Full wwPDB EM Validation Report ⓘ

May 2, 2024 – 05:29 PM JST

PDB ID	:	8H6L
EMDB ID	:	EMD-34508
Title	:	Cryo-EM structure of human exon-defined spliceosome in the early B state.
Authors	:	Zhang, W.; Zhan, X.; Zhang, X.; Bai, R.; Lei, J.; Yan, C.; Shi, Y.
Deposited on	:	2022-10-18
Resolution	:	2.60 Å(reported)

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

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

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

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

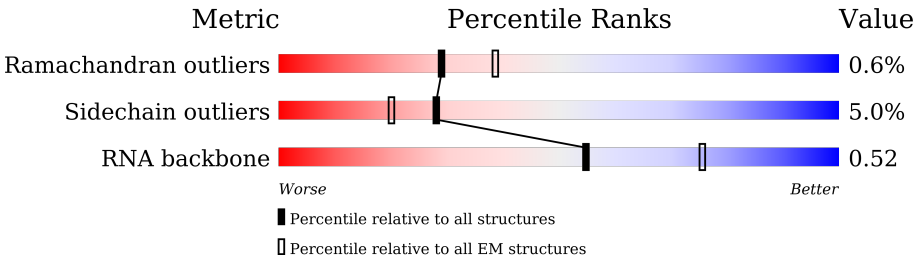
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	144	29% 12% 26% 60%
2	5A	117	38% 72% 26%
3	5B	2335	92%
4	5C	972	80% 5% 16%
5	5D	2136	57% 78% 21%
6	5E	357	80% 81% 16%
7	2a	231	37% 37% 63%
7	4a	231	28% 28% 72%

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Mol	Chain	Length	Quality of chain
7	5a	231	28% 36% 64%
8	2b	119	69% 69% 31%
8	4b	119	68% 69% 31%
8	5b	119	60% 69% 31%
9	2c	118	72% 71% 28%
9	4c	118	59% 63% 37%
9	5c	118	70% 81% 18%
10	2d	86	86% 86% 14%
10	4d	86	81% 83% 17%
10	5d	86	76% 86% 14%
11	2e	92	86% 86% 14%
11	4e	92	85% 85% 15%
11	5e	92	70% 86% 14%
12	2f	76	89% 89% 11%
12	4f	76	92% 96%
12	5f	76	75% 95% 5%
13	2g	126	63% 63% 37%
13	4g	126	56% 56% 44%
13	5g	126	44% 60% 40%
14	6A	107	15% 42% 13% 45%
15	6a	95	95% 91% 5%
16	6b	102	73% 70% 27%
17	6c	139	53% 53% 47%
18	6d	91	79% 78% 21%
19	6e	80	88% 85% 12%

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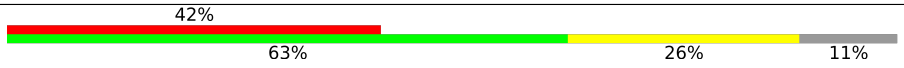
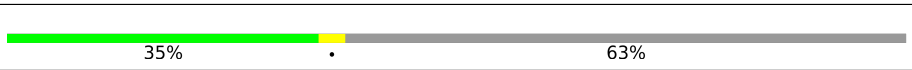
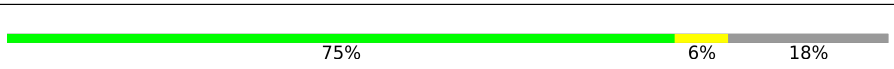
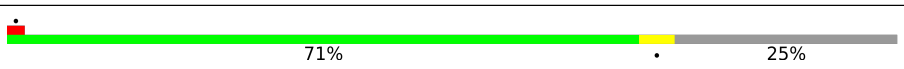
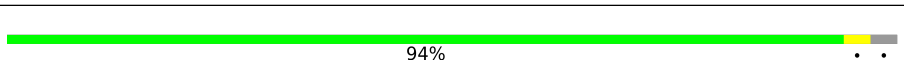
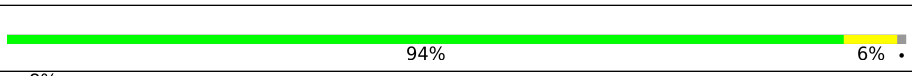
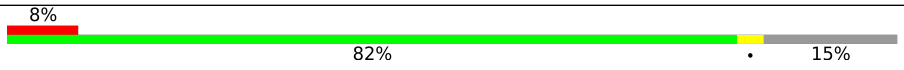
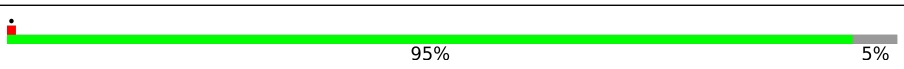
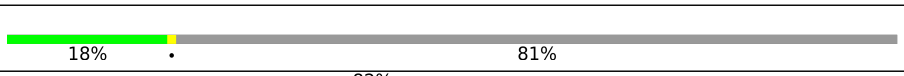
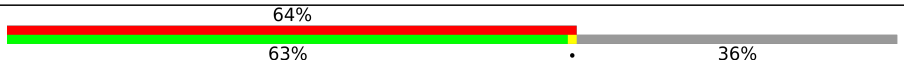
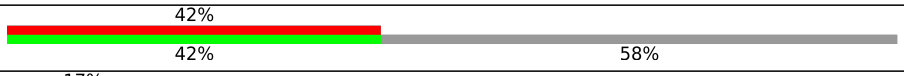
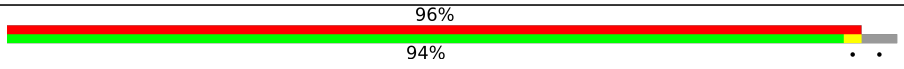
Mol	Chain	Length	Quality of chain
20	6f	103	
21	6g	96	
22	4A	145	
23	4B	683	
24	4C	522	
25	4D	499	
26	4E	128	
27	4F	142	
28	4G	941	
29	4H	177	
30	4I	376	
31	4J	800	
32	4Z	513	
33	2A	188	
34	2B	255	
35	2C	225	
36	2D	793	
37	2E	464	
38	2F	501	
39	2G	1304	
40	2H	895	
41	2I	1217	
42	2J	424	
43	2K	125	
44	2L	110	

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Mol	Chain	Length	Quality of chain
45	2M	86	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 94667 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 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	57	Total	C	N	O	P	0	0
			1187	531	183	416	57		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	115	Total	C	N	O	P	0	0
			2420	1084	403	818	115		

- Molecule 3 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	2253	Total	C	N	O	S	0	0
			18642	11992	3250	3319	81		

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5C	818	Total	C	N	O	S	0	0
			6436	4114	1085	1205	32		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5D	1696	Total	C	N	O	S	0	0
			13633	8715	2329	2519	70		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5E	299	Total	C	N	O	0	0
			1196	598	299	299		

- Molecule 7 is a protein called Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5a	84	Total 336	C 168	N 84	O 84	0	0
7	4a	64	Total 256	C 128	N 64	O 64	0	0
7	2a	86	Total 344	C 172	N 86	O 86	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	5b	82	Total 328	C 164	N 82	O 82	0	0
8	4b	82	Total 334	C 170	N 82	O 82	0	0
8	2b	82	Total 328	C 164	N 82	O 82	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	5c	97	Total 388	C 194	N 97	O 97	0	0
9	4c	74	Total 300	C 152	N 74	O 74	0	0
9	2c	85	Total 340	C 170	N 85	O 85	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	5d	74	Total 296	C 148	N 74	O 74	0	0
10	4d	71	Total 292	C 150	N 71	O 71	0	0
10	2d	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	5e	79	Total 316	C 158	N 79	O 79	0	0
11	4e	78	Total 314	C 158	N 78	O 78	0	0
11	2e	79	Total 316	C 158	N 79	O 79	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	5f	72	Total 288	C 144	N 72	O 72	0	0
12	4f	73	Total 298	C 152	N 73	O 73	0	0
12	2f	68	Total 272	C 136	N 68	O 68	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	5g	76	Total 304	C 152	N 76	O 76	0	0
13	4g	71	Total 288	C 146	N 71	O 71	0	0
13	2g	80	Total 320	C 160	N 80	O 80	0	0

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6A	59	Total 1251	C 558	N 230	O 404	P 59	0	0

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	6a	90	Total 360	C 180	N 90	O 90	0	0

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	6b	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6c	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	6d	72	Total 288	C 144	N 72	O 72	0	0

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	6e	70	Total 280	C 140	N 70	O 70	0	0

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	6f	65	Total 260	C 130	N 65	O 65	0	0

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	6g	61	Total 244	C 122	N 61	O 61	0	0

- Molecule 22 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4A	129	Total 2744	C 1225	N 472	O 917	P 130	0	0

- Molecule 23 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4B	256	Total	C	N	O	S	0	0
			2076	1316	385	367	8		

- Molecule 24 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4C	426	Total	C	N	O	S	0	0
			3370	2118	612	620	20		

- Molecule 25 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4D	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

- Molecule 26 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4E	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 27 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4F	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 28 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4G	801	Total	C	N	O	S	0	0
			5504	3419	1043	1026	16		

- Molecule 29 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4H	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 30 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4I	75	Total	C	N	O	S	0	0
			494	304	96	91	3		

- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4J	153	Total	C	N	O	S	0	0
			1153	715	206	230	2		

- Molecule 32 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4Z	420	Total	C	N	O	0	0
			2093	1253	420	420		

- Molecule 33 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2A	109	Total	C	N	O	P	0	0
			2311	1032	396	774	109		

- Molecule 34 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	2B	162	Total	C	N	O	0	0
			648	324	162	162		

- Molecule 35 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
35	2C	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 36 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2D	236	Total	C	N	O	S	0	0
			1380	793	285	299	3		

- Molecule 37 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	2E	94	Total 376	C 188	N 94	O 94	0	0

- Molecule 38 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2F	423	Total 1693	C 847	N 423	O 423	0	0

- Molecule 39 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	2G	1048	Total 4192	C 2096	N 1048	O 1048	0	0

- Molecule 40 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2H	213	Total 959	C 510	N 220	O 226	S 3	0	0

- Molecule 41 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	2I	1168	Total 4672	C 2336	N 1168	O 1168	0	0

- Molecule 42 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2J	78	Total 312	C 156	N 78	O 78	0	0

- Molecule 43 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2K	108	Total 432	C 216	N 108	O 108	0	0

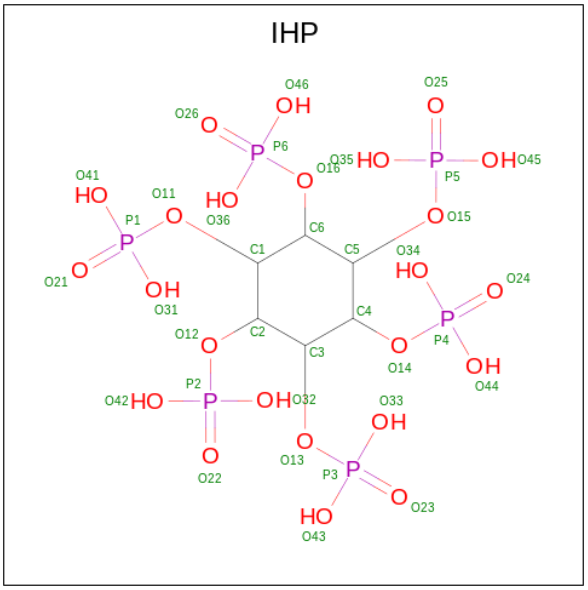
- Molecule 44 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2L	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 45 is a protein called Splicing factor 3B subunit 5.

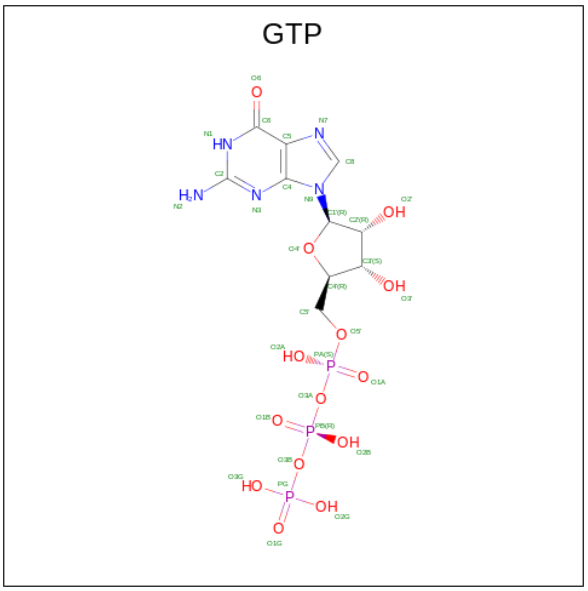
Mol	Chain	Residues	Atoms				AltConf	Trace
45	2M	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 46 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
46	5B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
47	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	5C	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

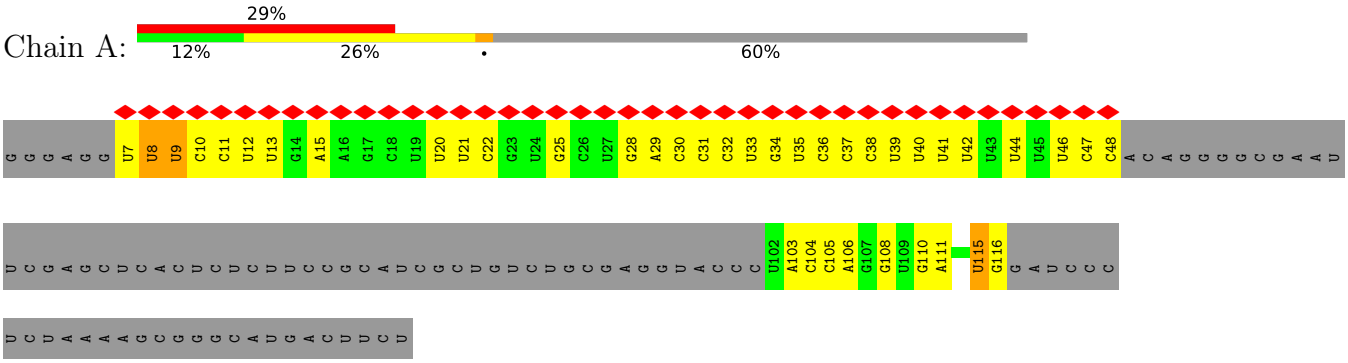
Mol	Chain	Residues	Atoms		AltConf
49	4I	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

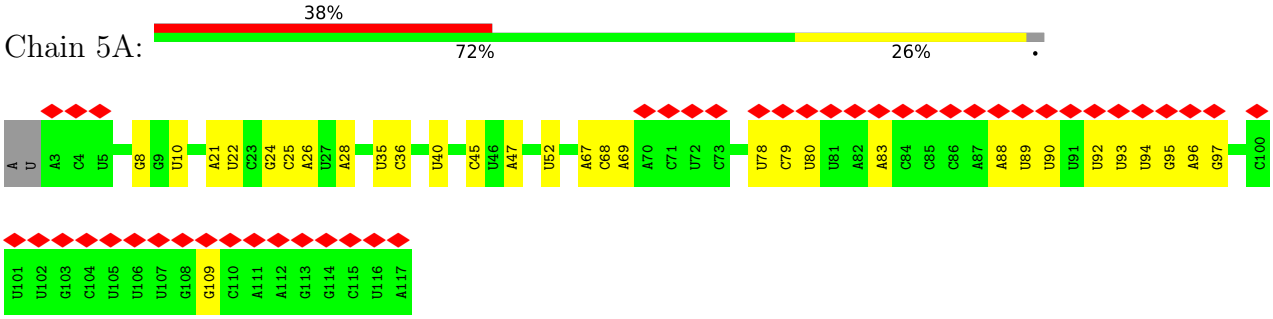
• Molecule 1: pre-mRNA

Chain A:



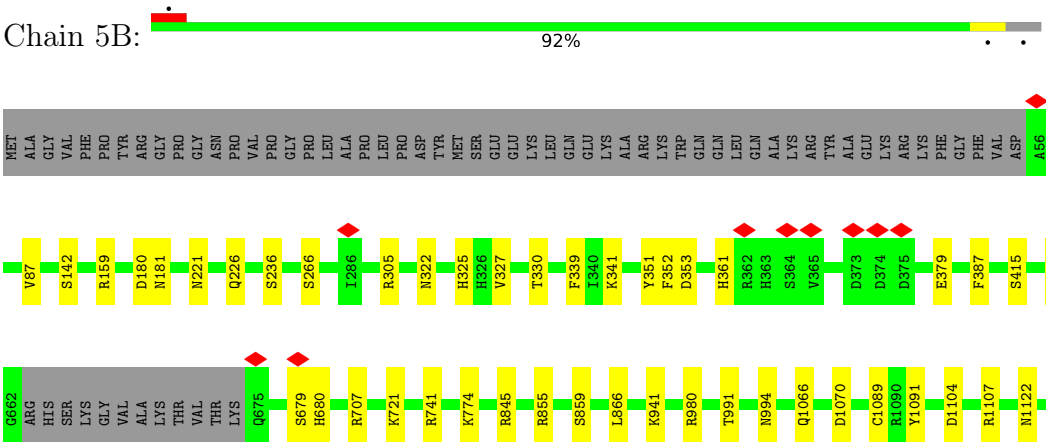
• Molecule 2: U5 snRNA

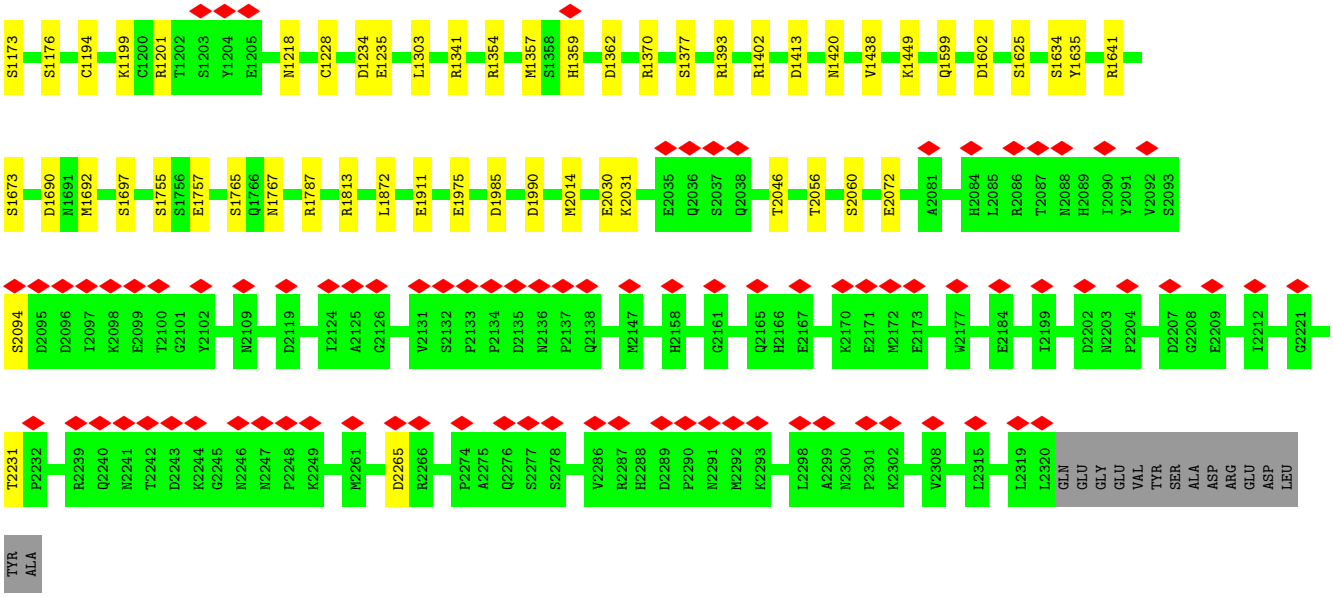
Chain 5A:



• Molecule 3: Pre-mRNA-processing-splicing factor 8

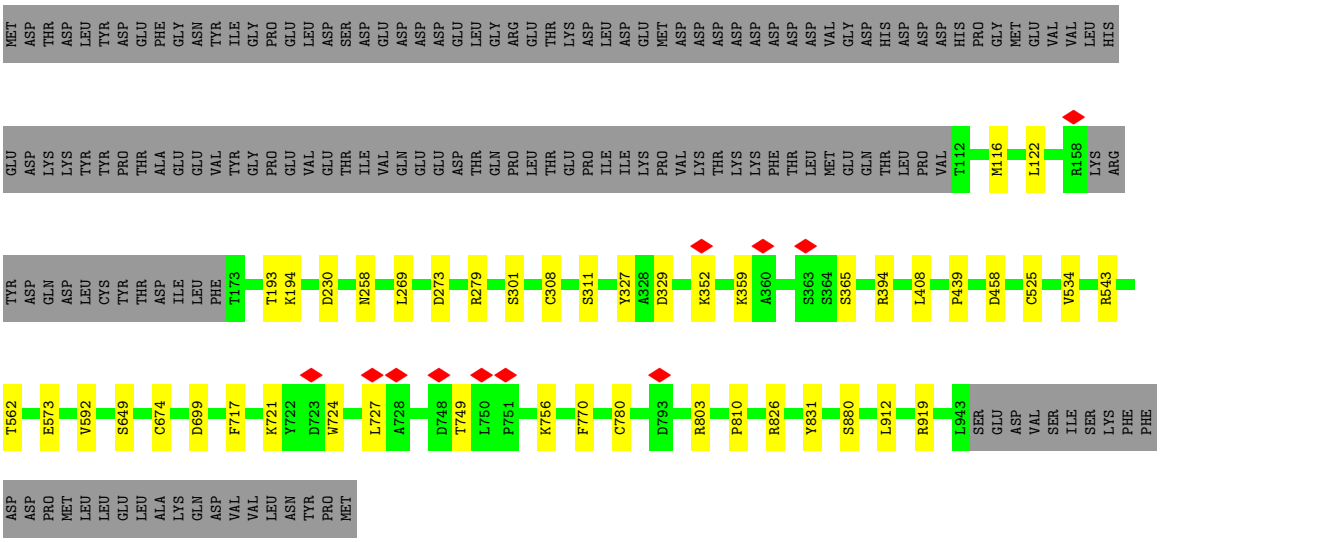
Chain 5B:





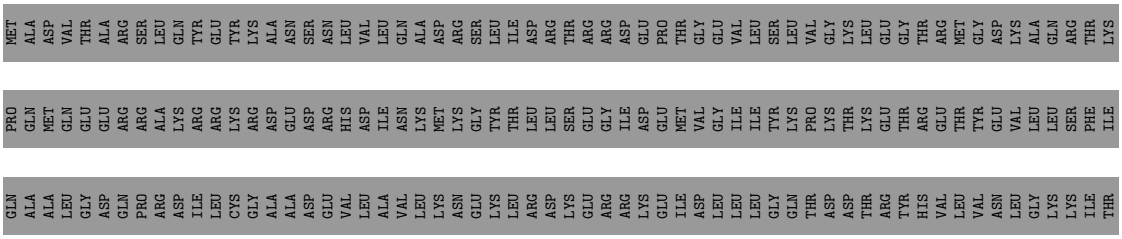
• Molecule 4: 116 kDa U5 small nuclear ribonucleoprotein component

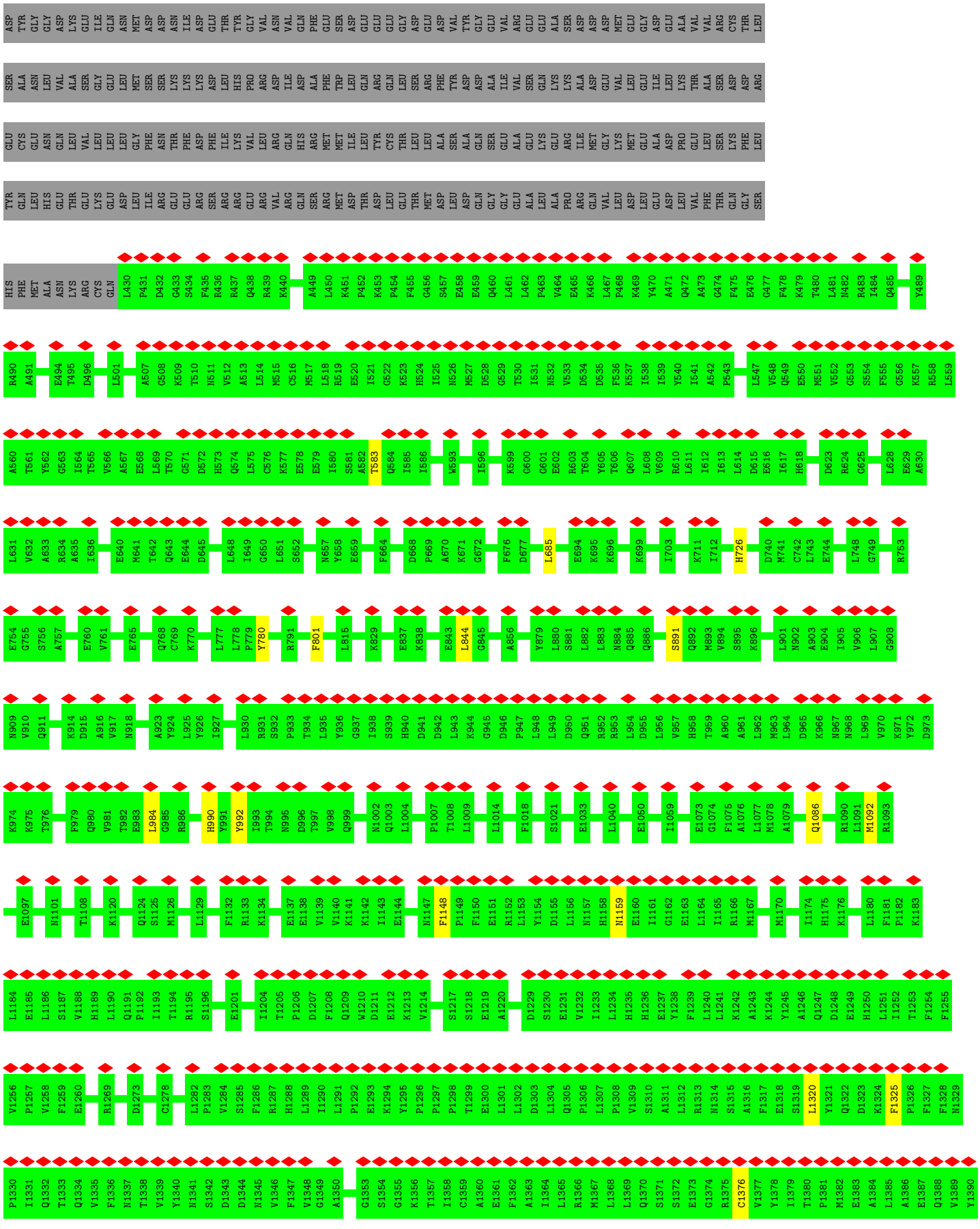
Chain 5C:



• Molecule 5: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain 5D:

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SER ALA ASN LEU VAL ALA SER GLY GLU LEU MET SER SER LYS LYS LYS ASP LEU HIS PRO ARG ASP ILE ASP ALA PHE TRP LEU GLN ARG GLN LEU GLU LEU MET ILE LEU TYR CYS THR LEU LEU ALA SER ALA ASP GLN SER GLU ALA GLU LYS GLU ARG GLN LEU ASP LEU VAL PHE THR GLN GLY SER
GLU CYS GLU ASN GLN LEU VAL LEU LEU LEU GLY PHE ASN THR PHE ASP PHE ILE LYS VAL LEU ARG GLN HIS ARG MET MET ILE LEU TYR CYS THR LEU LEU ALA SER ALA GLN SER GLU ALA GLU LYS GLU ARG GLN LEU ASP LEU ALA ILE MET GLY LYS MET GLU LEU ALA ASP PRO GLU LEU SER LYS PHE LEU
TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP LEU ASP GLN GLY GLY GLU ALA LEU ALA PRO ARG GLN VAL LEU ASP LEU GLU ASP LEU VAL PHE THR GLN GLY SER
HIS PHE MET ALA ASN LYS ARG CYS GLN L430 P431 D432 G433 S434 F435 R436 R437 Q438 R439 K440 A449 L450 K451 P452 K453 P454 F455 G456 S457 E458 E459 Q460 L461 L462 P463 V464 E465 K466 L467 P468 K469 Y470 A471 Q472 A473 G474 F475 E476 G477 F478 K479 T480 L481 N482 R483 I484 Q485 Y489
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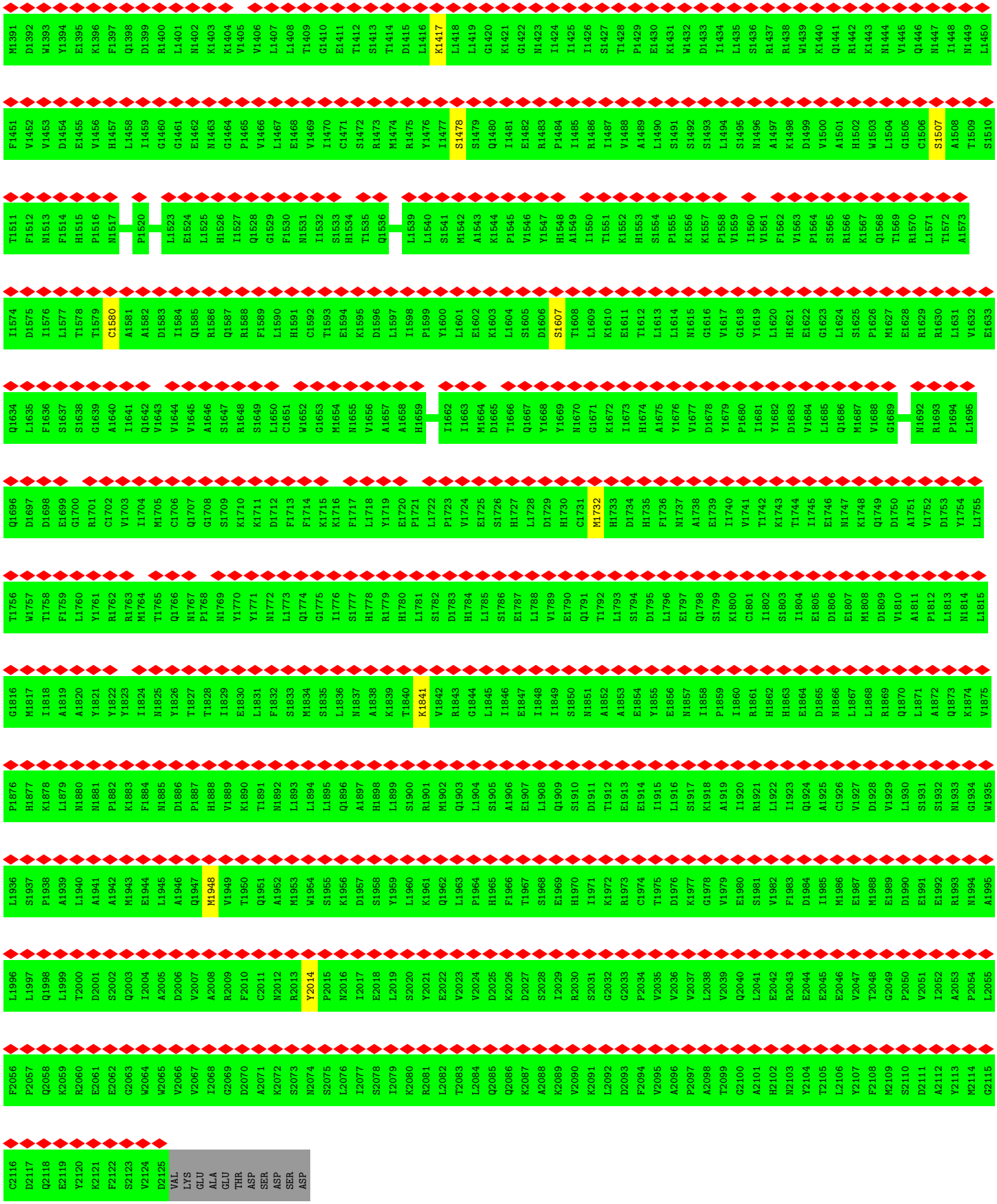
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C2116 D2117 Q2118 E2119 Y2120 K2121 F2122 S2123 V2124 D2125 VAL LYS GLU ALA GLU THR ASP SER ASP SER ASP

• Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

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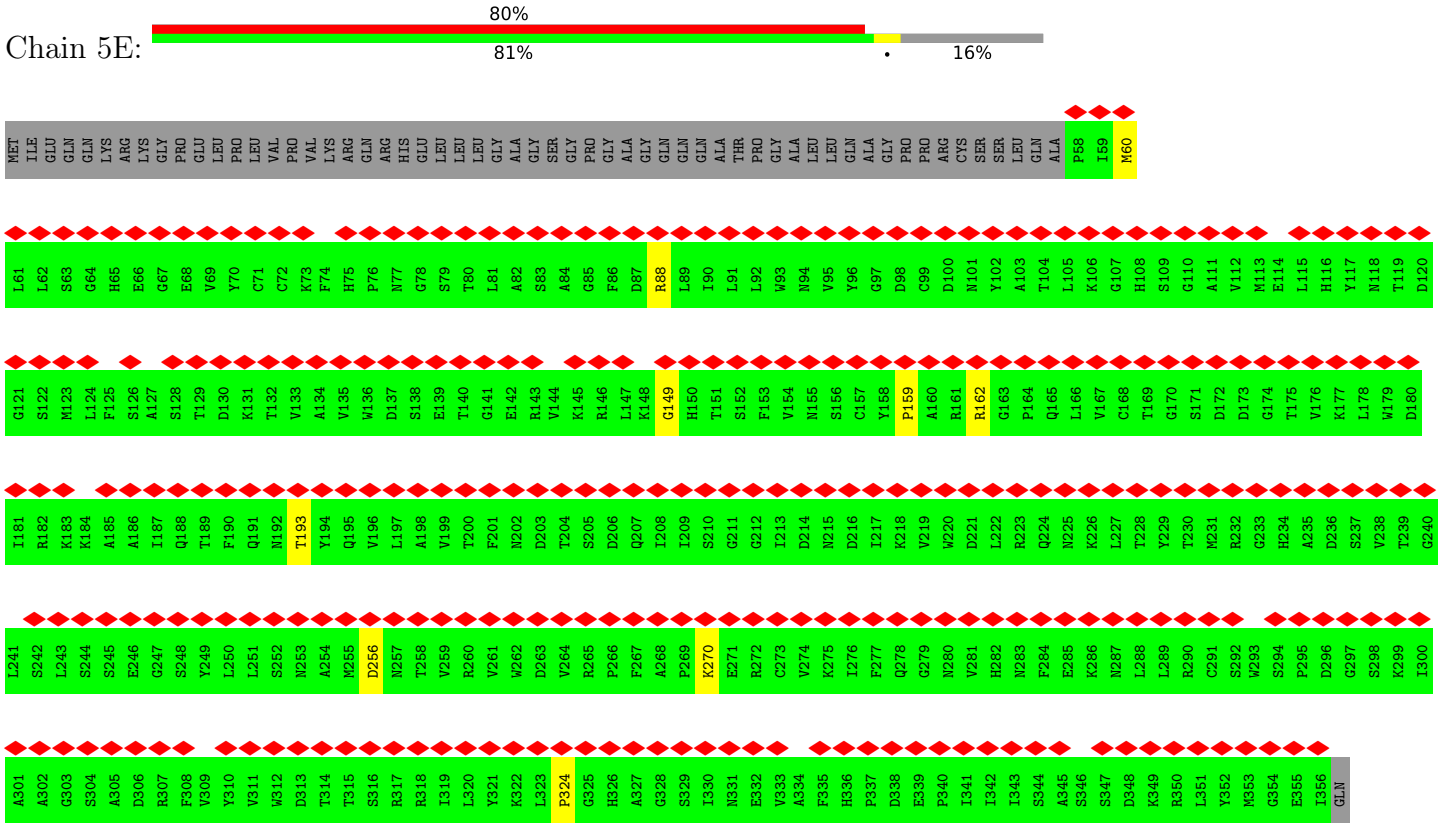
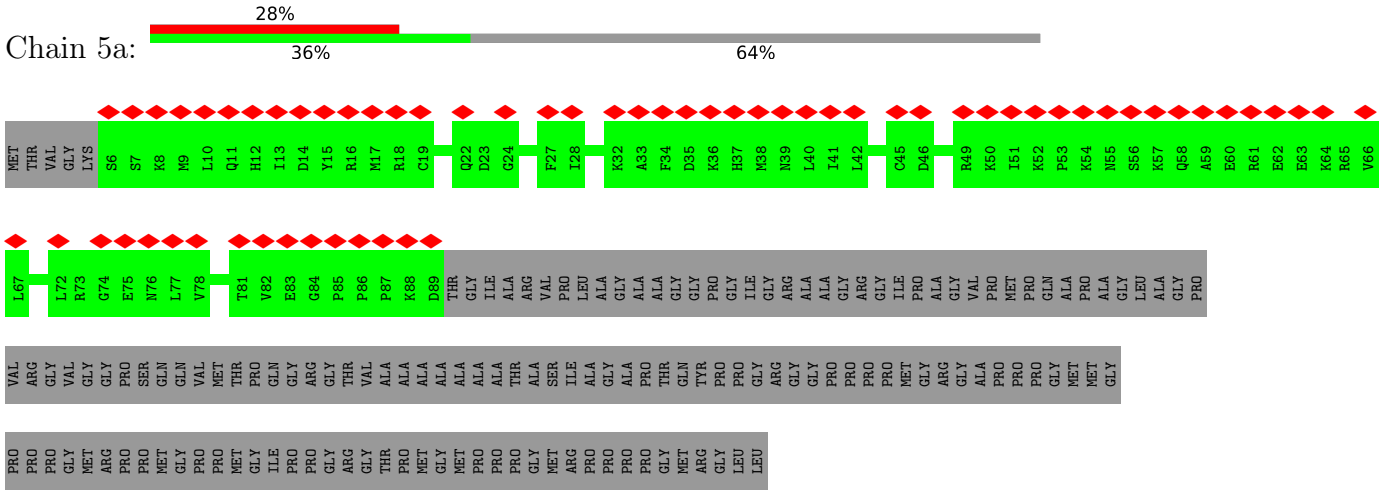


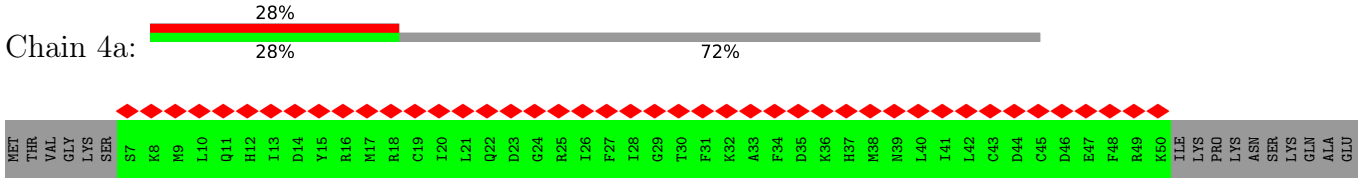
• Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

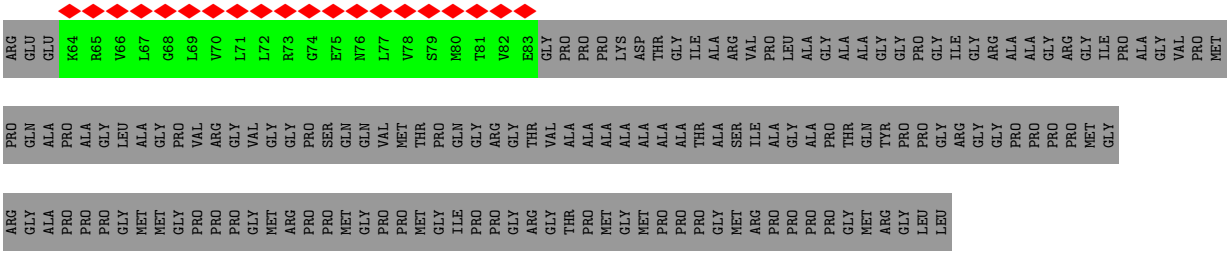
Chain 5a:



• Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

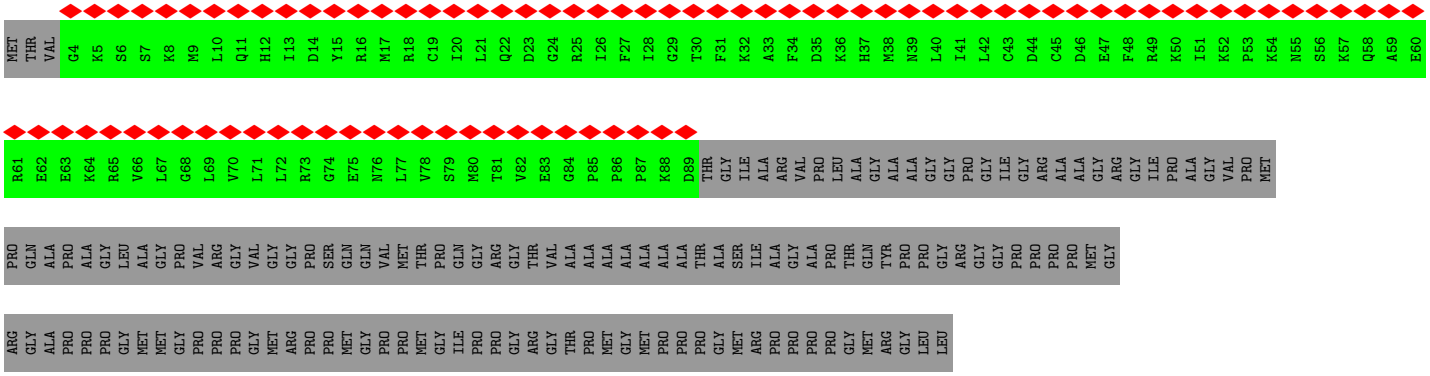
Chain 4a:





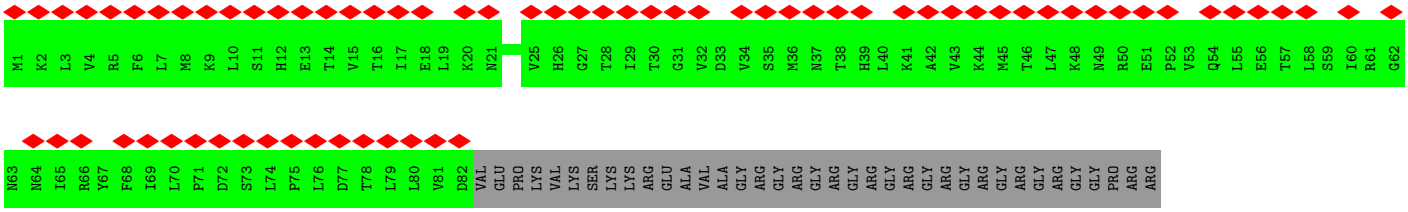
• Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 2a:



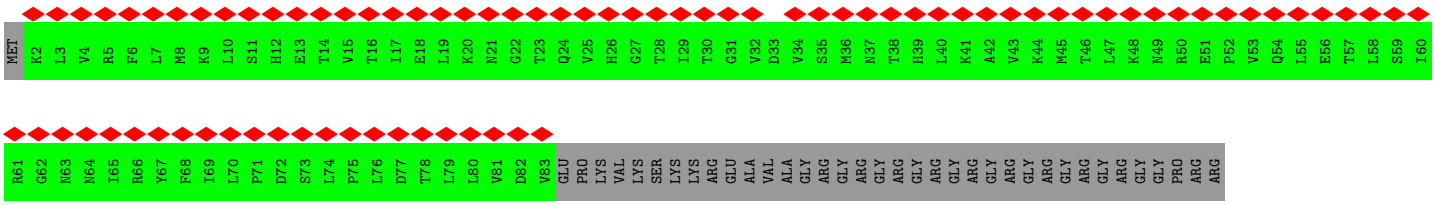
• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain 5b:



• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain 4b:



• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain 2b:

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R61 G62 N63 N64 I65 R66 Y67 F68 I69 L70 P71 D72 S73 L74 P75 L76 D77 T78 L79 L80 V81 D82 VAL GLU PRO LYS VAL LYS SER LYS LYS ARG GLU ALA VAL ALA GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY PRO ARG ARG

- Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain 5c: 70% / 81% • 18%

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG E20 E21 E22 E23 F24 N25 T26 G27 P28 L29 S30 V31 L32 T33 Q34 S35 V36 K37 N38 N39 T40 Q41 V42 L43 I44 N45 K50 K51 L52 L53 G54 R55 V56 K57 A58 F59 D60 R61 H62 C63

N64 M65 V66 L67 E68 N69 V70 K71 E72 M73 W74 T75 E76 V77 P78 K79 S80 G81 K82 G83 K84 K85 K86 S87 K88 P89 V90 N91 K92 D93 R94 S97 K98 M99 F100 L101 R102 G103 D104 S105 V106 I107 V108 V109 L110 R111 N112 P113 L114 I115 A116 GLY LYS

- Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain 4c: 59% / 63% 37%

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG GLU GLU GLU PHE ASN T26 G27 P28 L29 S30 V31 L32 T33 Q34 S35 V36 K37 N38 N39 T40 Q41 V42 L43 I44 N45 C46 R47 N48 N49 K50 K51 L52 L53 G54 R55 V56 K57 A58 F59 D60

R61 H62 C63 N64 M65 V66 L67 E68 N69 V70 K71 E72 M73 W74 T75 GLU VAL PRO LYS SER GLY LYS GLY LYS LYS LYS SER LYS PRO VAL N91 K92 D93 R94 Y95 I96 S97 K98 M99 F100 L101 R102 G103 D104 S105 V106 I107 V108 V109 L110 R111 N112 P113 L114 ILE ALA GLY LYS

- Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain 2c: 72% / 71% • 28%

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG E20 E21 E22 E23 F24 N25 T26 G27 P28 L29 S30 V31 L32 T33 Q34 S35 V36 K37 N38 N39 T40 Q41 V42 L43 I44 N45 C46 R47 N48 N49 K50 K51 L52 L53 G54 R55 V56 K57 A58 F59 D60

R61 H62 C63 N64 M65 V66 L67 E68 N69 V70 K71 E72 M73 W74 T75 E76 VAL PRO LYS SER GLY LYS GLY LYS LYS LYS SER LYS P89 V90 N91 K92 D93 R94 Y95 I96 S97 K98 M99 F100 L101 R102 G103 D104 S105 V106 I107 V108 V109 L110 R111 N112 P113 L114 I115 A116 GLY LYS

- Molecule 10: Small nuclear ribonucleoprotein F

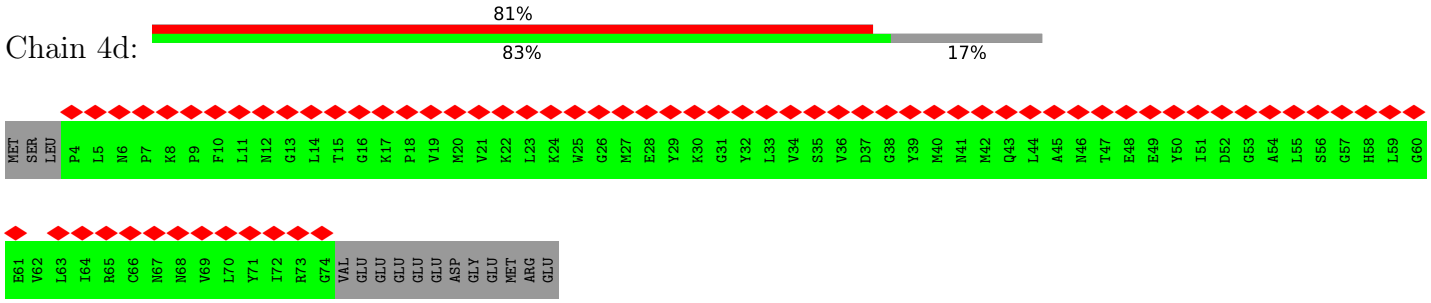
Chain 5d: 76% / 86% 14%

MET S2 L3 P4 L5 N6 P7 K8 P9 F10 L11 N12 G13 L14 T15 G16 K17 P18 V19 M20 V21 K22 L23 K24 W25 G26 M27 E28 Y29 K30 G31 Y32 L33 V34 S35 V36 D37 G38 Y39 M40 N41 M42 Q43 L44 A45 N46 T47 E48 E49 Y50 I51 D52 G53 A54 L55 S56 G57 H58 L59 G60

E61 V62 L63 I64 R65 C66 N67 N68 V69 L70 Y71 I72 R73 G74 V75 GLU GLU GLU GLU GLU ASP GLY GLU MET ARG GLU

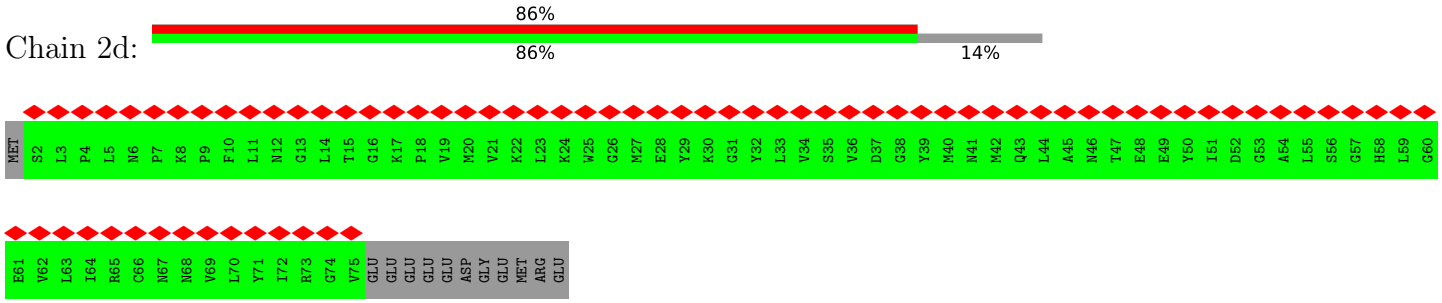
• Molecule 10: Small nuclear ribonucleoprotein F

Chain 4d:



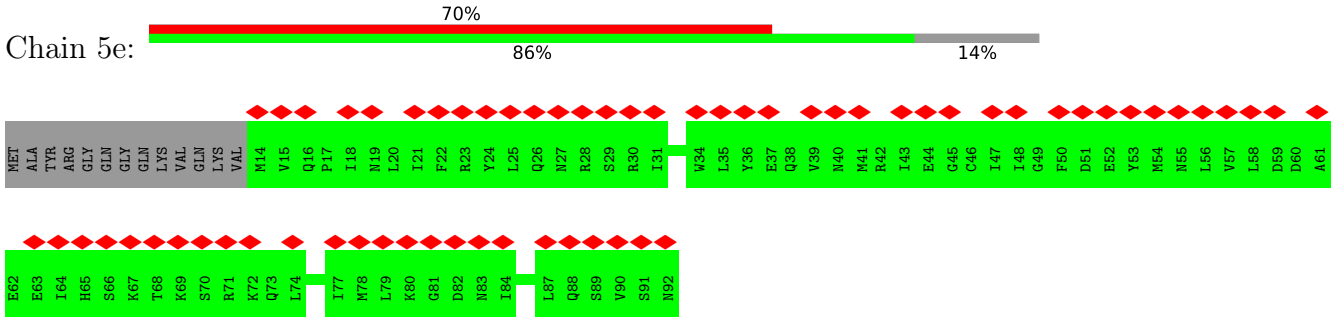
• Molecule 10: Small nuclear ribonucleoprotein F

Chain 2d:



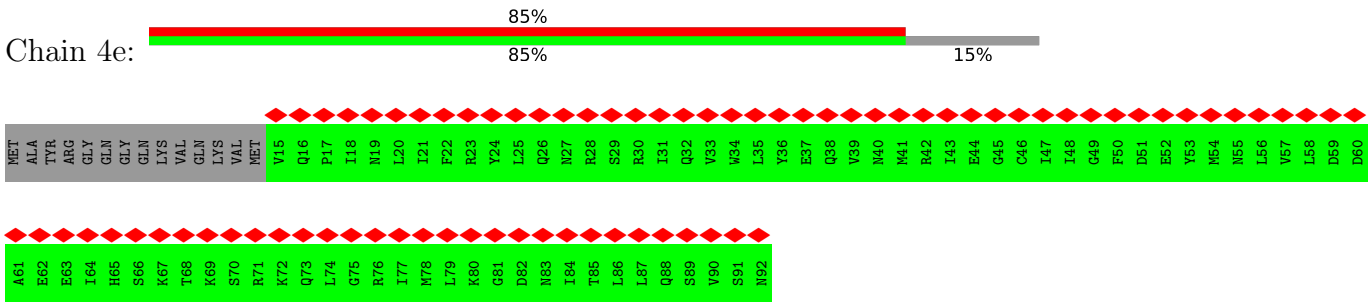
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 5e:



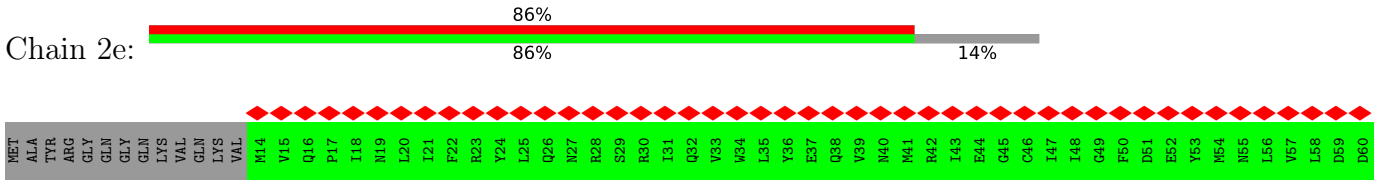
• Molecule 11: Small nuclear ribonucleoprotein E

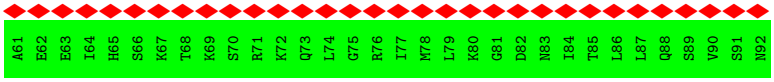
Chain 4e:



• Molecule 11: Small nuclear ribonucleoprotein E

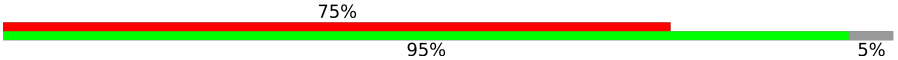
Chain 2e:





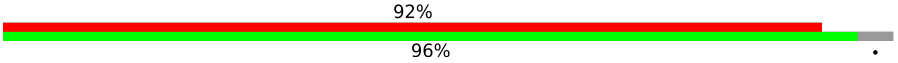
• Molecule 12: Small nuclear ribonucleoprotein G

Chain 5f:



• Molecule 12: Small nuclear ribonucleoprotein G

Chain 4f:

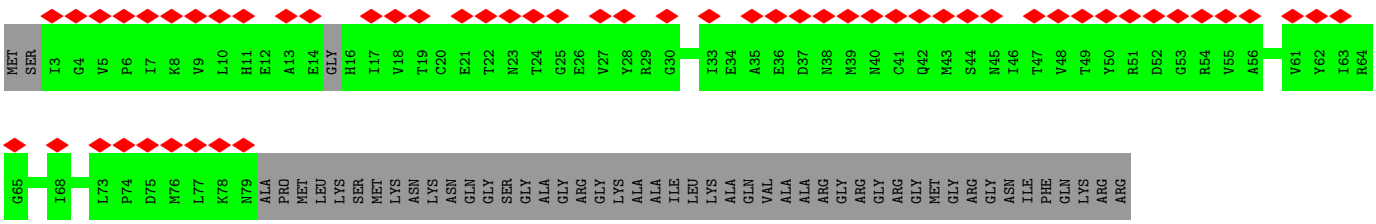


• Molecule 12: Small nuclear ribonucleoprotein G

Chain 2f:

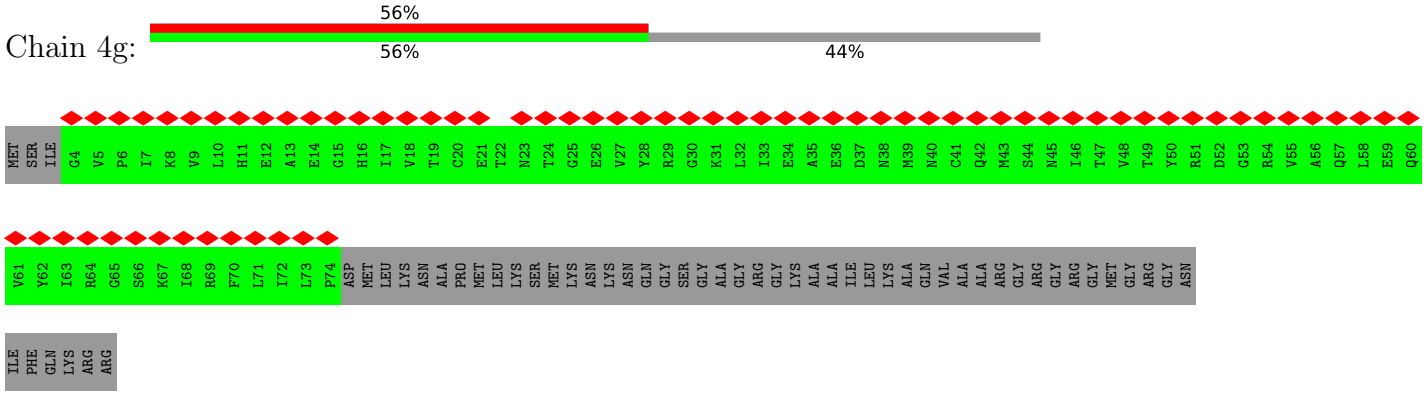
• Molecule 13: Small nuclear ribonucleoprotein Sm D3

Chain 5g:



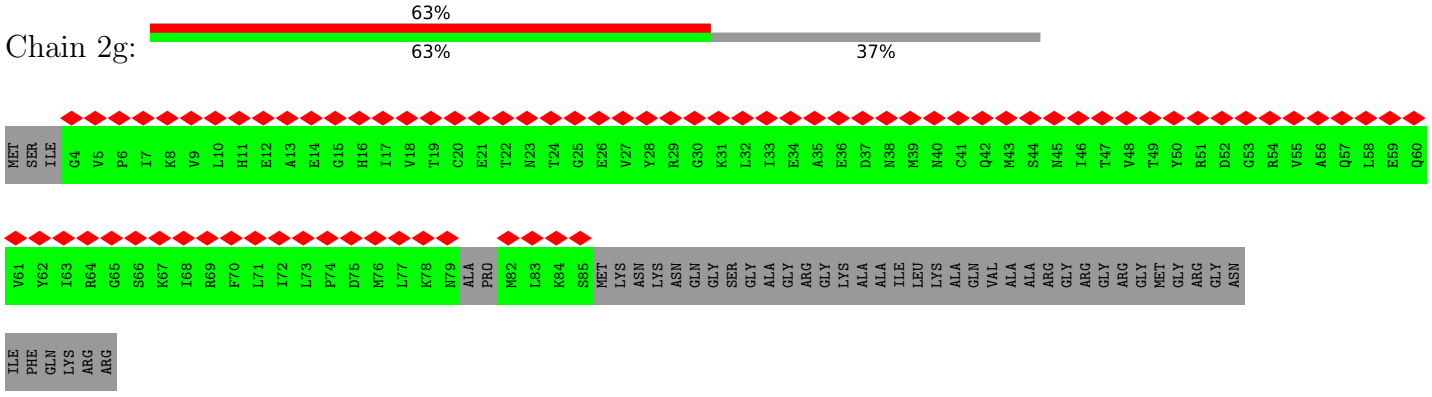
• Molecule 13: Small nuclear ribonucleoprotein Sm D3

Chain 4g:



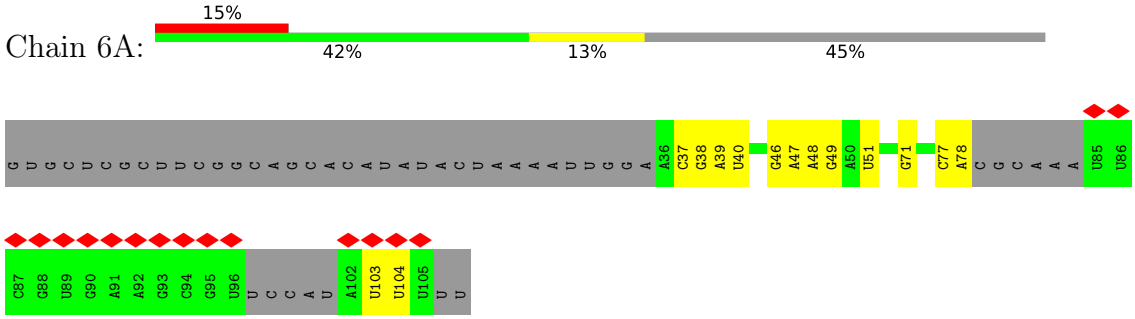
• Molecule 13: Small nuclear ribonucleoprotein Sm D3

Chain 2g:



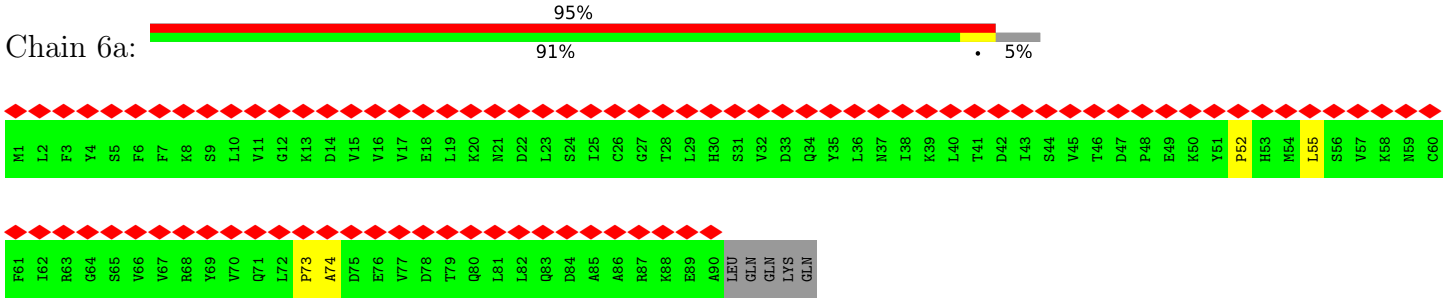
• Molecule 14: U6 snRNA

Chain 6A:



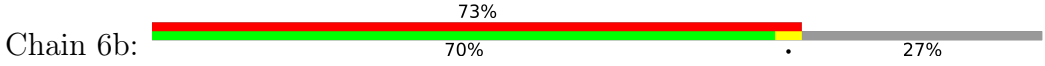
• Molecule 15: U6 snRNA-associated Sm-like protein LSm2

Chain 6a:

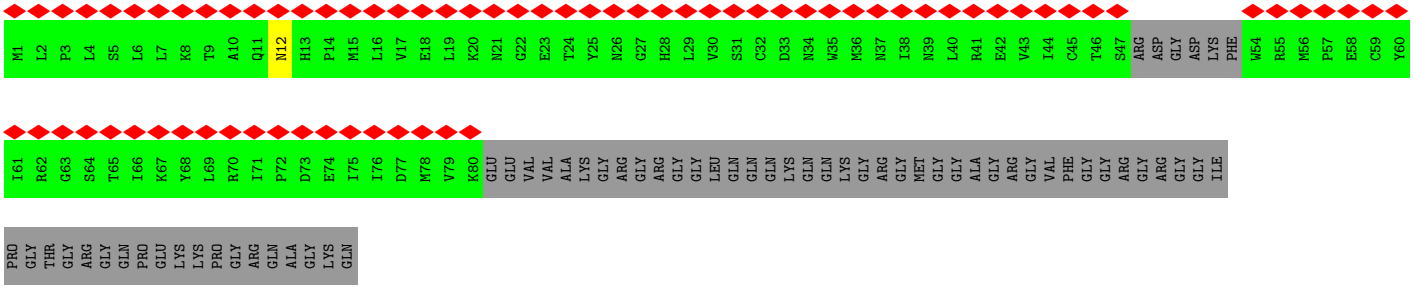


• Molecule 16: U6 snRNA-associated Sm-like protein LSm3

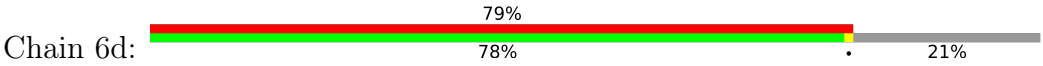
Chain 6b:

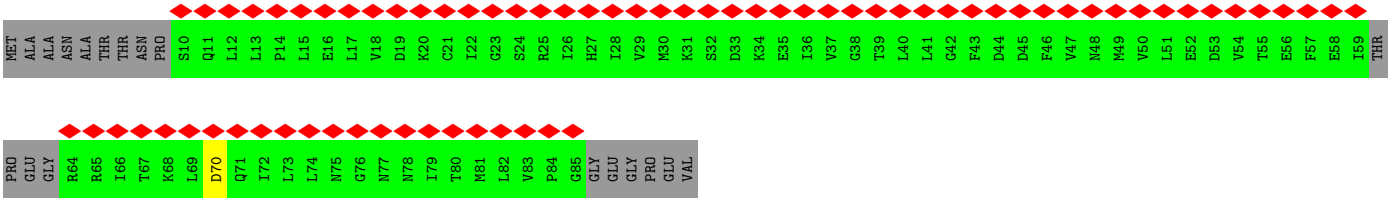


• Molecule 17: U6 snRNA-associated Sm-like protein LSm4

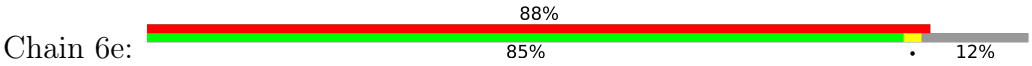


• Molecule 18: U6 snRNA-associated Sm-like protein LSm5

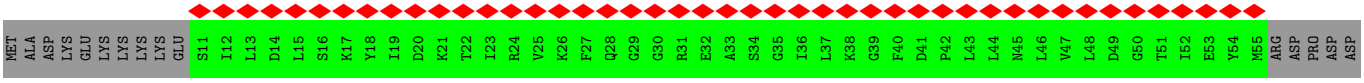


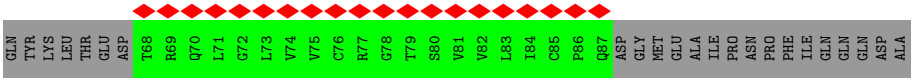


• Molecule 19: U6 snRNA-associated Sm-like protein LSm6



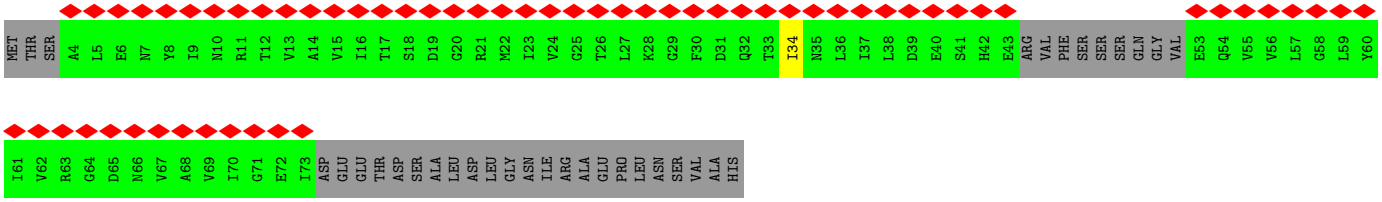
• Molecule 20: U6 snRNA-associated Sm-like protein LSm7





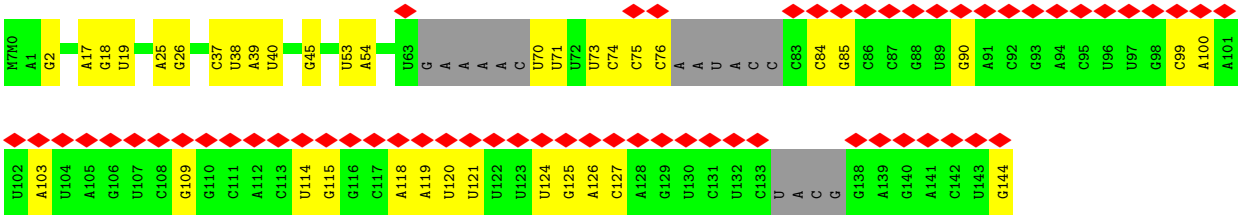
• Molecule 21: U6 snRNA-associated Sm-like protein LSm8

Chain 6g:



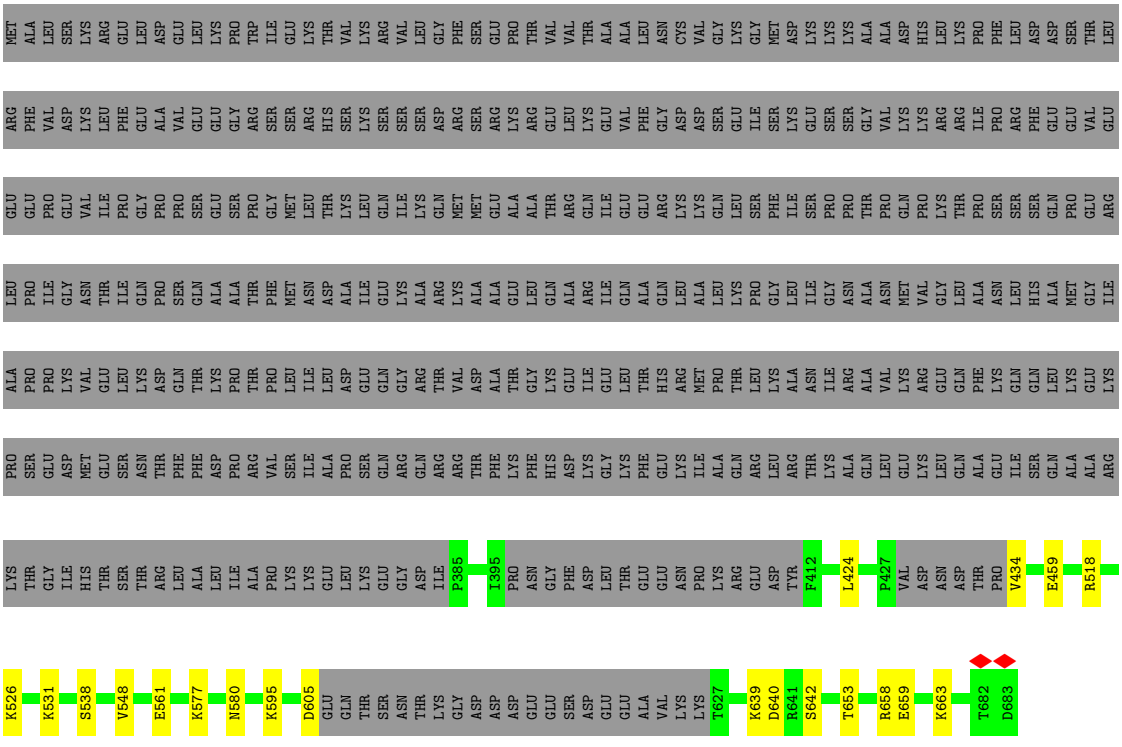
• Molecule 22: U4 snRNA

Chain 4A:



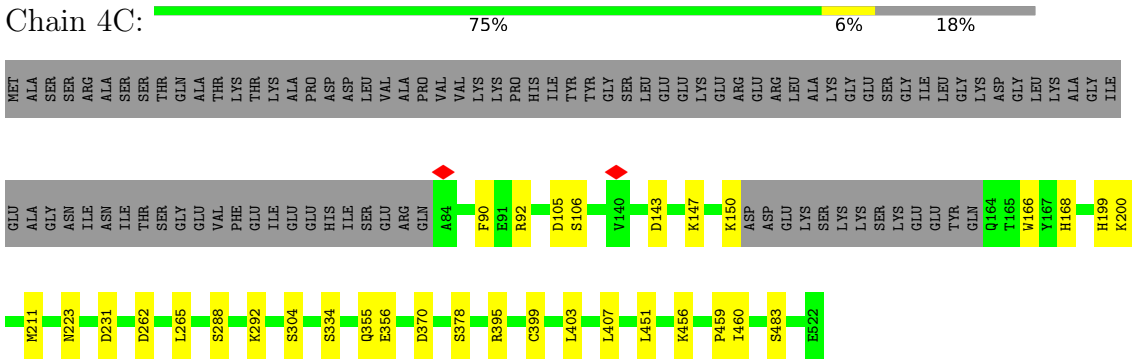
• Molecule 23: U4/U6 small nuclear ribonucleoprotein Prp3

Chain 4B:



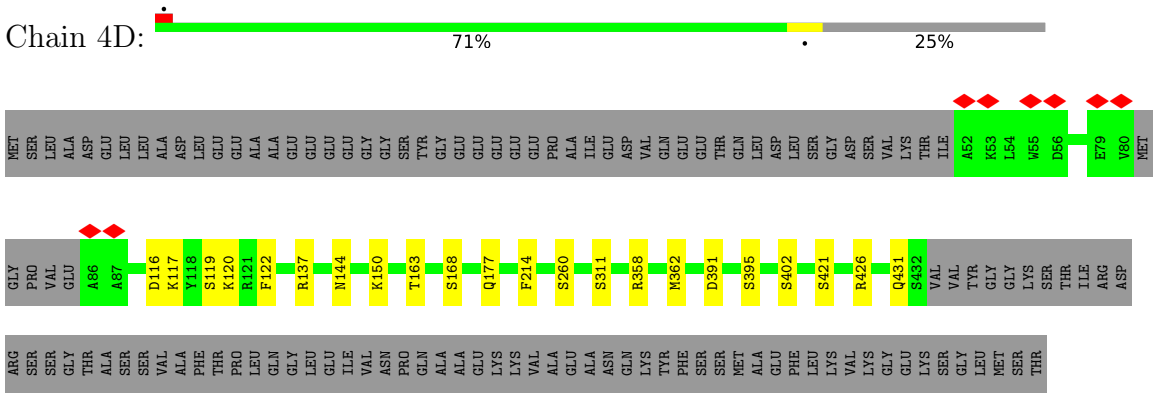
• Molecule 24: U4/U6 small nuclear ribonucleoprotein Prp4

Chain 4C:



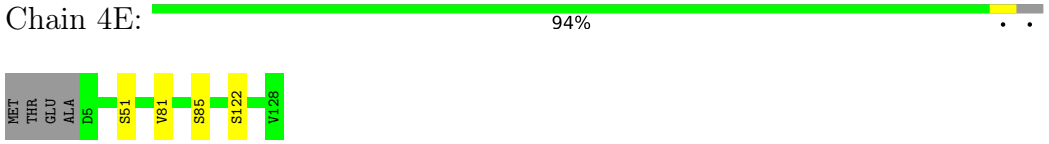
• Molecule 25: U4/U6 small nuclear ribonucleoprotein Prp31

Chain 4D:



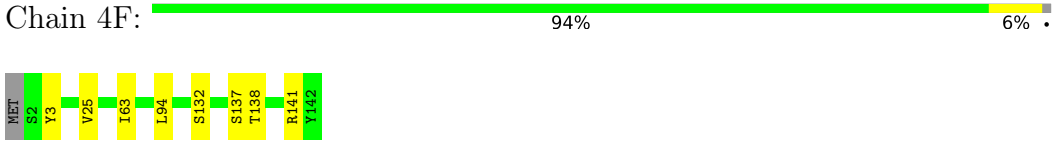
• Molecule 26: NHP2-like protein 1

Chain 4E:



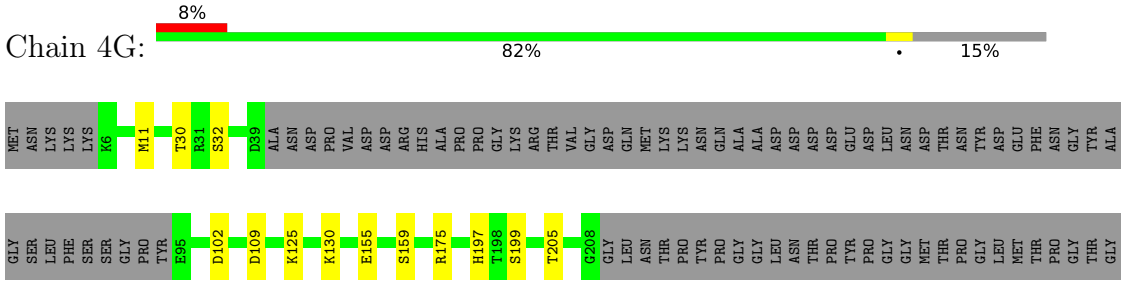
• Molecule 27: Thioredoxin-like protein 4A

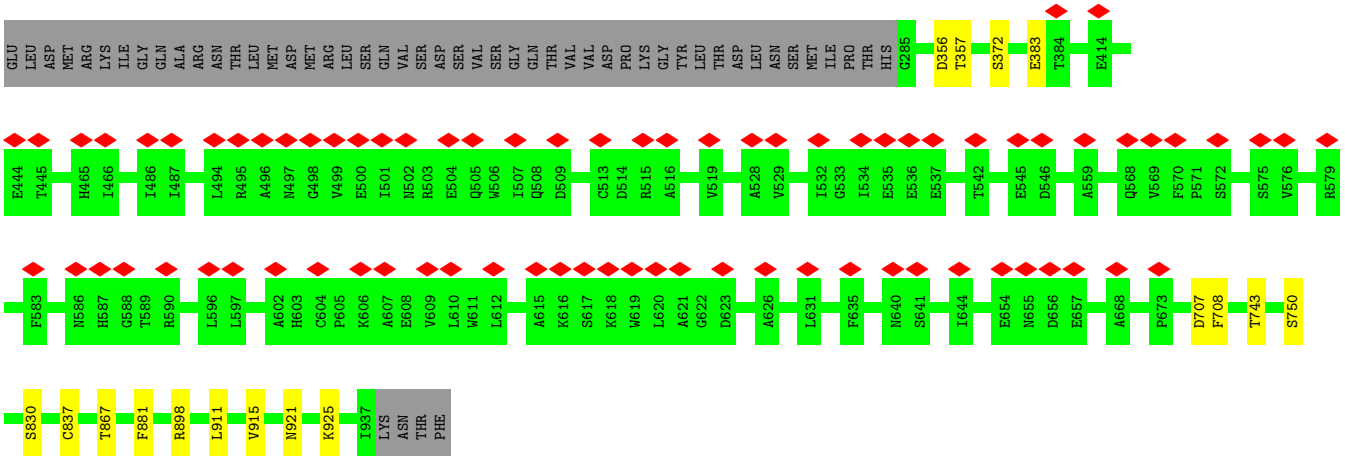
Chain 4F:



• Molecule 28: Pre-mRNA-processing factor 6

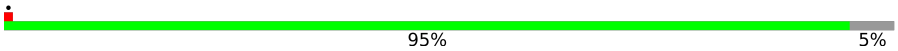
Chain 4G:

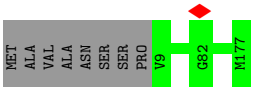




• Molecule 29: Peptidyl-prolyl cis-trans isomerase H

Chain 4H:



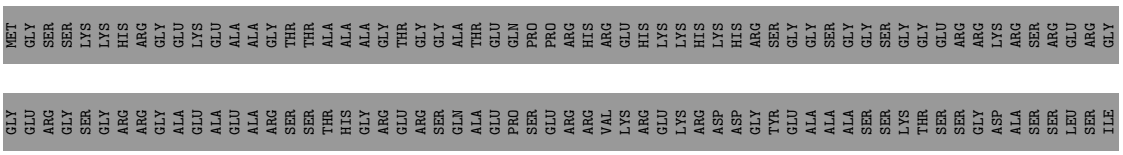


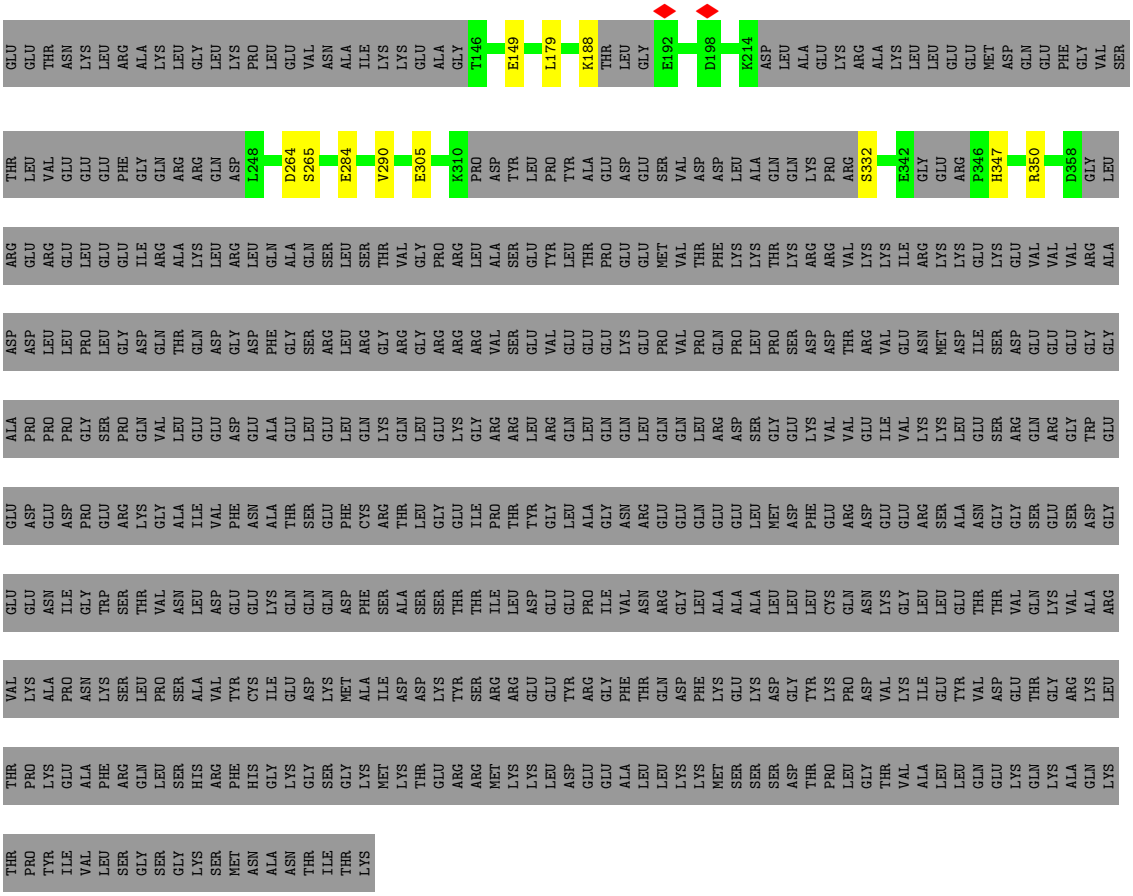
• Molecule 30: WW domain-binding protein 4

Chain 4I:

• Molecule 31: U4/U6.U5 tri-snRNP-associated protein 1

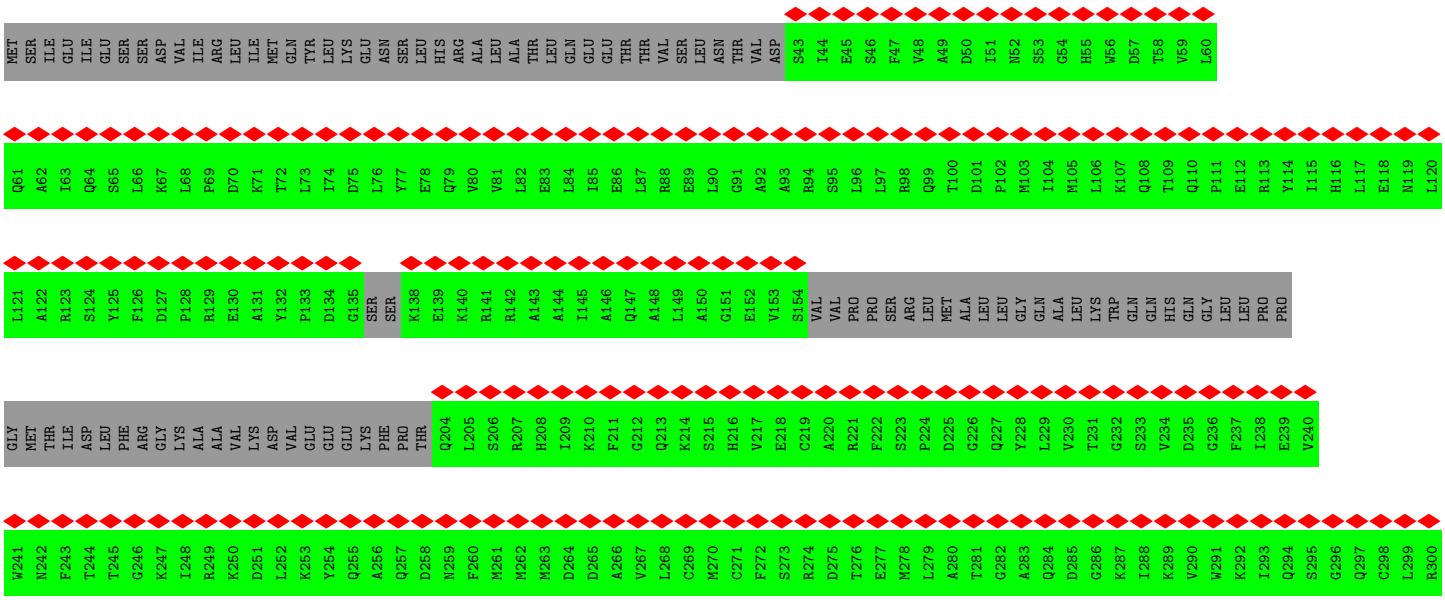
Chain 4J:

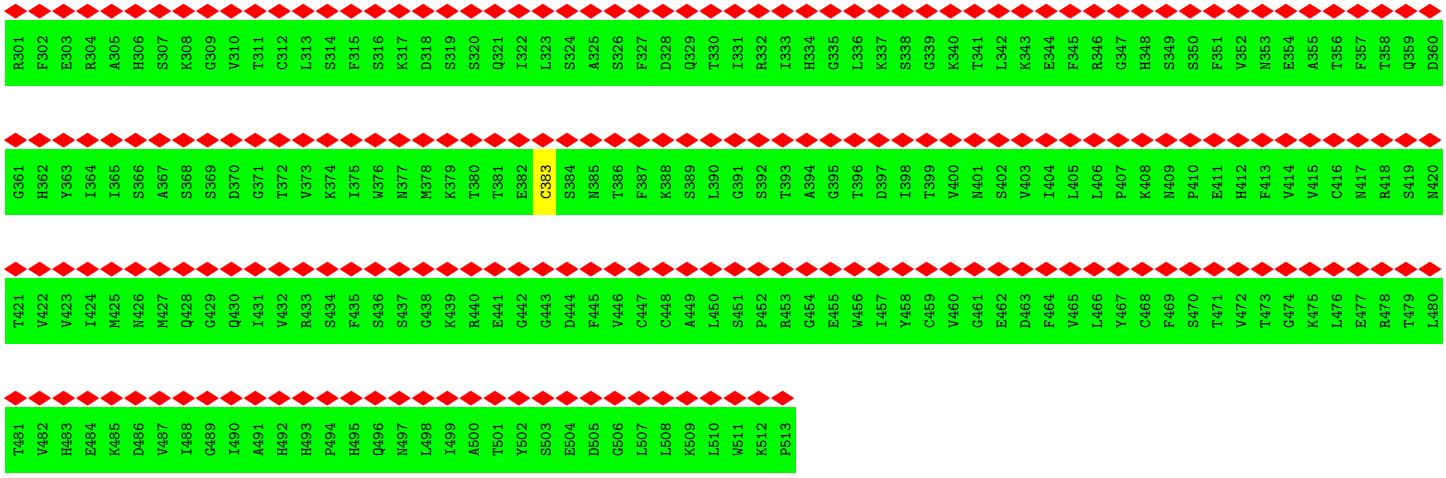




• Molecule 32: WD40 repeat-containing protein SMU1

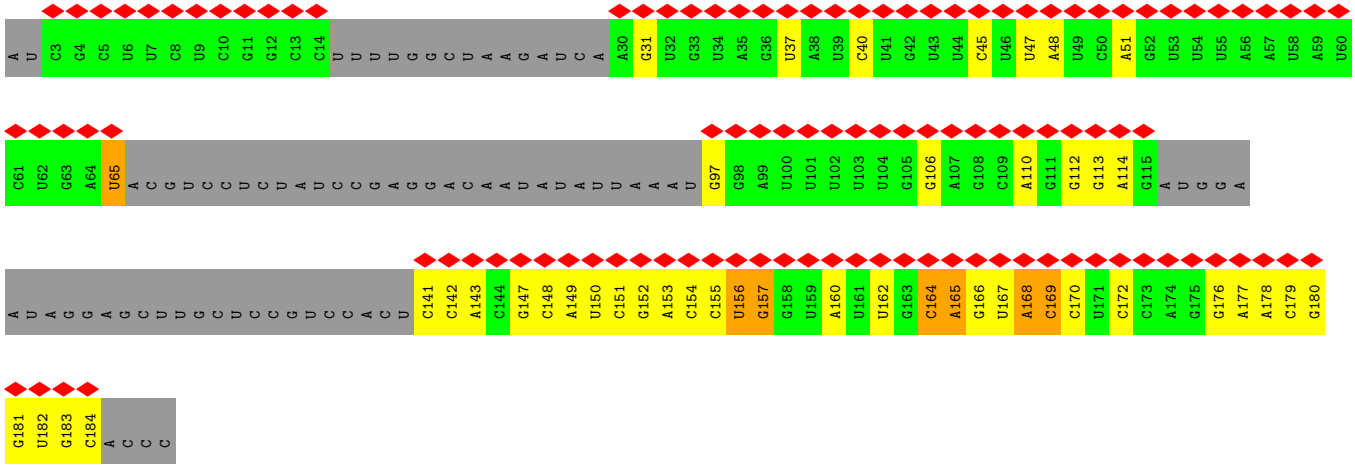
Chain 4Z:





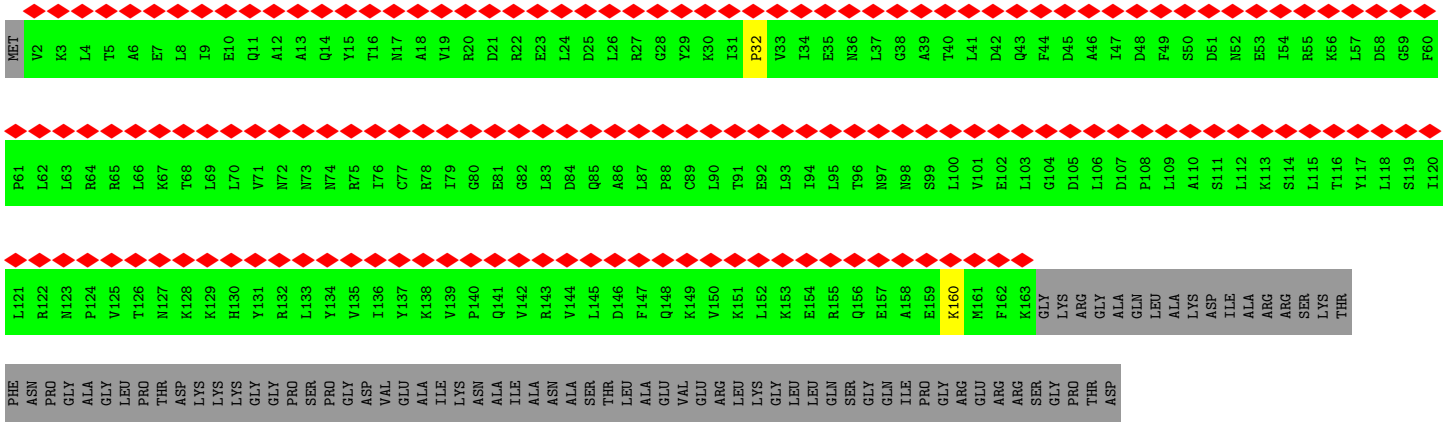
• Molecule 33: U2 snRNA

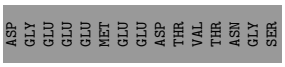
Chain 2A:



• Molecule 34: U2 small nuclear ribonucleoprotein A'

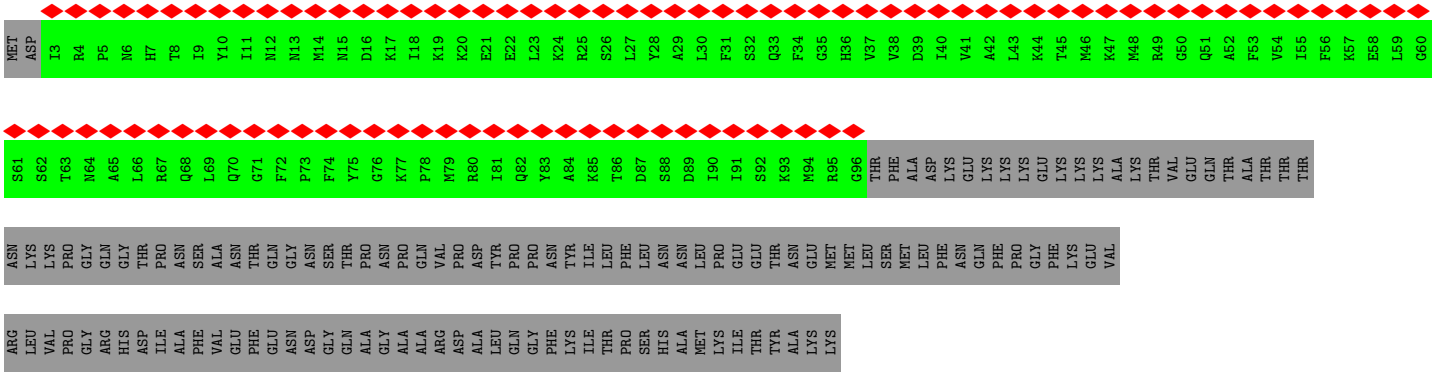
Chain 2B:





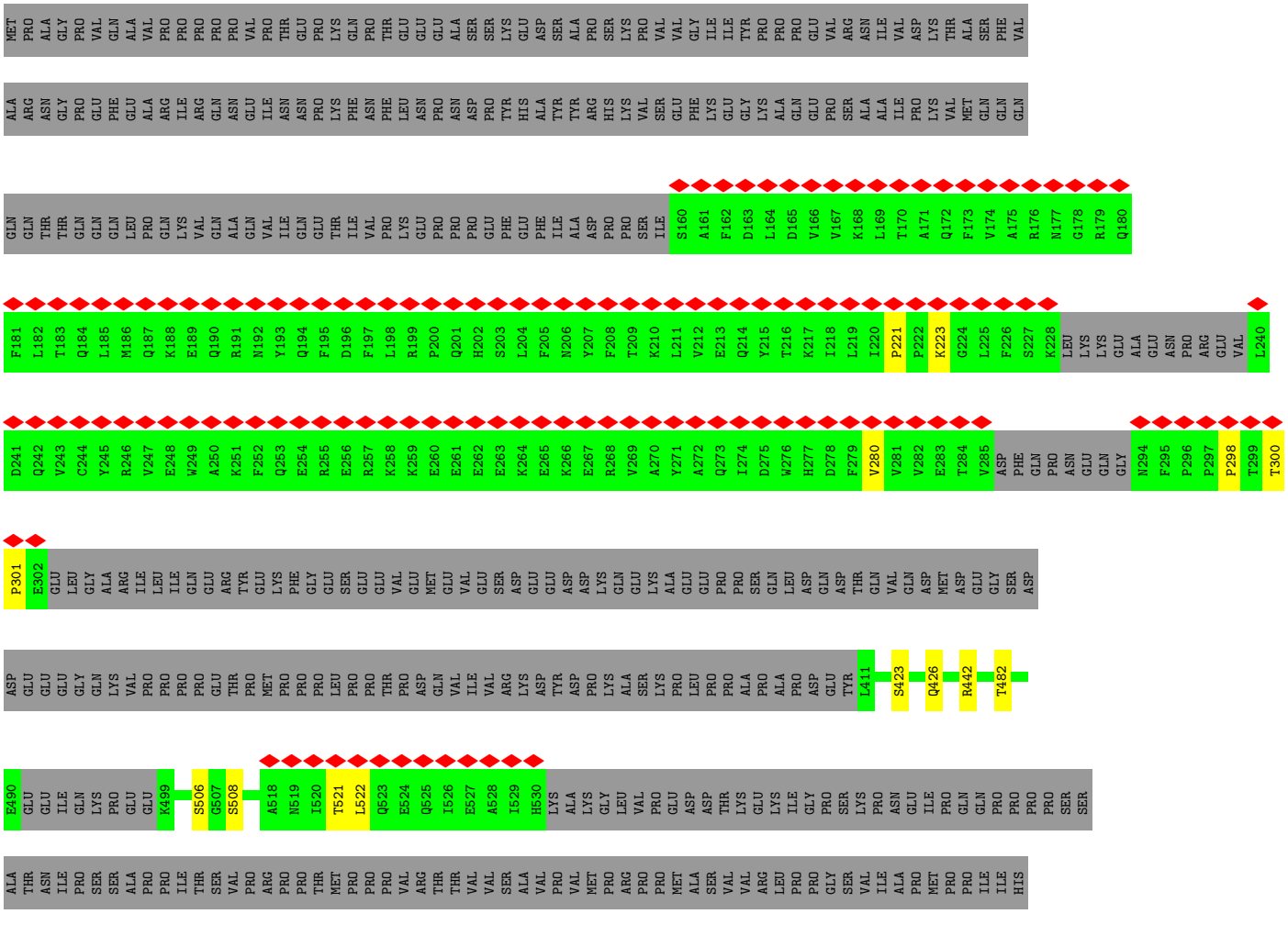
• Molecule 35: U2 small nuclear ribonucleoprotein B"

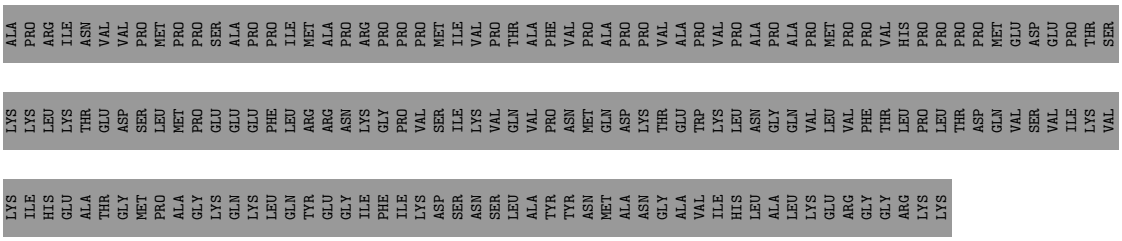
Chain 2C:



• Molecule 36: Splicing factor 3A subunit 1

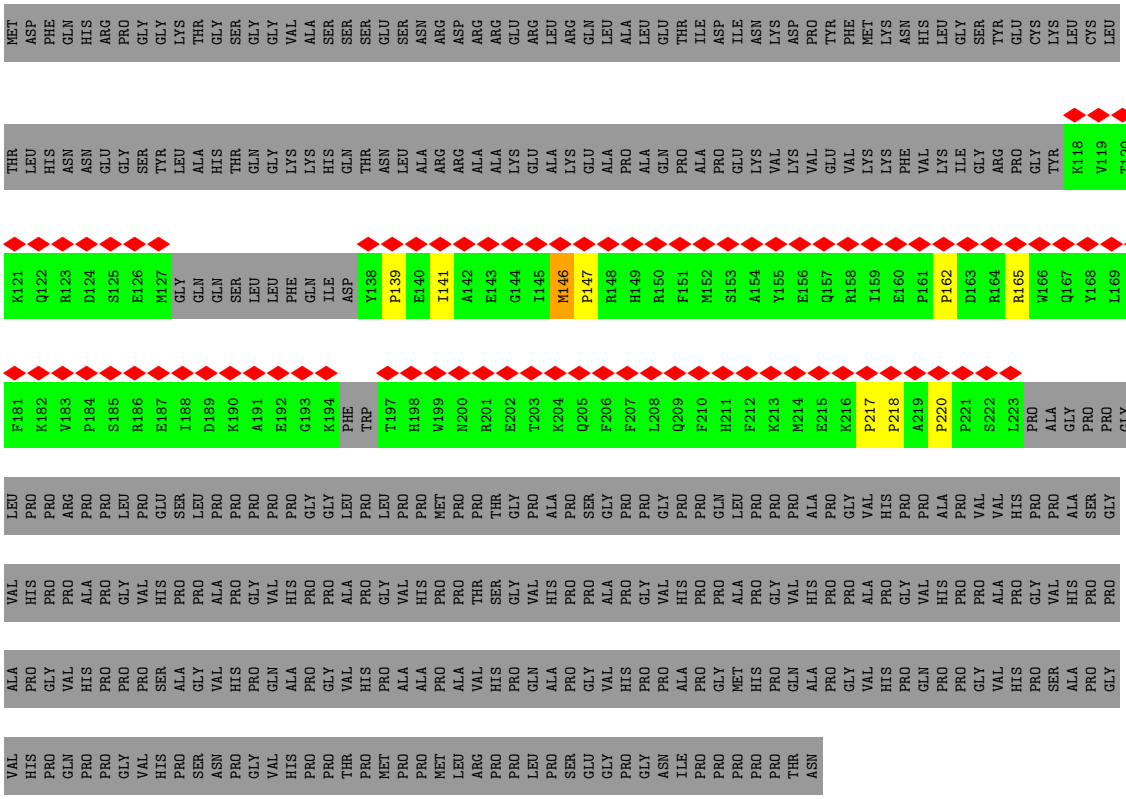
Chain 2D:





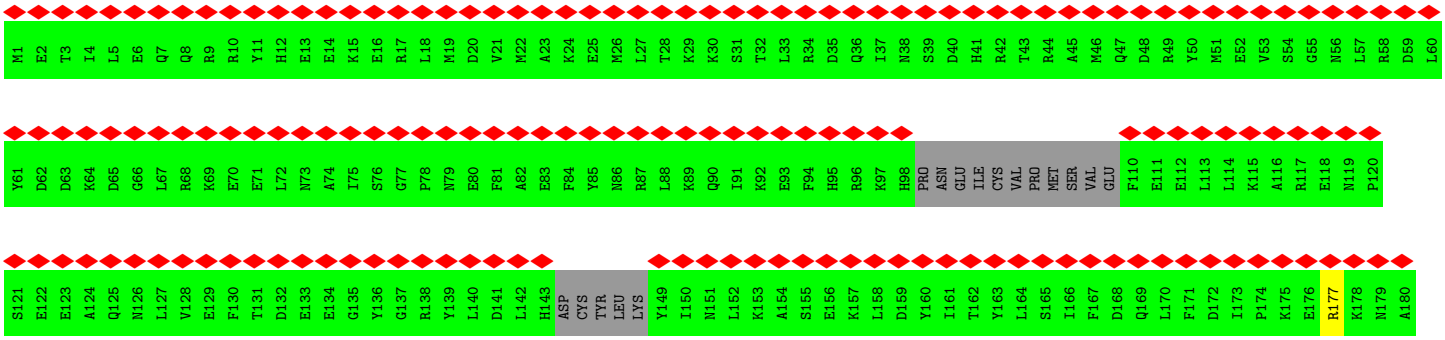
• Molecule 37: Splicing factor 3A subunit 2

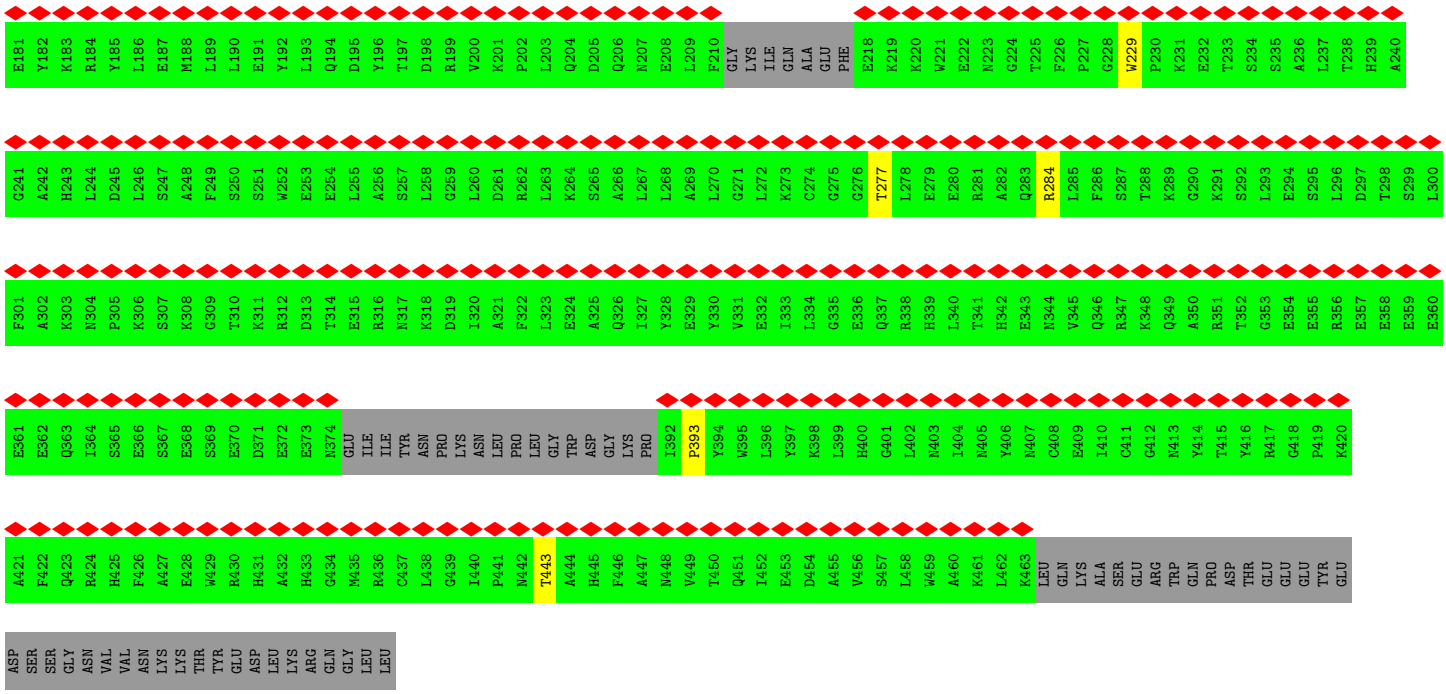
Chain 2E:



• Molecule 38: Splicing factor 3A subunit 3

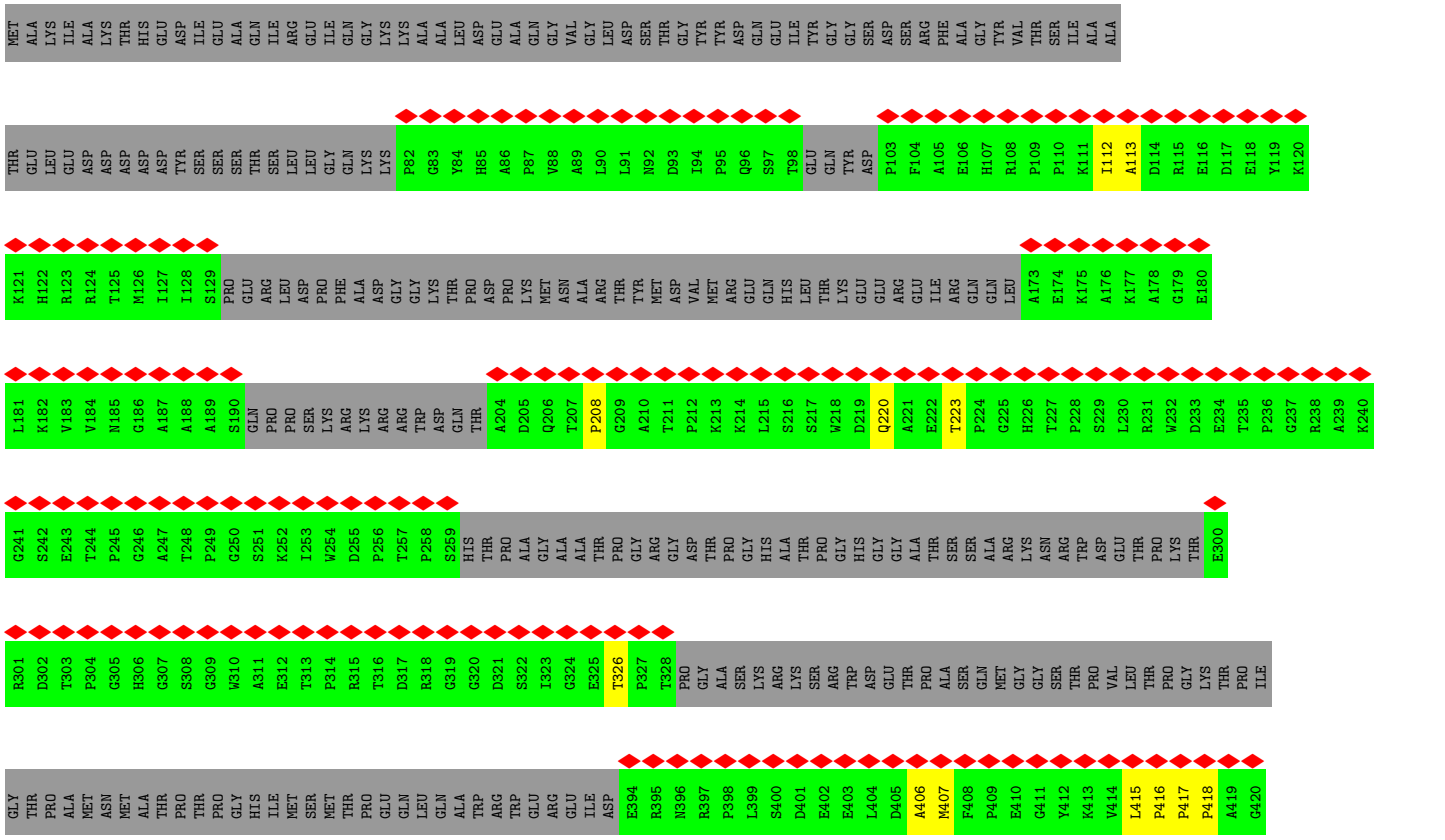
Chain 2F:

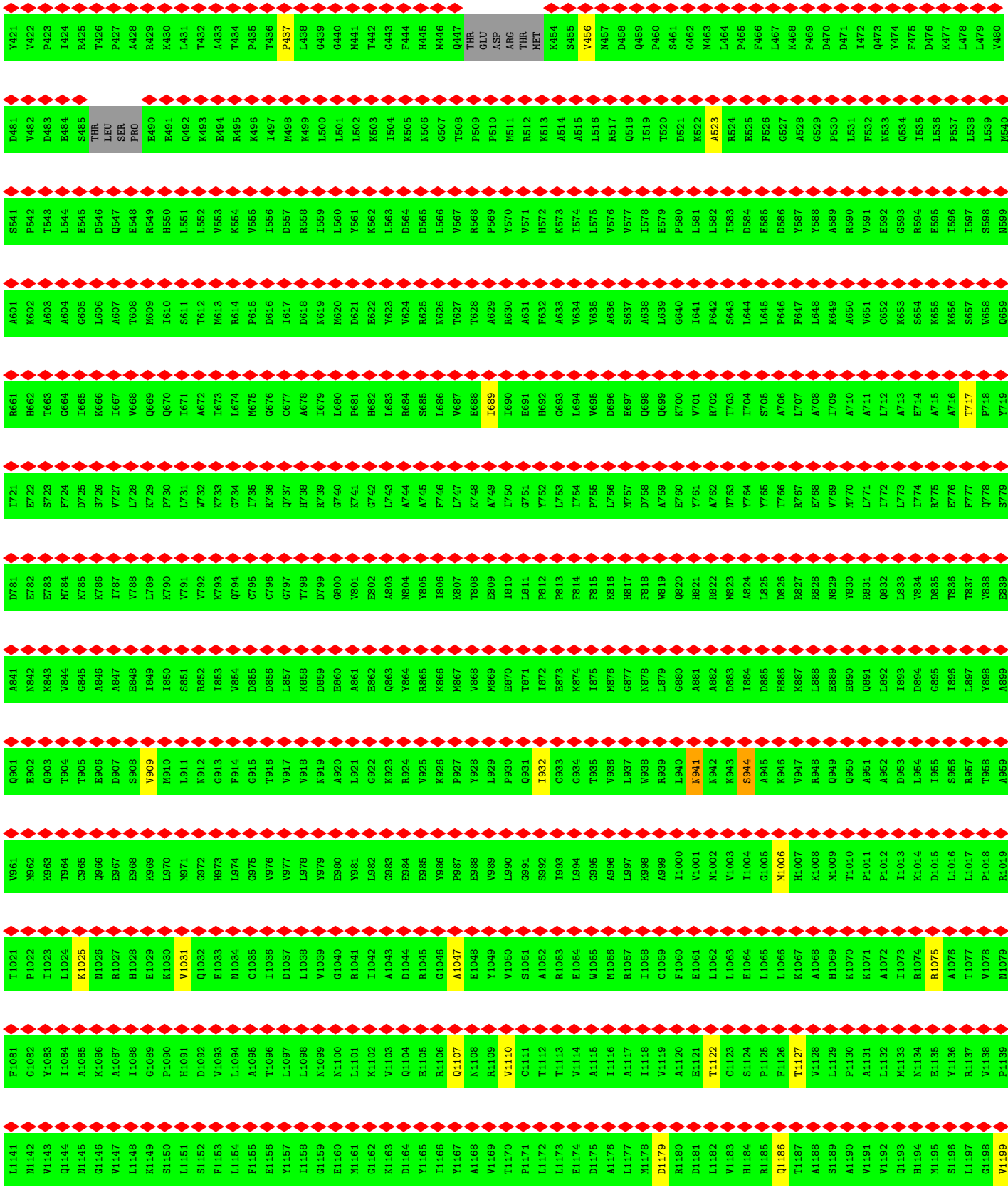




- Molecule 39: Splicing factor 3B subunit 1

Chain 2G:

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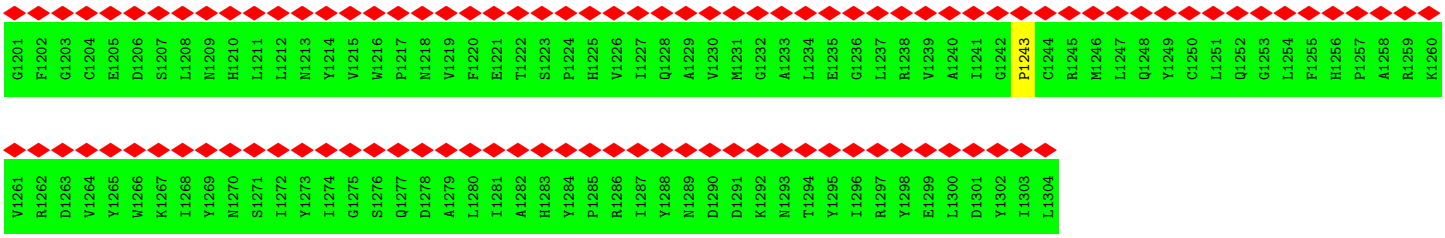
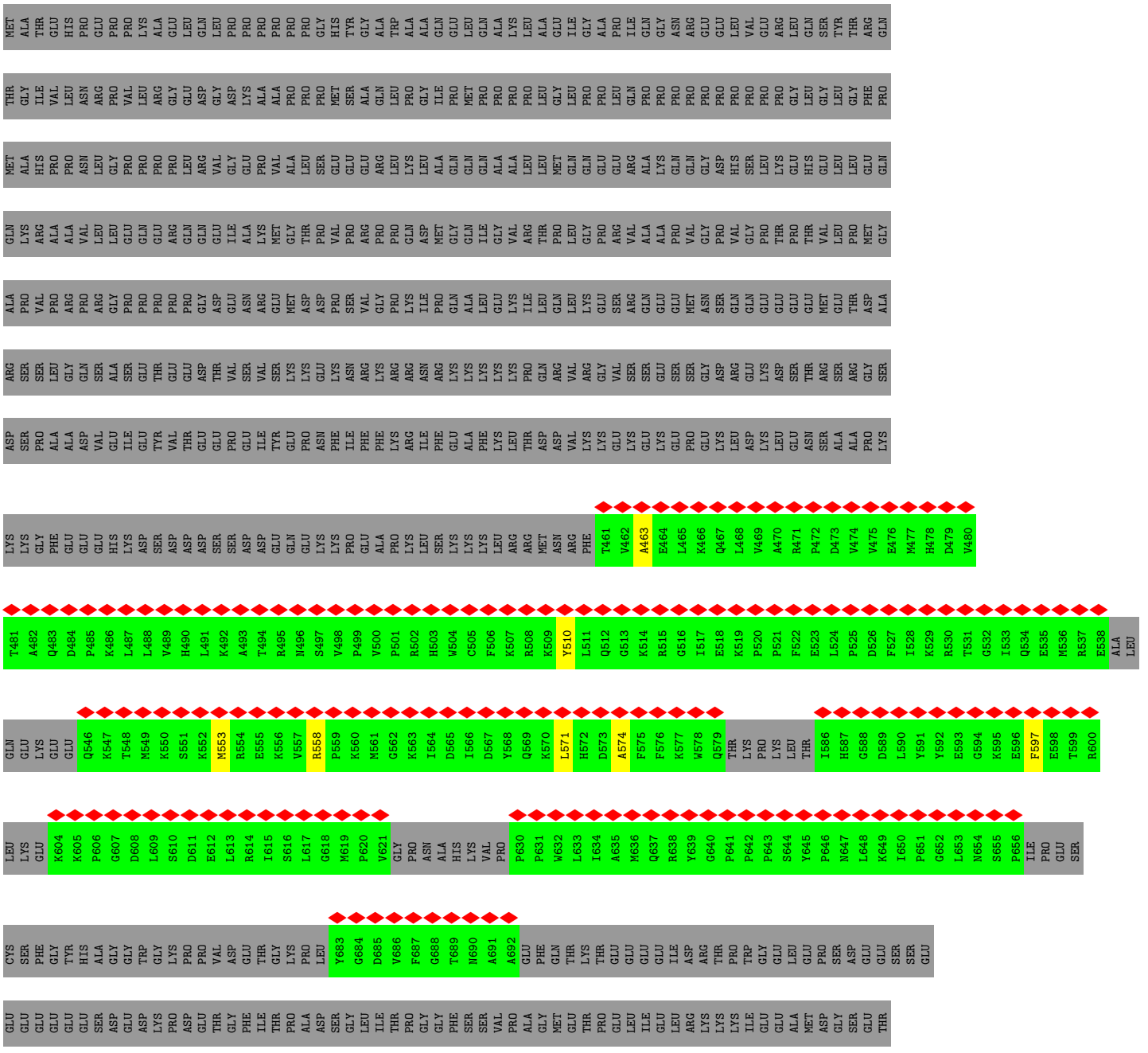
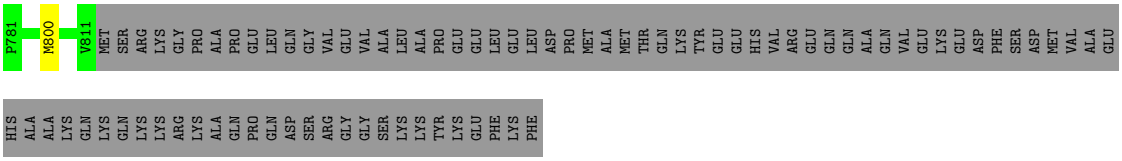
D481 V482 D483 E484 S485 THR LEU SER PRO E490 E491 Q492 K493 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 N506 G507 T508 P509 P510 M511 R512 K513 A514 A515 L516 R517 Q518 I519 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 F532 N533 Q534 I535 L536 P537 L538 L539 N540
S541 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 E588 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 P755 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 P1060 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



• Molecule 40: Splicing factor 3B subunit 2

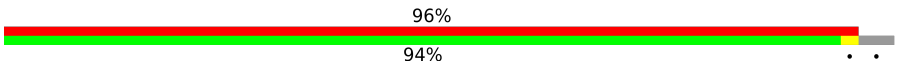
Chain 2H:

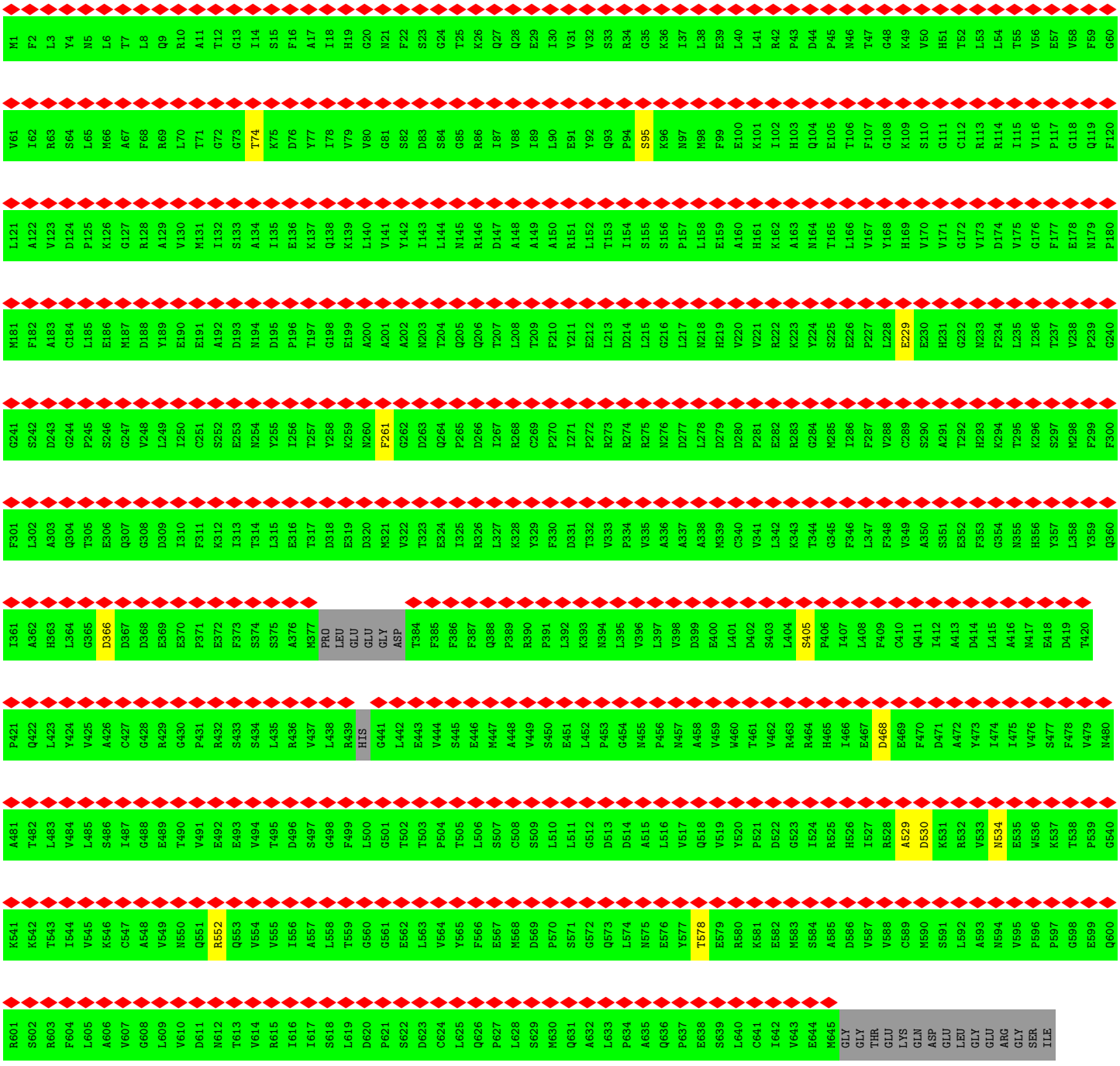


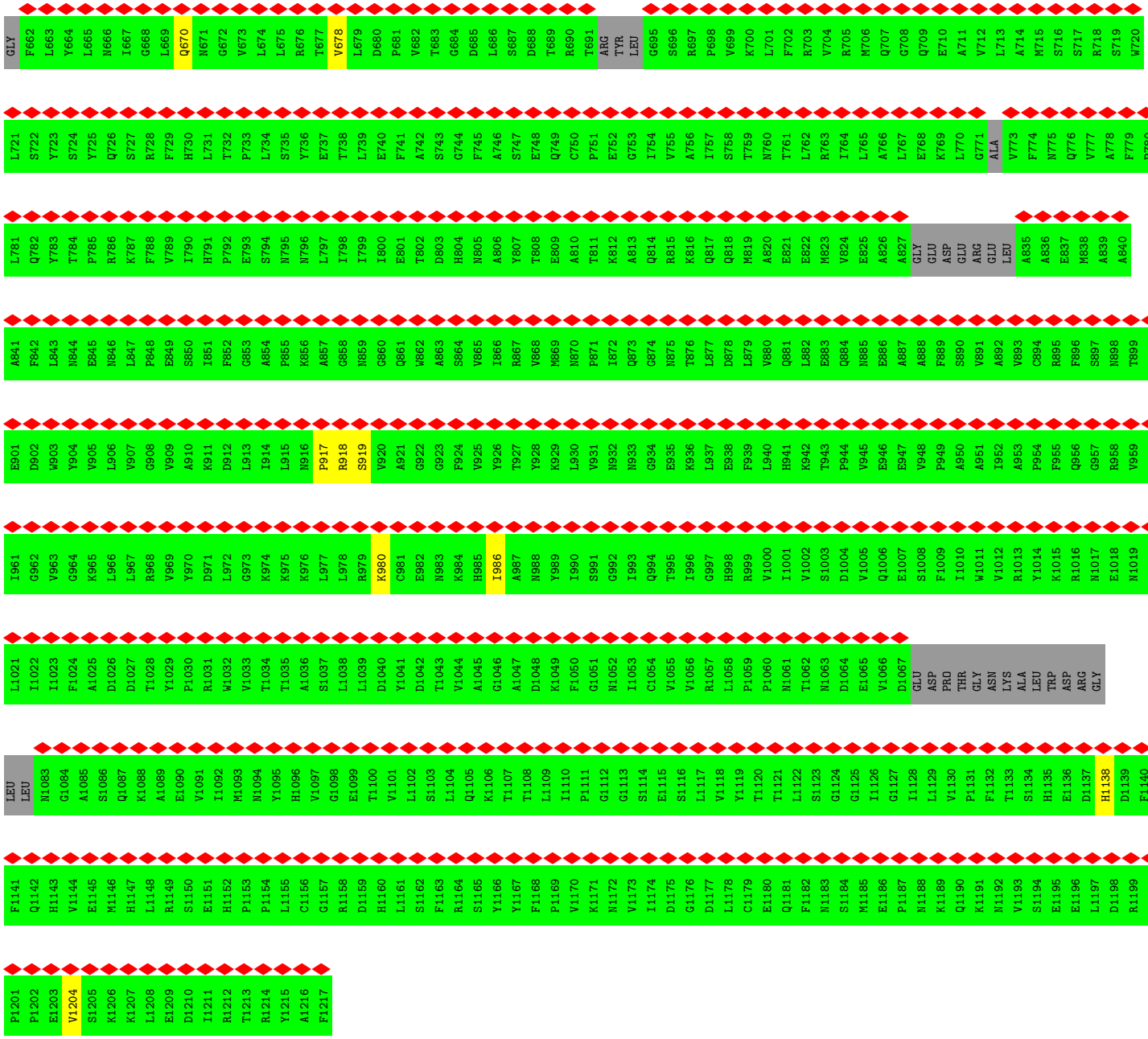


• Molecule 41: Splicing factor 3B subunit 3

Chain 2I:

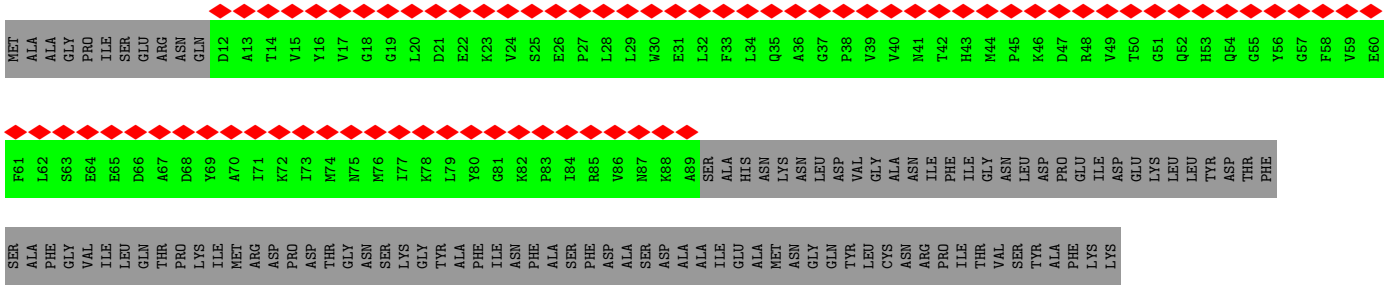


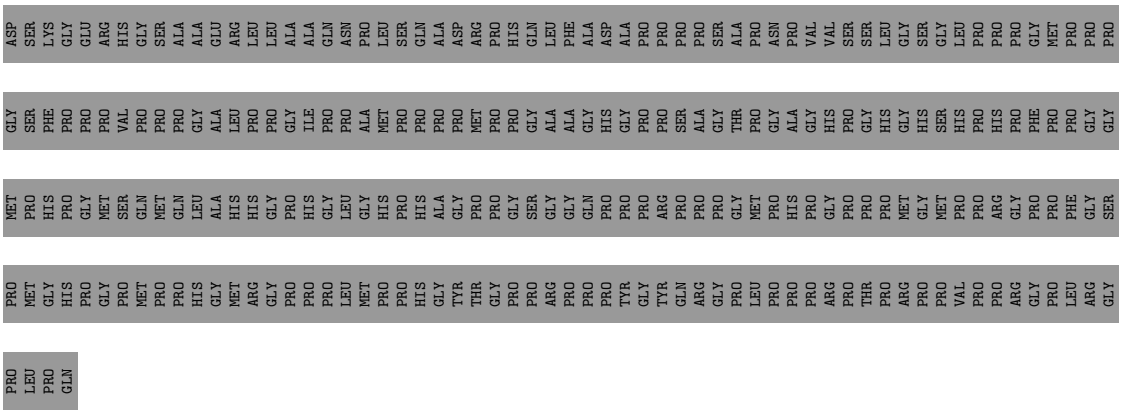




• Molecule 42: Splicing factor 3B subunit 4

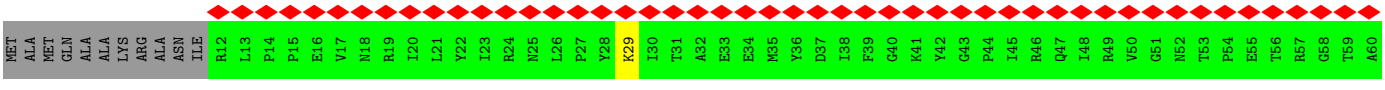
Chain 2J:

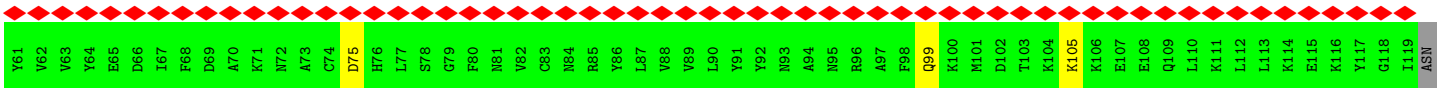




• Molecule 43: Splicing factor 3B subunit 6

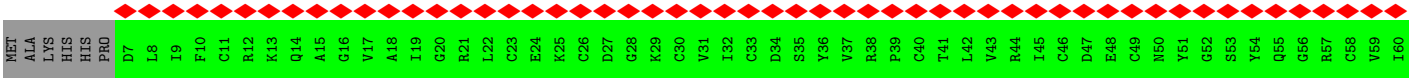
Chain 2K:

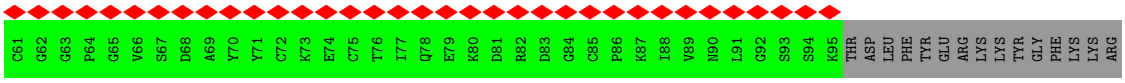




• Molecule 44: PHD finger-like domain-containing protein 5A

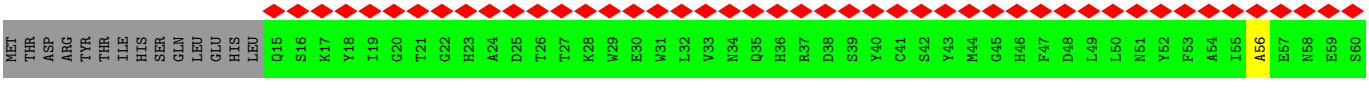
Chain 2L:

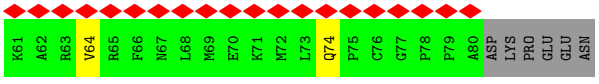




• Molecule 45: Splicing factor 3B subunit 5

Chain 2M:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	716083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	3/1317 (0.2%)	0.90	1/2042 (0.0%)
2	5A	0.29	0/2698	0.82	0/4195
3	5B	0.28	1/19157 (0.0%)	0.51	2/26004 (0.0%)
4	5C	0.27	1/6580 (0.0%)	0.56	3/8938 (0.0%)
5	5D	0.26	0/13923	0.49	1/18868 (0.0%)
6	5E	0.67	0/1195	0.71	0/1492
7	2a	0.50	0/343	0.69	0/427
7	4a	0.22	0/254	0.48	0/314
7	5a	0.50	0/335	0.68	0/417
8	2b	0.56	0/327	0.68	0/407
8	4b	0.22	0/333	0.48	0/416
8	5b	0.57	0/327	0.67	0/407
9	2c	0.70	0/338	0.73	0/419
9	4c	0.23	0/298	0.48	0/370
9	5c	0.69	0/387	0.72	0/482
10	2d	0.77	0/295	0.76	0/367
10	4d	0.24	0/291	0.49	0/363
10	5d	0.77	0/295	0.76	0/367
11	2e	0.64	0/315	0.75	0/392
11	4e	0.22	0/313	0.49	0/390
11	5e	0.65	0/315	0.74	0/392
12	2f	0.55	0/270	0.63	0/334
12	4f	0.24	0/297	0.51	0/371
12	5f	0.54	0/287	0.61	0/357
13	2g	0.47	0/318	0.56	0/394
13	4g	0.23	0/287	0.49	0/358
13	5g	0.46	0/302	0.56	0/374
14	6A	0.30	0/1398	0.81	0/2172
15	6a	0.43	0/359	0.67	0/447
16	6b	0.46	0/294	0.75	0/364
17	6c	0.34	0/294	0.61	0/364
18	6d	0.43	0/286	0.59	0/354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	6e	0.43	0/279	0.72	0/347
20	6f	0.38	0/258	0.61	0/319
21	6g	0.41	0/242	0.64	0/299
22	4A	0.31	0/3025	0.77	1/4702 (0.0%)
23	4B	0.25	0/2114	0.50	0/2836
24	4C	0.25	0/3452	0.53	0/4675
25	4D	0.25	0/2912	0.50	0/3924
26	4E	0.25	0/974	0.47	0/1316
27	4F	0.28	0/1198	0.50	0/1620
28	4G	0.24	0/5592	0.48	1/7615 (0.0%)
29	4H	0.24	0/853	0.45	0/1188
30	4I	0.28	0/502	0.62	2/683 (0.3%)
31	4J	0.25	0/1158	0.52	0/1553
32	4Z	0.24	0/2101	0.45	0/2928
33	2A	0.86	11/2576 (0.4%)	1.43	55/4003 (1.4%)
34	2B	0.63	0/647	1.42	0/807
35	2C	0.61	0/375	1.20	0/467
36	2D	0.23	0/1388	0.48	0/1813
37	2E	0.22	0/373	0.58	1/461 (0.2%)
38	2F	0.25	0/1688	0.47	0/2102
39	2G	1.04	4/4184 (0.1%)	0.83	2/5216 (0.0%)
40	2H	0.65	0/957	0.67	0/1209
41	2I	0.85	0/4664	0.76	0/5816
42	2J	0.62	0/311	0.64	0/387
43	2K	0.79	0/431	0.79	0/537
44	2L	0.74	0/355	0.68	0/442
45	2M	1.01	0/263	0.77	0/327
All	All	0.45	20/96900 (0.0%)	0.65	69/130950 (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
3	5B	0	1
9	2c	0	1
9	5c	0	1
25	4D	0	1
38	2F	0	1
39	2G	0	11
40	2H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	2I	0	11
43	2K	0	1
45	2M	0	1
All	All	0	32

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2G	407	MET	N-CA	12.36	1.71	1.46
39	2G	406	ALA	C-N	7.94	1.52	1.34
33	2A	142	C	C1'-N1	7.32	1.59	1.48
39	2G	1243	PRO	N-CA	-7.11	1.35	1.47
33	2A	182	U	C1'-N1	6.94	1.59	1.48
33	2A	150	U	C1'-N1	6.74	1.58	1.48
33	2A	151	C	C1'-N1	6.53	1.58	1.48
33	2A	97	G	C1'-N9	-6.41	1.37	1.46
33	2A	141	C	C1'-N1	6.38	1.58	1.48
33	2A	184	C	C1'-N1	6.35	1.58	1.48
33	2A	148	C	C1'-N1	6.33	1.58	1.48
39	2G	944	SER	N-CA	-5.72	1.34	1.46
33	2A	65	U	C1'-N1	5.54	1.57	1.48
3	5B	1228	CYS	CB-SG	5.51	1.91	1.82
33	2A	48	A	C1'-N9	-5.48	1.39	1.46
4	5C	810	PRO	CG-CD	-5.20	1.33	1.50
1	A	9	U	C1'-N1	5.14	1.56	1.48
1	A	8	U	C1'-N1	5.13	1.56	1.48
1	A	7	U	C1'-N1	5.13	1.56	1.48
33	2A	110	A	C1'-N9	-5.08	1.39	1.46

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5C	810	PRO	CA-N-CD	-14.23	91.58	111.50
33	2A	167	U	C5-C4-O4	11.61	132.87	125.90
39	2G	406	ALA	C-N-CA	10.28	147.39	121.70
33	2A	164	C	N1-C2-O2	-10.12	112.83	118.90
3	5B	1194	CYS	CA-CB-SG	9.56	131.21	114.00
33	2A	162	U	N3-C2-O2	-8.97	115.92	122.20
33	2A	164	C	C5'-C4'-O4'	-8.21	99.25	109.10
33	2A	169	C	P-O3'-C3'	8.20	129.54	119.70
33	2A	166	G	O4'-C1'-N9	8.03	114.62	108.20
33	2A	167	U	N3-C4-O4	-7.89	113.88	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2A	164	C	P-O3'-C3'	7.54	128.75	119.70
33	2A	167	U	N1-C2-O2	7.41	127.98	122.80
33	2A	164	C	N3-C2-O2	7.38	127.07	121.90
4	5C	810	PRO	N-CD-CG	-7.37	92.14	103.20
33	2A	113	G	OP2-P-O3'	7.26	121.17	105.20
33	2A	149	A	OP2-P-O3'	7.26	121.16	105.20
33	2A	141	C	OP2-P-O3'	7.24	121.13	105.20
33	2A	114	A	OP2-P-O3'	7.24	121.12	105.20
33	2A	183	G	OP2-P-O3'	7.22	121.08	105.20
33	2A	181	G	OP2-P-O3'	7.21	121.07	105.20
33	2A	182	U	OP2-P-O3'	7.21	121.07	105.20
33	2A	180	G	OP2-P-O3'	7.21	121.06	105.20
33	2A	150	U	OP2-P-O3'	7.20	121.05	105.20
33	2A	148	C	OP2-P-O3'	7.18	121.00	105.20
33	2A	168	A	P-O5'-C5'	-7.14	109.47	120.90
30	4I	25	PRO	N-CD-CG	-6.97	92.74	103.20
33	2A	167	U	N3-C2-O2	-6.96	117.33	122.20
33	2A	180	G	O3'-P-O5'	-6.83	91.02	104.00
33	2A	149	A	O3'-P-O5'	-6.83	91.03	104.00
39	2G	406	ALA	CA-C-O	-6.82	105.77	120.10
33	2A	155	C	P-O3'-C3'	6.82	127.88	119.70
33	2A	182	U	O3'-P-O5'	-6.81	91.06	104.00
4	5C	308	CYS	CA-CB-SG	6.79	126.22	114.00
33	2A	183	G	O3'-P-O5'	-6.79	91.11	104.00
33	2A	148	C	O3'-P-O5'	-6.78	91.12	104.00
33	2A	141	C	O3'-P-O5'	-6.77	91.14	104.00
33	2A	150	U	O3'-P-O5'	-6.75	91.17	104.00
33	2A	113	G	O3'-P-O5'	-6.75	91.19	104.00
33	2A	181	G	O3'-P-O5'	-6.74	91.19	104.00
33	2A	114	A	O3'-P-O5'	-6.73	91.21	104.00
30	4I	25	PRO	CA-N-CD	-6.53	102.36	111.50
33	2A	165	A	O4'-C1'-N9	-6.19	103.25	108.20
33	2A	166	G	N9-C4-C5	6.14	107.86	105.40
33	2A	166	G	C8-N9-C4	-6.11	103.96	106.40
1	A	115	U	P-O3'-C3'	6.11	127.03	119.70
33	2A	162	U	N1-C2-O2	6.07	127.05	122.80
33	2A	166	G	N3-C4-C5	-6.01	125.60	128.60
33	2A	168	A	C5'-C4'-C3'	-5.93	106.51	116.00
33	2A	172	C	P-O3'-C3'	5.80	126.66	119.70
33	2A	156	U	P-O3'-C3'	-5.77	112.78	119.70
37	2E	146	MET	C-N-CA	5.75	146.17	122.00
5	5D	583	THR	C-N-CA	5.75	136.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2A	167	U	O3'-P-O5'	-5.74	93.09	104.00
33	2A	164	C	C5-C4-N4	-5.72	116.20	120.20
28	4G	707	ASP	C-N-CA	5.66	135.84	121.70
33	2A	157	G	O4'-C1'-N9	-5.50	103.80	108.20
33	2A	166	G	C6-N1-C2	-5.46	121.83	125.10
33	2A	106	G	O5'-P-OP1	5.41	117.19	110.70
3	5B	1194	CYS	N-CA-CB	5.28	120.11	110.60
33	2A	156	U	OP2-P-O3'	5.28	116.82	105.20
33	2A	160	A	P-O5'-C5'	-5.27	112.46	120.90
33	2A	170	C	O4'-C1'-C2'	-5.23	100.57	105.80
22	4A	70	U	C2-N1-C1'	5.20	123.94	117.70
33	2A	164	C	C6-N1-C2	5.17	122.37	120.30
33	2A	157	G	P-O5'-C5'	-5.15	112.66	120.90
33	2A	170	C	N3-C4-C5	-5.14	119.84	121.90
33	2A	156	U	C4'-C3'-C2'	5.08	107.69	102.60
33	2A	162	U	C2-N3-C4	-5.03	123.98	127.00
33	2A	176	G	N9-C4-C5	5.01	107.41	105.40

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	2F	443	THR	Peptide
39	2G	1025	LYS	Peptide
39	2G	1122	THR	Peptide
39	2G	1127	THR	Peptide
39	2G	1179	ASP	Peptide
39	2G	1199	VAL	Peptide
39	2G	220	GLN	Peptide
39	2G	415	LEU	Mainchain,Peptide
39	2G	689	ILE	Peptide
39	2G	941	ASN	Peptide
39	2G	944	SER	Peptide
40	2H	553	MET	Peptide
40	2H	558	ARG	Peptide
40	2H	571	LEU	Peptide
41	2I	261	PHE	Peptide
41	2I	366	ASP	Peptide
41	2I	468	ASP	Peptide
41	2I	530	ASP	Peptide
41	2I	534	ASN	Peptide
41	2I	552	ARG	Peptide

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Mol	Chain	Res	Type	Group
41	2I	670	GLN	Peptide
41	2I	678	VAL	Peptide
41	2I	74	THR	Peptide
41	2I	980	LYS	Peptide
41	2I	986	ILE	Peptide
43	2K	29	LYS	Peptide
45	2M	74	GLN	Peptide
9	2c	112	ASN	Peptide
25	4D	358	ARG	Sidechain
3	5B	941	LYS	Peptide
9	5c	112	ASN	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	5B	2249/2335 (96%)	2145 (95%)	104 (5%)	0	100 100
4	5C	814/972 (84%)	745 (92%)	68 (8%)	1 (0%)	51 75
5	5D	1694/2136 (79%)	1618 (96%)	75 (4%)	1 (0%)	51 75
6	5E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	4 7
7	2a	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
7	4a	60/231 (26%)	57 (95%)	3 (5%)	0	100 100
7	5a	82/231 (36%)	80 (98%)	2 (2%)	0	100 100
8	2b	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
8	4b	80/119 (67%)	76 (95%)	4 (5%)	0	100 100
8	5b	80/119 (67%)	77 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2c	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
9	4c	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
9	5c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
10	2d	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
10	4d	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
10	5d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
11	2e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	4e	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
11	5e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	2f	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
12	4f	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
12	5f	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
13	2g	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
13	4g	69/126 (55%)	69 (100%)	0	0	100	100
13	5g	72/126 (57%)	70 (97%)	2 (3%)	0	100	100
15	6a	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	3
16	6b	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	3
17	6c	70/139 (50%)	63 (90%)	6 (9%)	1 (1%)	11	22
18	6d	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	10	21
19	6e	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	4	7
20	6f	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
21	6g	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	8	16
23	4B	248/683 (36%)	229 (92%)	19 (8%)	0	100	100
24	4C	422/522 (81%)	388 (92%)	33 (8%)	1 (0%)	47	71
25	4D	372/499 (74%)	354 (95%)	18 (5%)	0	100	100
26	4E	122/128 (95%)	112 (92%)	10 (8%)	0	100	100
27	4F	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
28	4G	795/941 (84%)	745 (94%)	50 (6%)	0	100	100
29	4H	167/177 (94%)	156 (93%)	11 (7%)	0	100	100
30	4I	73/376 (19%)	71 (97%)	2 (3%)	0	100	100
31	4J	143/800 (18%)	136 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	4Z	414/513 (81%)	401 (97%)	12 (3%)	1 (0%)	47 71
34	2B	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12 24
35	2C	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
36	2D	226/793 (28%)	208 (92%)	12 (5%)	6 (3%)	5 8
37	2E	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0 0
38	2F	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	13 27
39	2G	1032/1304 (79%)	844 (82%)	166 (16%)	22 (2%)	7 13
40	2H	199/895 (22%)	179 (90%)	16 (8%)	4 (2%)	7 14
41	2I	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	17 35
42	2J	76/424 (18%)	75 (99%)	1 (1%)	0	100 100
43	2K	106/125 (85%)	85 (80%)	18 (17%)	3 (3%)	5 7
44	2L	87/110 (79%)	74 (85%)	13 (15%)	0	100 100
45	2M	64/86 (74%)	55 (86%)	7 (11%)	2 (3%)	4 6
All	All	13703/20230 (68%)	12707 (93%)	908 (7%)	88 (1%)	29 47

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	5D	1086	GLN
6	5E	193	THR
15	6a	55	LEU
16	6b	84	MET
18	6d	70	ASP
19	6e	52	VAL
19	6e	55	GLN
24	4C	459	PRO
32	4Z	383	CYS
36	2D	301	PRO
37	2E	139	PRO
37	2E	141	ILE
37	2E	146	MET
37	2E	162	PRO
37	2E	165	ARG
37	2E	218	PRO
38	2F	284	ARG
39	2G	208	PRO
39	2G	416	PRO

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Mol	Chain	Res	Type
39	2G	418	PRO
39	2G	456	VAL
39	2G	717	THR
39	2G	941	ASN
39	2G	1107	GLN
41	2I	405	SER
41	2I	919	SER
43	2K	99	GLN
43	2K	105	LYS
15	6a	74	ALA
16	6b	97	PRO
17	6c	12	ASN
34	2B	160	LYS
36	2D	223	LYS
36	2D	280	VAL
38	2F	277	THR
39	2G	113	ALA
39	2G	1110	VAL
40	2H	597	PHE
41	2I	917	PRO
6	5E	60	MET
6	5E	88	ARG
6	5E	256	ASP
38	2F	177	ARG
38	2F	393	PRO
40	2H	510	TYR
6	5E	162	ARG
16	6b	96	ALA
34	2B	32	PRO
36	2D	300	THR
39	2G	112	ILE
39	2G	437	PRO
39	2G	523	ALA
39	2G	909	VAL
39	2G	1006	MET
40	2H	463	ALA
40	2H	574	ALA
41	2I	529	ALA
41	2I	578	THR
43	2K	75	ASP
6	5E	159	PRO
15	6a	73	PRO

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Mol	Chain	Res	Type
37	2E	147	PRO
37	2E	217	PRO
39	2G	1047	ALA
39	2G	1075	ARG
39	2G	1186	GLN
41	2I	95	SER
41	2I	229	GLU
6	5E	270	LYS
21	6g	34	ILE
37	2E	220	PRO
39	2G	326	THR
39	2G	932	ILE
41	2I	918	ARG
41	2I	1138	HIS
45	2M	56	ALA
6	5E	149	GLY
39	2G	417	PRO
36	2D	221	PRO
39	2G	223	THR
4	5C	439	PRO
38	2F	229	TRP
41	2I	1204	VAL
6	5E	324	PRO
36	2D	298	PRO
39	2G	1031	VAL
45	2M	64	VAL
15	6a	52	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	5B	2034/2108 (96%)	1932 (95%)	102 (5%)	24 47
4	5C	718/866 (83%)	676 (94%)	42 (6%)	20 40
5	5D	1517/1908 (80%)	1493 (98%)	24 (2%)	62 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	4B	225/599 (38%)	205 (91%)	20 (9%)	9 19
24	4C	362/442 (82%)	330 (91%)	32 (9%)	10 19
25	4D	299/424 (70%)	278 (93%)	21 (7%)	15 30
26	4E	108/111 (97%)	104 (96%)	4 (4%)	34 60
27	4F	129/130 (99%)	121 (94%)	8 (6%)	18 37
28	4G	417/792 (53%)	388 (93%)	29 (7%)	15 30
29	4H	10/148 (7%)	10 (100%)	0	100 100
30	4I	32/333 (10%)	28 (88%)	4 (12%)	4 8
31	4J	113/681 (17%)	102 (90%)	11 (10%)	8 15
32	4Z	11/450 (2%)	11 (100%)	0	100 100
36	2D	95/709 (13%)	87 (92%)	8 (8%)	11 21
40	2H	26/776 (3%)	25 (96%)	1 (4%)	33 59
All	All	6096/10477 (58%)	5790 (95%)	306 (5%)	28 47

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5B	68	LYS
3	5B	81	PHE
3	5B	87	VAL
3	5B	142	SER
3	5B	159	ARG
3	5B	180	ASP
3	5B	181	ASN
3	5B	221	ASN
3	5B	226	GLN
3	5B	236	SER
3	5B	266	SER
3	5B	305	ARG
3	5B	322	ASN
3	5B	325	HIS
3	5B	327	VAL
3	5B	330	THR
3	5B	339	PHE
3	5B	341	LYS
3	5B	351	TYR
3	5B	352	PHE
3	5B	353	ASP

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Mol	Chain	Res	Type
3	5B	361	HIS
3	5B	379	GLU
3	5B	387	PHE
3	5B	415	SER
3	5B	468	LYS
3	5B	486	LYS
3	5B	510	ARG
3	5B	679	SER
3	5B	680	HIS
3	5B	707	ARG
3	5B	721	LYS
3	5B	741	ARG
3	5B	774	LYS
3	5B	845	ARG
3	5B	855	ARG
3	5B	859	SER
3	5B	866	LEU
3	5B	980	ARG
3	5B	991	THR
3	5B	994	ASN
3	5B	1066	GLN
3	5B	1070	ASP
3	5B	1089	CYS
3	5B	1091	TYR
3	5B	1104	ASP
3	5B	1107	ARG
3	5B	1122	ASN
3	5B	1129	ASN
3	5B	1137	ASP
3	5B	1173	SER
3	5B	1176	SER
3	5B	1199	LYS
3	5B	1201	ARG
3	5B	1218	ASN
3	5B	1234	ASP
3	5B	1235	GLU
3	5B	1303	LEU
3	5B	1341	ARG
3	5B	1354	ARG
3	5B	1357	MET
3	5B	1359	HIS
3	5B	1362	ASP

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Mol	Chain	Res	Type
3	5B	1370	ARG
3	5B	1377	SER
3	5B	1393	ARG
3	5B	1402	ARG
3	5B	1413	ASP
3	5B	1420	ASN
3	5B	1438	VAL
3	5B	1449	LYS
3	5B	1599	GLN
3	5B	1602	ASP
3	5B	1625	SER
3	5B	1634	SER
3	5B	1635	TYR
3	5B	1641	ARG
3	5B	1673	SER
3	5B	1690	ASP
3	5B	1692	MET
3	5B	1697	SER
3	5B	1755	SER
3	5B	1757	GLU
3	5B	1765	SER
3	5B	1767	ASN
3	5B	1787	ARG
3	5B	1813	ARG
3	5B	1872	LEU
3	5B	1911	GLU
3	5B	1975	GLU
3	5B	1985	ASP
3	5B	1990	ASP
3	5B	2014	MET
3	5B	2030	GLU
3	5B	2031	LYS
3	5B	2046	THR
3	5B	2056	THR
3	5B	2060	SER
3	5B	2072	GLU
3	5B	2094	SER
3	5B	2231	THR
3	5B	2265	ASP
4	5C	116	MET
4	5C	122	LEU
4	5C	193	THR

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Mol	Chain	Res	Type
4	5C	194	LYS
4	5C	230	ASP
4	5C	258	ASN
4	5C	269	LEU
4	5C	273	ASP
4	5C	279	ARG
4	5C	301	SER
4	5C	311	SER
4	5C	327	TYR
4	5C	329	ASP
4	5C	352	LYS
4	5C	359	LYS
4	5C	365	SER
4	5C	394	ARG
4	5C	408	LEU
4	5C	458	ASP
4	5C	525	CYS
4	5C	534	VAL
4	5C	543	ARG
4	5C	562	THR
4	5C	573	GLU
4	5C	592	VAL
4	5C	649	SER
4	5C	674	CYS
4	5C	699	ASP
4	5C	717	PHE
4	5C	721	LYS
4	5C	724	TRP
4	5C	727	LEU
4	5C	749	THR
4	5C	756	LYS
4	5C	770	PHE
4	5C	780	CYS
4	5C	803	ARG
4	5C	826	ARG
4	5C	831	TYR
4	5C	880	SER
4	5C	912	LEU
4	5C	919	ARG
5	5D	685	LEU
5	5D	726	HIS
5	5D	780	TYR

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Mol	Chain	Res	Type
5	5D	801	PHE
5	5D	844	LEU
5	5D	891	SER
5	5D	984	LEU
5	5D	990	HIS
5	5D	992	TYR
5	5D	1092	MET
5	5D	1148	PHE
5	5D	1159	ASN
5	5D	1320	LEU
5	5D	1325	PHE
5	5D	1376	CYS
5	5D	1417	LYS
5	5D	1478	SER
5	5D	1507	SER
5	5D	1580	CYS
5	5D	1607	SER
5	5D	1732	MET
5	5D	1841	LYS
5	5D	1948	MET
5	5D	2014	TYR
23	4B	424	LEU
23	4B	434	VAL
23	4B	459	GLU
23	4B	518	ARG
23	4B	526	LYS
23	4B	531	LYS
23	4B	538	SER
23	4B	548	VAL
23	4B	561	GLU
23	4B	577	LYS
23	4B	580	ASN
23	4B	595	LYS
23	4B	605	ASP
23	4B	639	LYS
23	4B	640	ASP
23	4B	642	SER
23	4B	653	THR
23	4B	658	ARG
23	4B	659	GLU
23	4B	663	LYS
24	4C	90	PHE

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Mol	Chain	Res	Type
24	4C	92	ARG
24	4C	105	ASP
24	4C	106	SER
24	4C	143	ASP
24	4C	147	LYS
24	4C	150	LYS
24	4C	166	TRP
24	4C	168	HIS
24	4C	199	HIS
24	4C	200	LYS
24	4C	211	MET
24	4C	223	ASN
24	4C	231	ASP
24	4C	262	ASP
24	4C	265	LEU
24	4C	288	SER
24	4C	292	LYS
24	4C	304	SER
24	4C	334	SER
24	4C	355	GLN
24	4C	356	GLU
24	4C	370	ASP
24	4C	378	SER
24	4C	395	ARG
24	4C	399	CYS
24	4C	403	LEU
24	4C	407	LEU
24	4C	451	LEU
24	4C	456	LYS
24	4C	460	ILE
24	4C	483	SER
25	4D	116	ASP
25	4D	117	LYS
25	4D	119	SER
25	4D	120	LYS
25	4D	122	PHE
25	4D	137	ARG
25	4D	144	ASN
25	4D	150	LYS
25	4D	163	THR
25	4D	168	SER
25	4D	177	GLN

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Mol	Chain	Res	Type
25	4D	214	PHE
25	4D	260	SER
25	4D	311	SER
25	4D	362	MET
25	4D	391	ASP
25	4D	395	SER
25	4D	402	SER
25	4D	421	SER
25	4D	426	ARG
25	4D	431	GLN
26	4E	51	SER
26	4E	81	VAL
26	4E	85	SER
26	4E	122	SER
27	4F	3	TYR
27	4F	25	VAL
27	4F	63	ILE
27	4F	94	LEU
27	4F	132	SER
27	4F	137	SER
27	4F	138	THR
27	4F	141	ARG
28	4G	11	MET
28	4G	30	THR
28	4G	32	SER
28	4G	102	ASP
28	4G	109	ASP
28	4G	125	LYS
28	4G	130	LYS
28	4G	155	GLU
28	4G	159	SER
28	4G	175	ARG
28	4G	197	HIS
28	4G	199	SER
28	4G	205	THR
28	4G	356	ASP
28	4G	357	THR
28	4G	372	SER
28	4G	383	GLU
28	4G	708	PHE
28	4G	743	THR
28	4G	750	SER

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Mol	Chain	Res	Type
28	4G	830	SER
28	4G	837	CYS
28	4G	867	THR
28	4G	881	PHE
28	4G	898	ARG
28	4G	911	LEU
28	4G	915	VAL
28	4G	921	ASN
28	4G	925	LYS
30	4I	14	ASP
30	4I	24	ARG
30	4I	27	VAL
30	4I	29	PHE
31	4J	149	GLU
31	4J	179	LEU
31	4J	188	LYS
31	4J	264	ASP
31	4J	265	SER
31	4J	284	GLU
31	4J	290	VAL
31	4J	305	GLU
31	4J	332	SER
31	4J	347	HIS
31	4J	350	ARG
36	2D	423	SER
36	2D	426	GLN
36	2D	442	ARG
36	2D	482	THR
36	2D	506	SER
36	2D	508	SER
36	2D	521	THR
36	2D	522	LEU
40	2H	800	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
3	5B	73	HIS
3	5B	105	ASN
3	5B	545	HIS
3	5B	680	HIS
3	5B	1487	HIS

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Mol	Chain	Res	Type
3	5B	1563	HIS
3	5B	1791	HIS
3	5B	2166	HIS
4	5C	154	HIS
4	5C	208	HIS
4	5C	245	HIS
4	5C	502	HIS
4	5C	627	HIS
4	5C	642	HIS
5	5D	785	HIS
5	5D	911	GLN
5	5D	1515	HIS
23	4B	480	ASN
23	4B	511	HIS
23	4B	515	ASN
24	4C	282	HIS
24	4C	322	HIS
24	4C	364	HIS
24	4C	421	HIS
25	4D	270	HIS
26	4E	17	HIS
27	4F	89	HIS
28	4G	741	HIS
28	4G	908	HIS
31	4J	261	HIS
36	2D	505	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	55/144 (38%)	35 (63%)	10 (18%)
14	6A	55/107 (51%)	14 (25%)	2 (3%)
2	5A	114/117 (97%)	30 (26%)	5 (4%)
22	4A	124/145 (85%)	35 (28%)	4 (3%)
33	2A	105/188 (55%)	22 (20%)	3 (2%)
All	All	453/701 (64%)	136 (30%)	24 (5%)

All (136) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U

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Mol	Chain	Res	Type
1	A	9	U
1	A	10	C
1	A	11	C
1	A	12	U
1	A	13	U
1	A	15	A
1	A	20	U
1	A	21	U
1	A	22	C
1	A	25	G
1	A	29	A
1	A	30	C
1	A	31	C
1	A	32	C
1	A	33	U
1	A	34	G
1	A	35	U
1	A	36	C
1	A	37	C
1	A	39	U
1	A	41	U
1	A	42	U
1	A	44	U
1	A	46	U
1	A	47	C
1	A	48	C
1	A	103	A
1	A	104	C
1	A	105	C
1	A	106	A
1	A	108	G
1	A	110	G
1	A	111	A
1	A	116	G
2	5A	8	G
2	5A	10	U
2	5A	21	A
2	5A	22	U
2	5A	24	G
2	5A	25	C
2	5A	26	A
2	5A	28	A

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Mol	Chain	Res	Type
2	5A	35	U
2	5A	36	C
2	5A	40	U
2	5A	45	C
2	5A	47	A
2	5A	52	U
2	5A	68	C
2	5A	69	A
2	5A	78	U
2	5A	79	C
2	5A	80	U
2	5A	83	A
2	5A	88	A
2	5A	89	U
2	5A	90	U
2	5A	92	U
2	5A	93	U
2	5A	94	U
2	5A	95	G
2	5A	96	A
2	5A	97	G
2	5A	109	G
14	6A	37	C
14	6A	38	G
14	6A	39	A
14	6A	40	U
14	6A	46	G
14	6A	47	A
14	6A	48	A
14	6A	49	G
14	6A	51	U
14	6A	71	G
14	6A	77	C
14	6A	78	A
14	6A	103	U
14	6A	104	U
22	4A	2	G
22	4A	17	A
22	4A	18	G
22	4A	19	U
22	4A	25	A
22	4A	26	G

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Mol	Chain	Res	Type
22	4A	37	C
22	4A	38	U
22	4A	39	A
22	4A	40	U
22	4A	45	G
22	4A	53	U
22	4A	54	A
22	4A	71	U
22	4A	73	U
22	4A	74	C
22	4A	75	C
22	4A	76	C
22	4A	84	C
22	4A	85	G
22	4A	90	G
22	4A	100	A
22	4A	103	A
22	4A	109	G
22	4A	114	U
22	4A	115	G
22	4A	118	A
22	4A	119	A
22	4A	120	U
22	4A	121	U
22	4A	124	U
22	4A	125	G
22	4A	126	A
22	4A	127	C
22	4A	144	G
33	2A	31	G
33	2A	37	U
33	2A	40	C
33	2A	45	C
33	2A	47	U
33	2A	51	A
33	2A	65	U
33	2A	112	G
33	2A	143	A
33	2A	147	G
33	2A	152	G
33	2A	153	A
33	2A	154	C

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Mol	Chain	Res	Type
33	2A	156	U
33	2A	157	G
33	2A	164	C
33	2A	165	A
33	2A	168	A
33	2A	169	C
33	2A	177	A
33	2A	178	A
33	2A	179	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	21	U
1	A	28	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	38	C
1	A	40	U
1	A	41	U
1	A	115	U
2	5A	67	A
2	5A	78	U
2	5A	79	C
2	5A	94	U
2	5A	96	A
14	6A	37	C
14	6A	77	C
22	4A	18	G
22	4A	38	U
22	4A	99	C
22	4A	114	U
33	2A	156	U
33	2A	164	C
33	2A	168	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
47	GTP	5C	1500	48	26,34,34	1.13	2 (7%)	32,54,54	1.53	7 (21%)
46	IHP	5B	3000	-	36,36,36	0.73	0	54,60,60	1.07	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	5C	1500	48	-	6/18/38/38	0/3/3/3
46	IHP	5B	3000	-	-	3/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	5C	1500	GTP	C5-C6	-4.03	1.39	1.47
47	5C	1500	GTP	C2-N3	2.08	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	5C	1500	GTP	PB-O3B-PG	-3.28	121.57	132.83
47	5C	1500	GTP	C5-C6-N1	3.26	119.72	113.95
47	5C	1500	GTP	PA-O3A-PB	-3.15	122.01	132.83
47	5C	1500	GTP	C8-N7-C5	3.01	108.72	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	5C	1500	GTP	C2-N1-C6	-2.88	119.80	125.10
47	5C	1500	GTP	C3'-C2'-C1'	2.51	104.75	100.98
47	5C	1500	GTP	O6-C6-C5	-2.23	120.01	124.37
46	5B	3000	IHP	C6-C5-C4	2.08	114.96	110.41
46	5B	3000	IHP	C5-C4-C3	2.02	114.82	110.41

There are no chirality outliers.

All (9) torsion outliers are listed below:

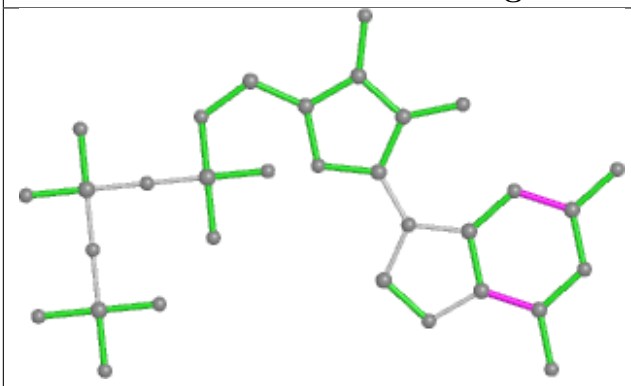
Mol	Chain	Res	Type	Atoms
46	5B	3000	IHP	C2-O12-P2-O42
46	5B	3000	IHP	C4-O14-P4-O44
47	5C	1500	GTP	PB-O3B-PG-O3G
47	5C	1500	GTP	C5'-O5'-PA-O1A
47	5C	1500	GTP	PB-O3A-PA-O5'
47	5C	1500	GTP	C5'-O5'-PA-O3A
47	5C	1500	GTP	C5'-O5'-PA-O2A
46	5B	3000	IHP	C5-O15-P5-O35
47	5C	1500	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

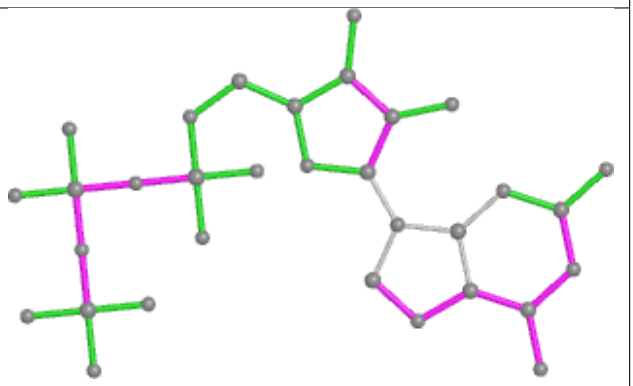
No monomer is involved in short contacts.

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.

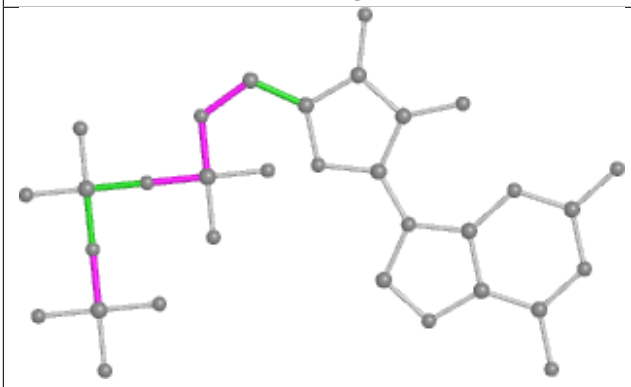
Ligand GTP 5C 1500



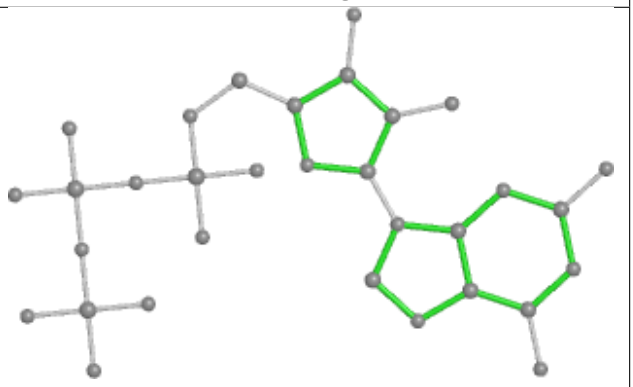
Bond lengths



Bond angles

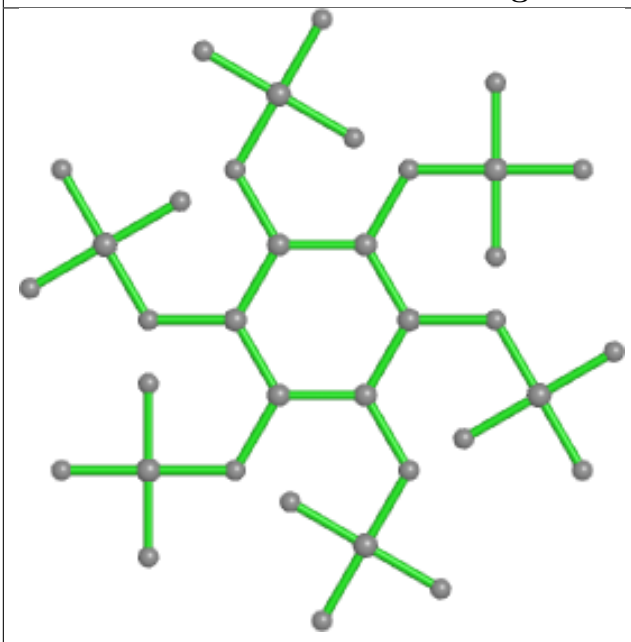


Torsions

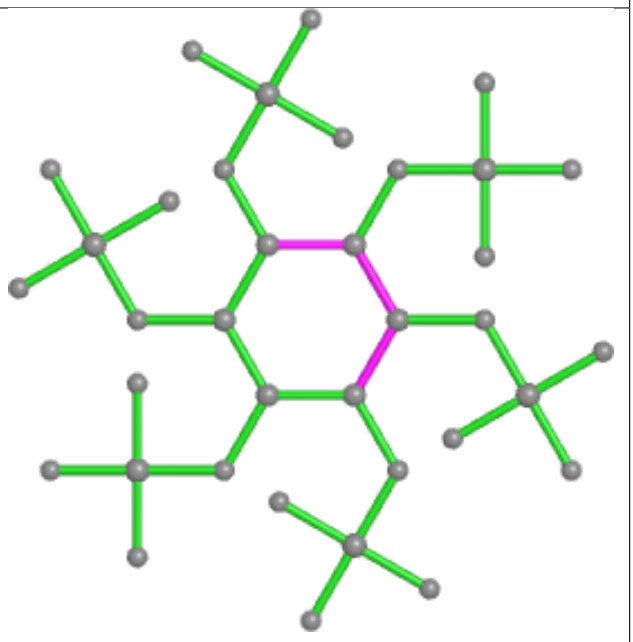


Rings

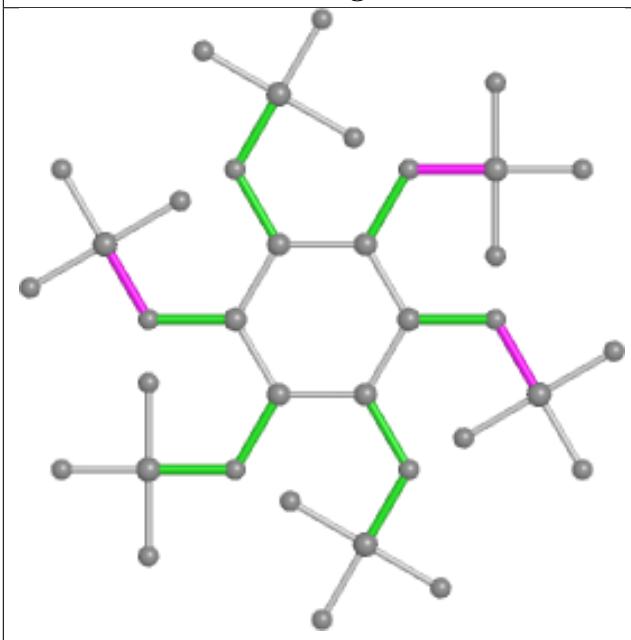
Ligand IHP 5B 3000



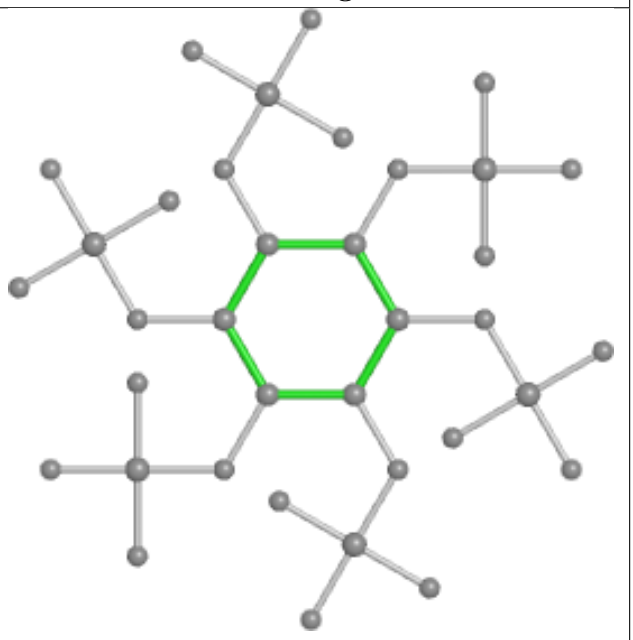
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

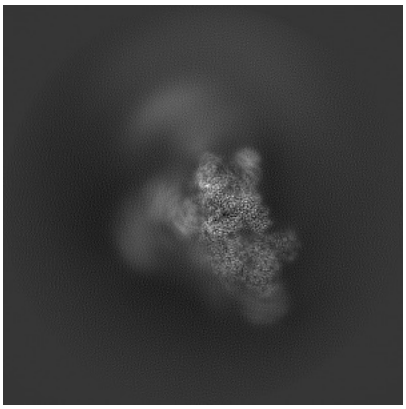
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34508. These allow visual inspection of the internal detail of the map and identification of artifacts.

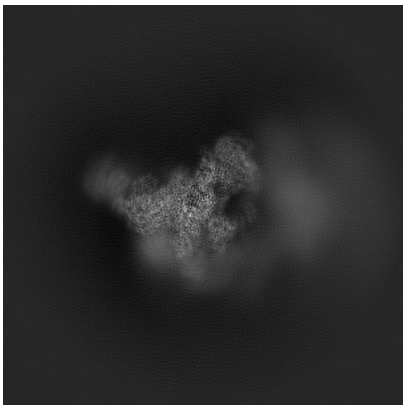
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

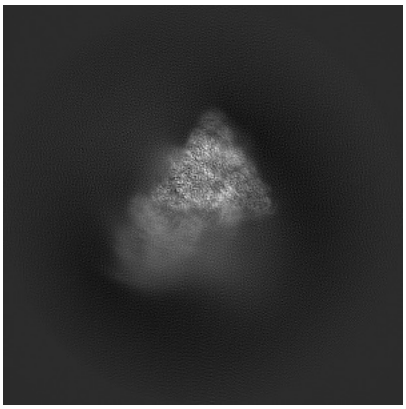
6.1.1 Primary map



X

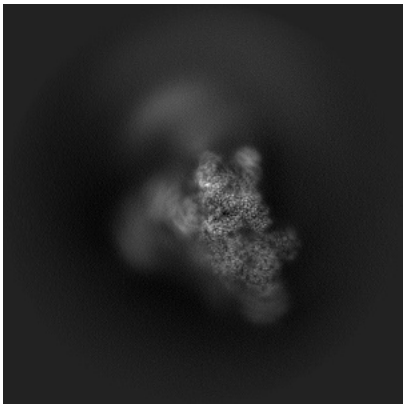


Y

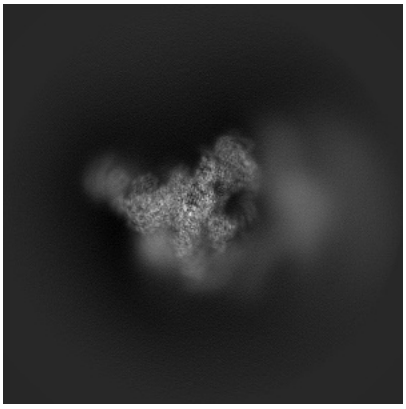


Z

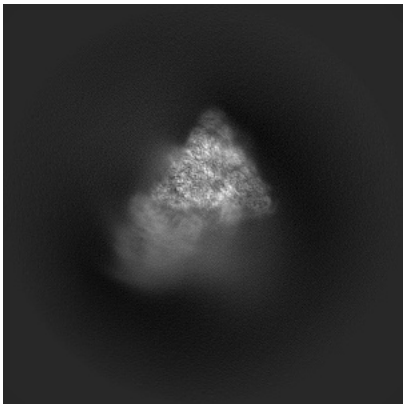
6.1.2 Raw map



X



Y

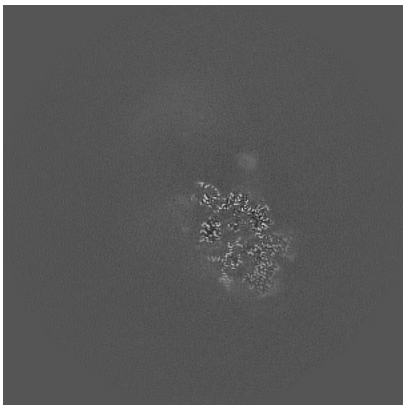


Z

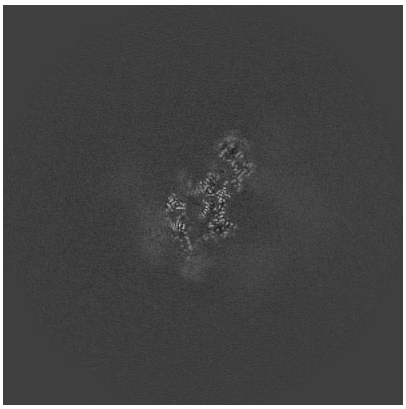
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

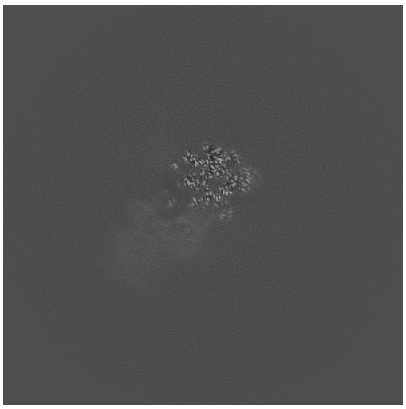
6.2.1 Primary map



X Index: 256

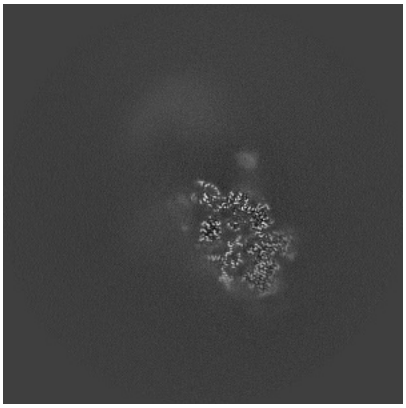


Y Index: 256

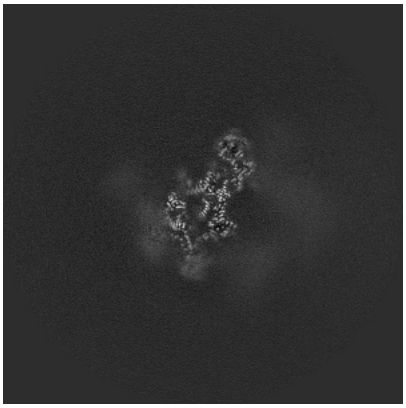


Z Index: 256

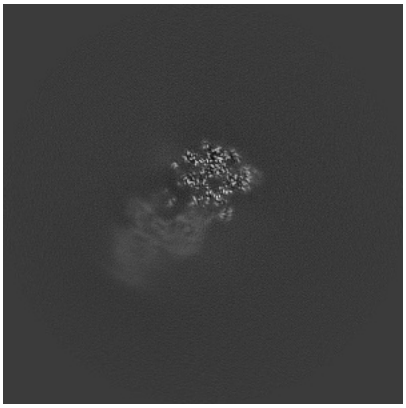
6.2.2 Raw map



X Index: 256



Y Index: 256

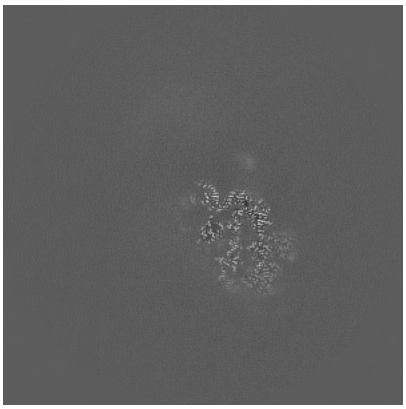


Z Index: 256

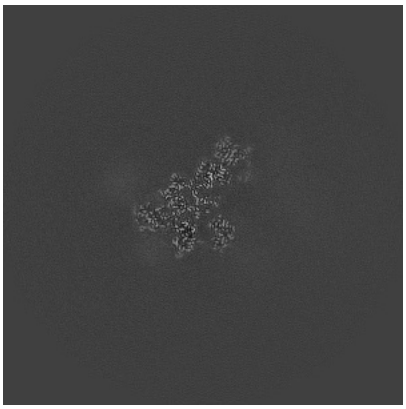
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

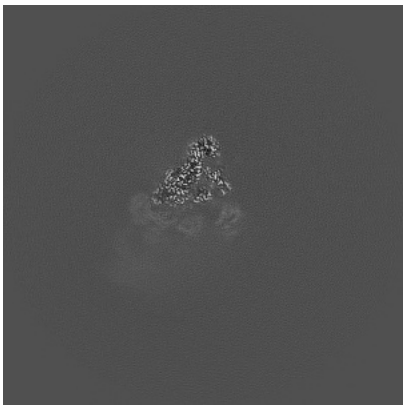
6.3.1 Primary map



X Index: 259

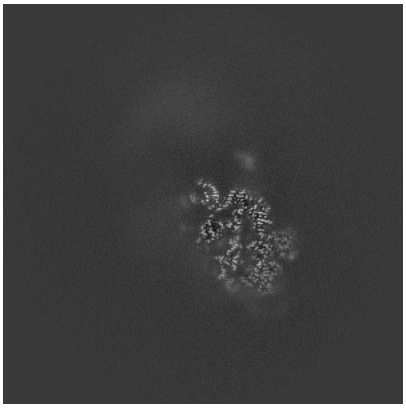


Y Index: 274

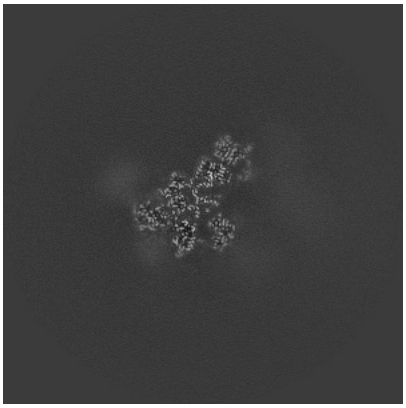


Z Index: 234

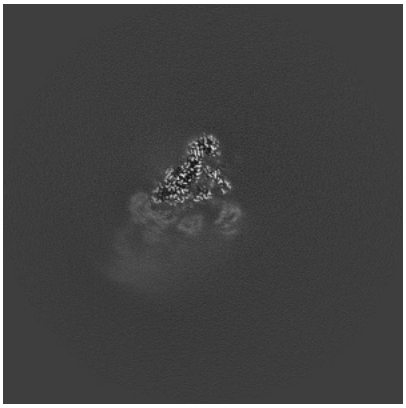
6.3.2 Raw map



X Index: 259



Y Index: 274

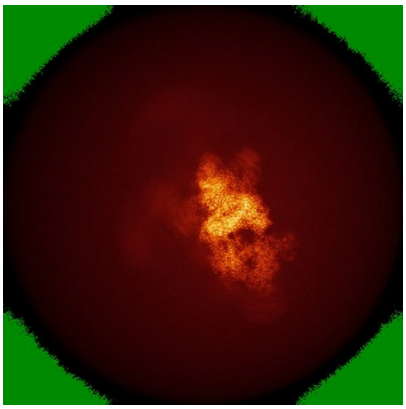


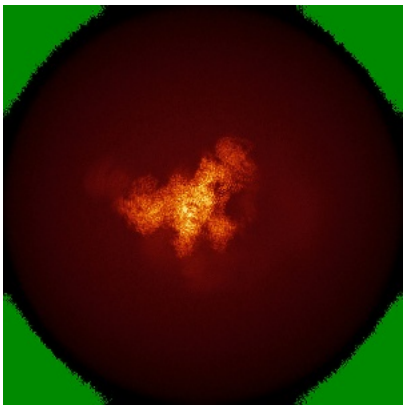
Z Index: 234

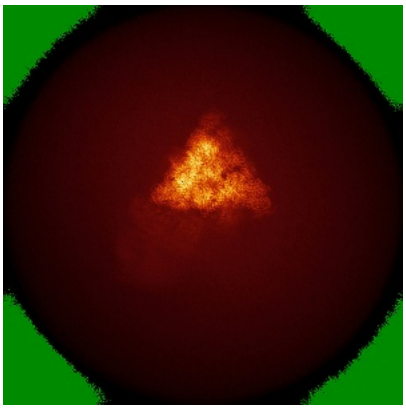
The images above show the largest variance slices of the map in three orthogonal directions.

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

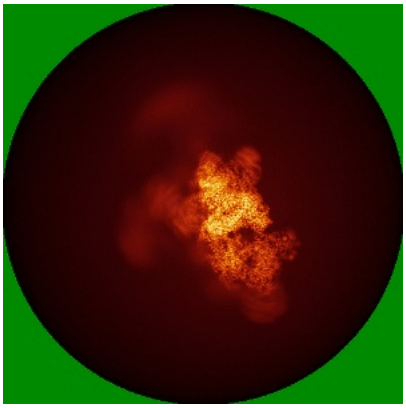
6.4.1 Primary map

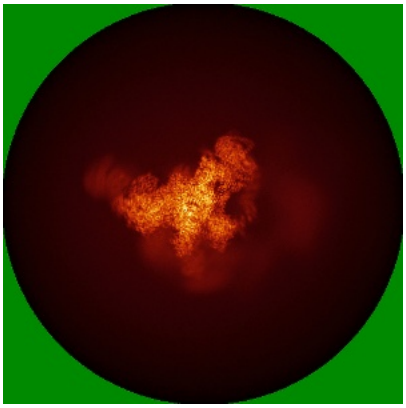

X

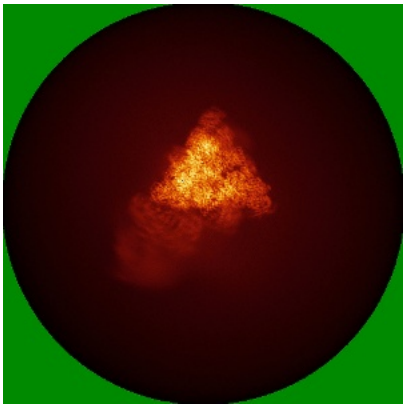

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

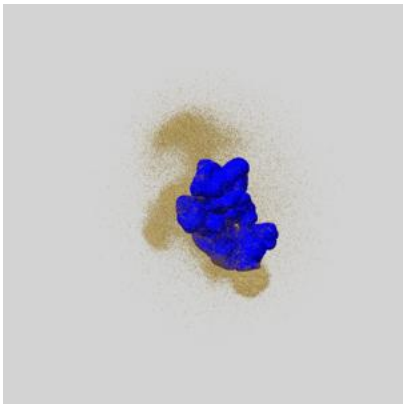
6.6 Mask visualisation

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

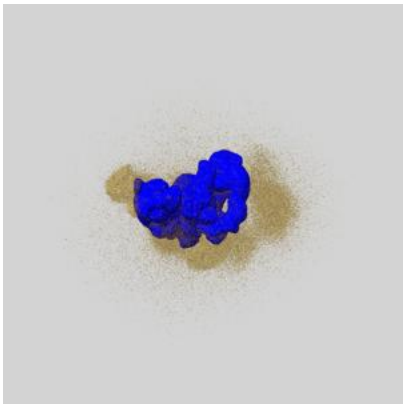
A mask typically either:

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

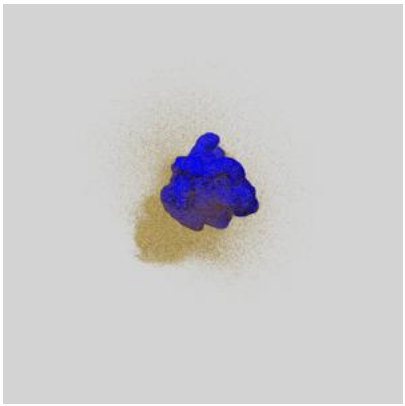
6.6.1 emd_34508_msk_1.map



X



Y

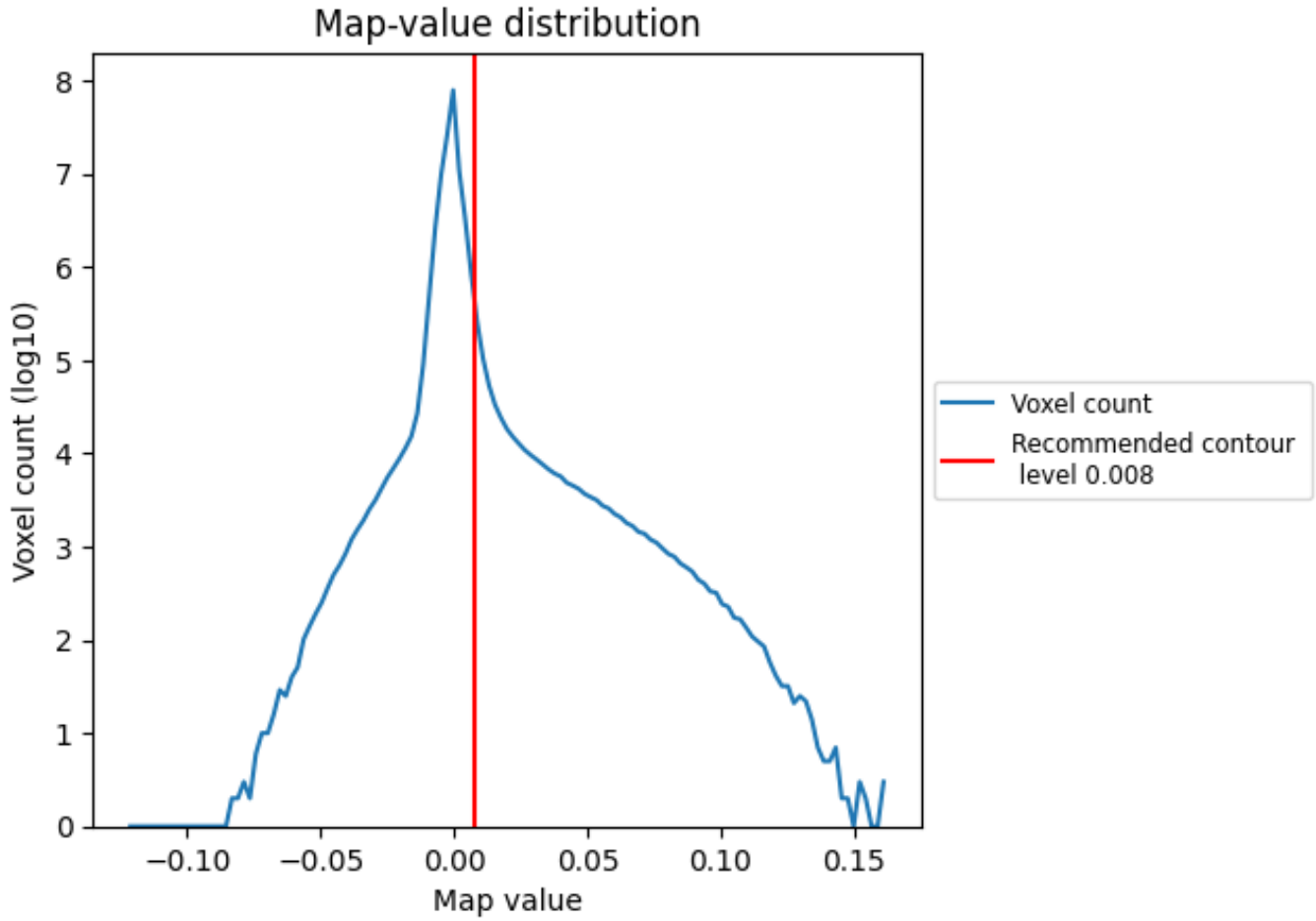


Z

7 Map analysis

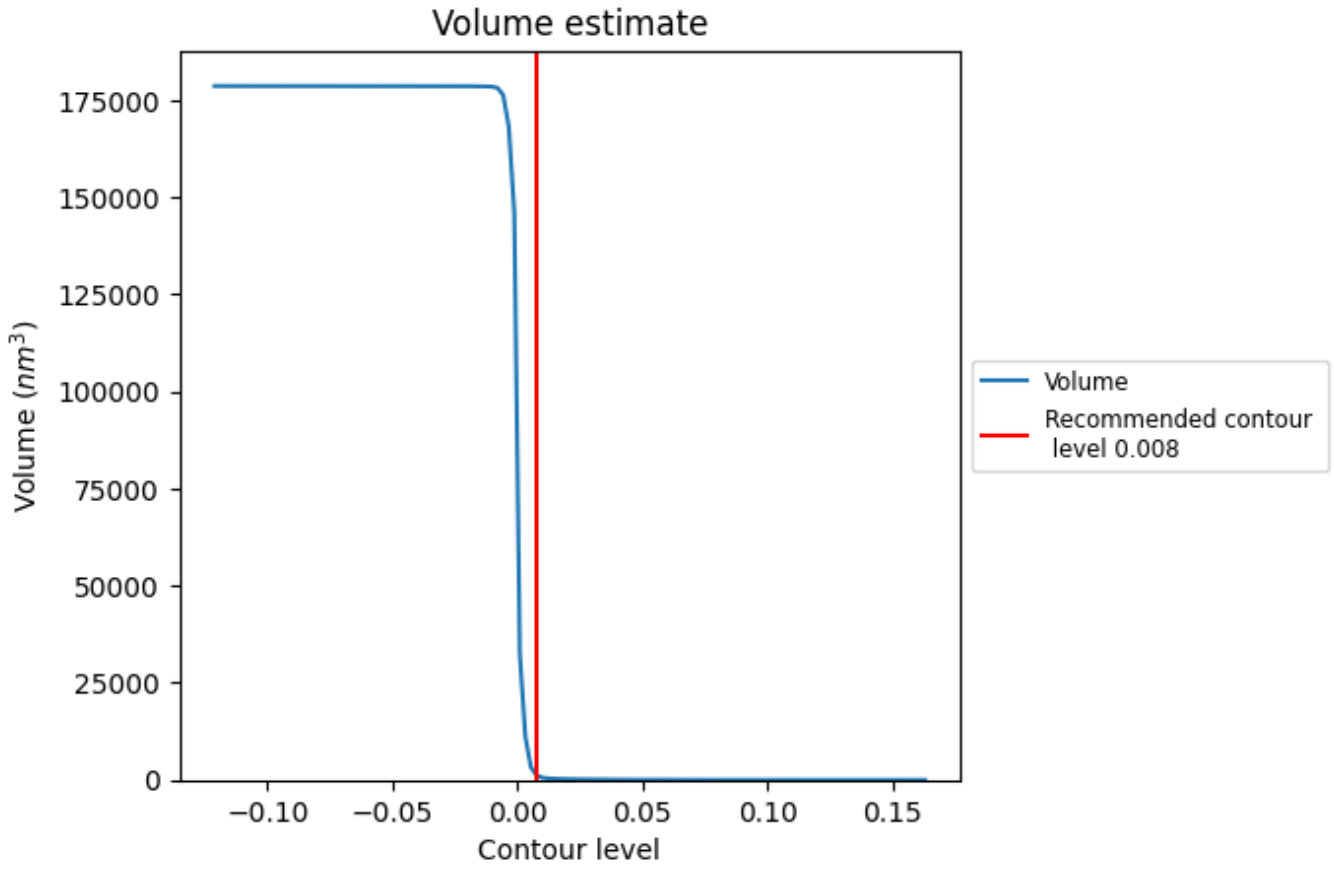
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

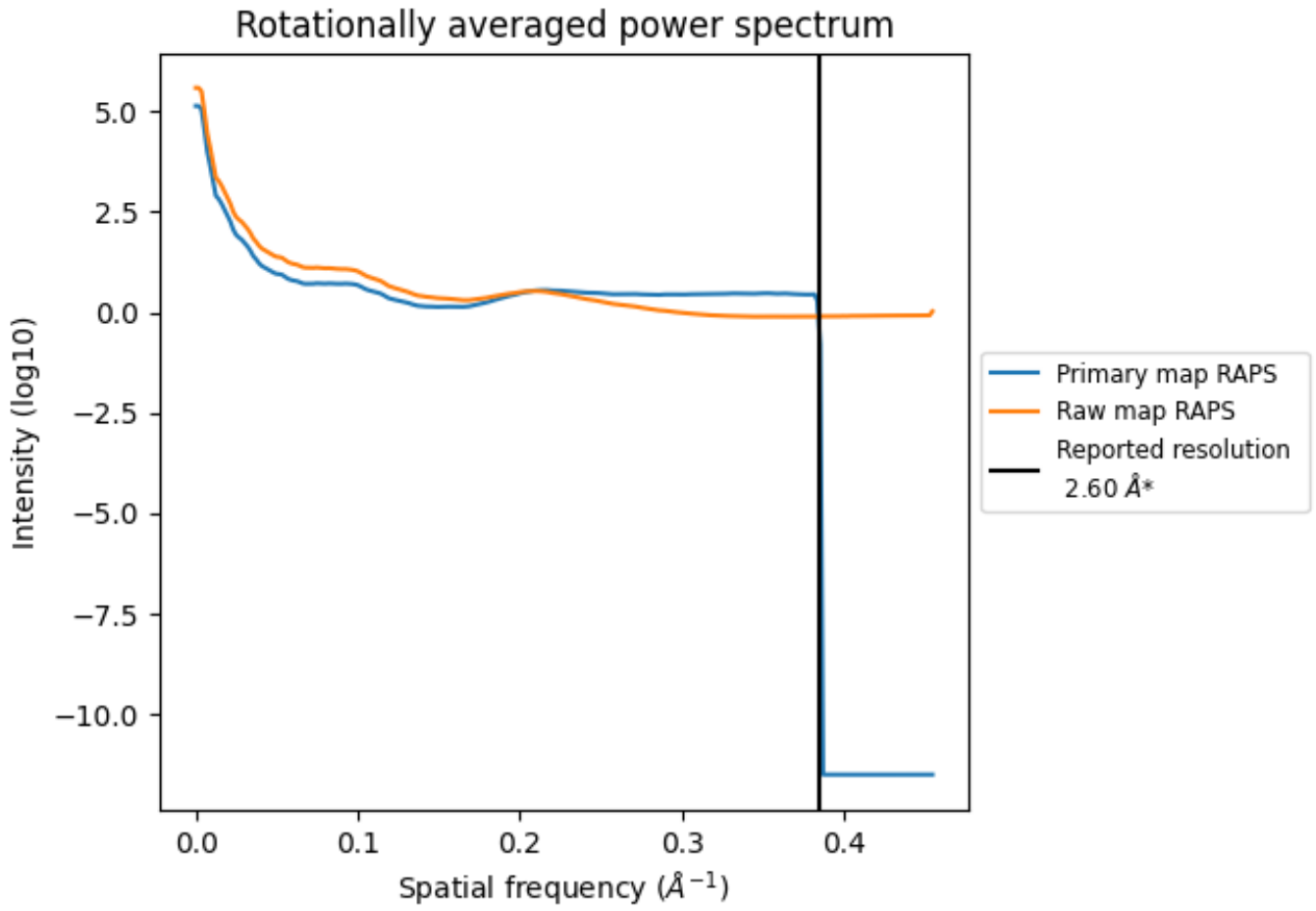
7.2 Volume estimate



The volume at the recommended contour level is 1104 nm^3; this corresponds to an approximate mass of 997 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)

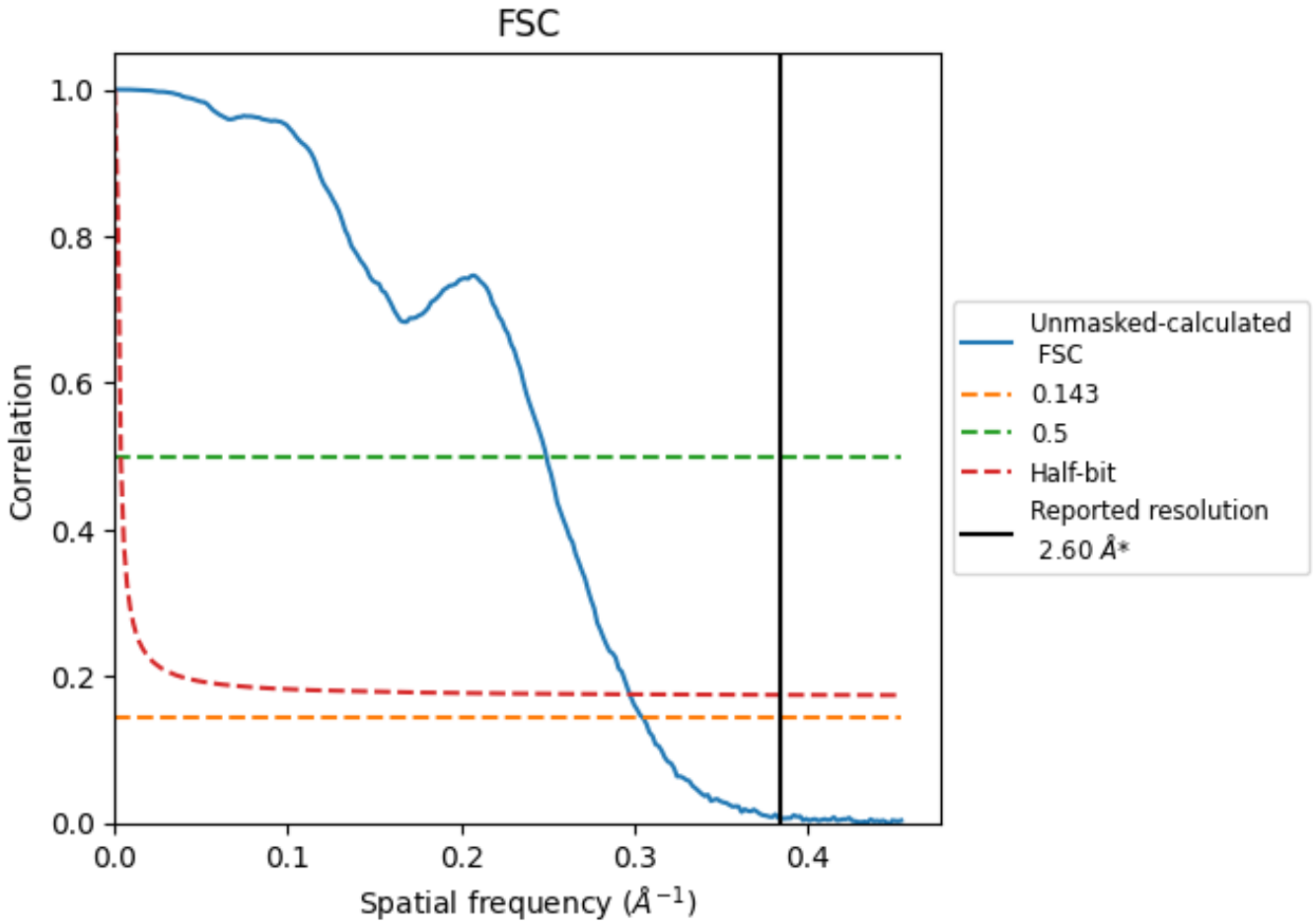


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

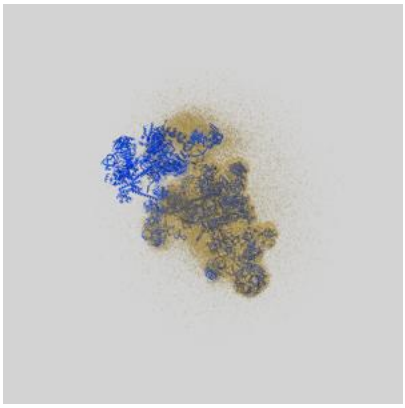
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.01	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.6 by more than 10 %

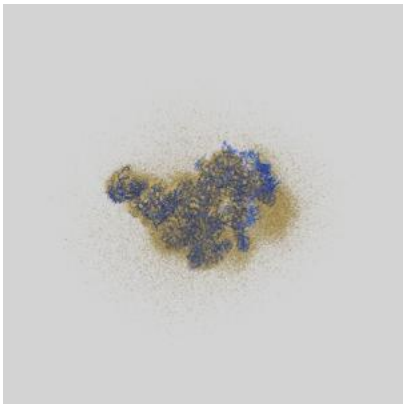
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34508 and PDB model 8H6L. Per-residue inclusion information can be found in section 3 on page 15.

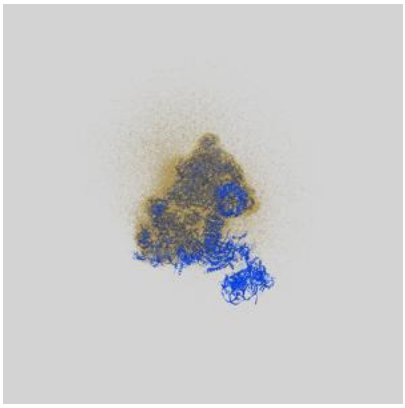
9.1 Map-model overlay



X



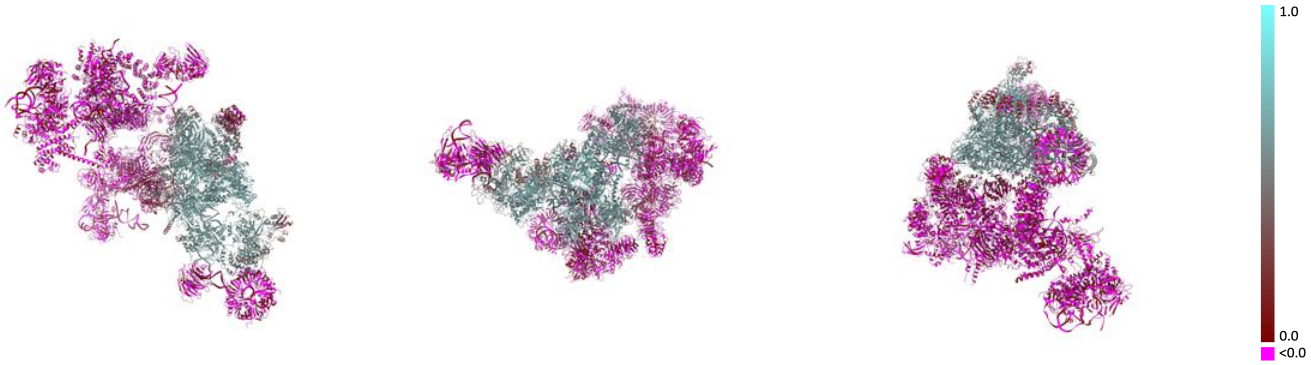
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

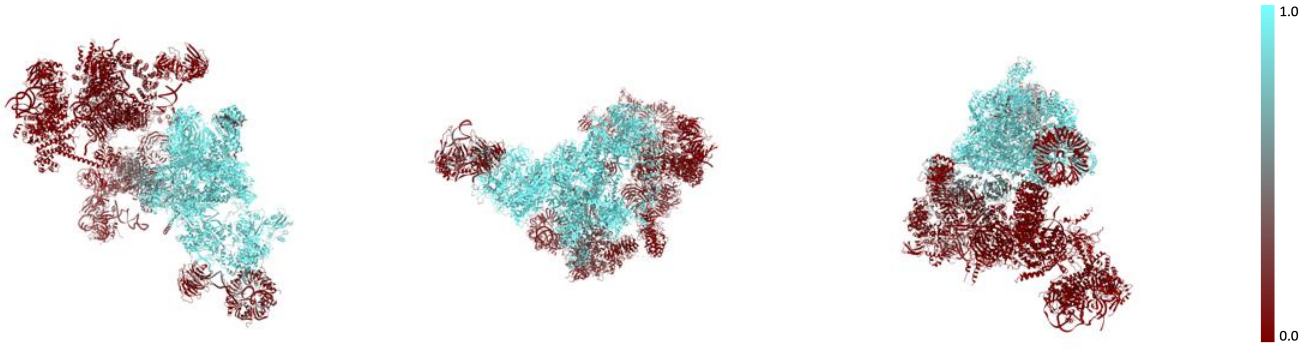
9.2 Q-score mapped to coordinate model (i)



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.

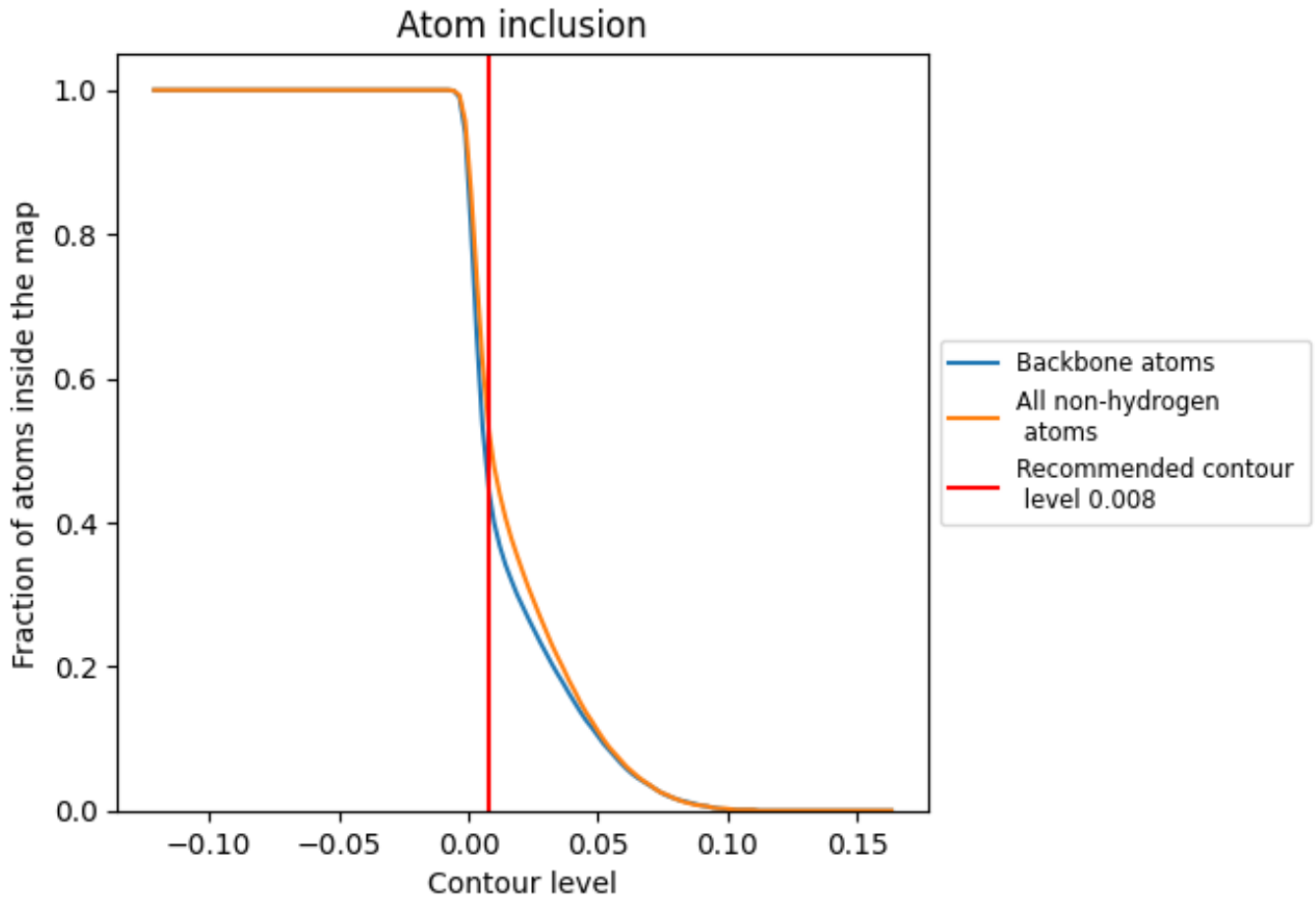
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 53% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5260	0.2830
2A	0.0030	0.0080
2B	0.0000	0.0230
2C	0.0000	0.0180
2D	0.5430	0.3300
2E	0.0000	0.0370
2F	0.0000	0.0030
2G	0.0050	0.0040
2H	0.2340	0.1520
2I	0.0010	0.0030
2J	0.0030	-0.0330
2K	0.0000	0.0130
2L	0.0000	-0.0350
2M	0.0110	0.0050
2a	0.0000	0.0390
2b	0.0000	-0.0010
2c	0.0000	-0.0030
2d	0.0000	0.0150
2e	0.0000	-0.0110
2f	0.0000	0.0220
2g	0.0000	-0.0050
4A	0.5380	0.3160
4B	0.9470	0.5370
4C	0.9600	0.5400
4D	0.9580	0.5830
4E	0.9860	0.6400
4F	0.9950	0.6570
4G	0.8880	0.4510
4H	0.9260	0.3380
4I	0.7670	0.3290
4J	0.9200	0.5340
4Z	0.0570	-0.0000
4a	0.0190	-0.0450
4b	0.0240	-0.0130
4c	0.0730	-0.0240

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Chain	Atom inclusion	Q-score
4d	0.0580	-0.0190
4e	0.0450	-0.0350
4f	0.0600	0.0000
4g	0.0620	0.0350
5A	0.6410	0.3220
5B	0.9230	0.5570
5C	0.9400	0.5080
5D	0.2680	0.0360
5E	0.0720	0.0020
5a	0.2230	-0.0220
5b	0.1550	-0.0160
5c	0.1470	0.0070
5d	0.1350	0.0090
5e	0.1610	-0.0140
5f	0.1980	-0.0280
5g	0.2570	-0.0050
6A	0.7150	0.4220
6a	0.0060	0.0080
6b	0.0030	-0.0140
6c	0.0030	0.0150
6d	0.0070	0.0160
6e	0.0210	0.0620
6f	0.0040	0.0110
6g	0.0080	-0.0300
A	0.2650	0.1630