wwPDB EM Validation Summary Report

Mar 13, 2024 – 07:23 PM JST

PDB ID	:	5WSG
EMDB ID	:	EMD-6684
Title	:	Cryo-EM structure of the Catalytic Step II spliceosome (C* complex) at 4.0 angstrom resolution
Authors	:	Yan, C.; Wan, R.; Bai, R.; Huang, G.; Shi, Y.
Deposited on	:	2016-12-07
Resolution	:	4.00 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:

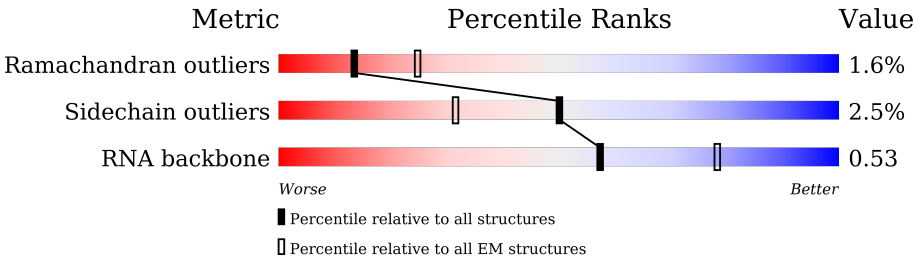
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2413	8% 77% 20%
2	C	1008	84% 13%
3	J	135	20% 80%
4	O	451	70% 25%
5	P	379	10% 50% 47%
6	Q	364	13% 48% 49%
7	R	339	75% 23%
8	S	175	9% 37% 61%

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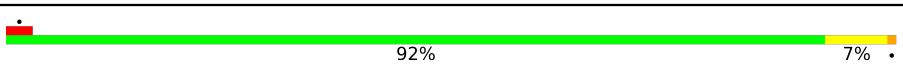
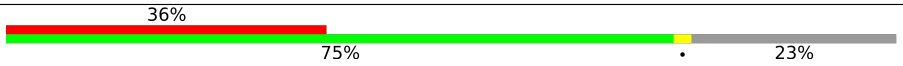
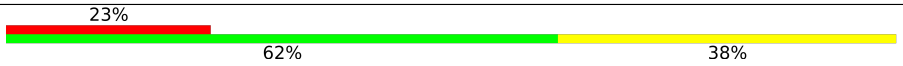
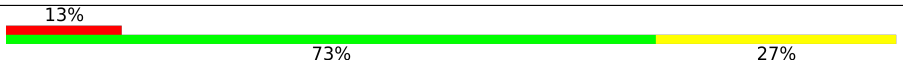
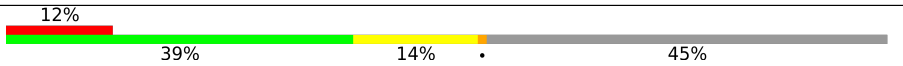
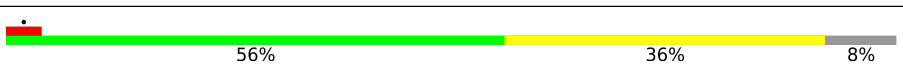
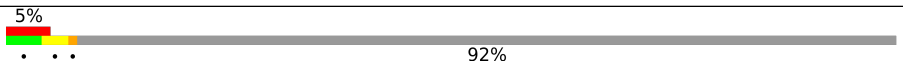
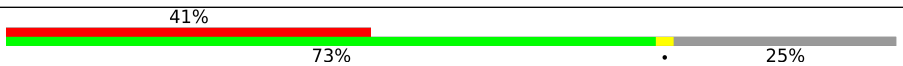
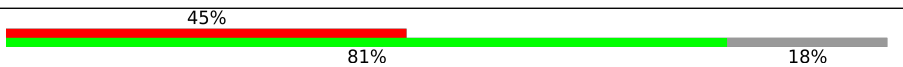
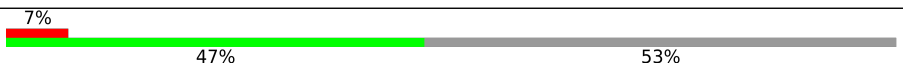
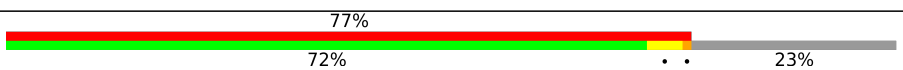
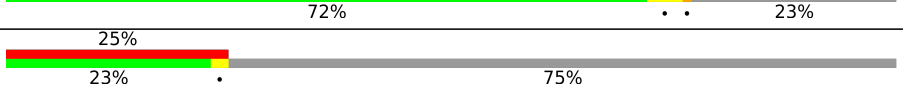
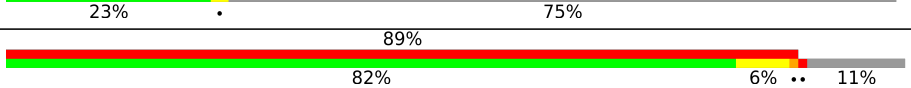
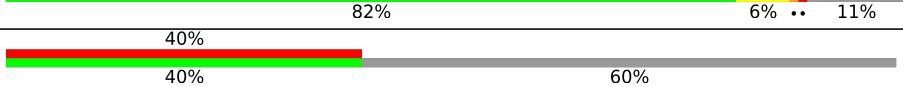
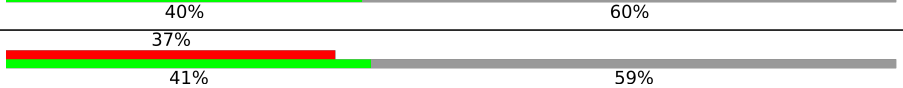
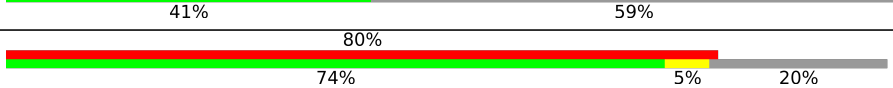
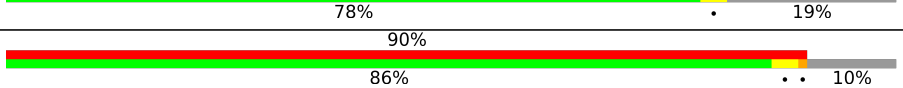
Mol	Chain	Length	Quality of chain
9	T	157	
10	Z	577	
11	B	13	
12	N	15	
13	D	214	
14	E	112	
15	L	1175	
16	M	23	
17	c	579	
18	d	652	
19	I	215	
20	v	858	
21	n	455	
22	o	503	
22	p	503	
22	q	503	
22	r	503	
23	t	175	
24	F	196	
24	k	196	
25	G	94	
25	i	94	
26	H	86	
26	h	86	
27	K	77	

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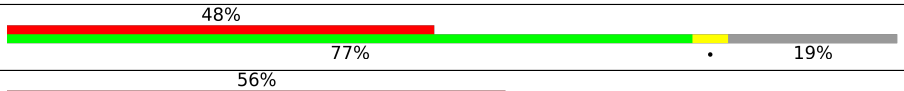
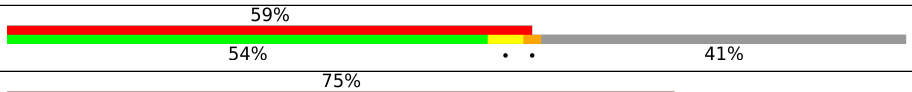
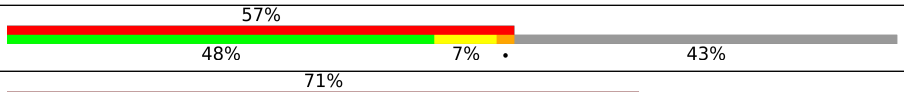
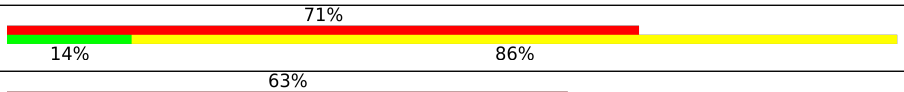
Mol	Chain	Length	Quality of chain
27	j	77	
28	U	101	
28	l	101	
29	V	146	
29	m	146	
30	W	110	
30	g	110	
31	X	111	
32	Y	238	
33	b	14	
34	e	1071	
35	f	251	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 76730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1931	15939	10244	2739	2898	58	0	0

- Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	878	7019	4529	1166	1295	29	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	27	190	112	38	40	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	337	2646	1669	466	501	10	0	0

- Molecule 5 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	201	1583	988	290	298	7	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	185	1472	930	256	271	15	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	69	Total	C	N	O	S	0	0
			560	351	112	96	1		

- Molecule 9 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 10 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	447	Total	C	N	O	S	0	0
			3651	2343	602	688	18		

- Molecule 11 is a RNA chain called 5'-exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	13	Total	C	N	O	P	0	0
			275	124	47	91	13		

- Molecule 12 is a RNA chain called 5'-intron-lariat.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	15	Total	C	N	O	P	0	0
			312	140	45	112	15		

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	117	Total	C	N	O	P	0	0
			2465	1104	414	830	117		

- Molecule 14 is a RNA chain called Saccharomyces cerevisiae S288c SNR6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 15 is a RNA chain called RNA (91-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	91	Total	C	N	O	P	0	0
			1909	854	309	655	91		

- Molecule 16 is a RNA chain called 3'-intron-lariat.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	23	Total	C	N	O	P	0	0
			486	219	86	158	23		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CEF1,Pre-mRNA-splicing factor CEF1,Cef1,Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	436	Total	C	N	O	S	0	0
			2971	1841	549	573	8		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CLF1,Pre-mRNA-splicing factor CLF1,Clf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	532	Total	C	N	O	S	0	0
			3506	2182	658	658	8		

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

- Molecule 20 is a protein called Syf1,Pre-mRNA-splicing factor SYF1,Syf1,Pre-mRNA-splici ng factor SYF1,Syf1,Pre-mRNA-splicing factor SYF1,Syf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	593	Total	C	N	O	S	0	0
			3183	1953	603	626	1		

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	296	Total	C	N	O	S	0	0
			1870	1162	337	365	6		

- Molecule 22 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	126	Total	C	N	O	S	0	0
			830	525	134	169	2		
22	p	128	Total	C	N	O	S	0	0
			843	532	136	173	2		
22	q	387	Total	C	N	O	S	0	0
			2345	1471	402	464	8		
22	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	156	Total	C	N	O	S	0	0
			926	585	160	180	1		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
24	F	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
25	G	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	70	Total	C	N	O	S	0	0
			554	355	98	100	1		
26	H	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	K	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	l	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
28	U	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
29	V	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	W	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
31	X	81	Total	C	N	O	0	0
			513	332	89	92		

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	135	Total	C	N	O	0	0
			841	538	142	161		

- Molecule 33 is a RNA chain called 3'-exon-intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	14	Total	C	N	O	P	0	0
			208	91	13	90	14		

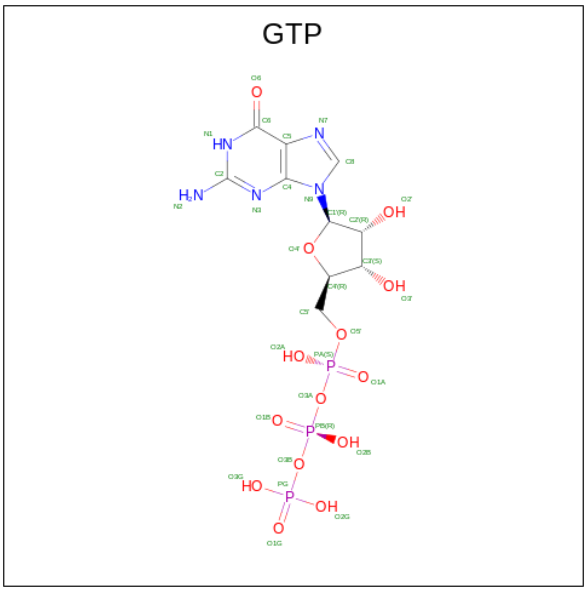
- Molecule 34 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	e	679	Total	C	N	O	0	0
			3360	2002	679	679		

- Molecule 35 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	148	Total	C	N	O	S	0	0
			1202	780	204	214	4		

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	E	4	Total	Mg	0
			4	4	

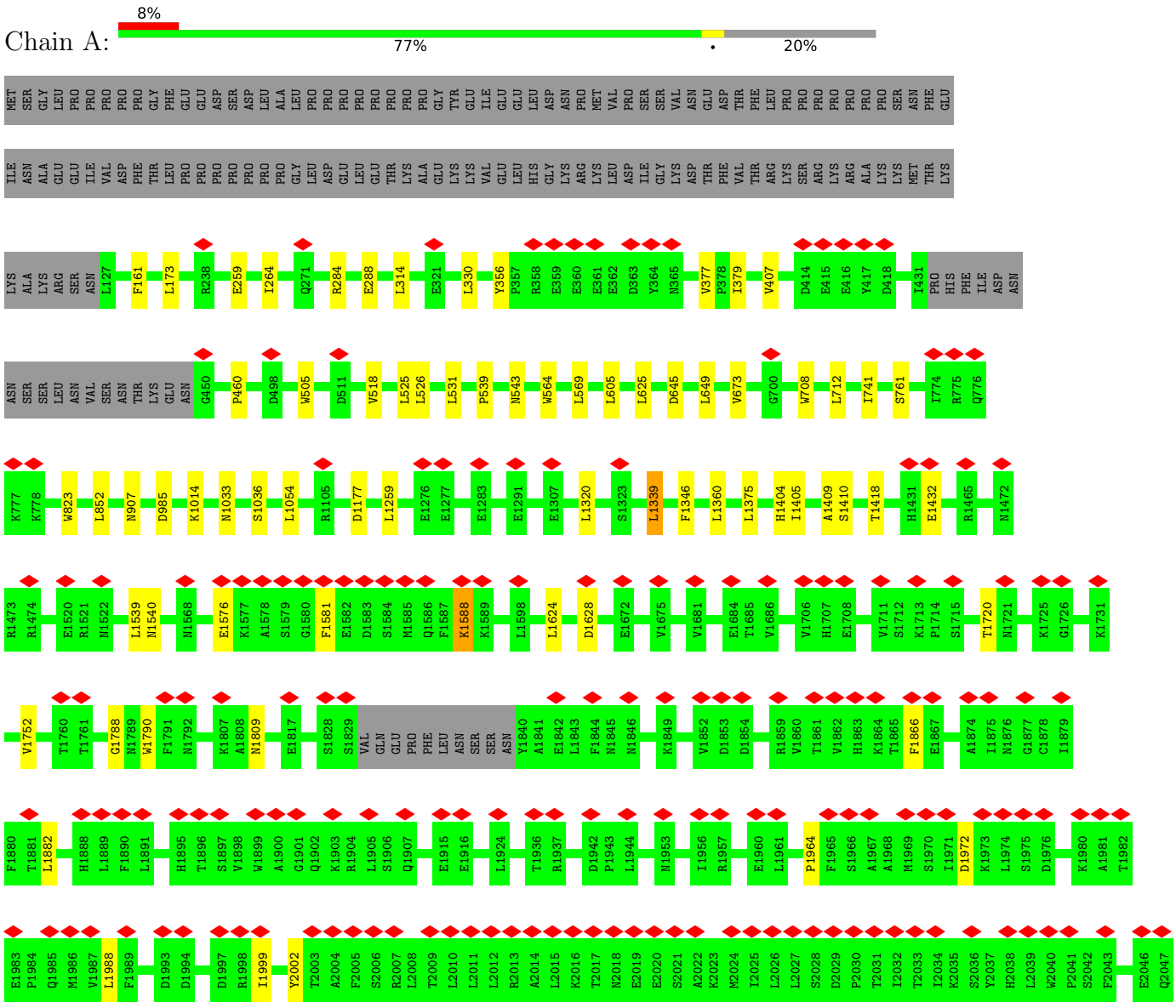
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

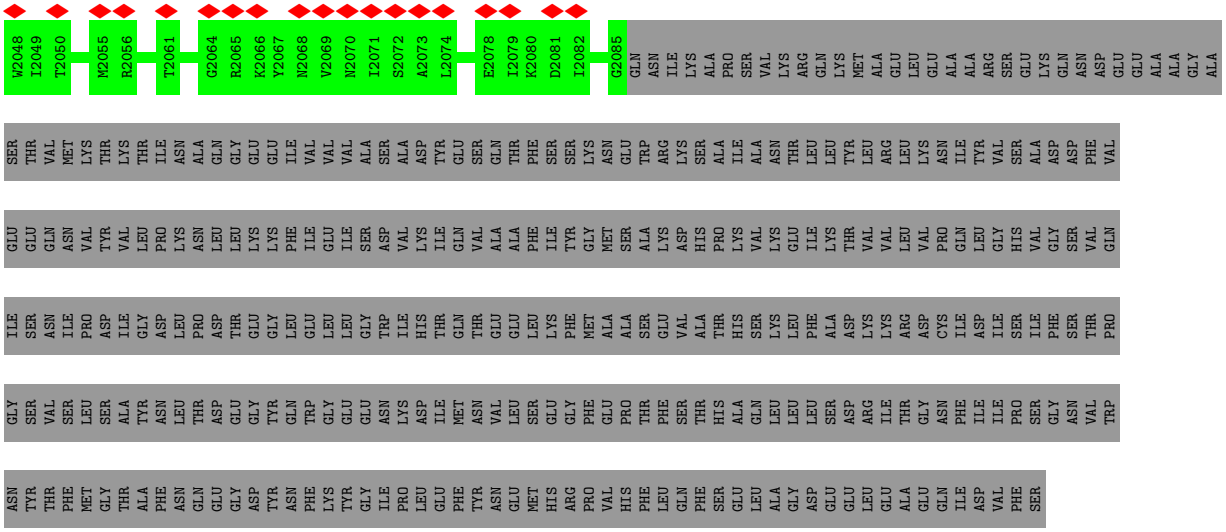
Mol	Chain	Residues	Atoms		AltConf
38	Q	2	Total	Zn	0
			2	2	
38	R	1	Total	Zn	0
			1	1	
38	T	3	Total	Zn	0
			3	3	

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.

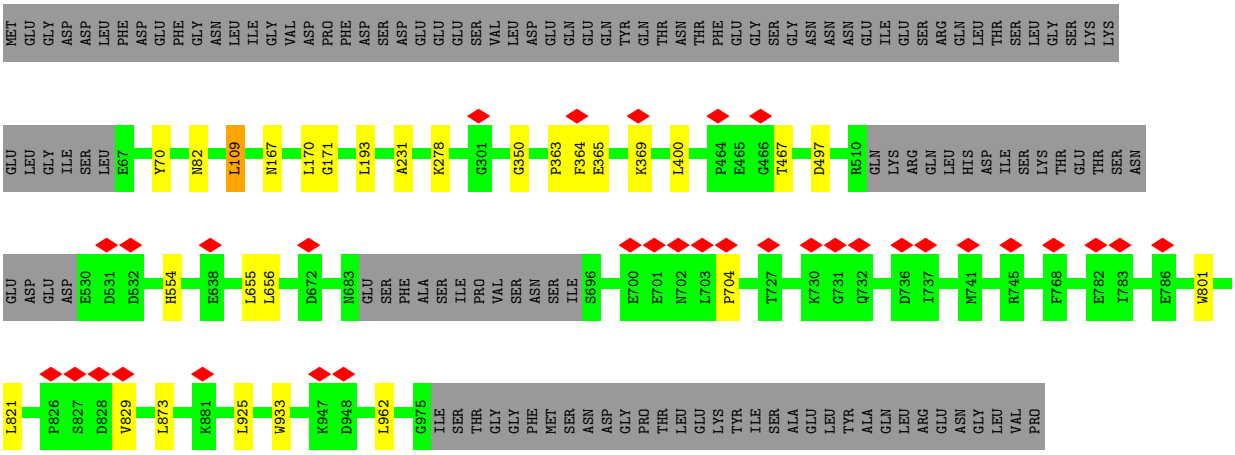
• Molecule 1: Pre-mRNA-splicing factor 8





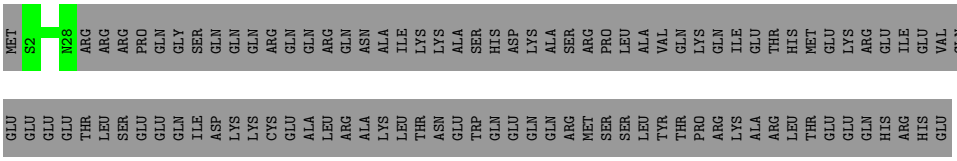
• Molecule 2: Pre-mRNA-splicing factor SNU114

Chain C:



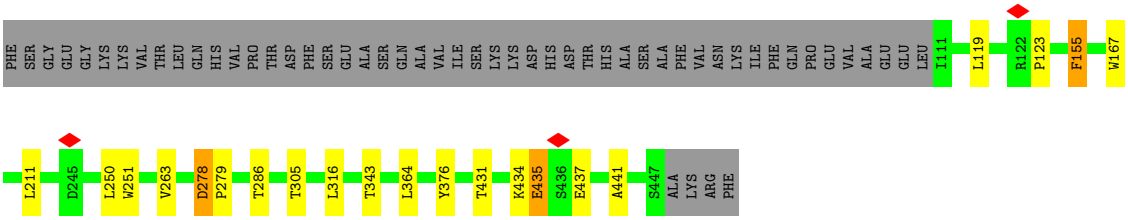
• Molecule 3: Pre-mRNA-splicing factor CWC21

Chain J:

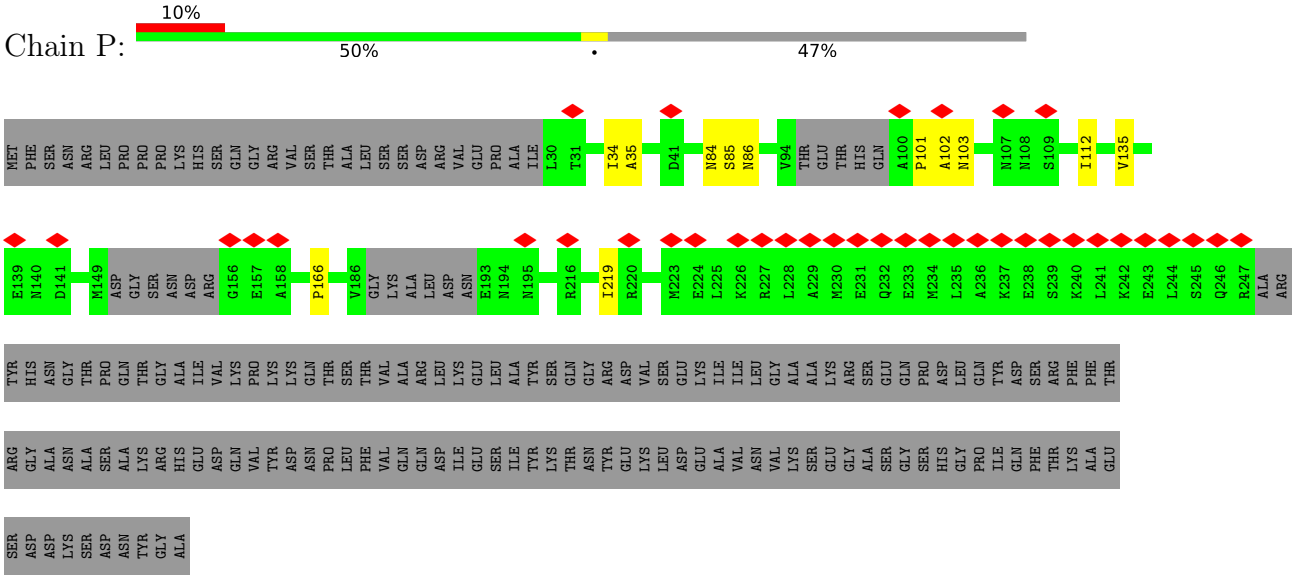


• Molecule 4: Pre-mRNA-splicing factor PRP46

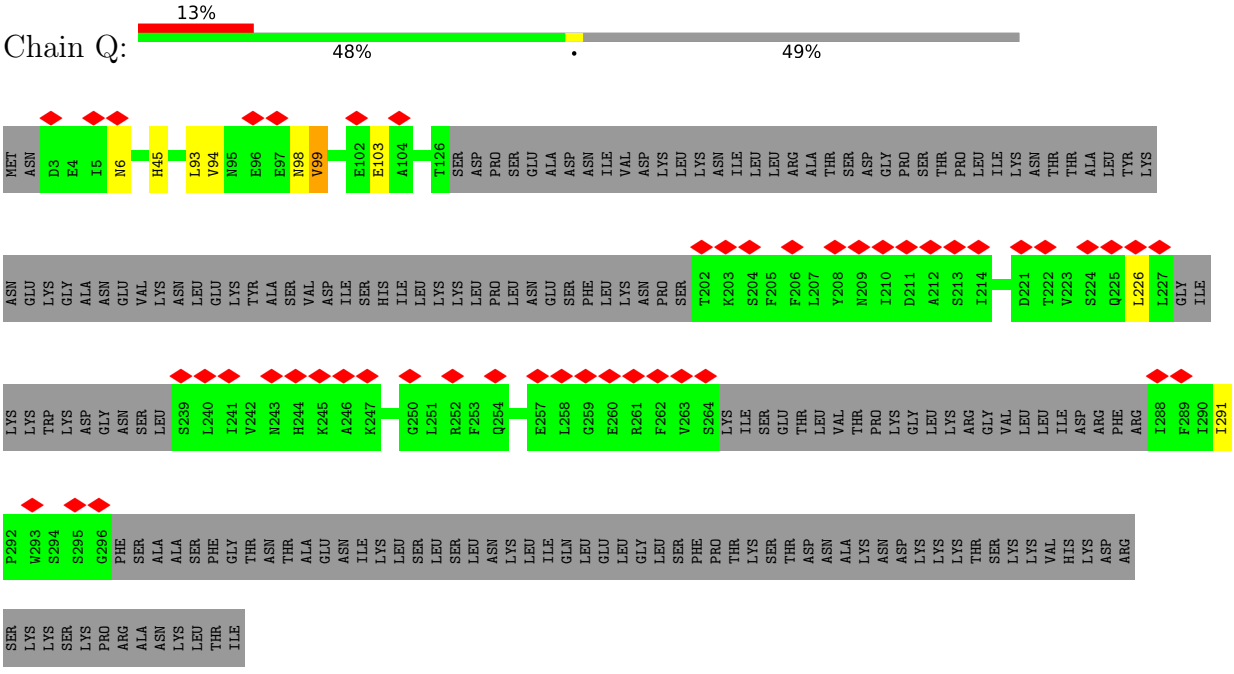
Chain O:



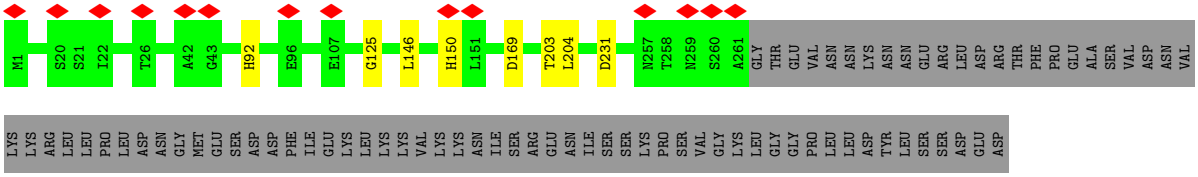
• Molecule 5: Pre-mRNA-processing protein 45



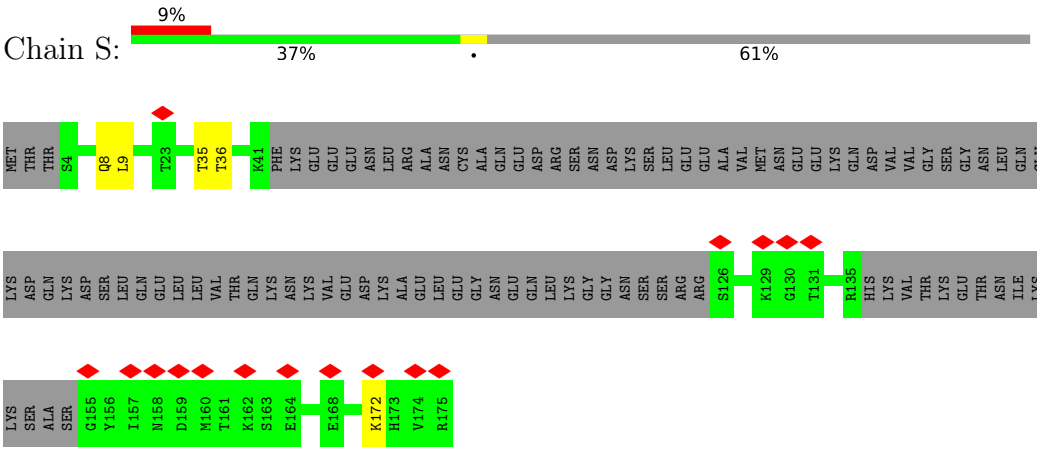
• Molecule 6: Pre-mRNA-splicing factor SLT11



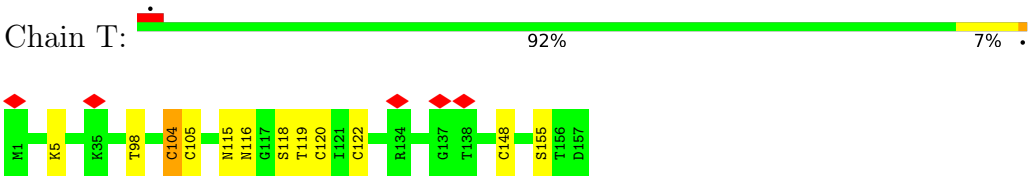
• Molecule 7: Pre-mRNA-splicing factor CWC2



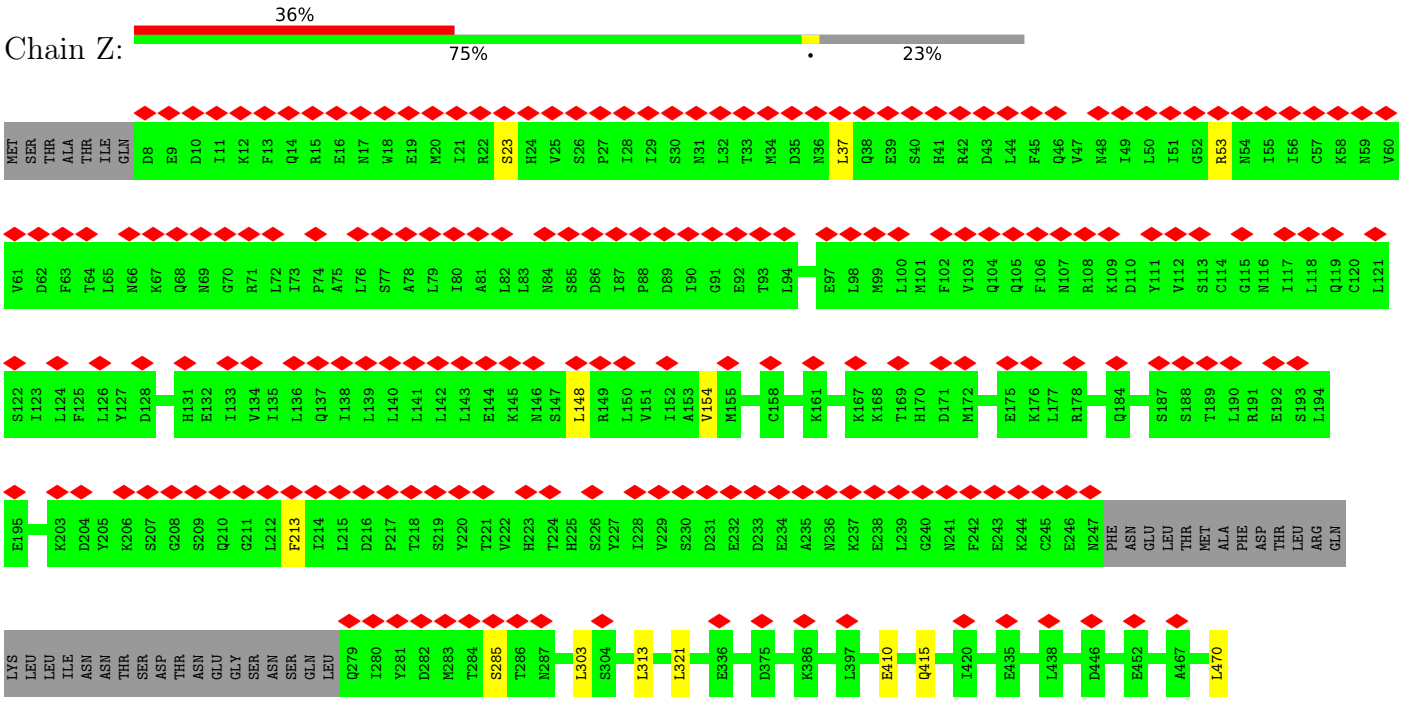
• Molecule 8: Pre-mRNA-splicing factor CWC15

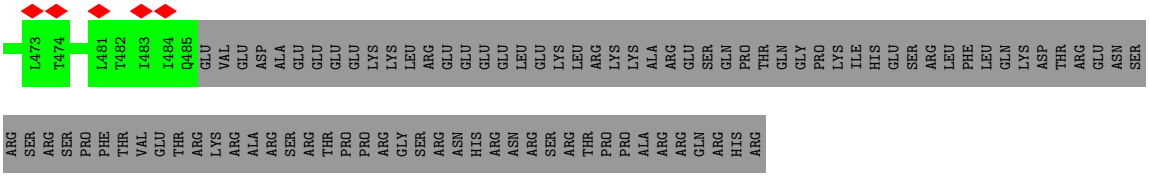


• Molecule 9: Pre-mRNA-splicing factor BUD31

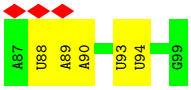


• Molecule 10: Pre-mRNA-splicing factor CWC22

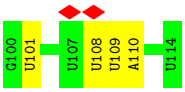




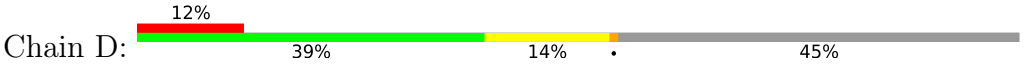
• Molecule 11: 5'-exon

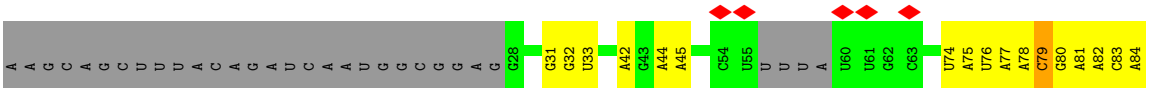


• Molecule 12: 5'-intron-lariat

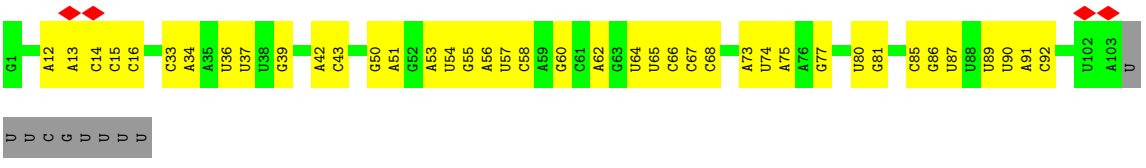


• Molecule 13: U5 snRNA

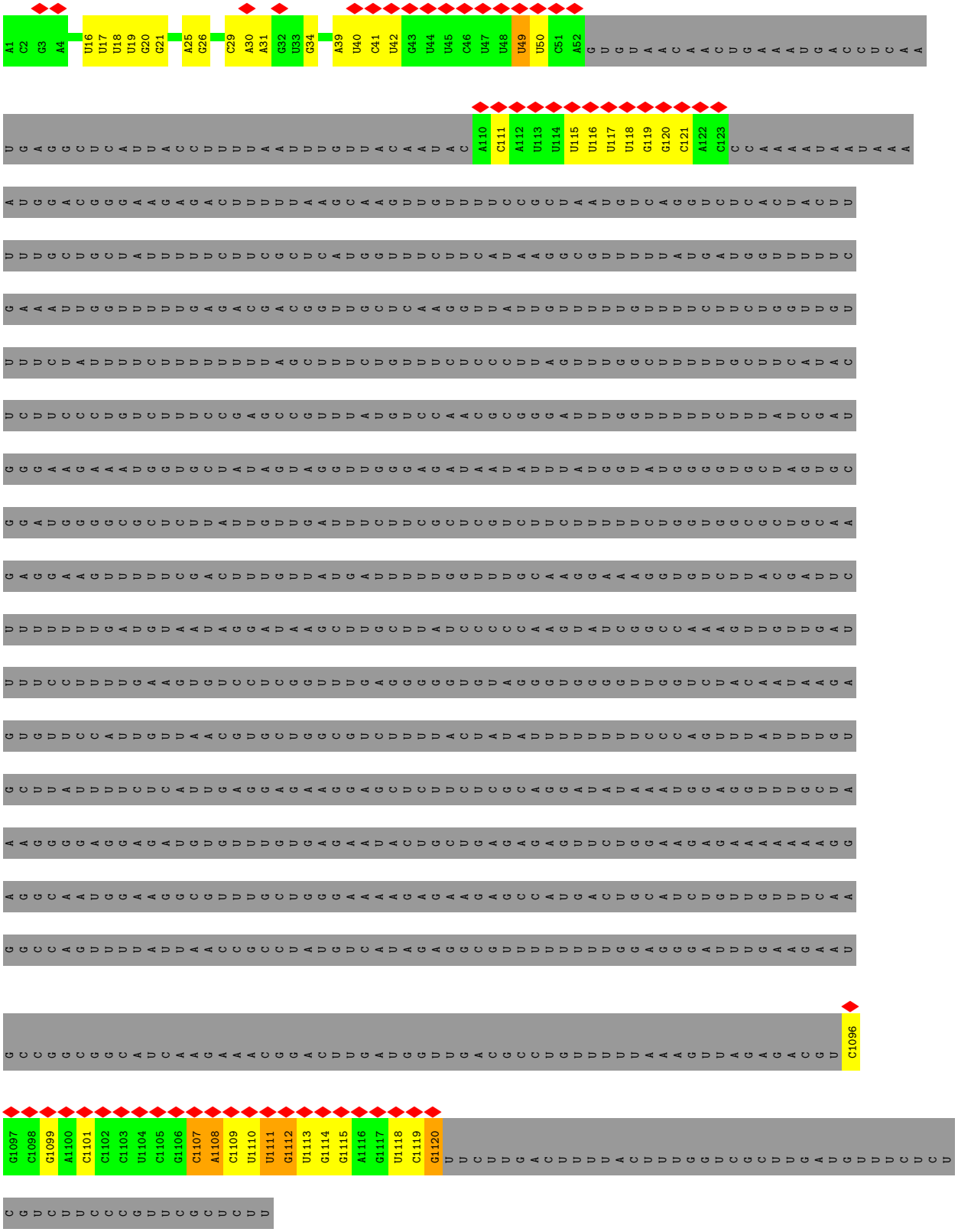




• Molecule 14: Saccharomyces cerevisiae S288c SNR6 snRNA

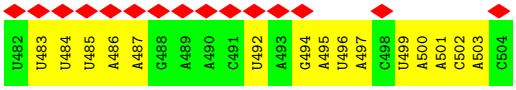


• Molecule 15: RNA (91-MER)



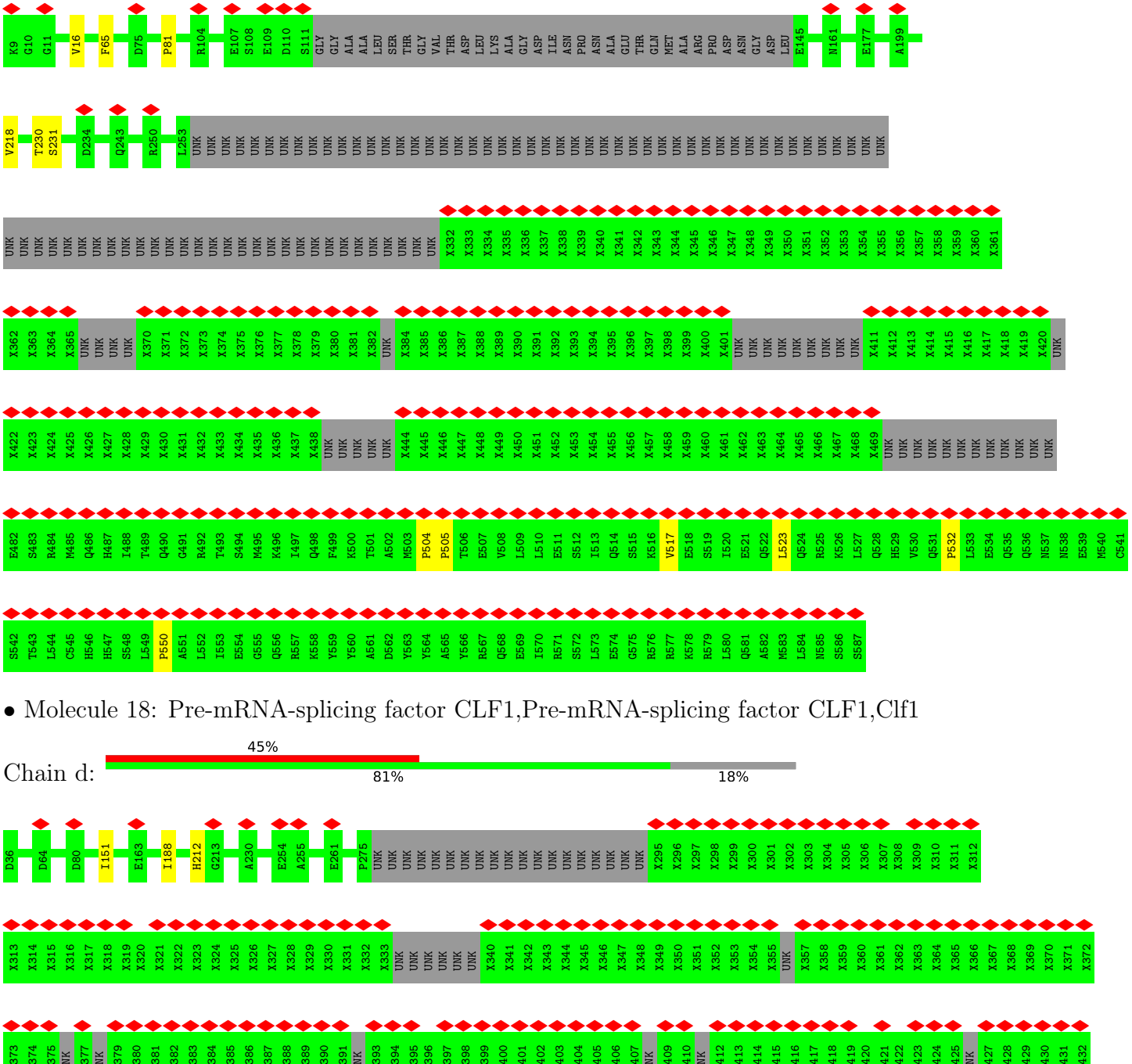
• Molecule 16: 3'-intron-lariat

Chain M:



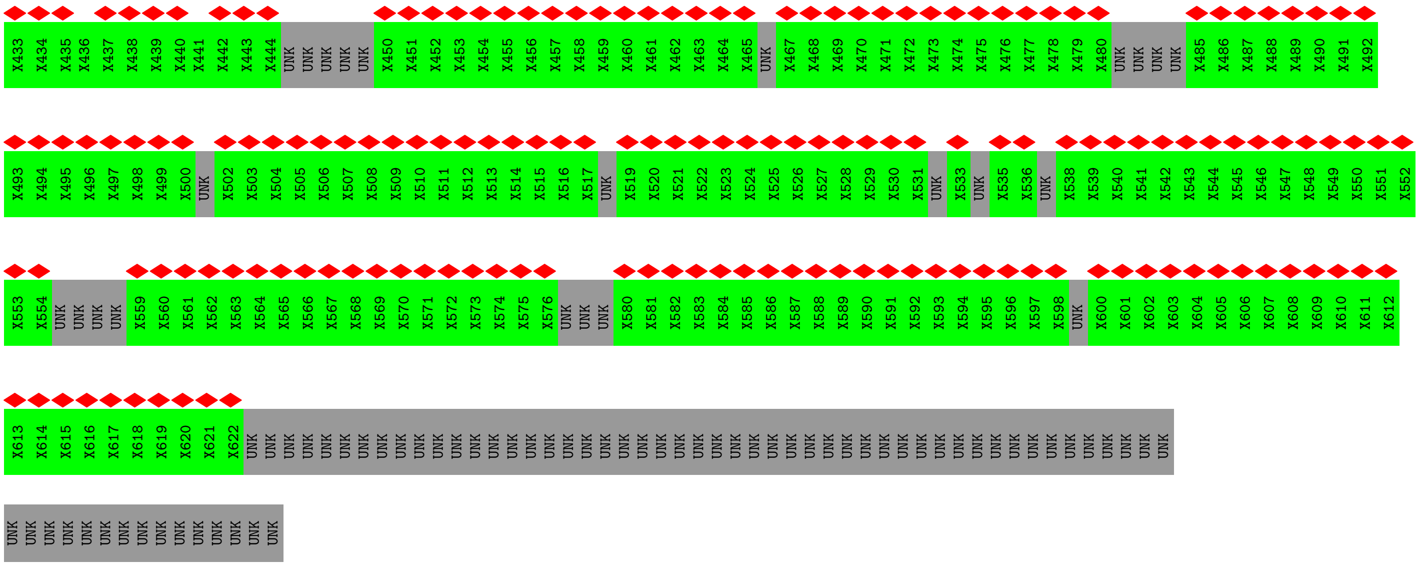
• Molecule 17: Pre-mRNA-splicing factor CEF1,Pre-mRNA-splicing factor CEF1,Cef1,Pre-mRNA-splicing factor CEF1

Chain c:

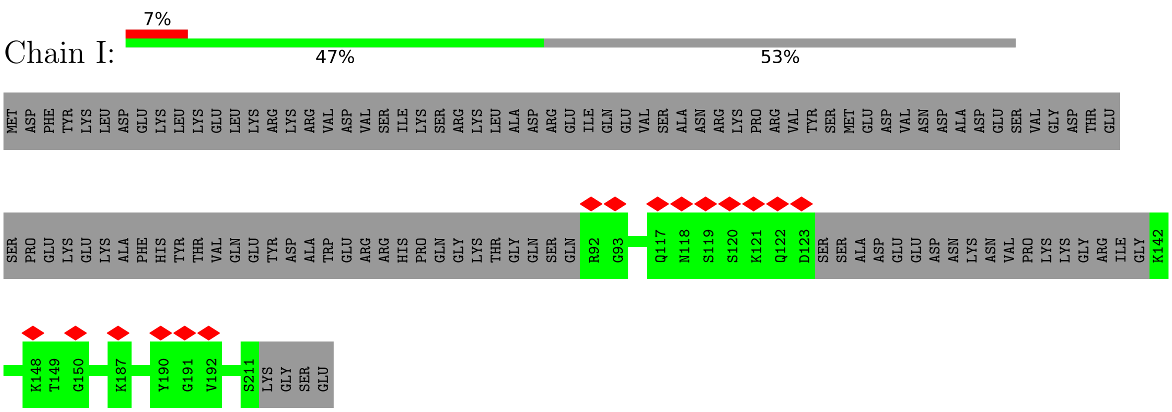


• Molecule 18: Pre-mRNA-splicing factor CLF1,Pre-mRNA-splicing factor CLF1,Clf1

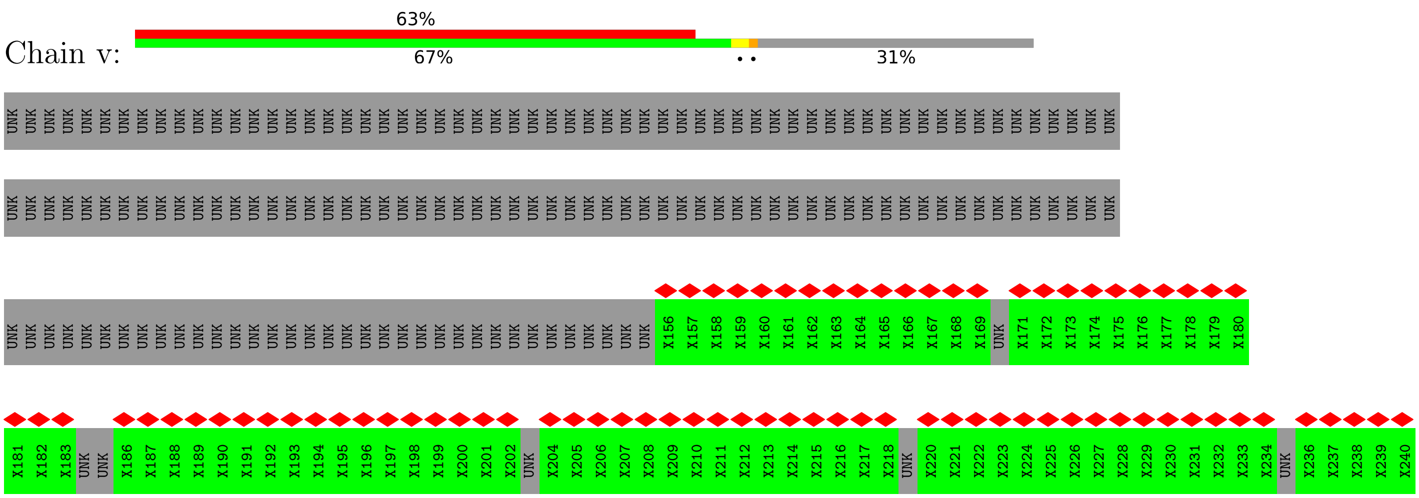
Chain d:

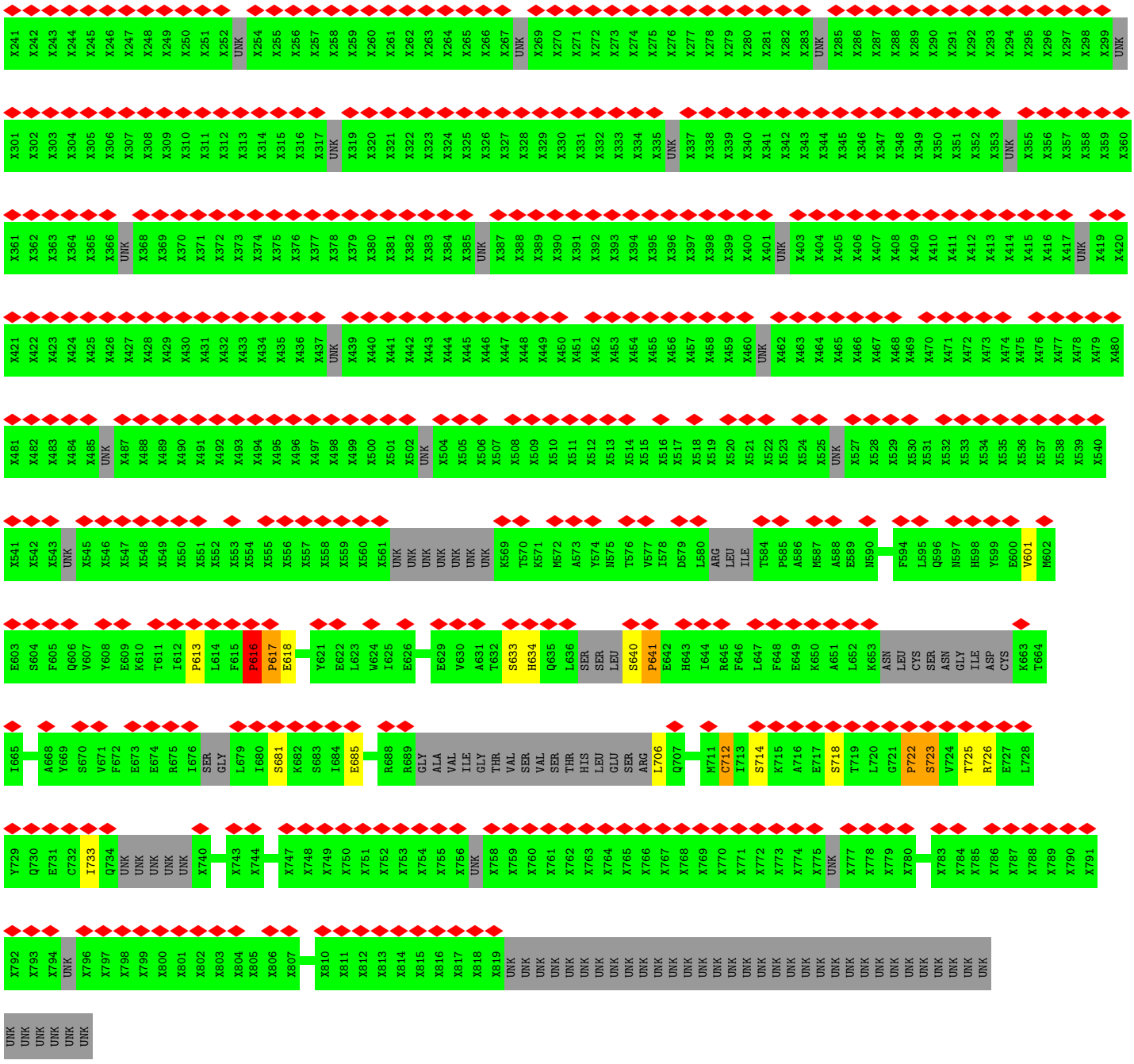


• Molecule 19: Pre-mRNA-splicing factor SYF2

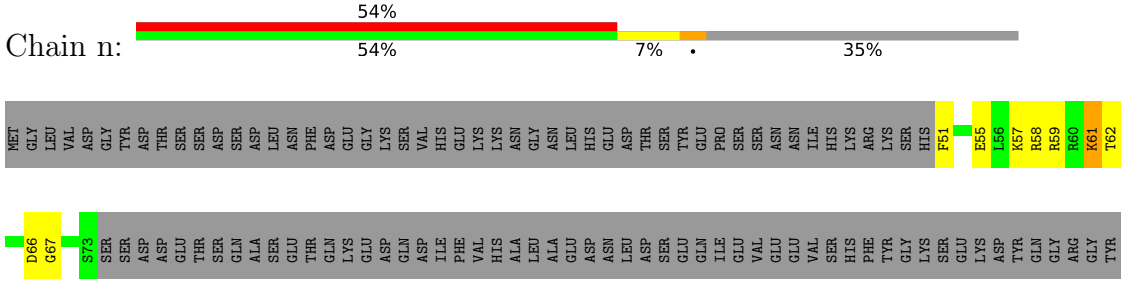


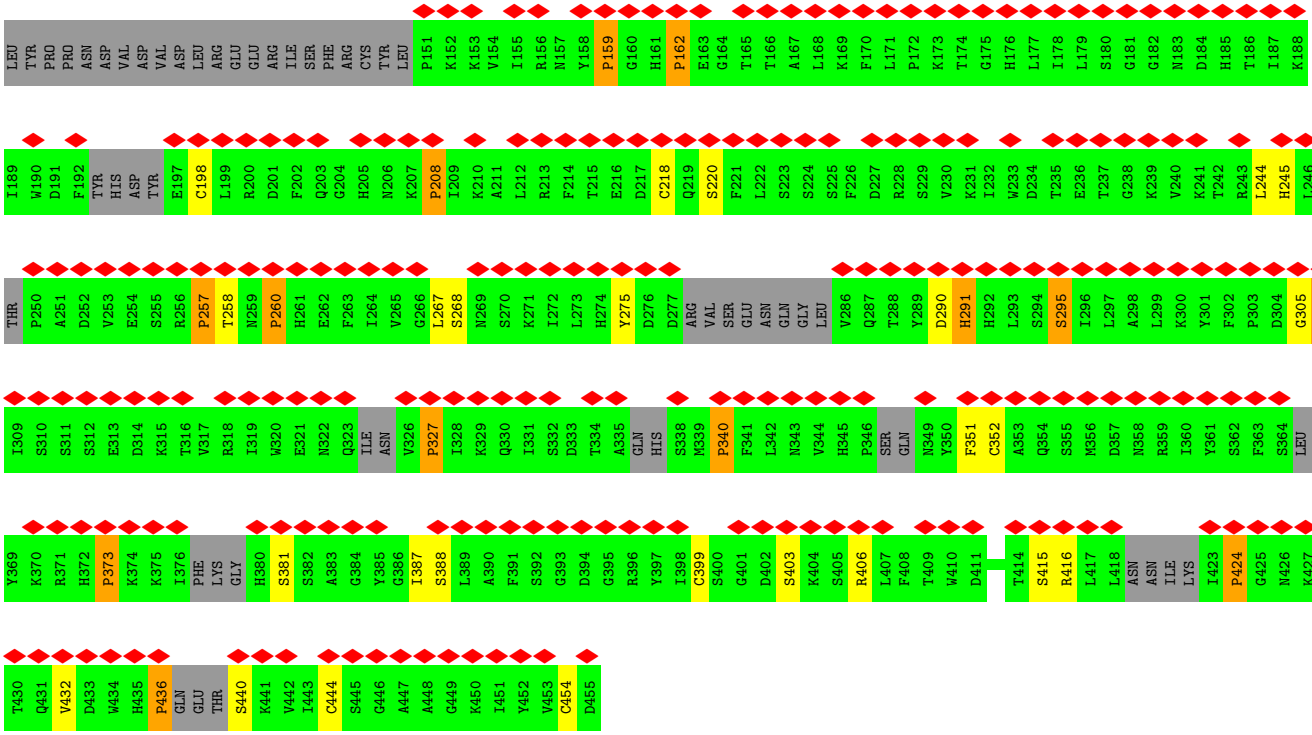
• Molecule 20: Syf1,Pre-mRNA-splicing factor SYF1,Syf1,Pre-mRNA-splicing factor SYF1,Syf1, Pre-mRNA-splicing factor SYF1,Syf1





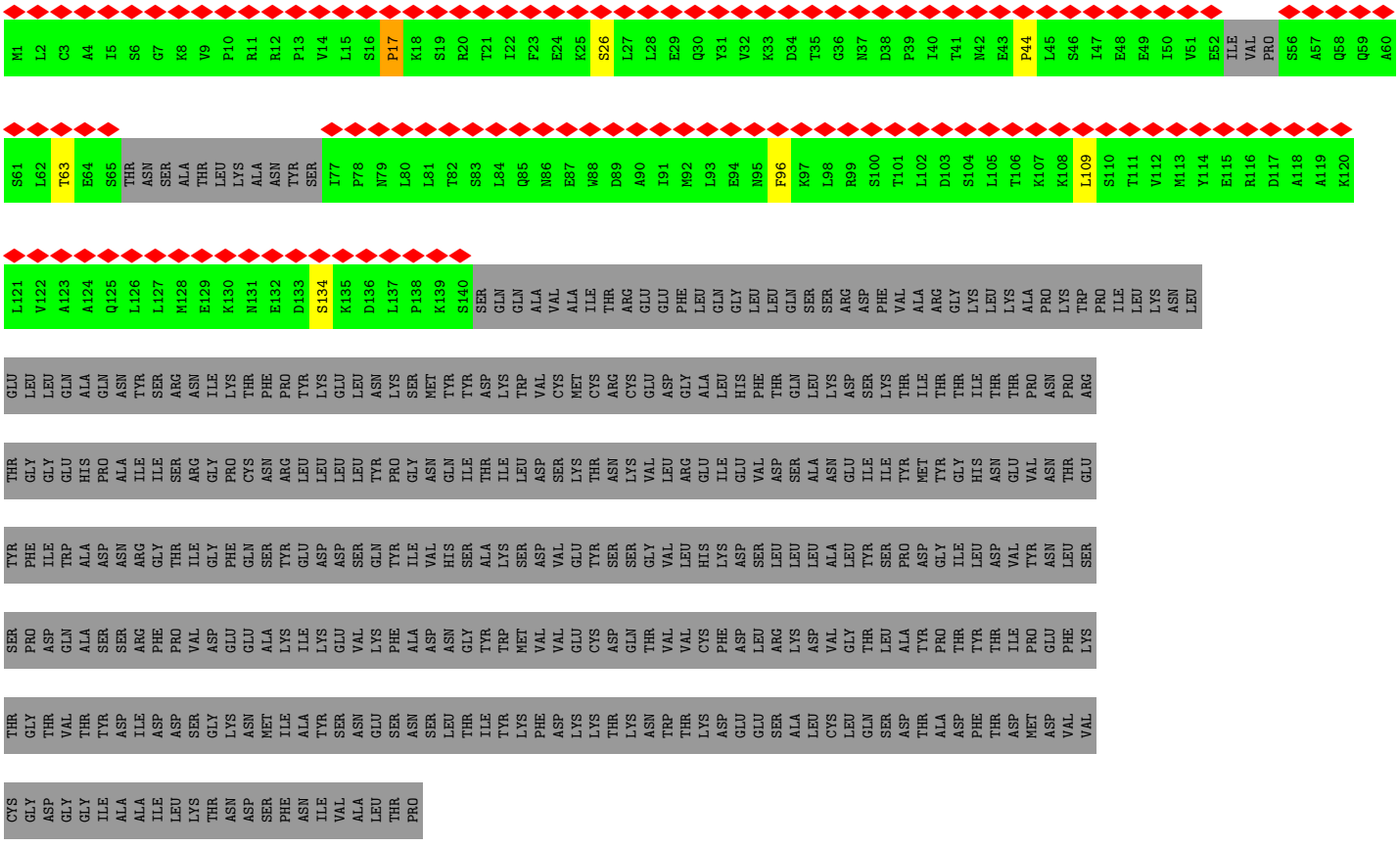
• Molecule 21: Pre-mRNA-processing factor 17





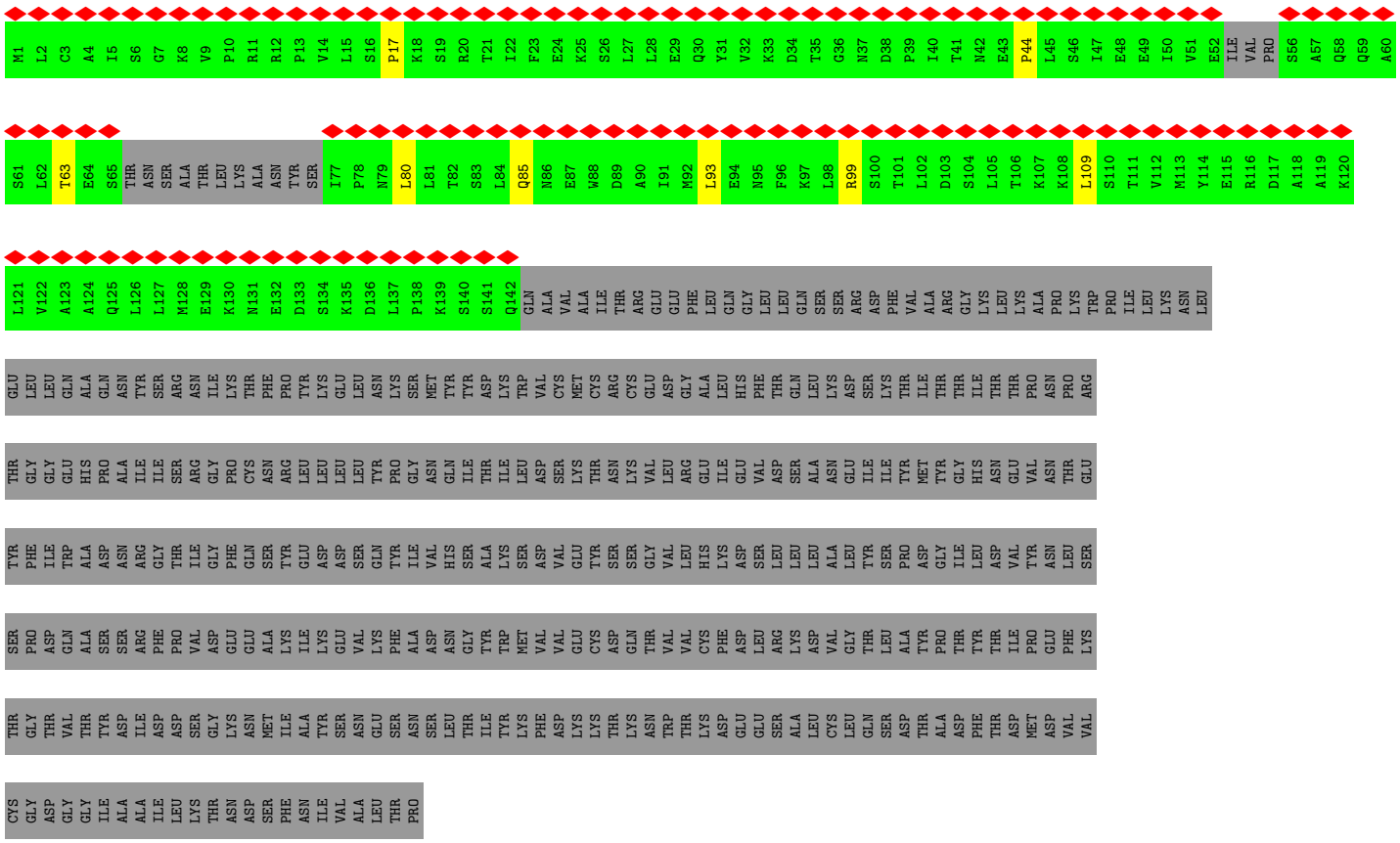
• Molecule 22: Pre-mRNA-processing factor 19

Chain o:



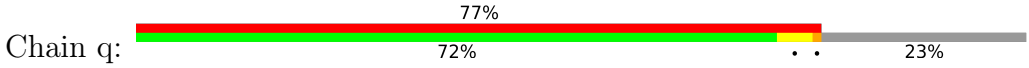
• Molecule 22: Pre-mRNA-processing factor 19

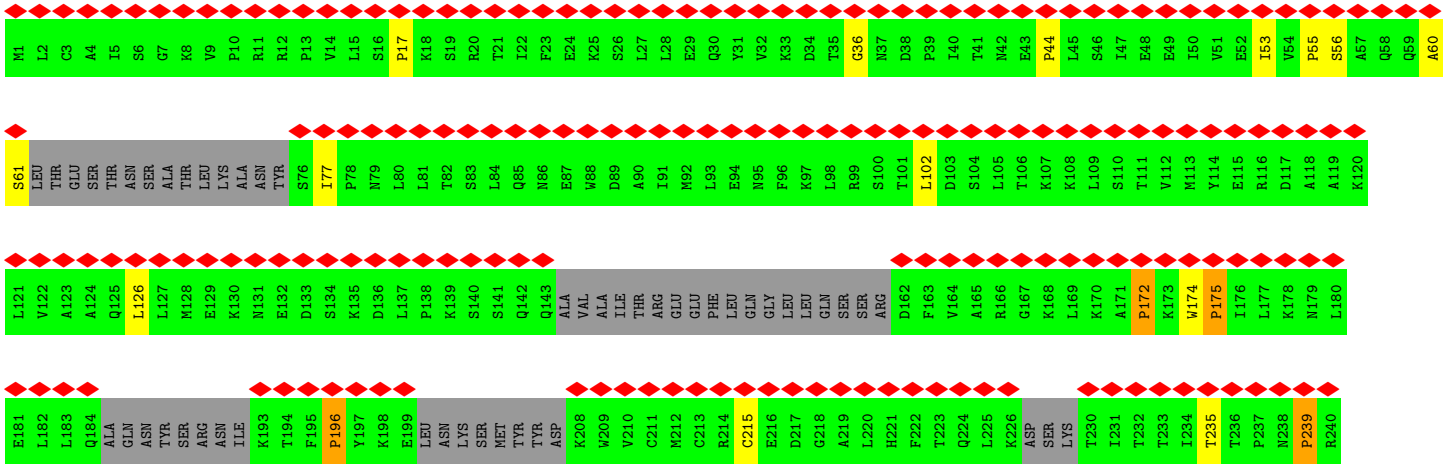
Chain p:

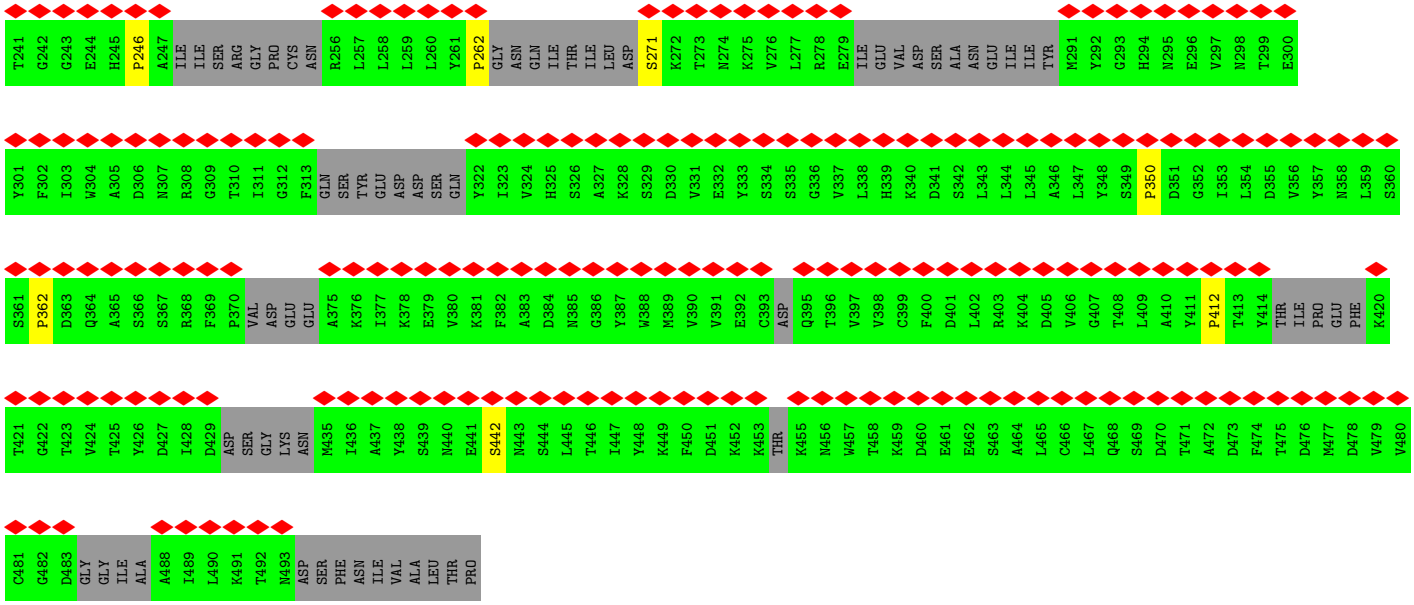


• Molecule 22: Pre-mRNA-processing factor 19

Chain q:





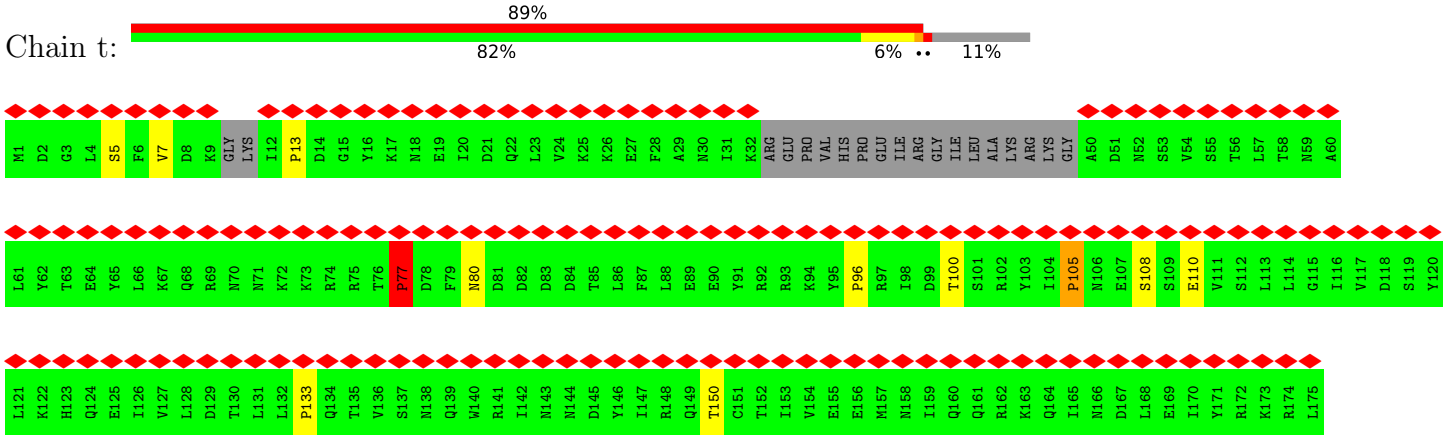


• Molecule 22: Pre-mRNA-processing factor 19

Chain r:

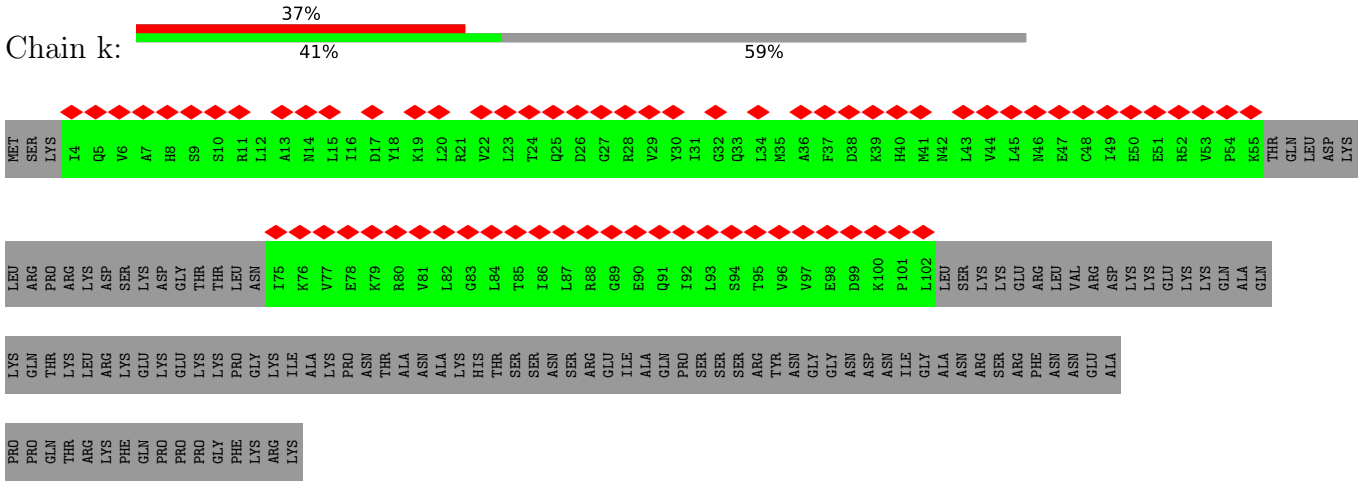
• Molecule 23: Pre-mRNA-splicing factor SNT309

Chain t:



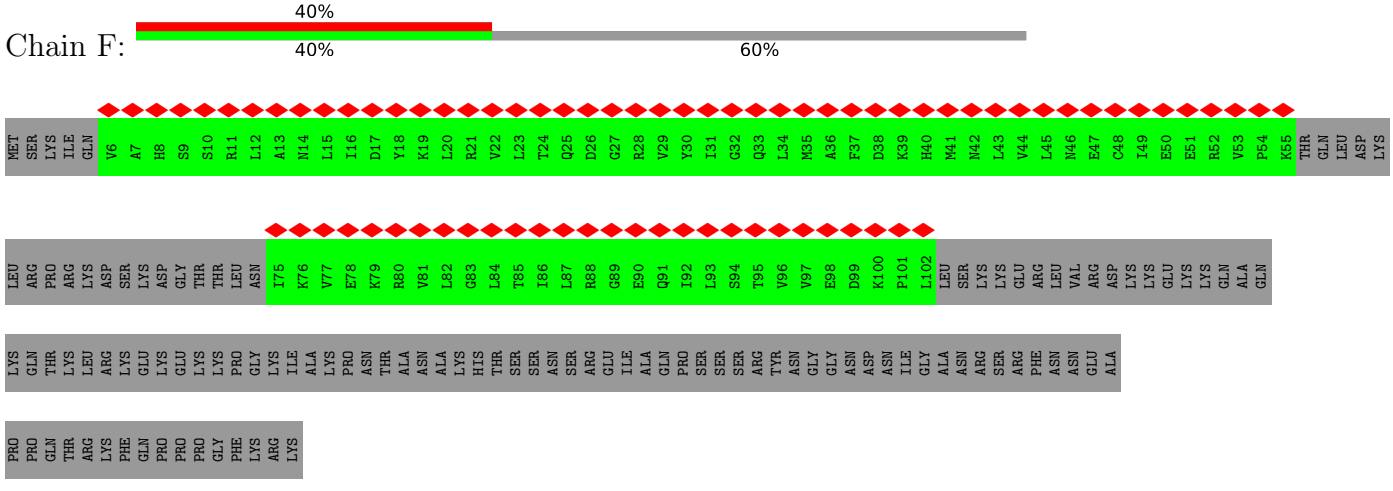
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B

Chain k:



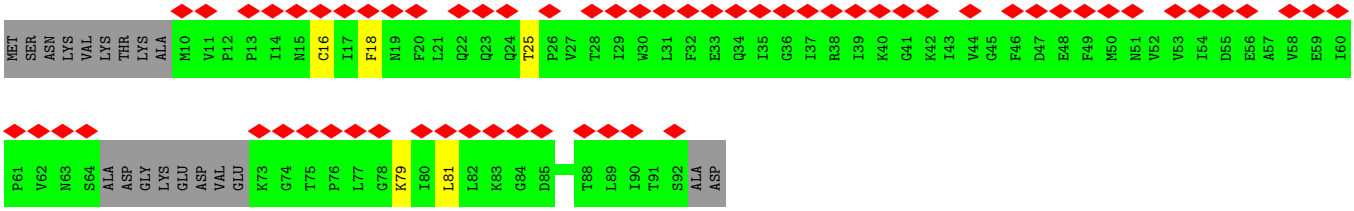
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B

Chain F:

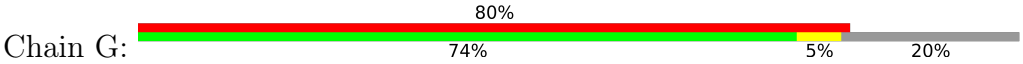


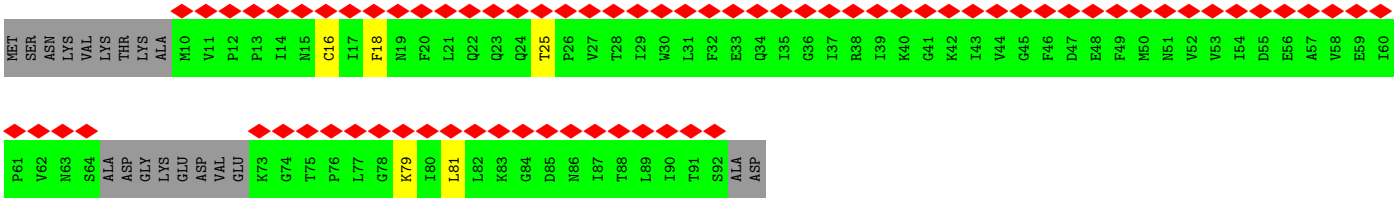
• Molecule 25: Small nuclear ribonucleoprotein E

Chain i:

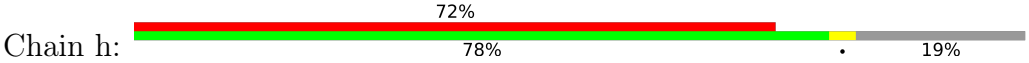


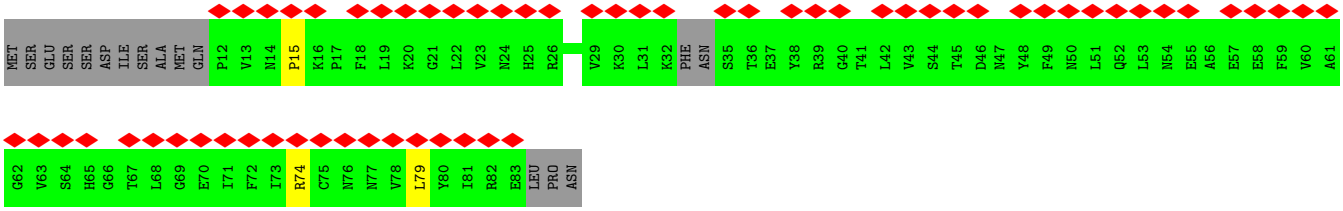
• Molecule 25: Small nuclear ribonucleoprotein E



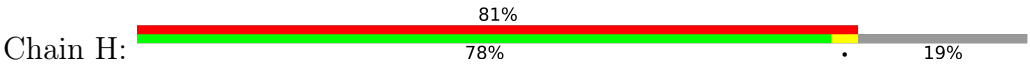


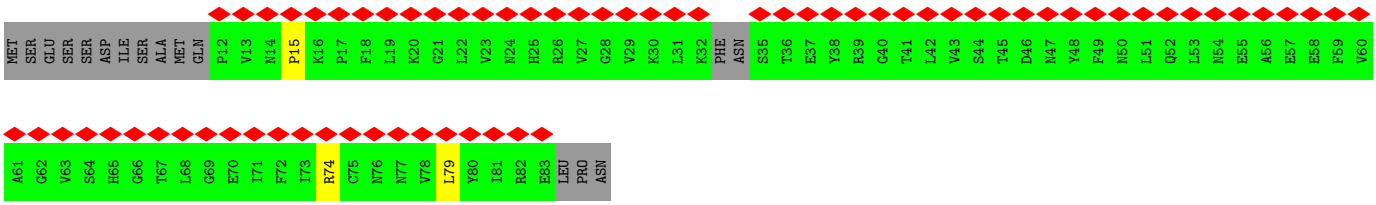
• Molecule 26: Small nuclear ribonucleoprotein F



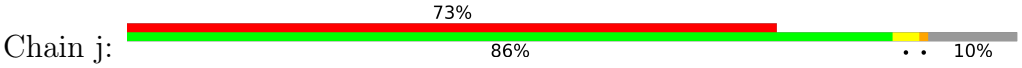


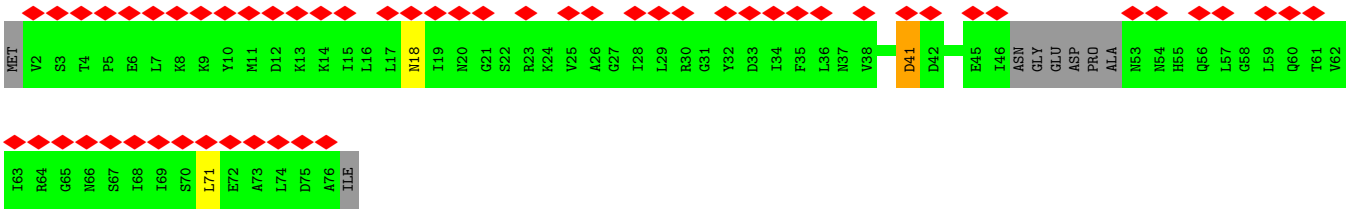
• Molecule 26: Small nuclear ribonucleoprotein F





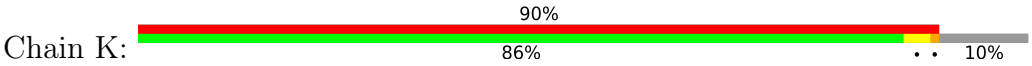
• Molecule 27: Small nuclear ribonucleoprotein G





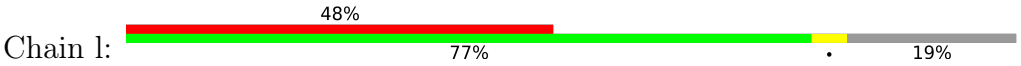
• Molecule 27: Small nuclear ribonucleoprotein G

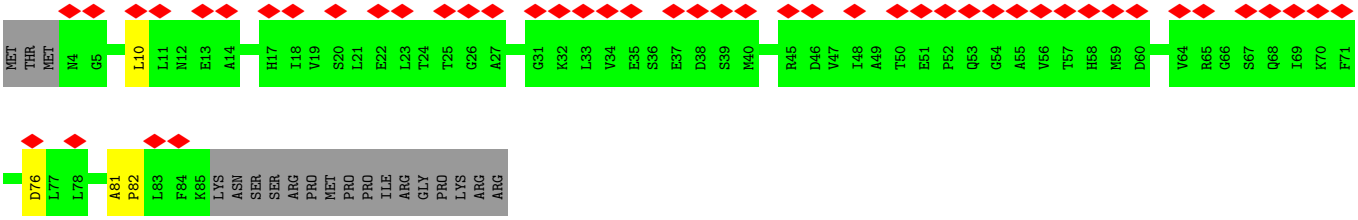
Chain K:



• Molecule 28: Small nuclear ribonucleoprotein Sm D3

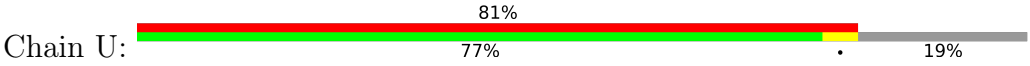
Chain l:

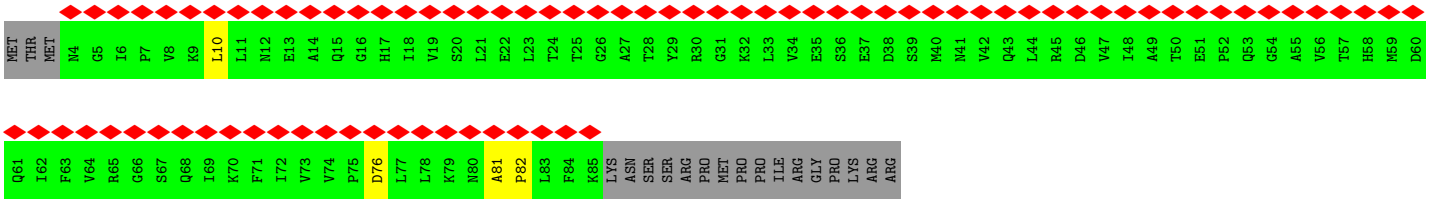




• Molecule 28: Small nuclear ribonucleoprotein Sm D3

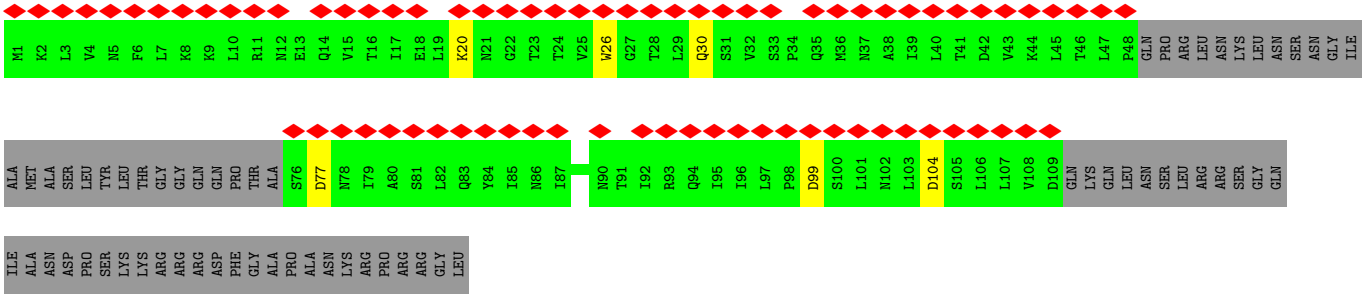
Chain U:





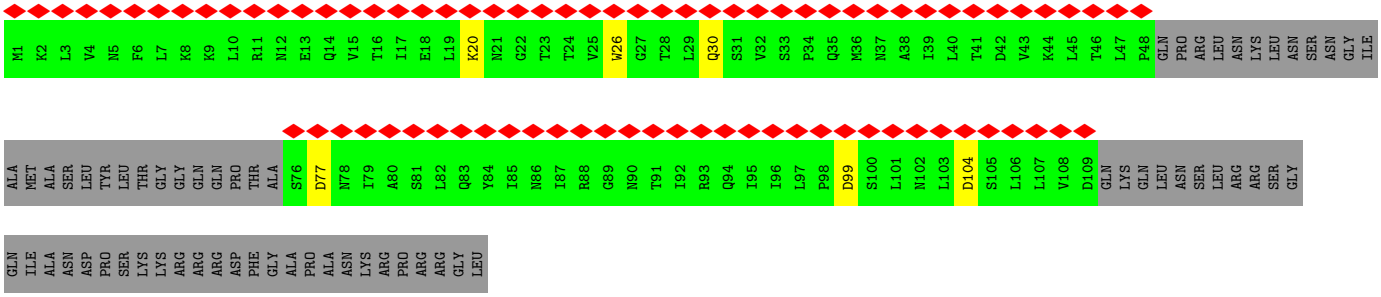
• Molecule 29: Small nuclear ribonucleoprotein Sm D1

Chain m:

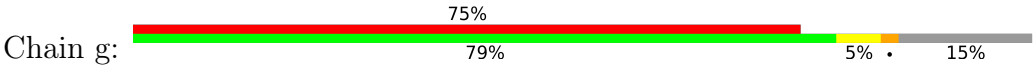


• Molecule 29: Small nuclear ribonucleoprotein Sm D1

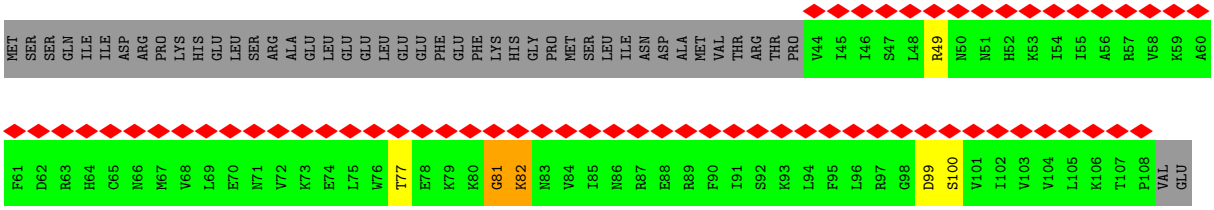
Chain V:



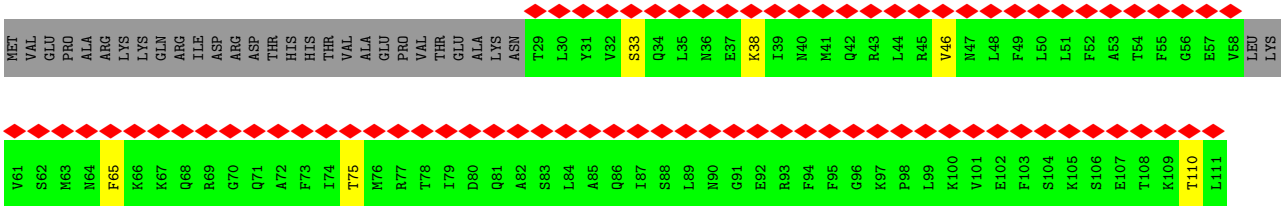
• Molecule 30: Small nuclear ribonucleoprotein Sm D2



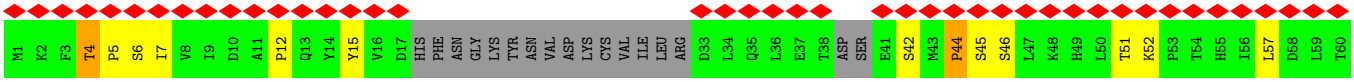
• Molecule 30: Small nuclear ribonucleoprotein Sm D2

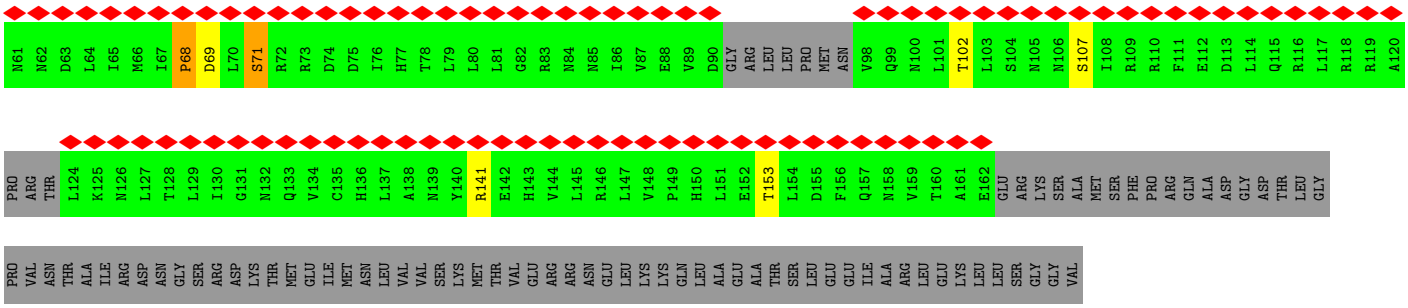


• Molecule 31: U2 small nuclear ribonucleoprotein B”



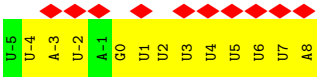
• Molecule 32: U2 small nuclear ribonucleoprotein A’





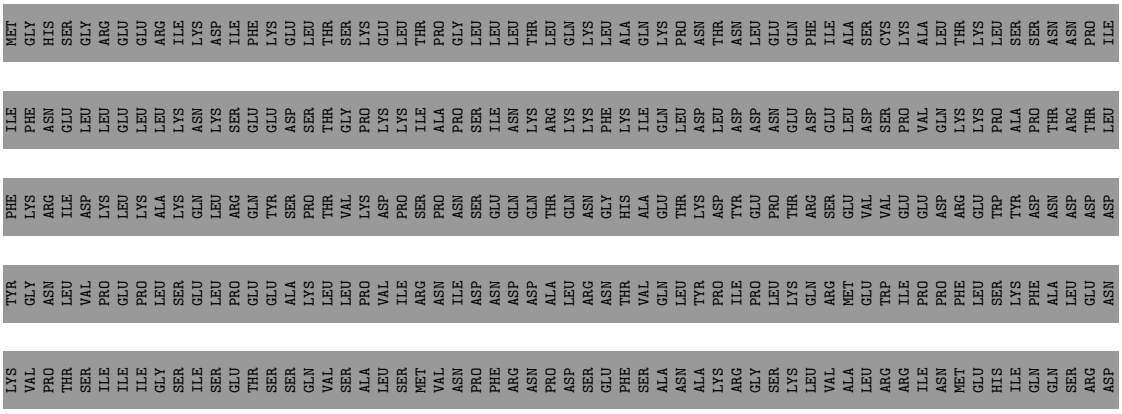
• Molecule 33: 3'-exon-intron

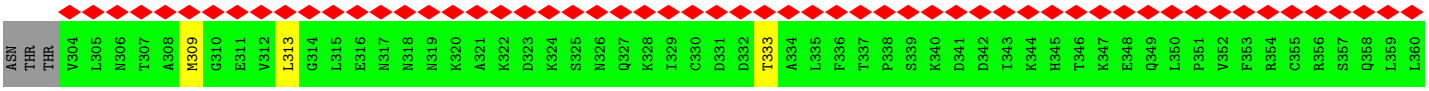
Chain b:

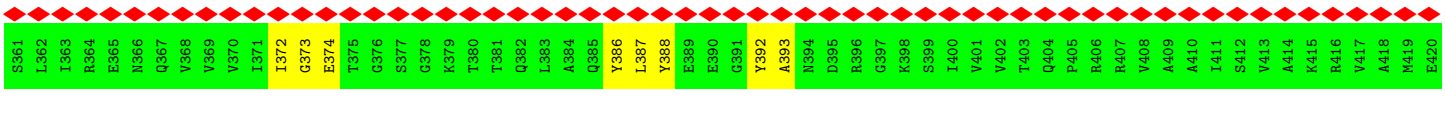


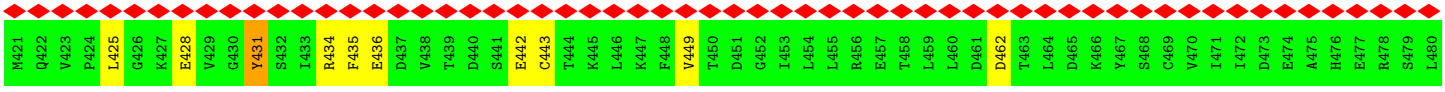
• Molecule 34: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

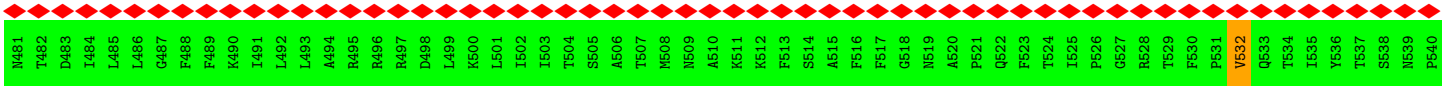
Chain e:

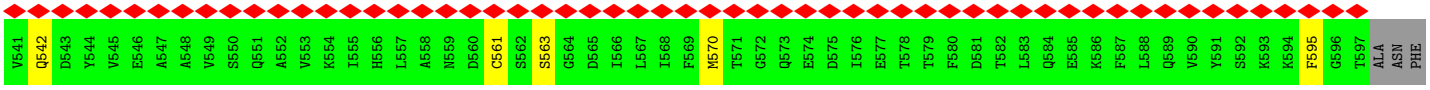


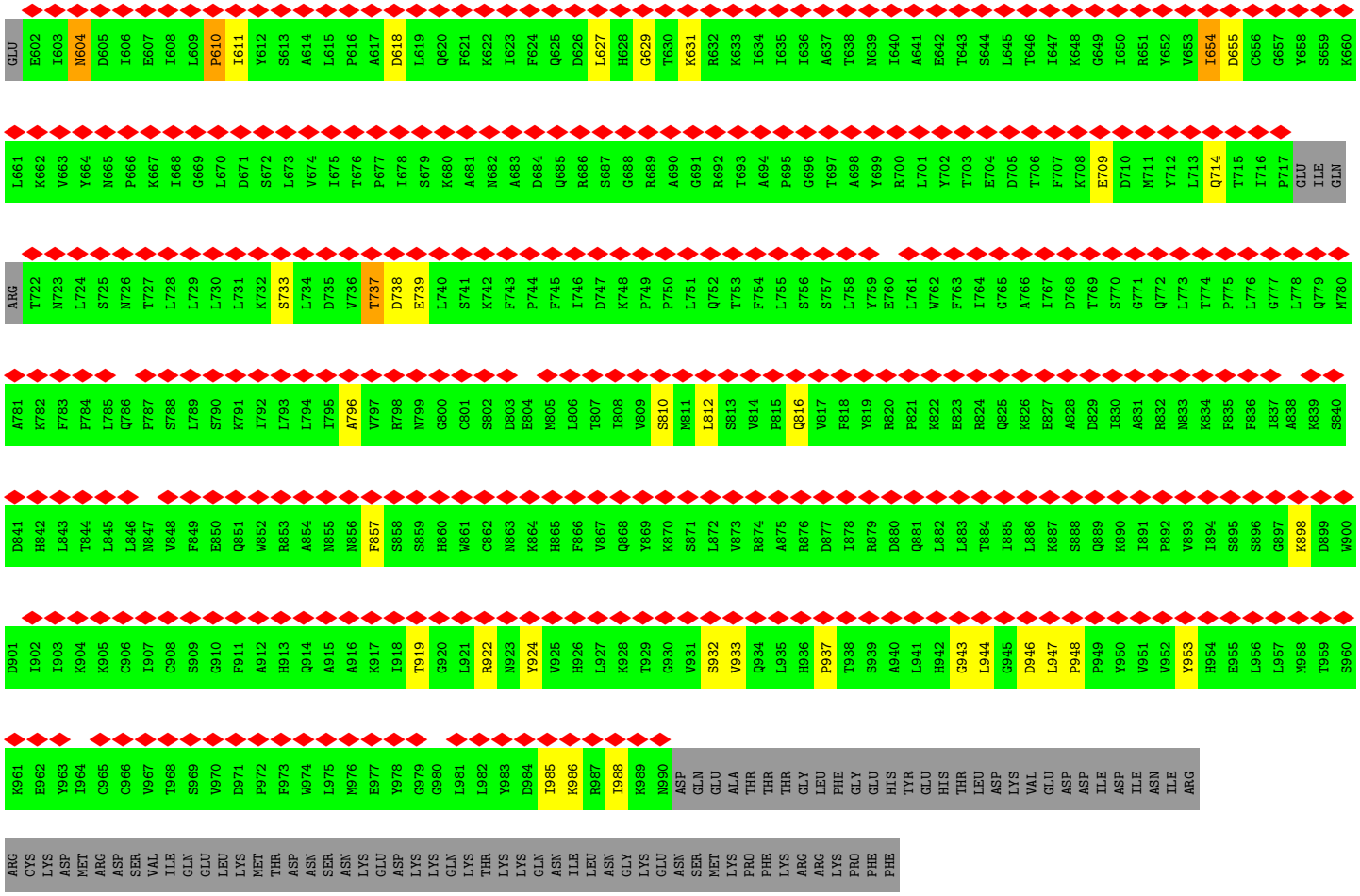






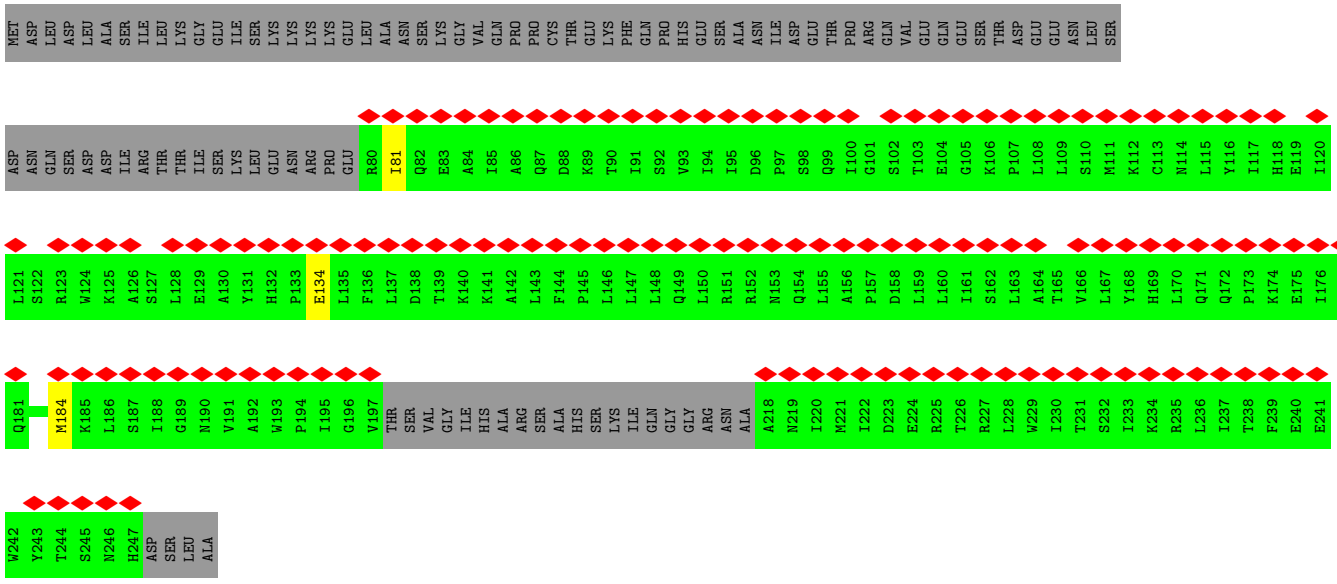






• Molecule 35: Pre-mRNA-splicing factor 18

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27558	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 ($e^-/Å^2$)	1.6	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	0.191	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0297	Depositor
Map size (Å)	522.4, 522.4, 522.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3060001, 1.3060001, 1.3060001	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: ZN, GTP, MG

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	0.81	5/16346 (0.0%)	0.81	19/22154 (0.1%)
2	C	0.79	1/7168 (0.0%)	0.80	7/9707 (0.1%)
3	J	0.70	0/191	0.80	0/254
4	O	0.98	3/2704 (0.1%)	0.89	5/3676 (0.1%)
5	P	0.66	0/1604	0.78	1/2160 (0.0%)
6	Q	0.64	0/1496	0.76	1/2014 (0.0%)
7	R	0.72	0/2135	0.76	2/2871 (0.1%)
8	S	0.70	0/574	0.85	0/766
9	T	0.81	3/1315 (0.2%)	0.79	0/1759
10	Z	0.55	0/3712	0.75	5/5004 (0.1%)
11	B	0.68	0/307	0.90	0/475
12	N	0.68	0/346	0.86	0/535
13	D	0.73	0/2747	0.92	3/4267 (0.1%)
14	E	0.72	0/2452	0.95	3/3817 (0.1%)
15	L	0.75	13/2123 (0.6%)	1.12	18/3295 (0.5%)
16	M	0.29	0/543	0.72	0/842
17	c	0.38	0/2405	0.54	0/3218
18	d	0.42	0/2107	0.54	0/2852
19	I	0.35	0/826	0.53	0/1097
20	v	1.05	8/905 (0.9%)	0.76	6/1214 (0.5%)
21	n	1.47	17/1878 (0.9%)	0.89	15/2503 (0.6%)
22	o	0.40	0/835	0.53	0/1126
22	p	0.40	0/848	0.55	0/1143
22	q	0.44	0/2342	0.65	0/3139
22	r	0.39	0/828	0.54	1/1117 (0.1%)
23	t	0.42	0/924	0.56	2/1244 (0.2%)
24	F	0.37	0/615	0.61	0/829
24	k	0.37	0/636	0.61	0/856
25	G	0.42	0/585	0.62	0/795
25	i	0.42	0/585	0.62	0/795
26	H	0.44	0/564	0.66	1/761 (0.1%)
26	h	0.44	0/564	0.65	1/761 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	K	0.37	0/532	0.60	0/715
27	j	0.37	0/532	0.60	0/715
28	U	0.40	0/634	0.70	0/859
28	l	0.40	0/634	0.70	0/859
29	V	0.41	0/649	0.61	0/880
29	m	0.41	0/649	0.61	0/880
30	W	0.43	0/535	0.66	2/717 (0.3%)
30	g	0.45	0/753	0.69	2/1013 (0.2%)
31	X	0.82	4/514 (0.8%)	1.32	2/686 (0.3%)
32	Y	1.03	9/839 (1.1%)	1.65	11/1127 (1.0%)
33	b	0.20	0/227	0.73	0/346
34	e	0.48	0/3357	1.09	4/4674 (0.1%)
35	f	0.29	0/1227	0.50	0/1665
All	All	0.71	63/74292 (0.1%)	0.81	111/102182 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	24
2	C	0	10
4	O	0	10
5	P	0	5
6	Q	0	6
7	R	0	3
8	S	0	1
9	T	0	5
10	Z	0	2
17	c	0	2
18	d	0	1
21	n	0	4
27	K	0	1
27	j	0	1
28	U	0	2
28	l	0	2
30	W	0	2
30	g	0	2
34	e	0	32
All	All	0	115

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	n	399	CYS	CB-SG	-24.14	1.41	1.82
21	n	444	CYS	CB-SG	-22.91	1.43	1.82
21	n	454	CYS	CB-SG	-19.93	1.48	1.82
21	n	218	CYS	CB-SG	-19.55	1.49	1.82
21	n	352	CYS	CB-SG	-18.81	1.50	1.82

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	1110	U	C5-C4-O4	11.94	133.07	125.90
15	L	1107	C	N1-C2-O2	-10.12	112.83	118.90
32	Y	44	PRO	N-CA-CB	8.85	113.92	103.30
15	L	1109	C	O4'-C1'-N1	8.79	115.23	108.20
2	C	656	LEU	CA-CB-CG	-8.46	95.84	115.30

There are no chirality outliers.

5 of 115 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	GLU	Peptide
1	A	288	GLU	Peptide
1	A	356	TYR	Peptide
1	A	460	PRO	Peptide
1	A	539	PRO	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
1	A	1925/2413 (80%)	1569 (82%)	339 (18%)	17 (1%)	17 55
2	C	872/1008 (86%)	735 (84%)	129 (15%)	8 (1%)	17 55
3	J	25/135 (18%)	21 (84%)	4 (16%)	0	100 100
4	O	335/451 (74%)	281 (84%)	49 (15%)	5 (2%)	10 45
5	P	193/379 (51%)	160 (83%)	27 (14%)	6 (3%)	4 31
6	Q	177/364 (49%)	145 (82%)	30 (17%)	2 (1%)	14 51
7	R	259/339 (76%)	218 (84%)	40 (15%)	1 (0%)	34 71
8	S	63/175 (36%)	49 (78%)	12 (19%)	2 (3%)	4 31
9	T	155/157 (99%)	123 (79%)	28 (18%)	4 (3%)	5 34
10	Z	443/577 (77%)	369 (83%)	68 (15%)	6 (1%)	11 46
17	c	312/579 (54%)	273 (88%)	35 (11%)	4 (1%)	12 48
18	d	238/652 (36%)	201 (84%)	35 (15%)	2 (1%)	19 58
19	I	98/215 (46%)	85 (87%)	13 (13%)	0	100 100
20	v	121/858 (14%)	110 (91%)	7 (6%)	4 (3%)	4 30
21	n	272/455 (60%)	234 (86%)	28 (10%)	10 (4%)	3 28
22	o	120/503 (24%)	115 (96%)	4 (3%)	1 (1%)	19 58
22	p	122/503 (24%)	116 (95%)	6 (5%)	0	100 100
22	q	355/503 (71%)	327 (92%)	16 (4%)	12 (3%)	3 30
22	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	5 35
23	t	150/175 (86%)	134 (89%)	13 (9%)	3 (2%)	7 40
24	F	74/196 (38%)	67 (90%)	7 (10%)	0	100 100
24	k	76/196 (39%)	69 (91%)	7 (9%)	0	100 100
25	G	71/94 (76%)	65 (92%)	6 (8%)	0	100 100
25	i	71/94 (76%)	65 (92%)	6 (8%)	0	100 100
26	H	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10 45
26	h	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10 45
27	K	65/77 (84%)	64 (98%)	1 (2%)	0	100 100
27	j	65/77 (84%)	64 (98%)	1 (2%)	0	100 100
28	U	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12 48
28	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12 48
29	V	78/146 (53%)	74 (95%)	4 (5%)	0	100 100
29	m	78/146 (53%)	74 (95%)	4 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	W	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	9 44
30	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	14 51
31	X	77/111 (69%)	75 (97%)	2 (3%)	0	100 100
32	Y	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	9 44
34	e	673/1071 (63%)	563 (84%)	75 (11%)	35 (5%)	2 21
35	f	144/251 (57%)	140 (97%)	4 (3%)	0	100 100
All	All	8398/14235 (59%)	7212 (86%)	1053 (12%)	133 (2%)	13 44

5 of 133 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	364	PHE
6	Q	99	VAL
10	Z	213	PHE
20	v	616	PRO
21	n	245	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
1	A	1753/2182 (80%)	1745 (100%)	8 (0%)	88 93
2	C	794/910 (87%)	791 (100%)	3 (0%)	91 94
3	J	21/121 (17%)	21 (100%)	0	100 100
4	O	295/397 (74%)	294 (100%)	1 (0%)	92 95
5	P	173/328 (53%)	173 (100%)	0	100 100
6	Q	171/332 (52%)	170 (99%)	1 (1%)	86 92
7	R	224/296 (76%)	222 (99%)	2 (1%)	78 88
8	S	56/151 (37%)	54 (96%)	2 (4%)	35 61
9	T	141/141 (100%)	140 (99%)	1 (1%)	84 90
10	Z	417/538 (78%)	417 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	c	212/308 (69%)	206 (97%)	6 (3%)	43 65
18	d	219/219 (100%)	219 (100%)	0	100 100
19	I	92/193 (48%)	92 (100%)	0	100 100
20	v	57/152 (38%)	47 (82%)	10 (18%)	2 12
21	n	122/413 (30%)	100 (82%)	22 (18%)	1 11
22	o	59/451 (13%)	52 (88%)	7 (12%)	5 24
22	p	62/451 (14%)	54 (87%)	8 (13%)	4 22
22	q	119/451 (26%)	102 (86%)	17 (14%)	3 19
22	r	60/451 (13%)	55 (92%)	5 (8%)	11 38
23	t	37/165 (22%)	27 (73%)	10 (27%)	0 3
24	F	67/176 (38%)	67 (100%)	0	100 100
24	k	70/176 (40%)	70 (100%)	0	100 100
25	G	65/83 (78%)	60 (92%)	5 (8%)	13 40
25	i	65/83 (78%)	60 (92%)	5 (8%)	13 40
26	H	61/77 (79%)	60 (98%)	1 (2%)	62 79
26	h	61/77 (79%)	60 (98%)	1 (2%)	62 79
27	K	58/66 (88%)	55 (95%)	3 (5%)	23 51
27	j	58/66 (88%)	55 (95%)	3 (5%)	23 51
28	U	69/89 (78%)	67 (97%)	2 (3%)	42 65
28	l	69/89 (78%)	67 (97%)	2 (3%)	42 65
29	V	77/129 (60%)	71 (92%)	6 (8%)	12 39
29	m	77/129 (60%)	71 (92%)	6 (8%)	12 39
30	W	59/103 (57%)	55 (93%)	4 (7%)	16 44
30	g	79/103 (77%)	74 (94%)	5 (6%)	18 46
31	X	26/100 (26%)	25 (96%)	1 (4%)	33 59
32	Y	47/219 (22%)	44 (94%)	3 (6%)	17 45
35	f	134/225 (60%)	131 (98%)	3 (2%)	52 71
All	All	6226/10640 (58%)	6073 (98%)	153 (2%)	50 68

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	m	26	TRP

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Mol	Chain	Res	Type
30	W	77	THR
29	m	104	ASP
26	H	79	LEU
35	f	81	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	4	ASN
7	R	91	HIS
25	G	34	GLN
4	O	223	HIS
5	P	103	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	B	12/13 (92%)	5 (41%)	0
12	N	14/15 (93%)	4 (28%)	1 (7%)
13	D	114/214 (53%)	31 (27%)	3 (2%)
14	E	102/112 (91%)	33 (32%)	6 (5%)
15	L	88/1175 (7%)	30 (34%)	8 (9%)
16	M	22/23 (95%)	13 (59%)	3 (13%)
33	b	12/14 (85%)	12 (100%)	0
All	All	364/1566 (23%)	128 (35%)	21 (5%)

5 of 128 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	B	88	U
11	B	89	A
11	B	90	A
11	B	93	U
11	B	94	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	L	41	C
15	L	1111	U

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Mol	Chain	Res	Type
16	M	499	U
16	M	483	U
15	L	1107	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
36	GTP	C	1500	37	26,34,34	1.67	4 (15%)	32,54,54	2.18	10 (31%)

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
36	GTP	C	1500	37	-	5/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	1500	GTP	C5-C6	-5.41	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	1500	GTP	C5-C4	-2.27	1.37	1.43
36	C	1500	GTP	O4'-C4'	-2.16	1.40	1.45
36	C	1500	GTP	C2'-C1'	-2.15	1.50	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	1500	GTP	PA-O3A-PB	-6.36	111.02	132.83
36	C	1500	GTP	PB-O3B-PG	-6.30	111.20	132.83
36	C	1500	GTP	O3G-PG-O3B	3.08	114.95	104.64
36	C	1500	GTP	C2-N1-C6	-3.00	119.57	125.10
36	C	1500	GTP	C8-N7-C5	2.75	108.23	102.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

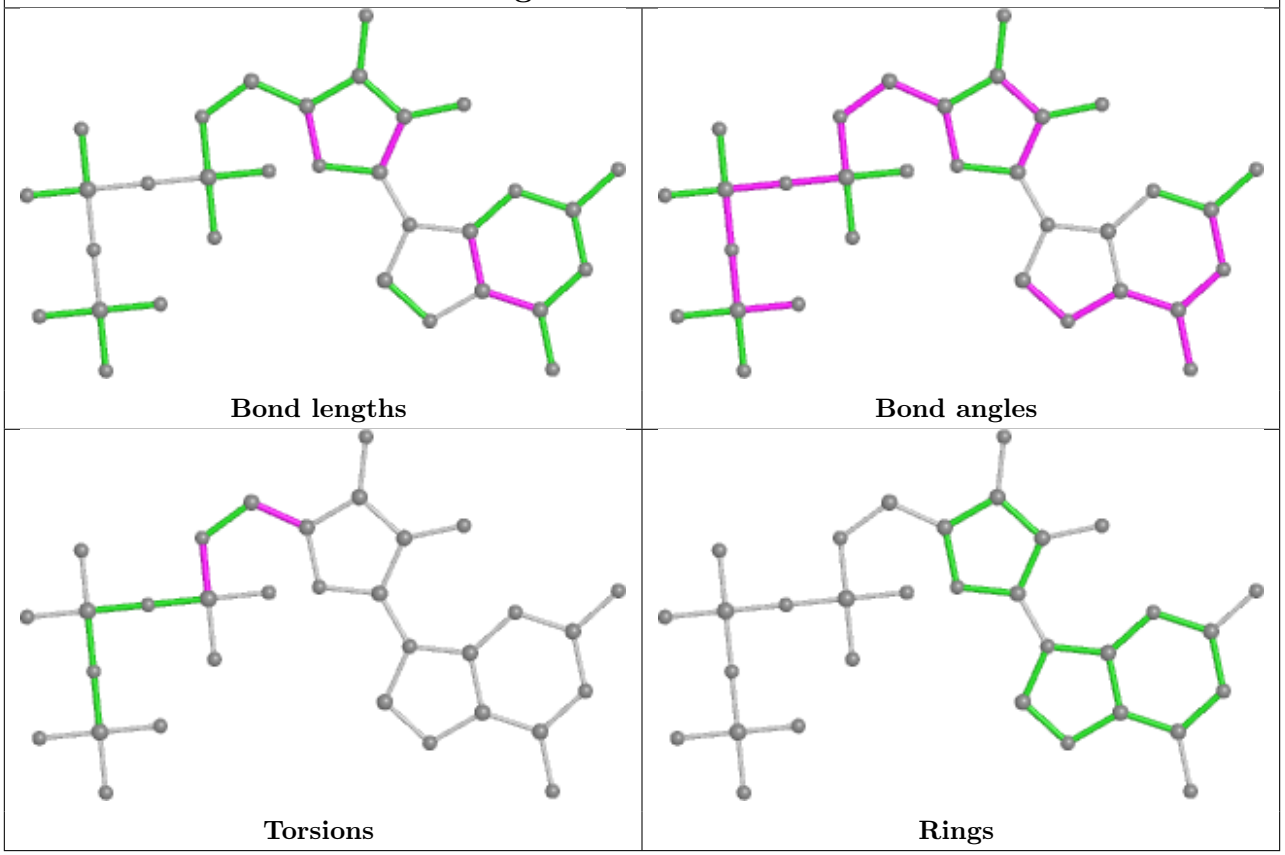
Mol	Chain	Res	Type	Atoms
36	C	1500	GTP	C5'-O5'-PA-O3A
36	C	1500	GTP	O4'-C4'-C5'-O5'
36	C	1500	GTP	C3'-C4'-C5'-O5'
36	C	1500	GTP	C5'-O5'-PA-O1A
36	C	1500	GTP	C5'-O5'-PA-O2A

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 C 1500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

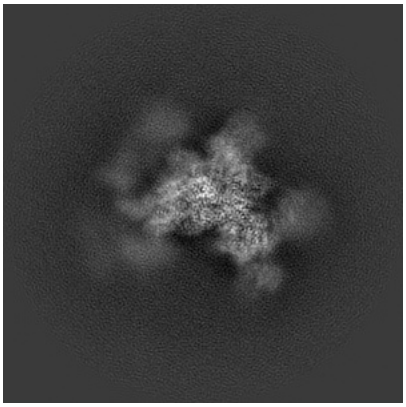
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6684. These allow visual inspection of the internal detail of the map and identification of artifacts.

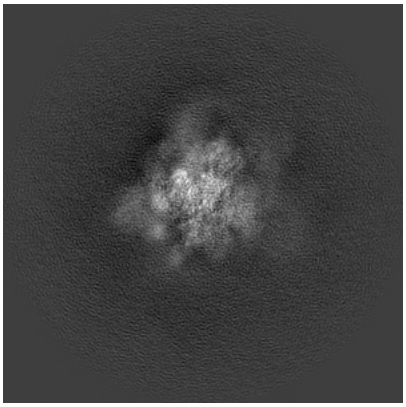
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

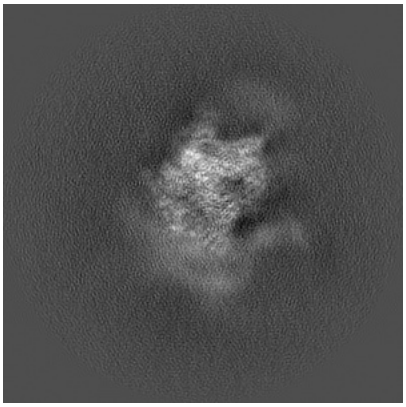
6.1.1 Primary map



X



Y

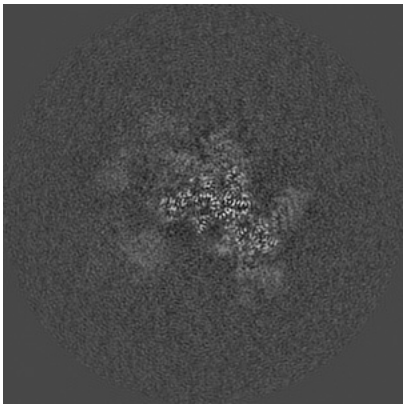


Z

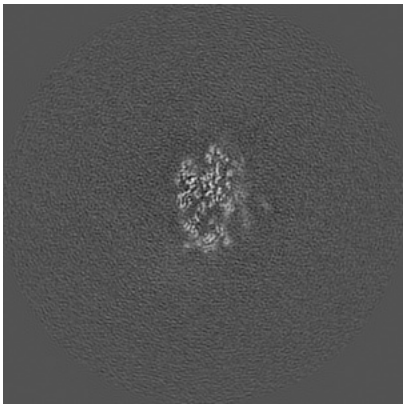
The images above show the map projected in three orthogonal directions.

6.2 Central slices

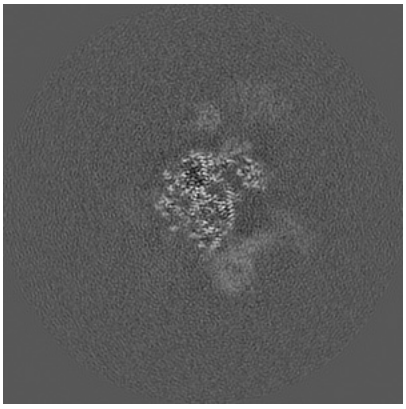
6.2.1 Primary map



X Index: 200



Y Index: 200

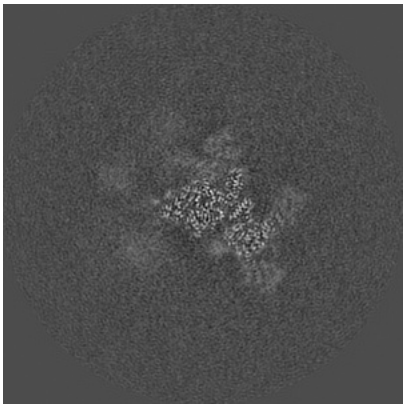


Z Index: 200

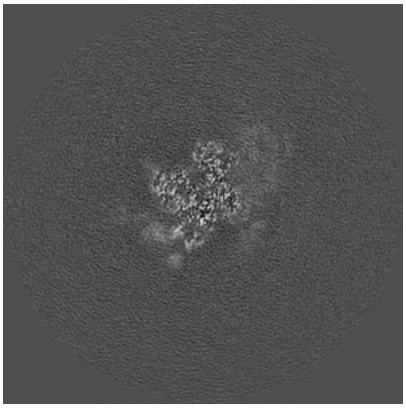
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

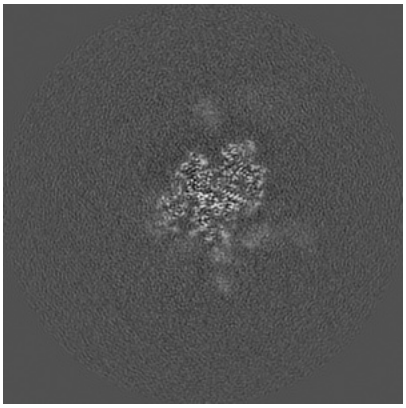
6.3.1 Primary map



X Index: 206



Y Index: 231

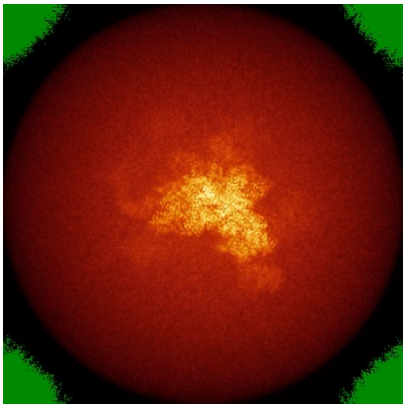


Z Index: 208

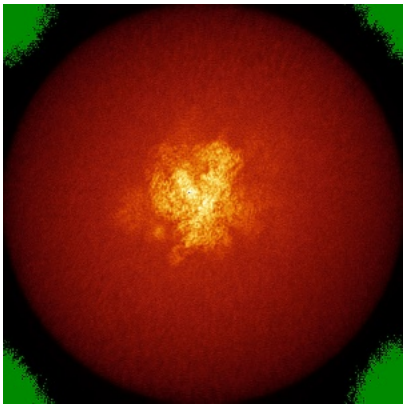
The images above show the largest variance slices of the map in three orthogonal directions.

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

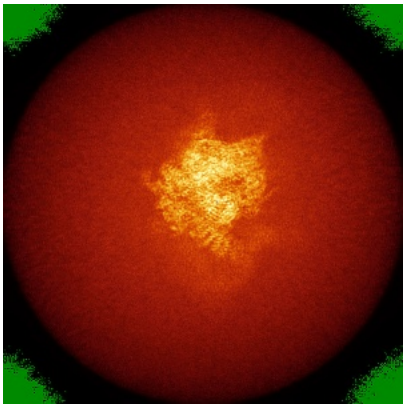
6.4.1 Primary map



X



Y

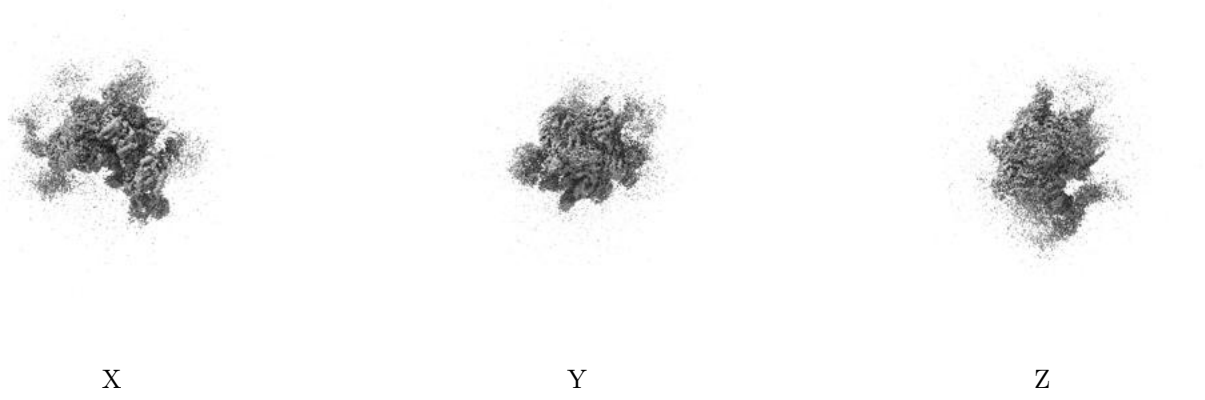


Z

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 0.0297. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

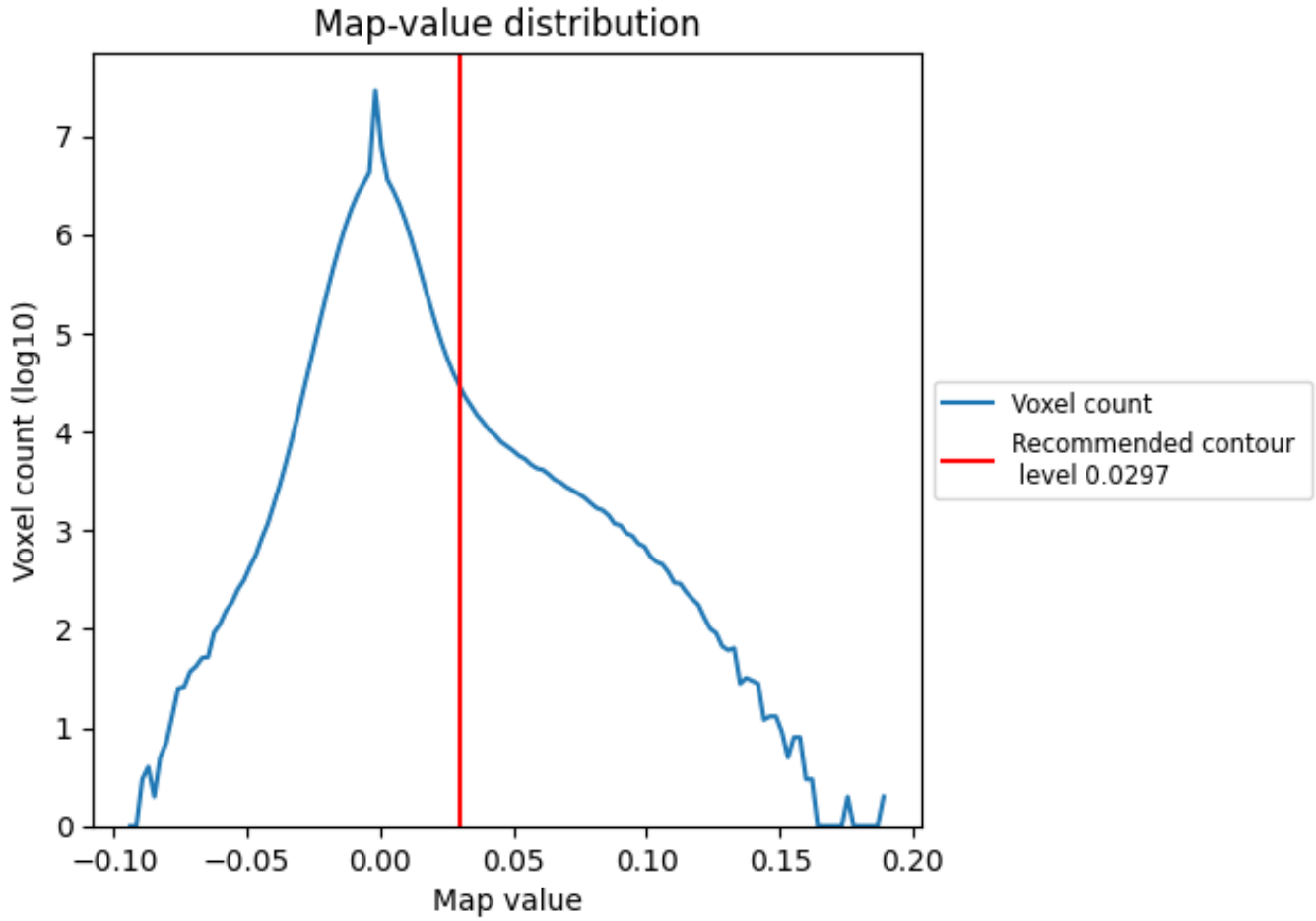
6.6 Mask visualisation (i)

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

7 Map analysis

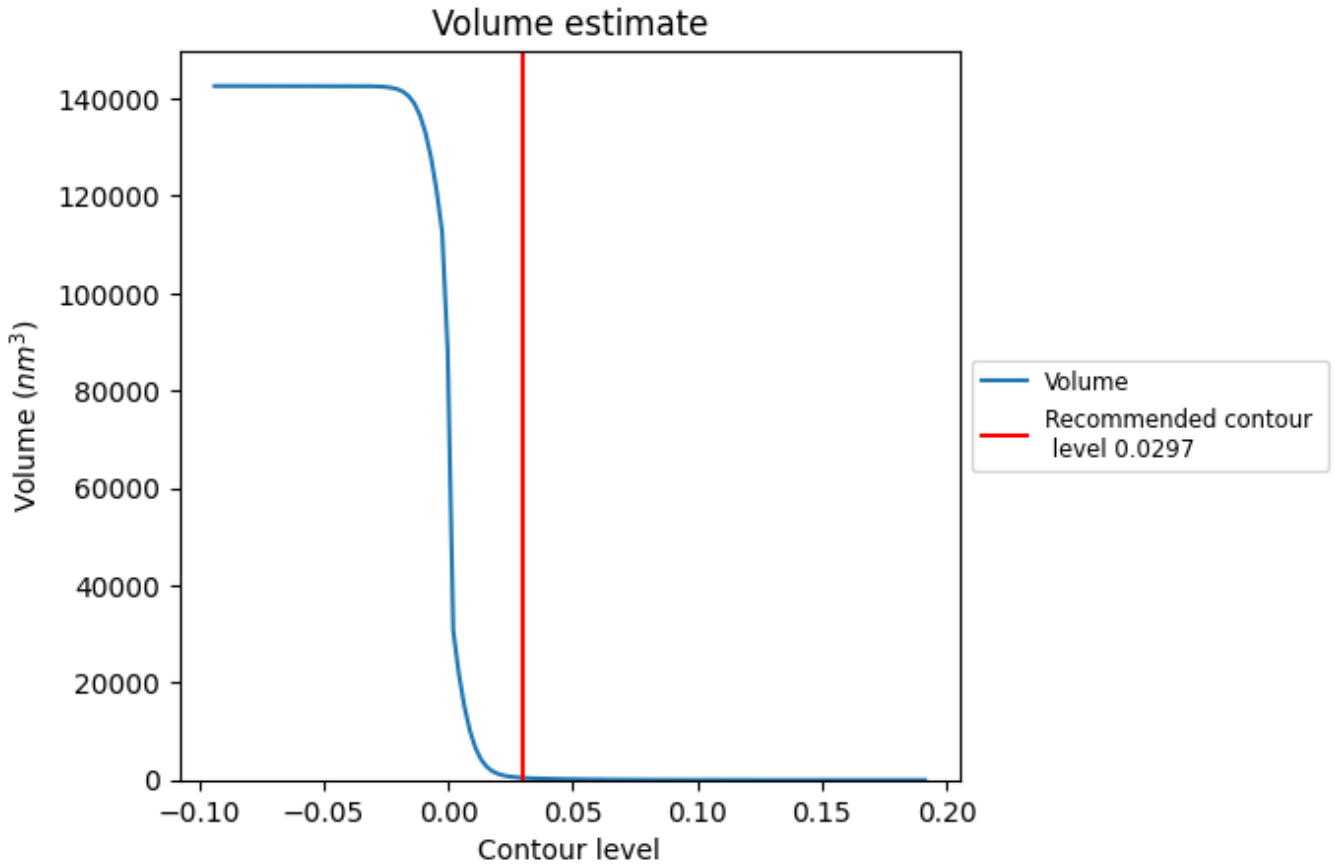
This section contains the results of statistical analysis of the map.

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.

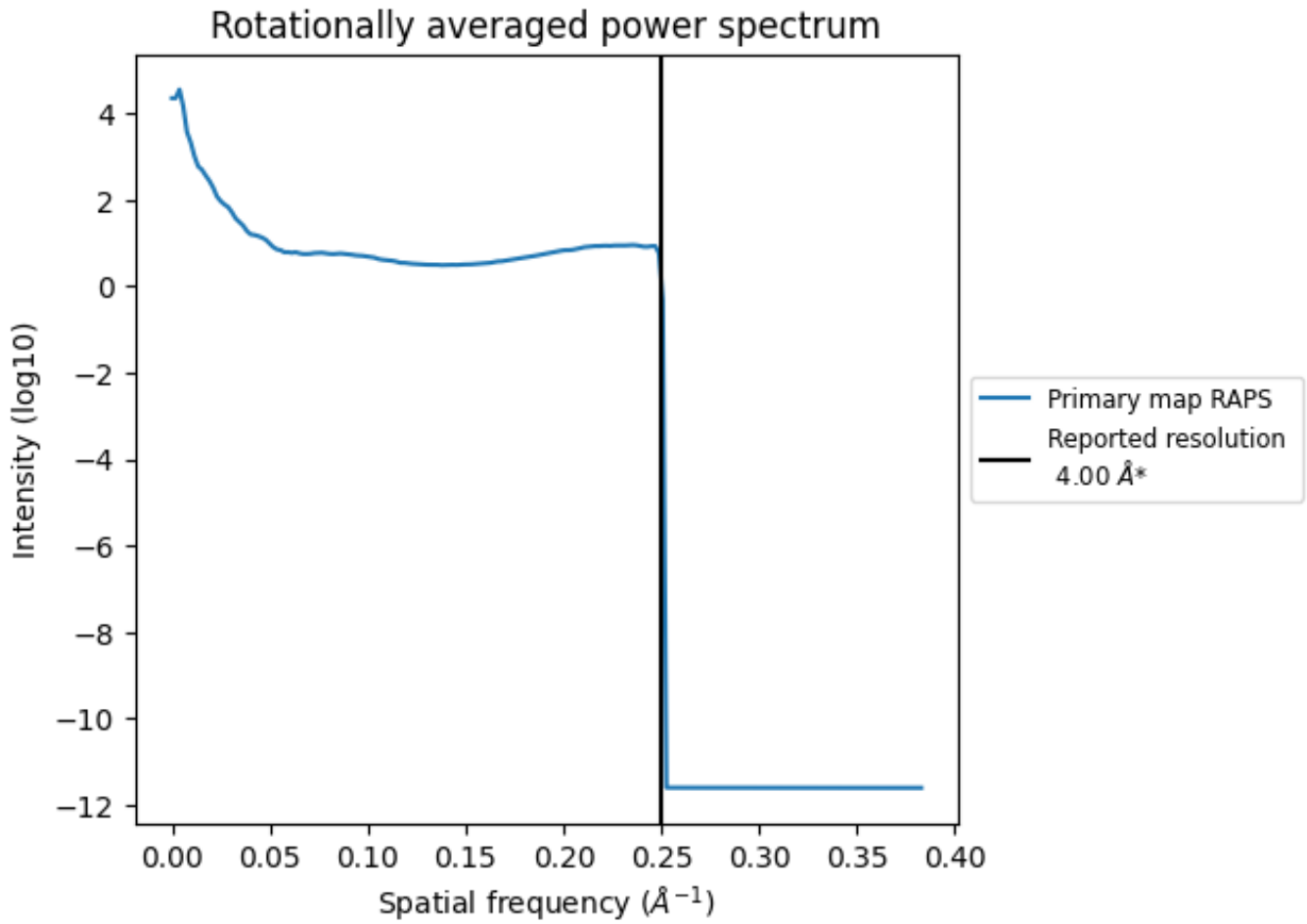
7.2 Volume estimate (i)



The volume at the recommended contour level is 445 nm^3; this corresponds to an approximate mass of 402 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 0.250 Å^{-1}

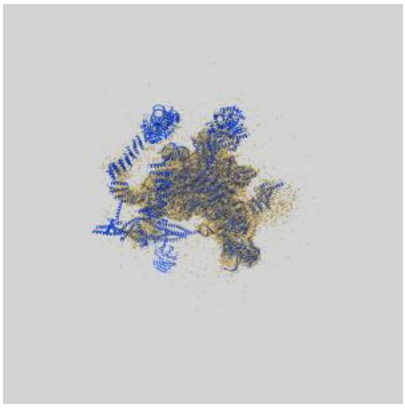
8 Fourier-Shell correlation (i)

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

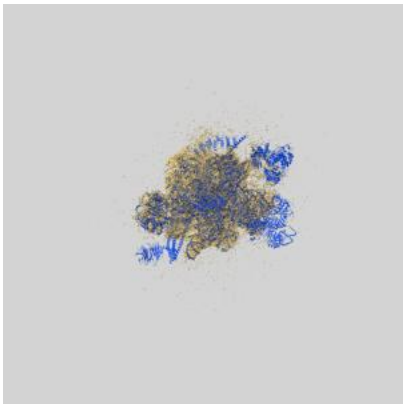
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6684 and PDB model 5WSG. Per-residue inclusion information can be found in section 3 on page 12.

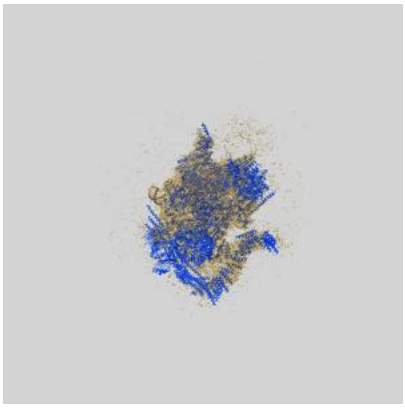
9.1 Map-model overlay



X



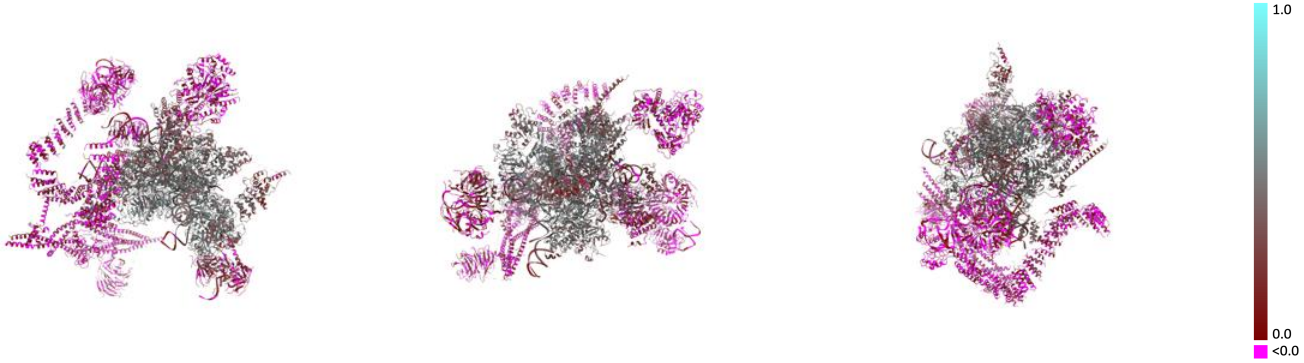
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0297 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.

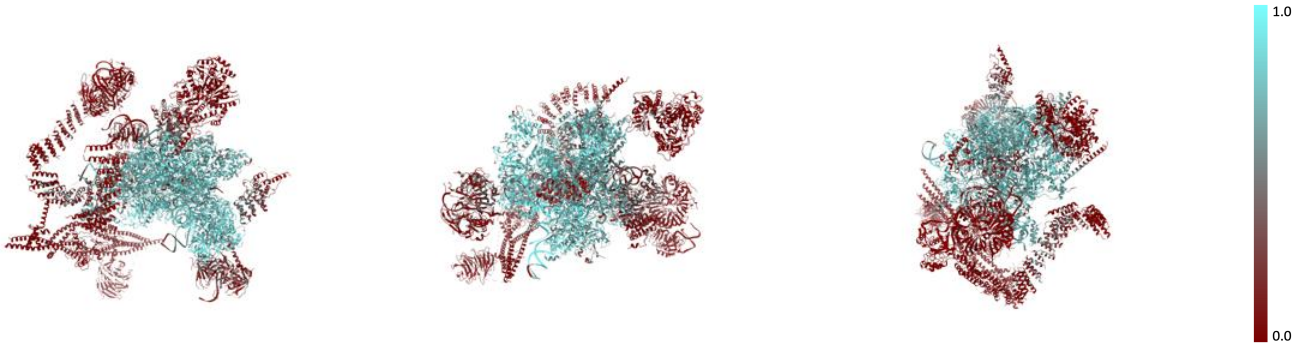
9.2 Q-score mapped to coordinate model (i)



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.

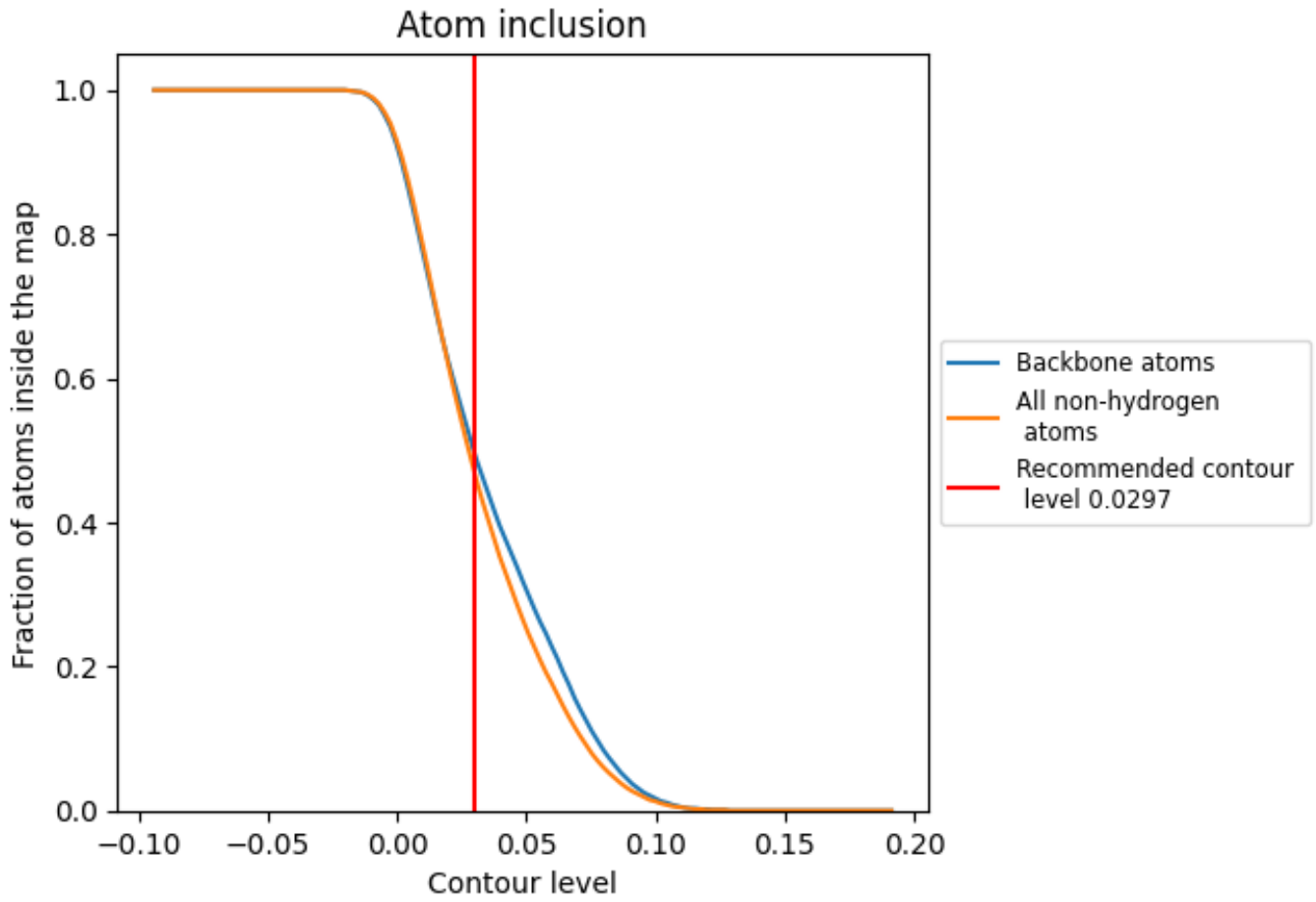
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0297).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 47% 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 (0.0297) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4730	0.2740
A	0.7330	0.4410
B	0.7390	0.3930
C	0.8060	0.4510
D	0.7220	0.3140
E	0.8230	0.3420
F	0.0020	0.0070
G	0.0040	0.0080
H	0.0000	-0.0050
I	0.6190	0.3700
J	0.7540	0.4820
K	0.0000	-0.0030
L	0.3220	0.1470
M	0.2550	0.1390
N	0.7080	0.3270
O	0.8350	0.4860
P	0.6520	0.4210
Q	0.6310	0.4150
R	0.7640	0.4190
S	0.6410	0.4670
T	0.7980	0.4470
U	0.0020	-0.0170
V	0.0020	-0.0300
W	0.0040	0.0200
X	0.0020	0.0070
Y	0.0000	-0.0230
Z	0.4450	0.3510
b	0.2600	0.3130
c	0.4110	0.2380
d	0.4710	0.2350
e	0.0370	0.0300
f	0.1000	0.1370
g	0.1550	0.1070
h	0.1620	0.0520
i	0.1910	0.1150

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Chain	Atom inclusion	Q-score
j	0.2110	0.1460
k	0.2060	0.1700
l	0.3380	0.2630
m	0.1410	0.0830
n	0.1980	0.0690
o	0.0120	0.0030
p	0.0060	-0.0080
q	0.0020	0.0120
r	0.0280	0.0490
t	0.0080	0.0200
v	0.1270	0.0360