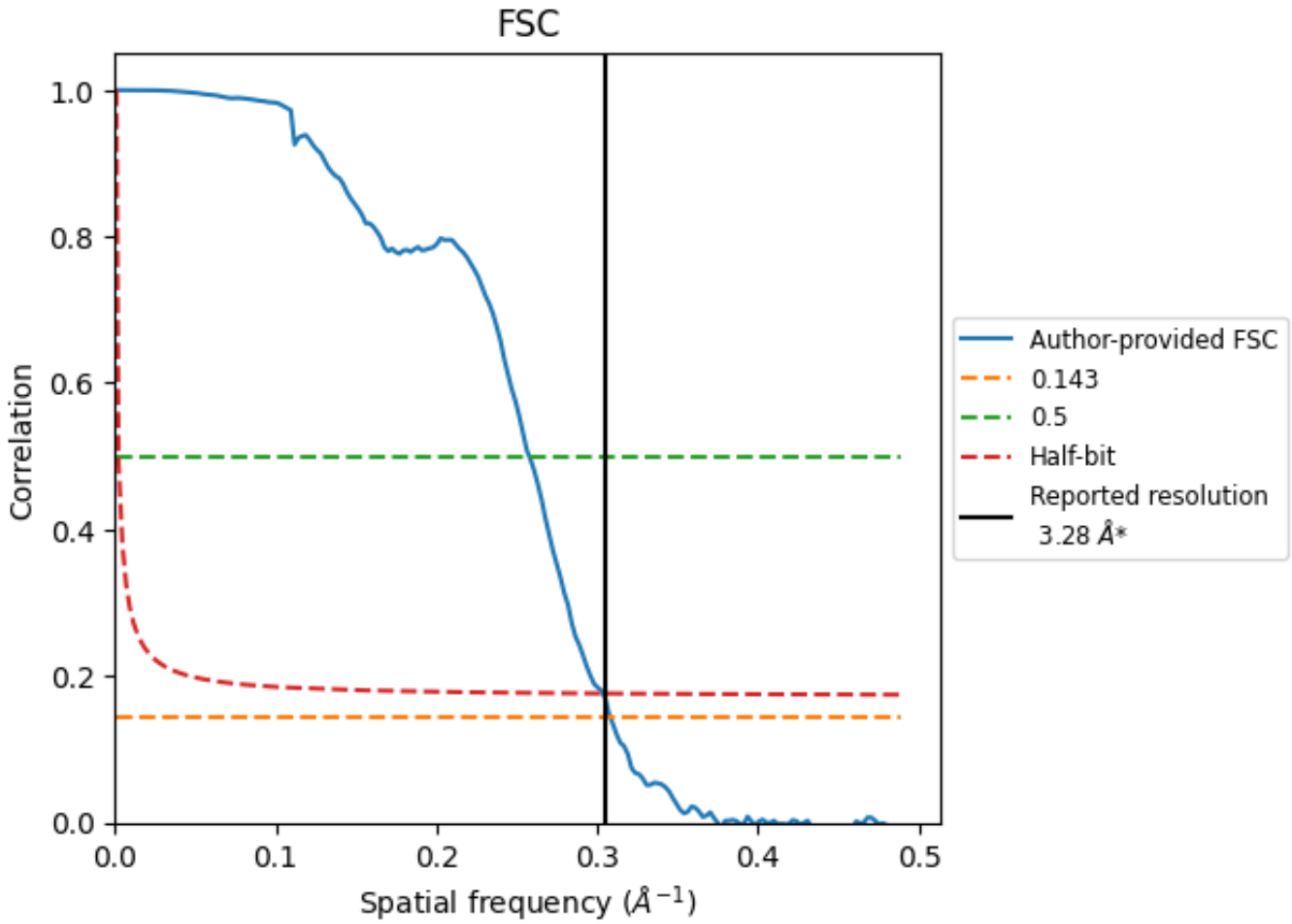


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

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 0.305 Å^{-1}

8.2 Resolution estimates (i)

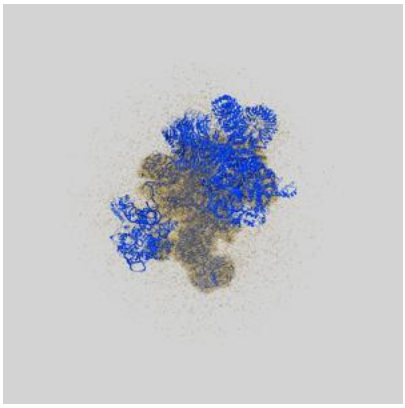
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.24	3.88	3.29
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

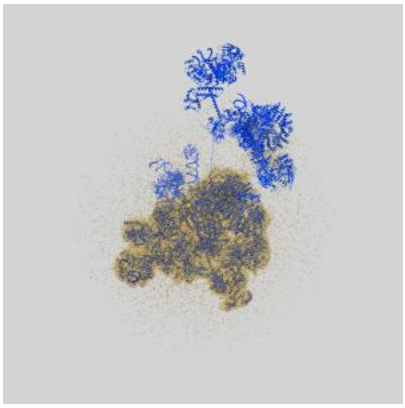
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4665 and PDB model 6QX9. Per-residue inclusion information can be found in section 3 on page 16.

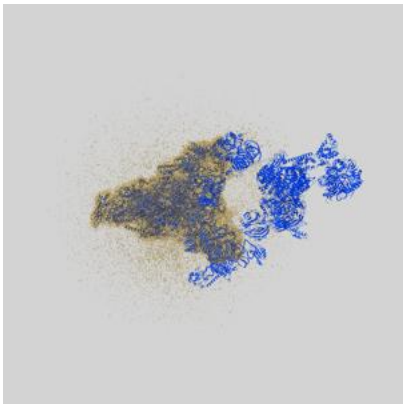
9.1 Map-model overlay



X



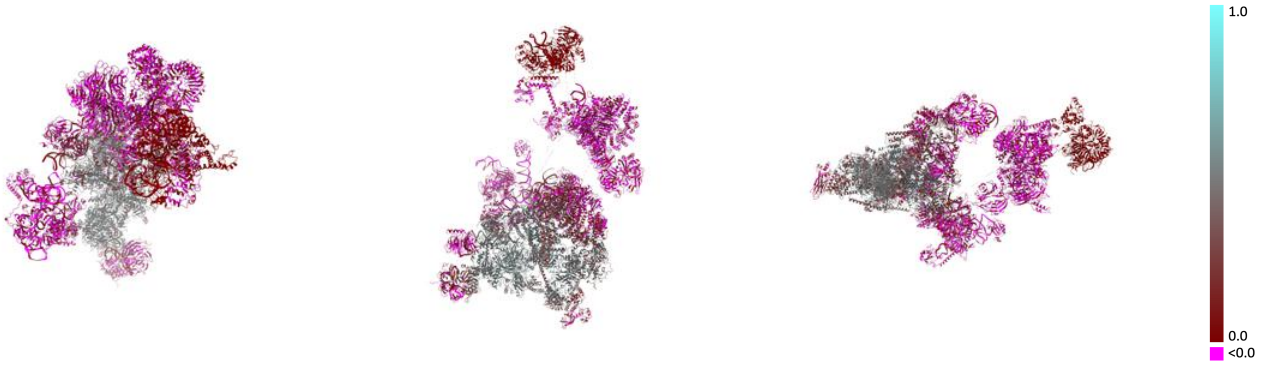
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

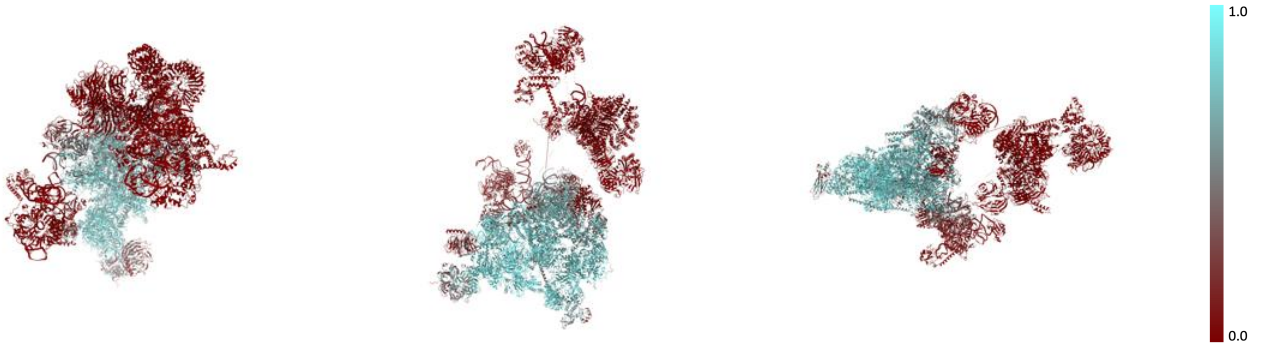
9.2 Q-score mapped to coordinate model (i)



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.

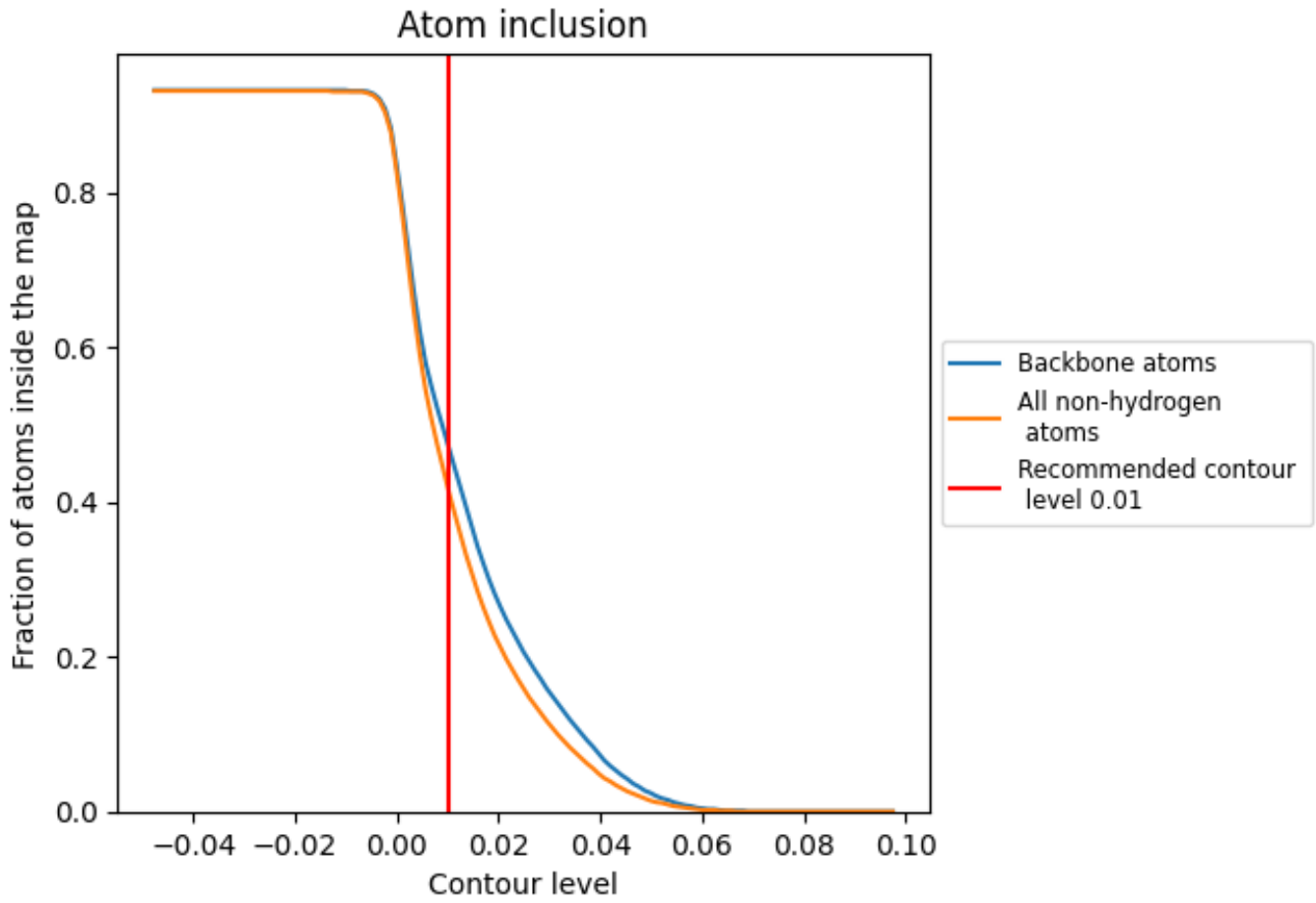
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 42% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4190	0.2070
1	0.0020	0.0030
11	0.0000	-0.0020
12	0.0000	0.0170
13	0.0000	-0.0140
1A	0.0000	0.0280
1C	0.0000	0.0100
1K	0.0010	-0.0000
1b	0.0030	0.0140
1e	0.0000	0.0140
1f	0.0020	0.0020
1g	0.0000	0.0360
2	0.0010	0.0120
21	0.0000	0.0000
22	0.0000	0.0000
23	0.0000	0.0000
2A	0.0000	0.0000
2B	0.0000	0.0000
2b	0.0000	0.0000
2e	0.0000	0.0000
2f	0.0000	0.0000
2g	0.0000	0.0000
4	0.6370	0.2230
41	0.4710	0.2010
42	0.4720	0.2320
43	0.2390	0.0480
4A	0.4880	0.1430
4B	0.5560	0.1550
4C	0.6880	0.3260
4D	0.6860	0.3020
4b	0.2840	0.0870
4e	0.2410	0.0760
4f	0.3330	0.1270
4g	0.2040	0.0230
5	0.7530	0.2980

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Chain	Atom inclusion	Q-score
51	0.4680	0.1340
52	0.4130	0.1040
53	0.7280	0.3830
5A	0.8230	0.4690
5B	0.7650	0.3870
5C	0.8730	0.5100
5D	0.8170	0.4650
5J	0.6500	0.2450
5O	0.1710	0.0160
5X	0.3060	0.1470
5b	0.5770	0.2660
5e	0.4730	0.1160
5f	0.3570	0.0930
5g	0.5680	0.2690
6	0.5610	0.1990
62	0.0050	0.0140
63	0.0100	-0.0020
64	0.0000	-0.0470
65	0.0020	0.0290
66	0.0000	-0.0070
67	0.0020	-0.0100
68	0.0010	0.0250
A1	0.1030	0.0580
A2	0.0000	-0.0020
A3	0.0000	0.0040
B1	0.0010	0.0020
B2	0.0020	0.0090
B3	0.0010	-0.0030
B4	0.0000	-0.0010
B5	0.0040	-0.0090
BP	0.0010	-0.0110
I	0.0040	-0.0000
K	0.0120	0.0130
R	0.6000	0.2310
S	0.6350	0.3130
U	0.8800	0.5060
X	0.5430	0.2760