



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 01:59 PM EST

PDB ID : 6BK8
EMDB ID : EMD-7109
Title : *S. cerevisiae* spliceosomal post-catalytic P complex
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2017-11-07
Resolution : 3.30 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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

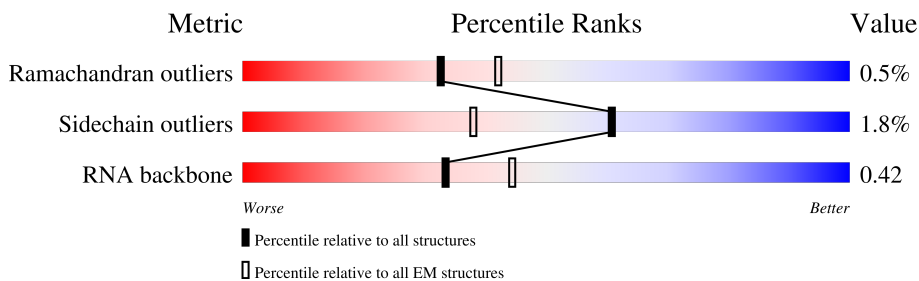
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 $\leq 5\%$. 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	2	1175	
2	5	214	
3	6	112	
4	e	34	
5	i	59	
6	A	2413	
7	B	1008	
8	D	451	

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Mol	Chain	Length	Quality of chain
9	E	379	7% 48% 51%
10	F	364	19% 54% 45%
11	G	339	7% 73% 25%
12	H	175	17% 37% 60%
13	I	157	99% 99%
14	K	135	36% 60% 39%
15	L	577	36% 71% 29%
16	M	455	24% 70% 28%
17	N	251	16% 66% 33%
18	O	382	24% 59% 40%
19	P	1145	51% 57% 43%
20	R	215	8% 46% 53%
21	S	590	40% 60%
22	T	687	33% 70% 30%
23	U	859	72% 73% 26%
24	X	219	60% 100%
25	Y	16	62% 100%
26	a	110	85% 85% 15%
26	q	110	82% 84% 15%
27	b	86	84% 84% 16%
27	m	86	81% 84% 16%
28	c	94	80% 78% 20%
28	l	94	80% 73% 6% 20%
29	d	77	90% 88% 10%
29	n	77	90% 88% 10%

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Mol	Chain	Length	Quality of chain
30	f	196	
30	k	196	
31	g	101	
31	o	101	
32	h	146	
32	p	146	
33	r	111	
34	s	238	
35	u	503	
35	v	503	
35	w	503	
35	x	503	
36	y	175	

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 82745 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 U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	135	2848	1272	472	969	135	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	103	2173	973	367	730	103	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	102	2170	972	386	710	102	0	0

- Molecule 4 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	e	34	707	319	107	247	34	0	0

- Molecule 5 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	i	59	1239	558	202	420	59	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	1960	16159	10381	2786	2933	59	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	899	7179	4638	1191	1321	29	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	359	2826	1786	497	533	10	0	0

- Molecule 9 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	186	1494	939	276	273	6	0	0

- Molecule 10 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	199	1576	991	277	293	15	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	255	2048	1297	362	378	11	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	70	570	357	113	99	1	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	156	1283	803	239	231	10	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	82	Total	C	N	O	S	0	0
			550	332	106	111	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	412	Total	C	N	O	S	0	0
			3353	2160	556	620	17		

- Molecule 16 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	326	Total	C	N	O	S	0	0
			2607	1649	465	485	8		

- Molecule 17 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	167	Total	C	N	O	S	0	0
			1326	856	233	233	4		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	229	Total	C	N	O	S	0	0
			1935	1211	347	368	9		

- Molecule 19 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	653	Total	C	N	O	S	0	0
			3872	2393	736	740	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	101	Total	C	N	O	S	0	0
			813	499	150	163	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	238	Total	C	N	O	S	0	0
			1948	1218	355	368	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	483	Total	C	N	O	S	0	0
			3370	2113	624	625	8		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	637	Total	C	N	O	S	0	0
			3625	2226	689	703	7		

- Molecule 24 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	219	Total	C	N	O	0	0
			1095	657	219	219		

- Molecule 25 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
26	q	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
27	m	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
28	l	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
29	n	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
30	k	78	Total	C	N	O	S	0	0
			610	389	109	109	3		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	o	78	Total	C	N	O	S	0	0
			600	384	104	110	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
32	p	79	Total	C	N	O	S	0	0
			618	393	107	116	2		

- Molecule 33 is a protein called Lea1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	r	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 34 is a protein called Msl1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 35 is a protein called Pre-mRNA-processing factor Prp19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	u	435	Total	C	N	O	0	0
			2156	1286	435	435		
35	v	118	Total	C	N	O	0	0
			588	352	118	118		
35	w	438	Total	C	N	O	0	0
			2171	1295	438	438		
35	x	116	Total	C	N	O	0	0
			578	346	116	116		

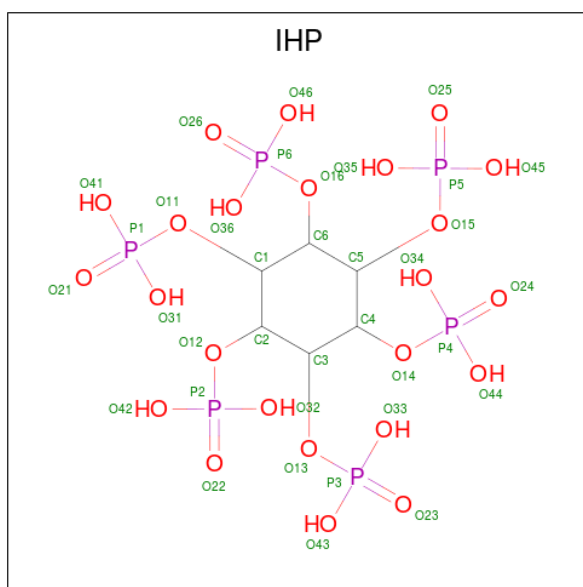
- Molecule 36 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	110	Total	C	N	O	0	0
			548	328	110	110		

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

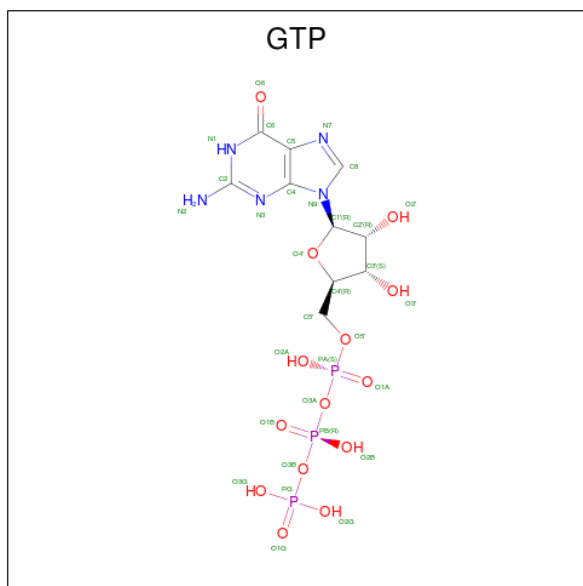
Mol	Chain	Residues	Atoms		AltConf
37	6	4	Total	Mg	0
			4	4	
37	B	1	Total	Mg	0
			1	1	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

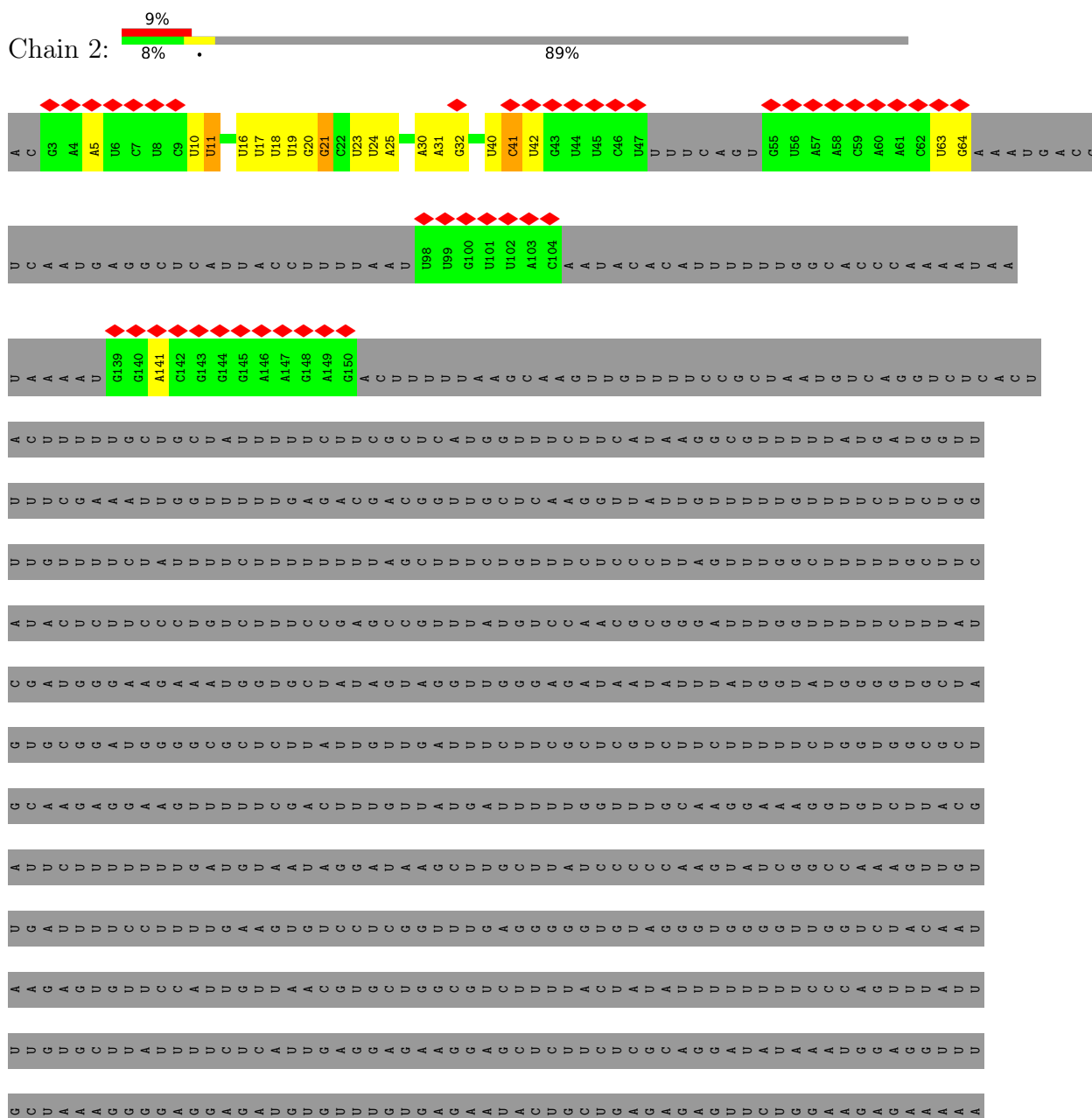
- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

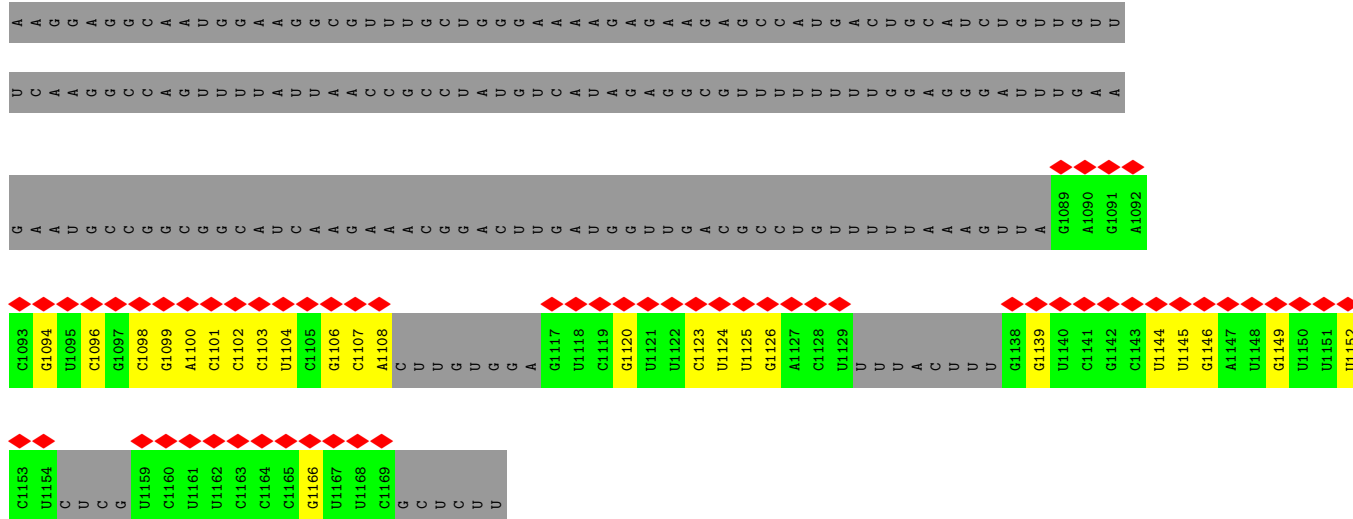
Mol	Chain	Residues	Atoms		AltConf
40	F	2	Total 2	Zn 2	0
40	G	1	Total 1	Zn 1	0
40	I	3	Total 3	Zn 3	0
40	O	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

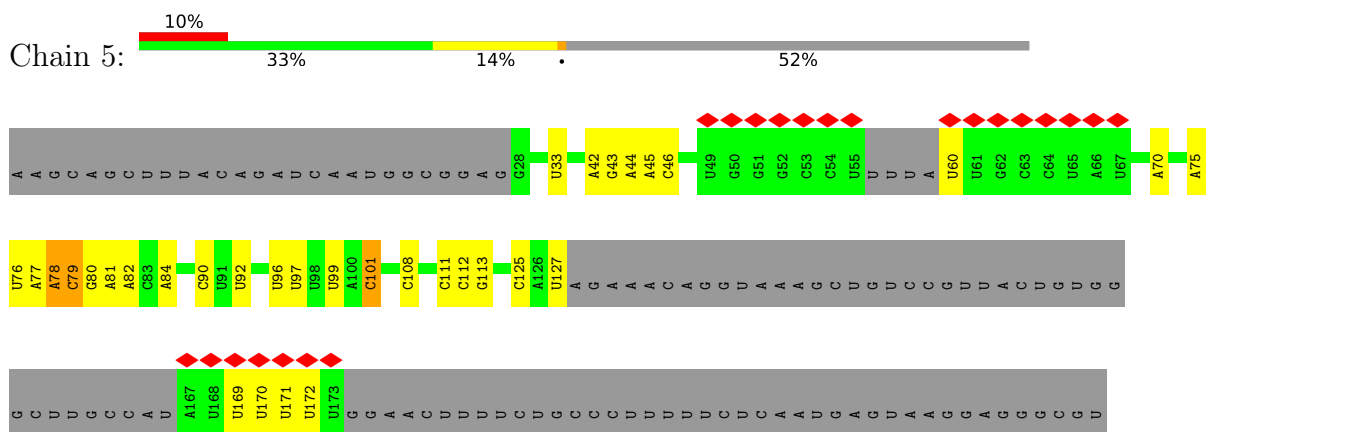
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U2 snRNA

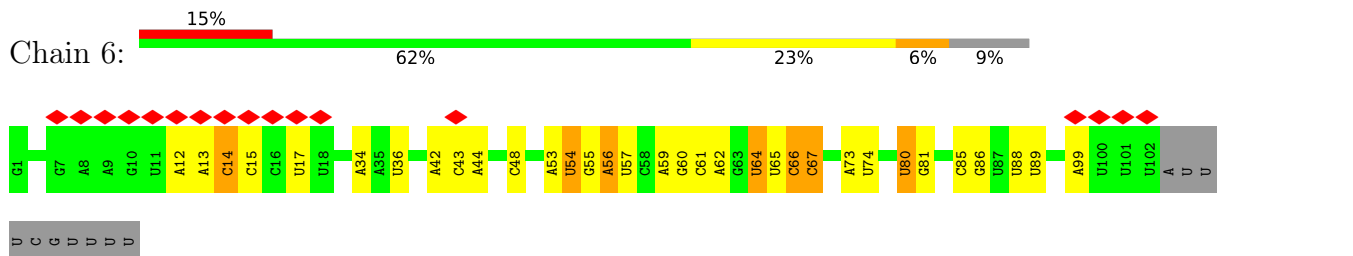




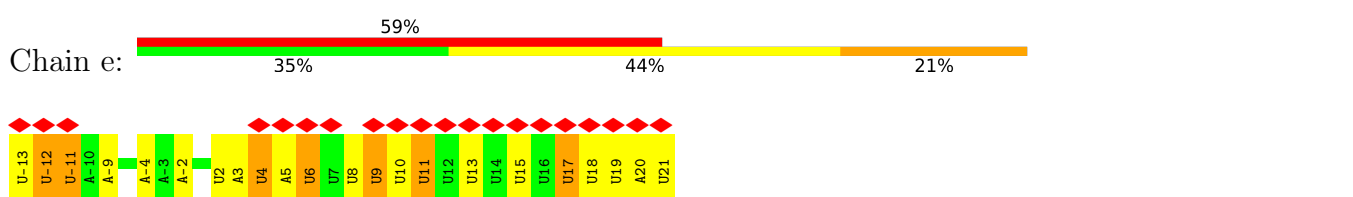
• Molecule 2: U5 snRNA



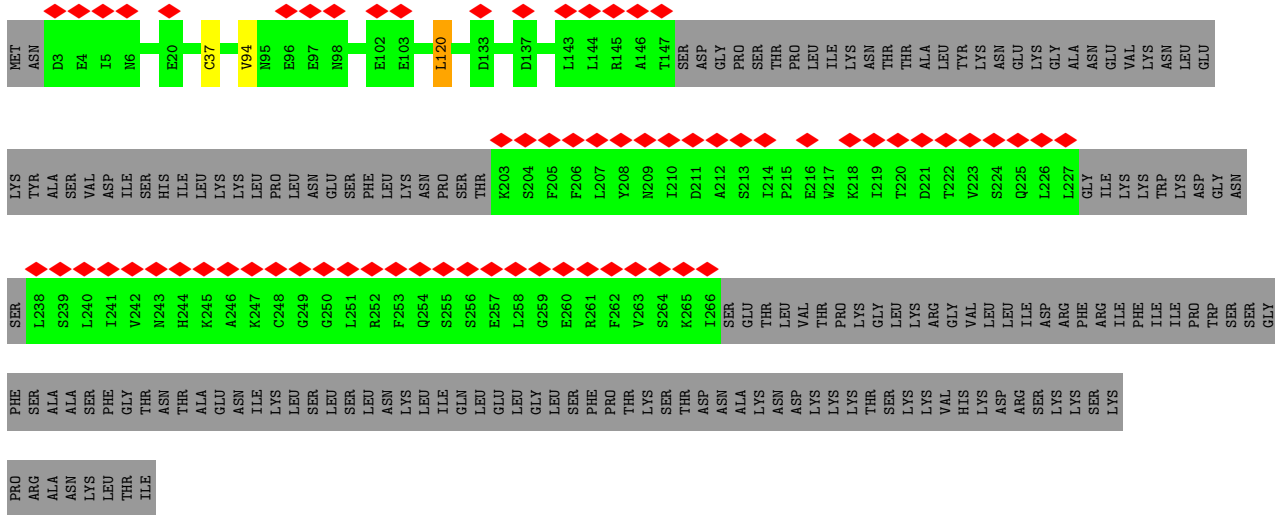
• Molecule 3: U6 snRNA



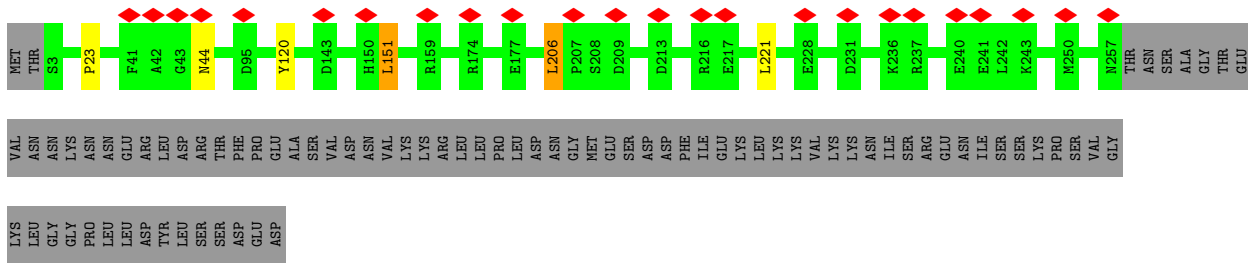
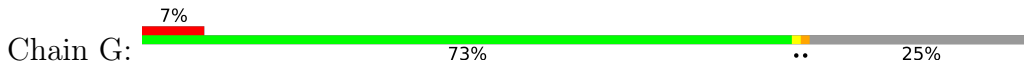
• Molecule 4: RNA (34-MER)



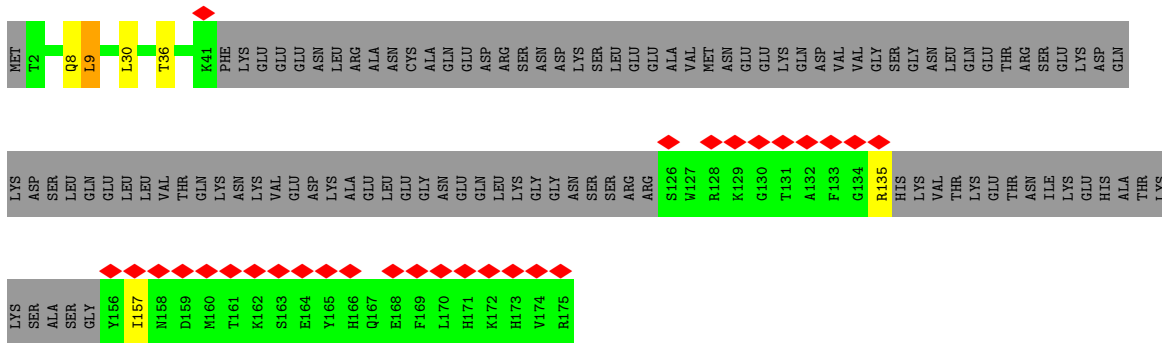
• Molecule 5: RNA (59-MER)



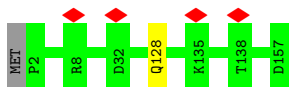
• Molecule 11: Pre-mRNA-splicing factor CWC2



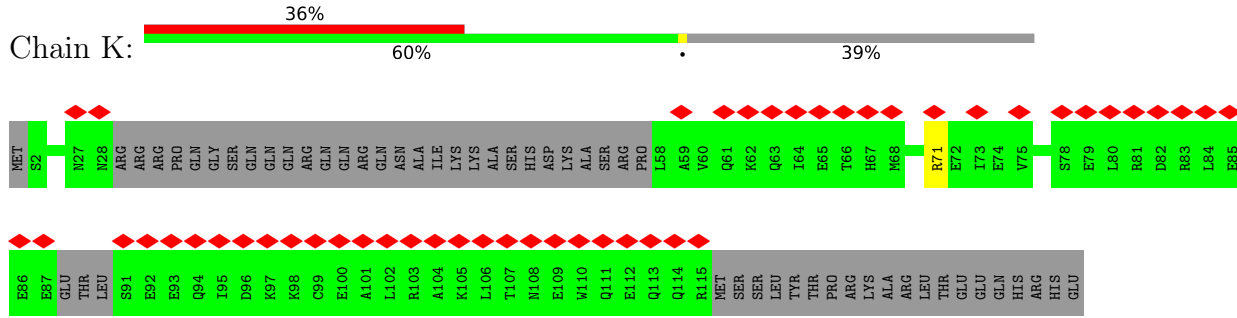
• Molecule 12: Pre-mRNA-splicing factor CWC15



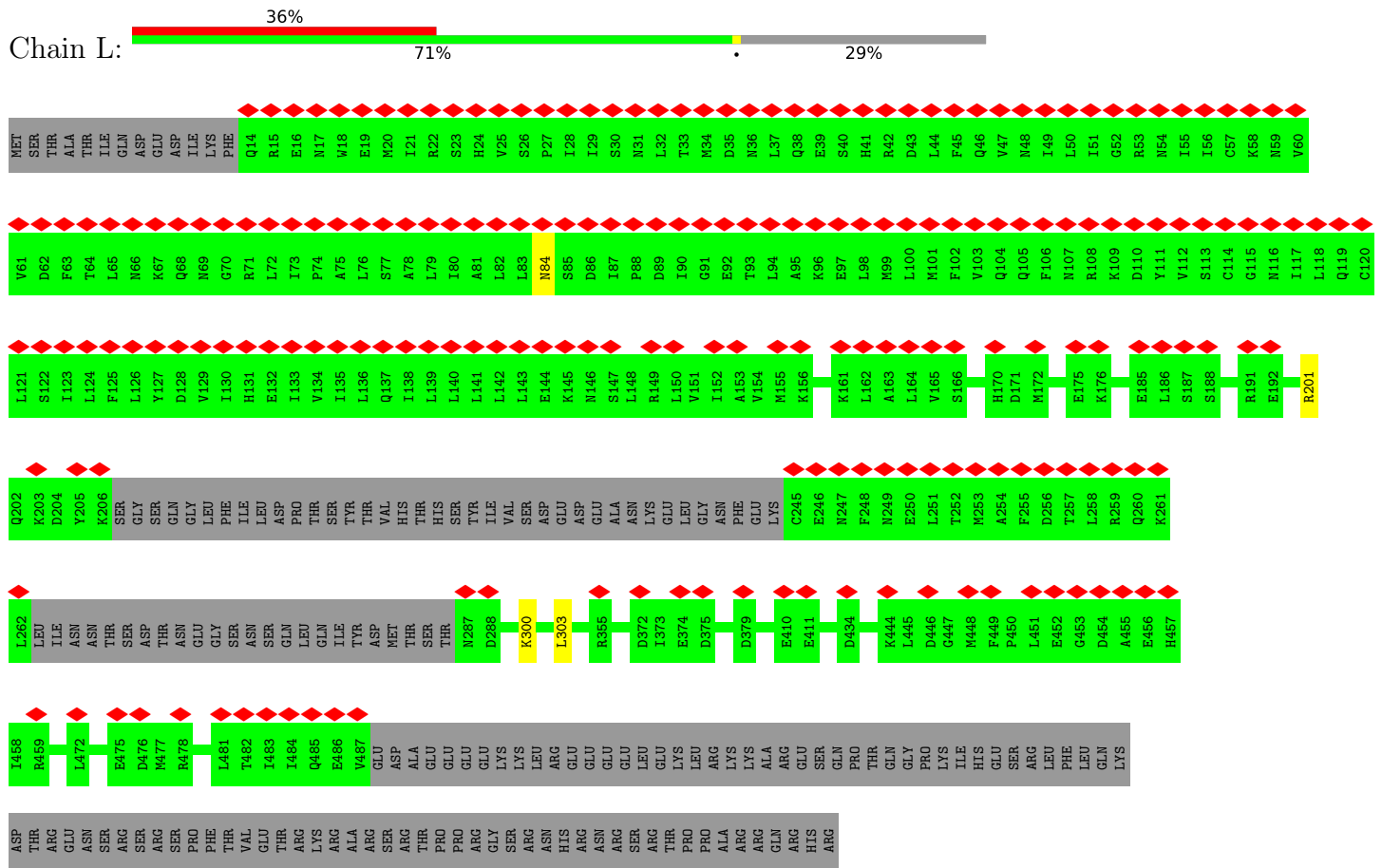
• Molecule 13: Pre-mRNA-splicing factor BUD31



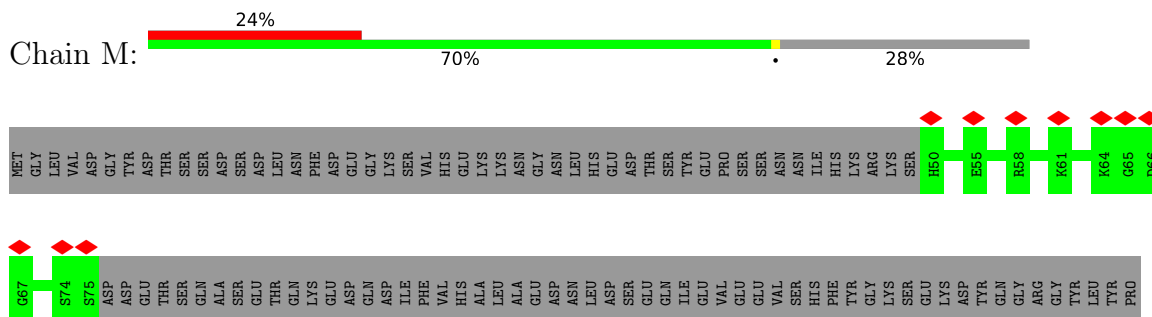
• Molecule 14: Pre-mRNA-splicing factor CWC21

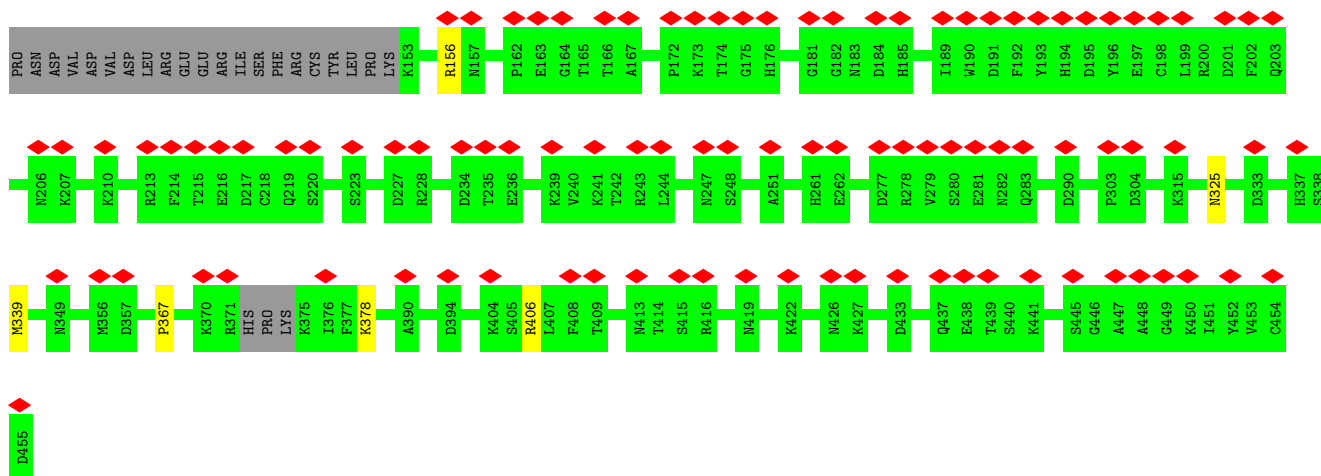


• Molecule 15: Pre-mRNA-splicing factor CWC22

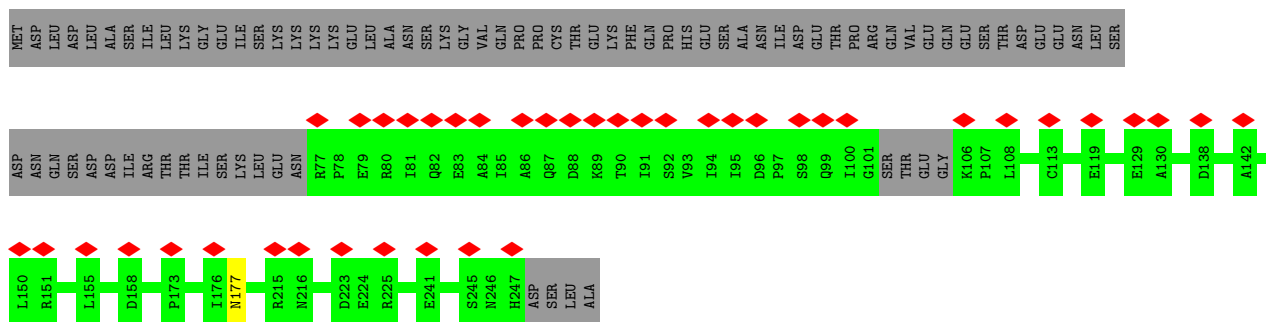


• Molecule 16: Pre-mRNA-processing factor Prp17

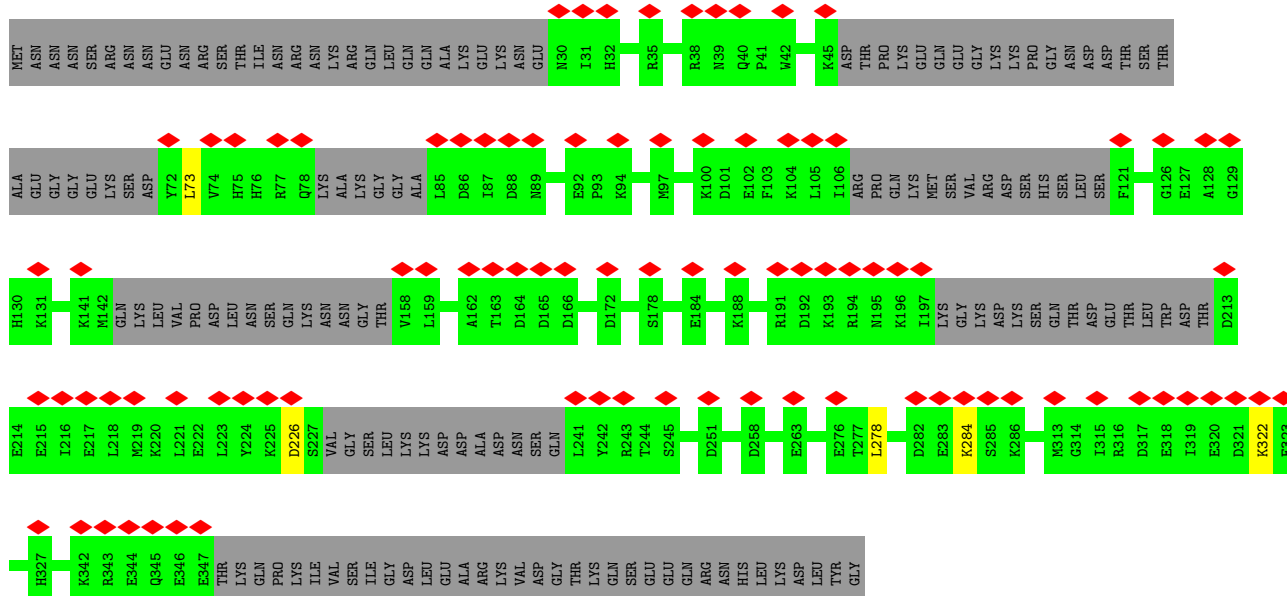


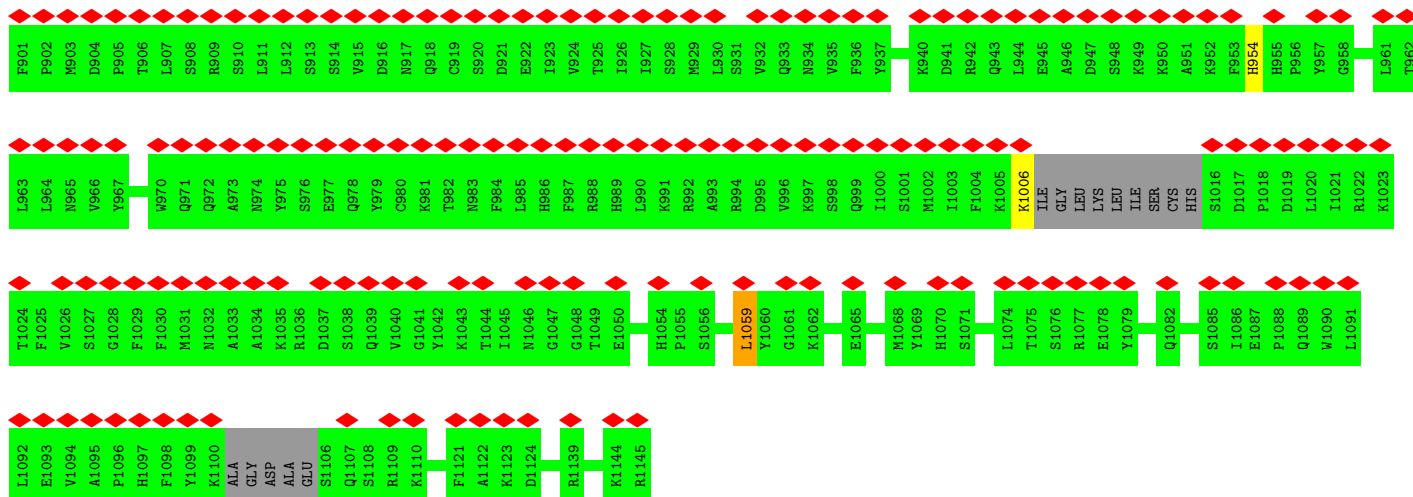


• Molecule 17: Pre-mRNA-splicing factor Prp18

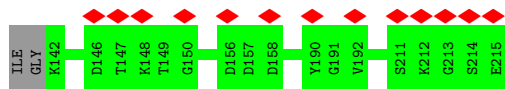


• Molecule 18: Pre-mRNA-splicing factor SLU7

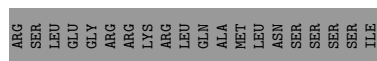
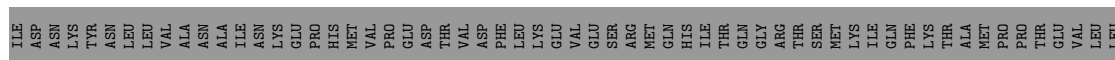
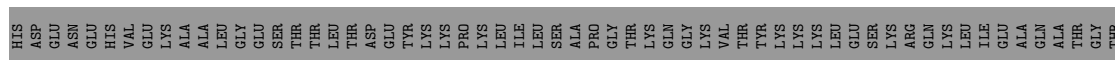
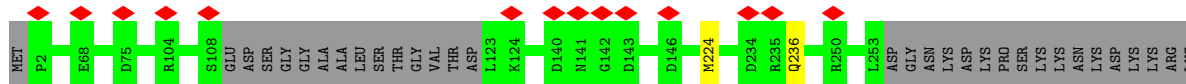




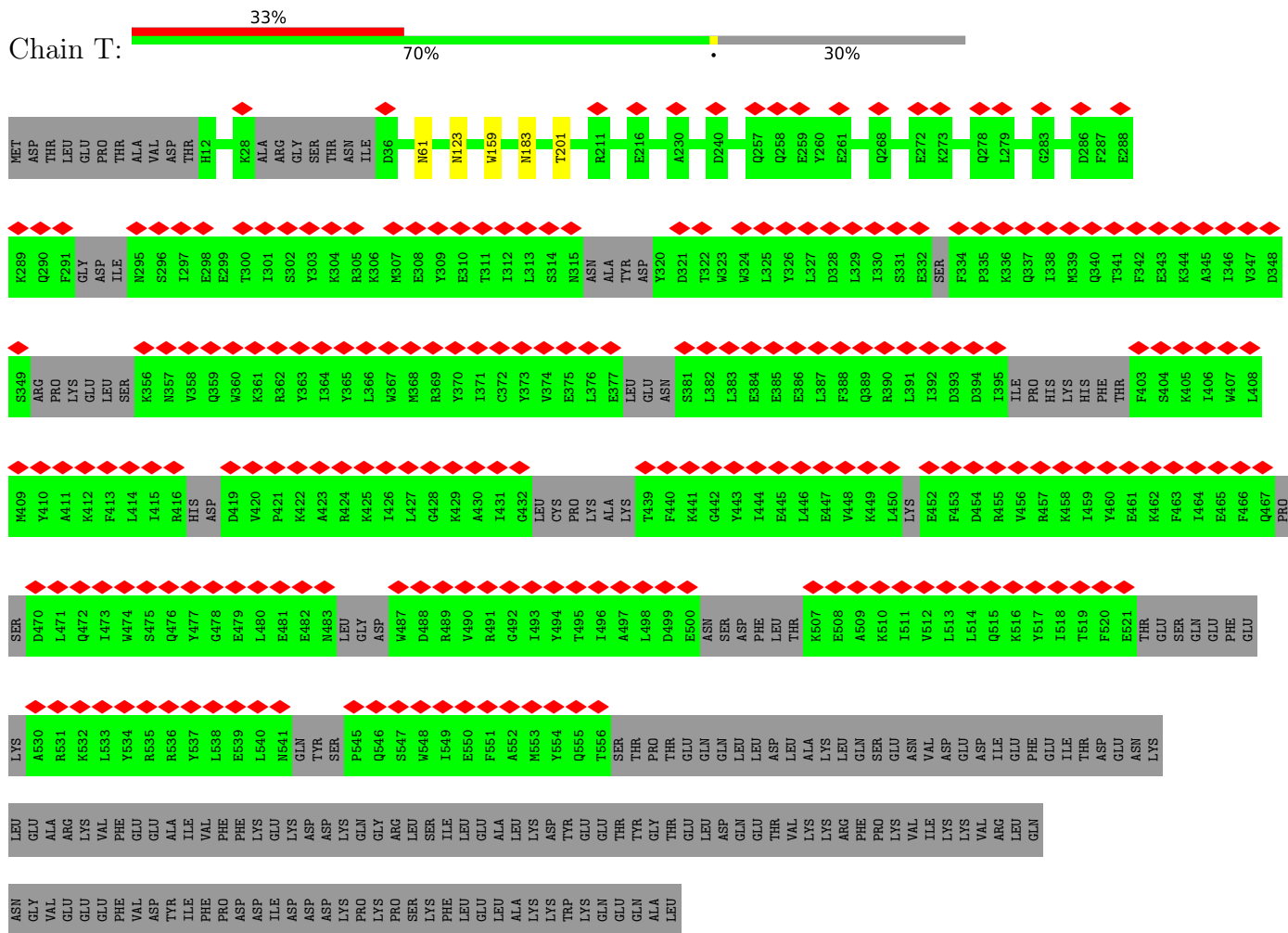
• Molecule 20: Pre-mRNA-splicing factor SYF2



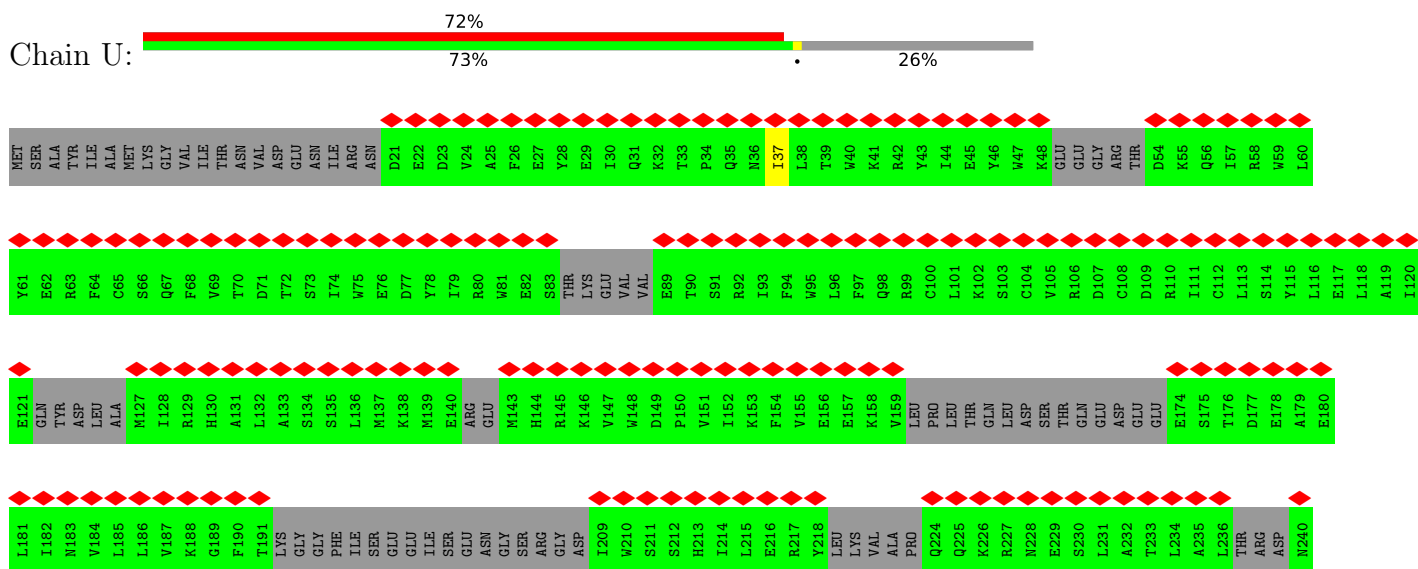
• Molecule 21: Pre-mRNA-splicing factor CEF1

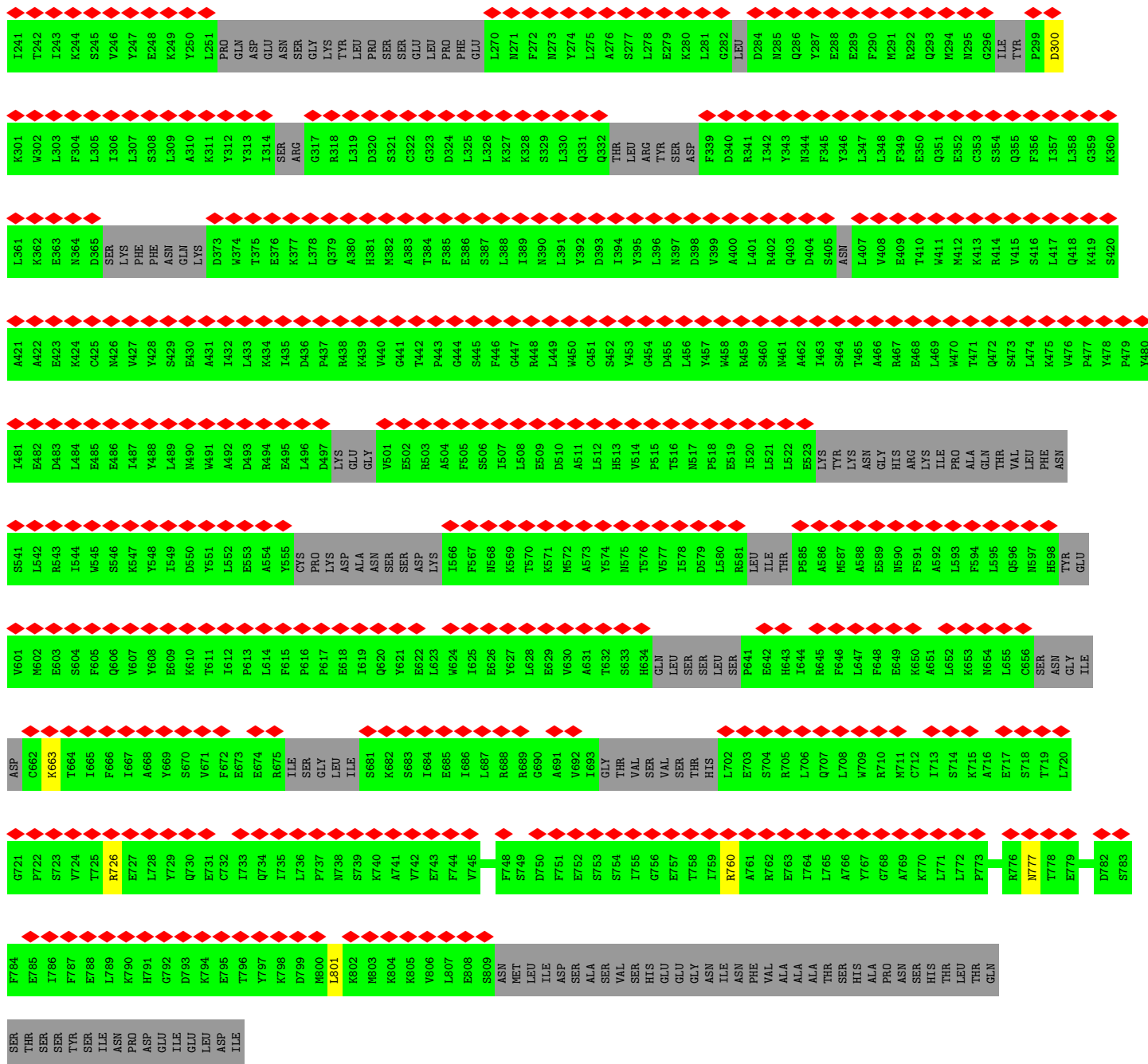


• Molecule 22: Pre-mRNA-splicing factor CLF1

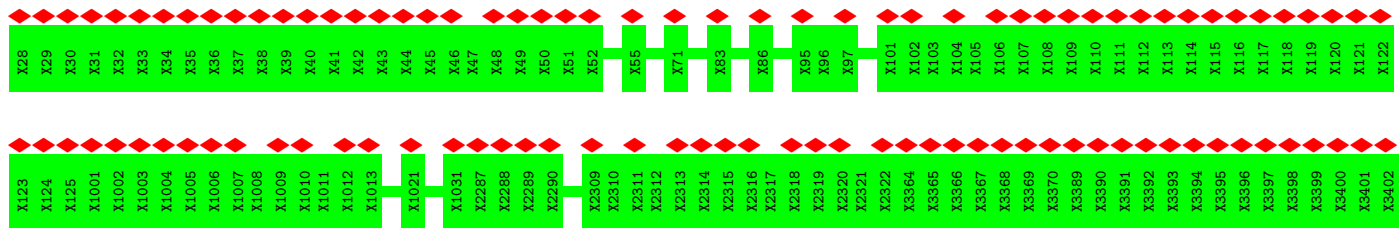


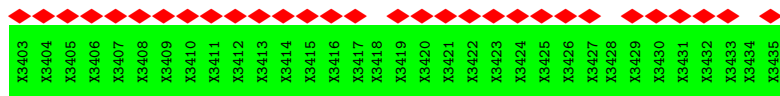
• Molecule 23: Pre-mRNA-splicing factor SYF1



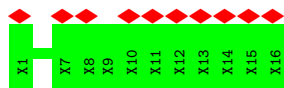


● Molecule 24: Unknown protein fragment

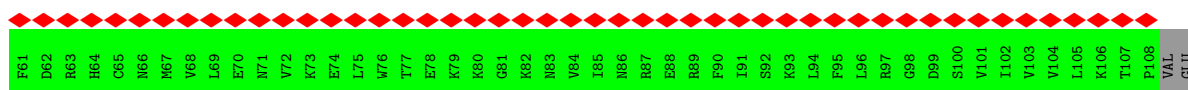
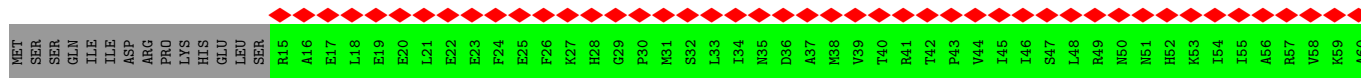
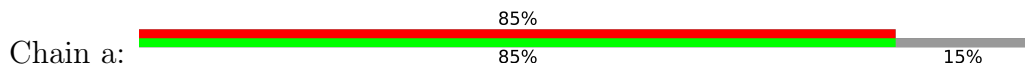




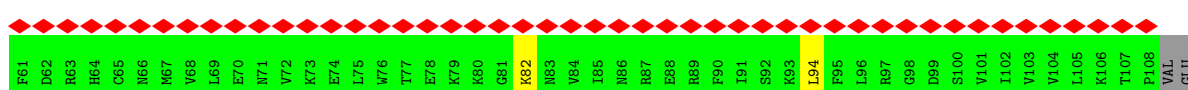
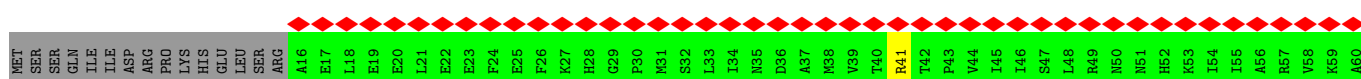
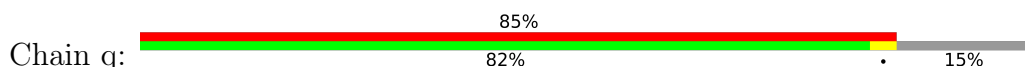
• Molecule 25: Unknown protein fragment



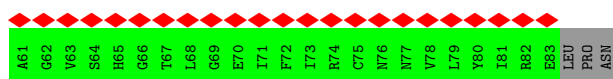
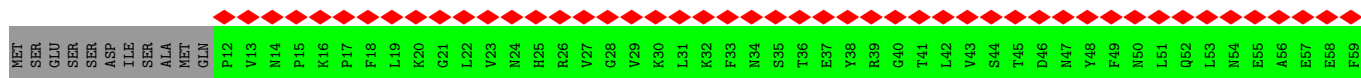
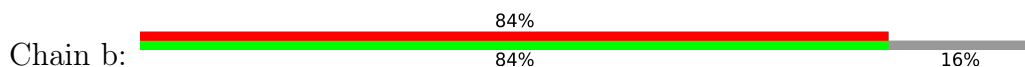
• Molecule 26: Small nuclear ribonucleoprotein Sm D2



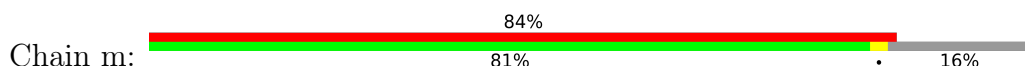
• Molecule 26: Small nuclear ribonucleoprotein Sm D2

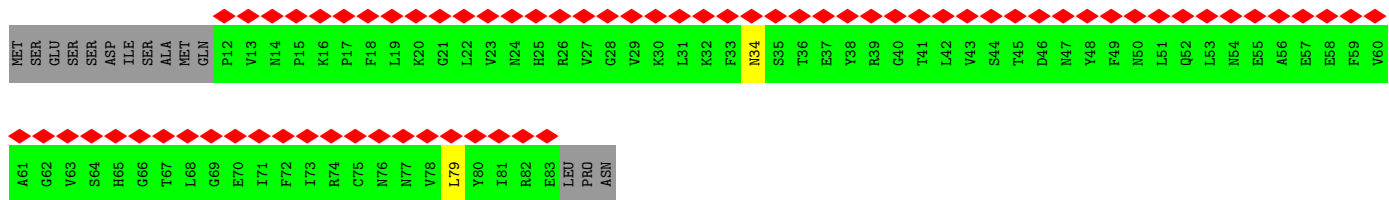


• Molecule 27: Small nuclear ribonucleoprotein F

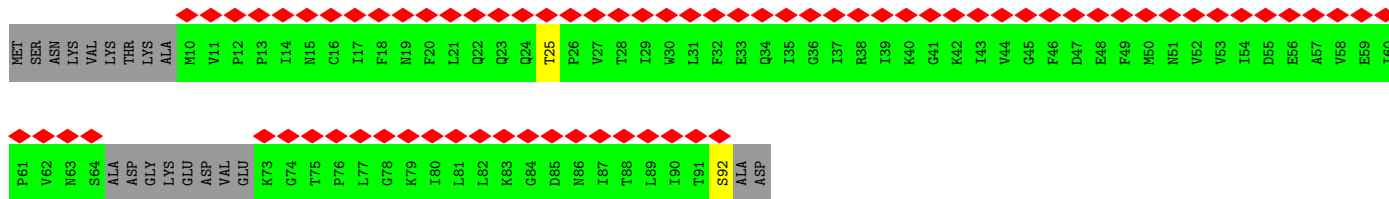
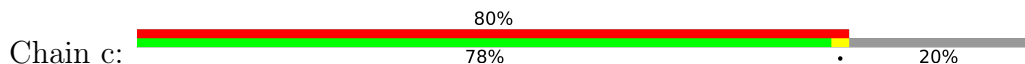


• Molecule 27: Small nuclear ribonucleoprotein F

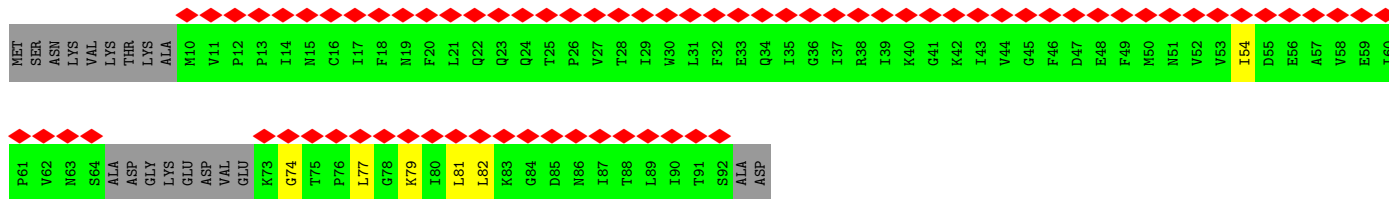
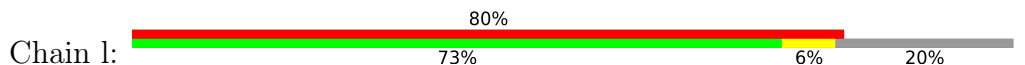




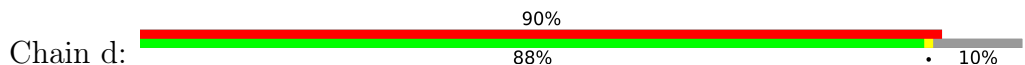
• Molecule 28: Small nuclear ribonucleoprotein E



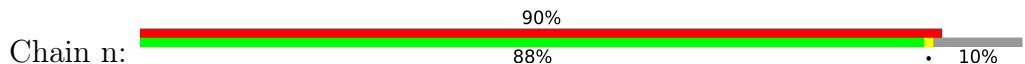
• Molecule 28: Small nuclear ribonucleoprotein E



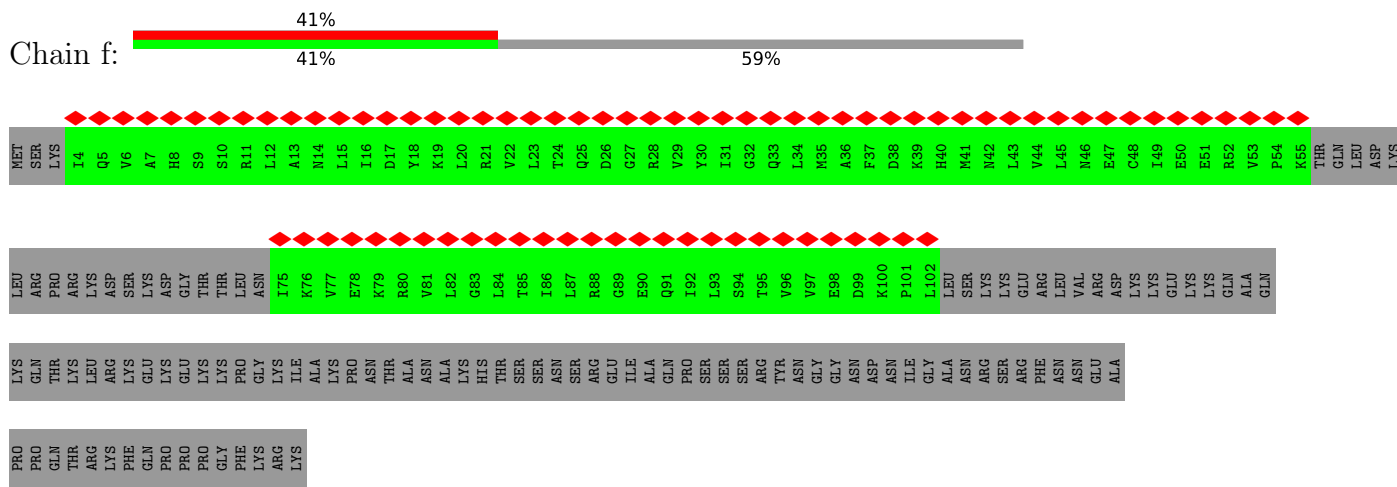
• Molecule 29: Small nuclear ribonucleoprotein G



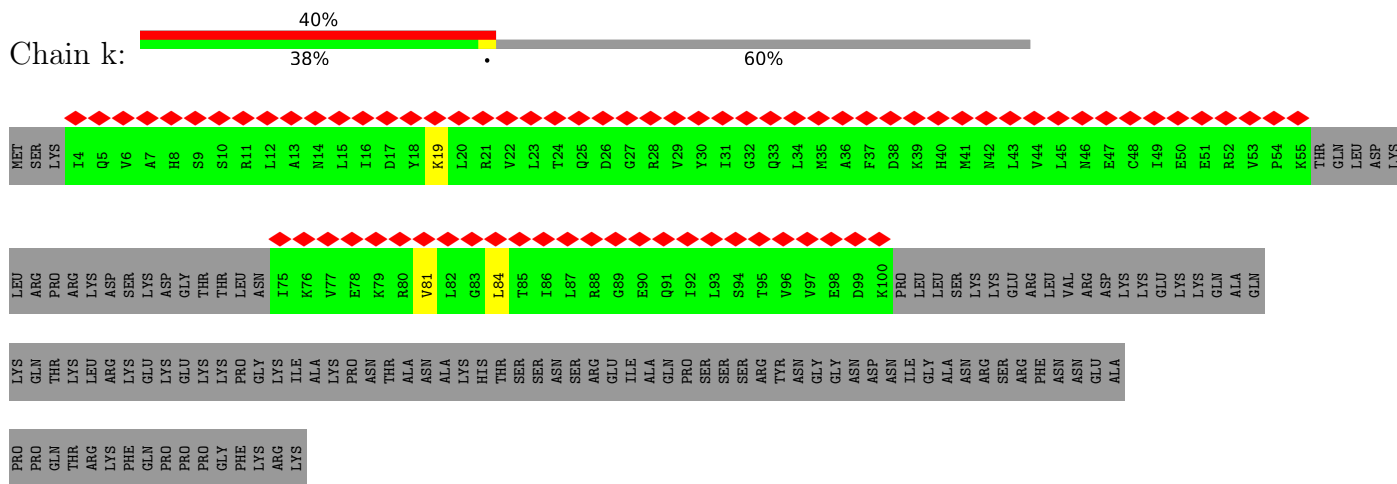
• Molecule 29: Small nuclear ribonucleoprotein G



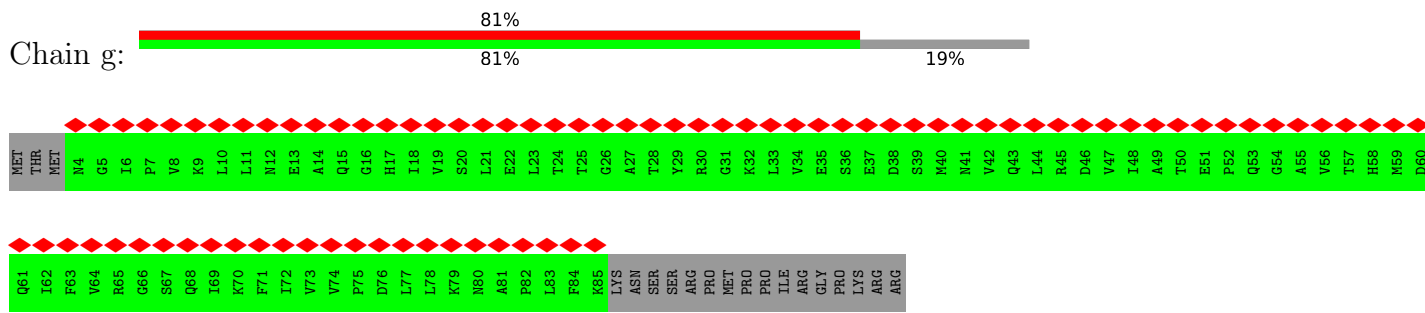
• Molecule 30: Small nuclear ribonucleoprotein-associated protein B



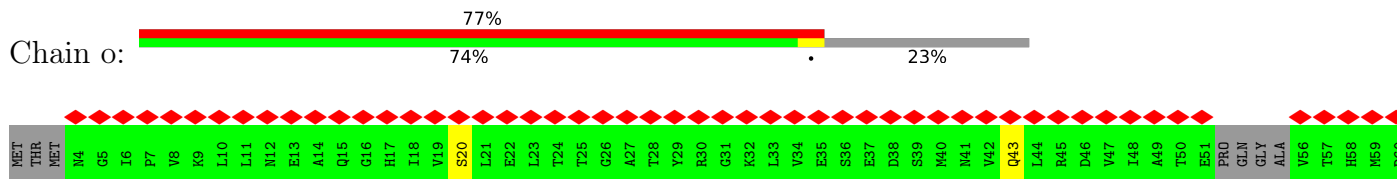
• Molecule 30: Small nuclear ribonucleoprotein-associated protein B

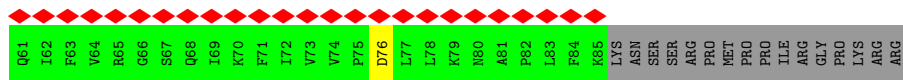


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

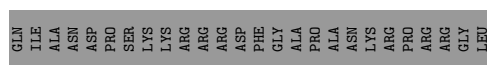
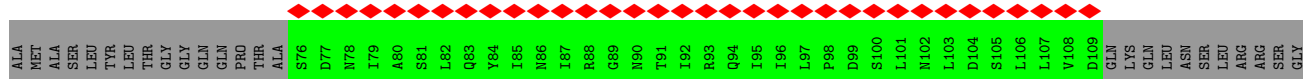
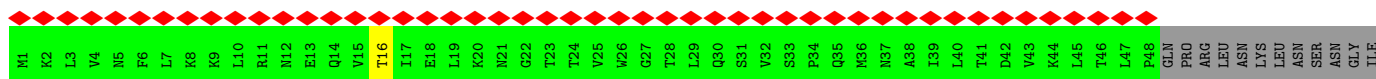


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

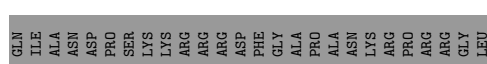




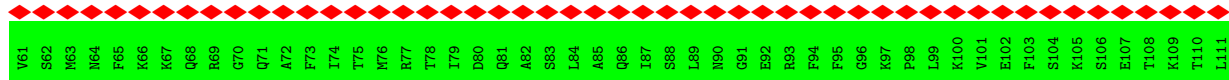
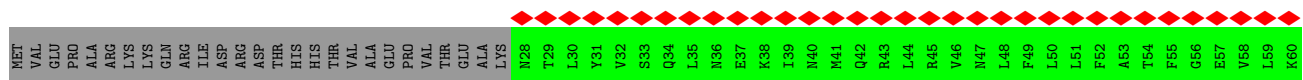
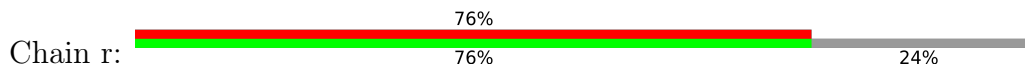
• Molecule 32: Small nuclear ribonucleoprotein Sm D1



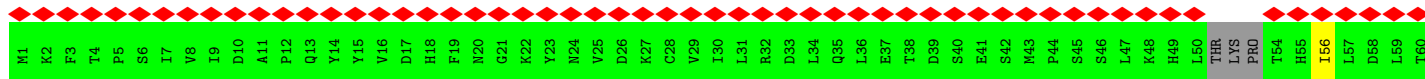
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

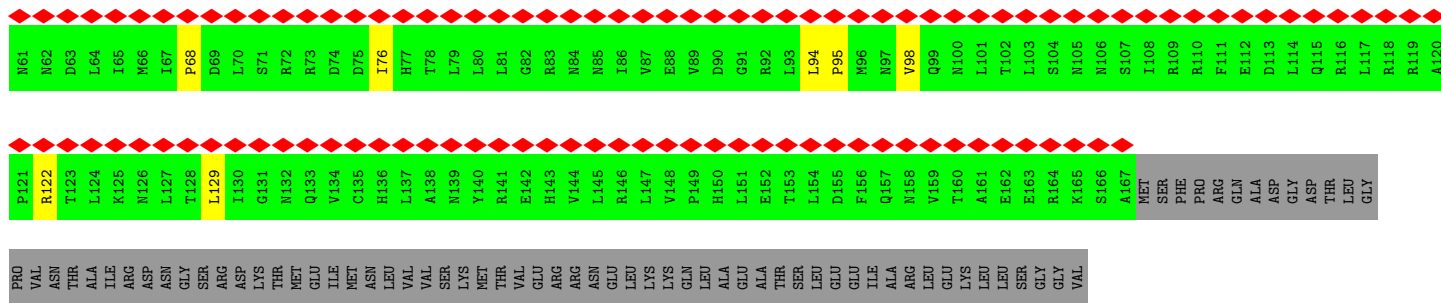


• Molecule 33: Lea1

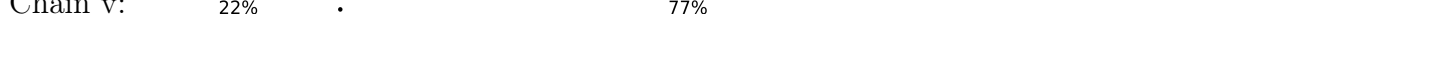
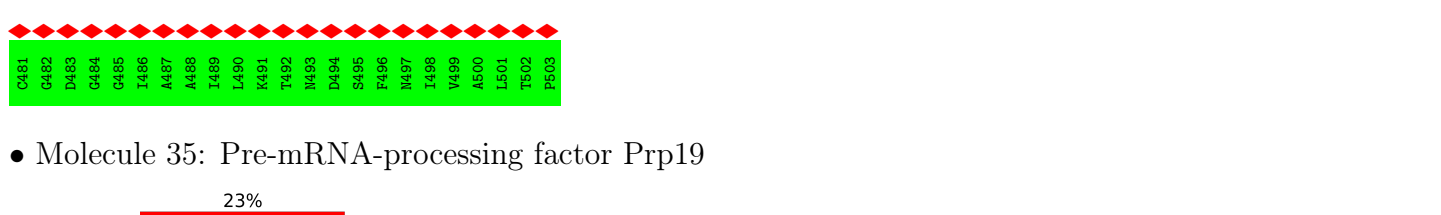
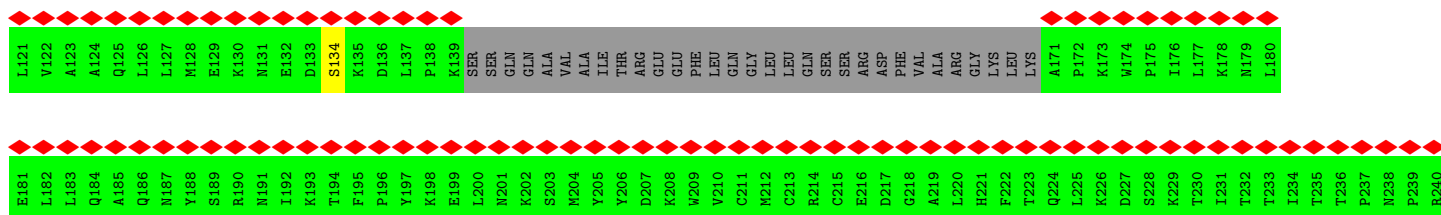
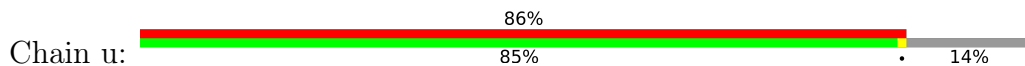


• Molecule 34: Msl1

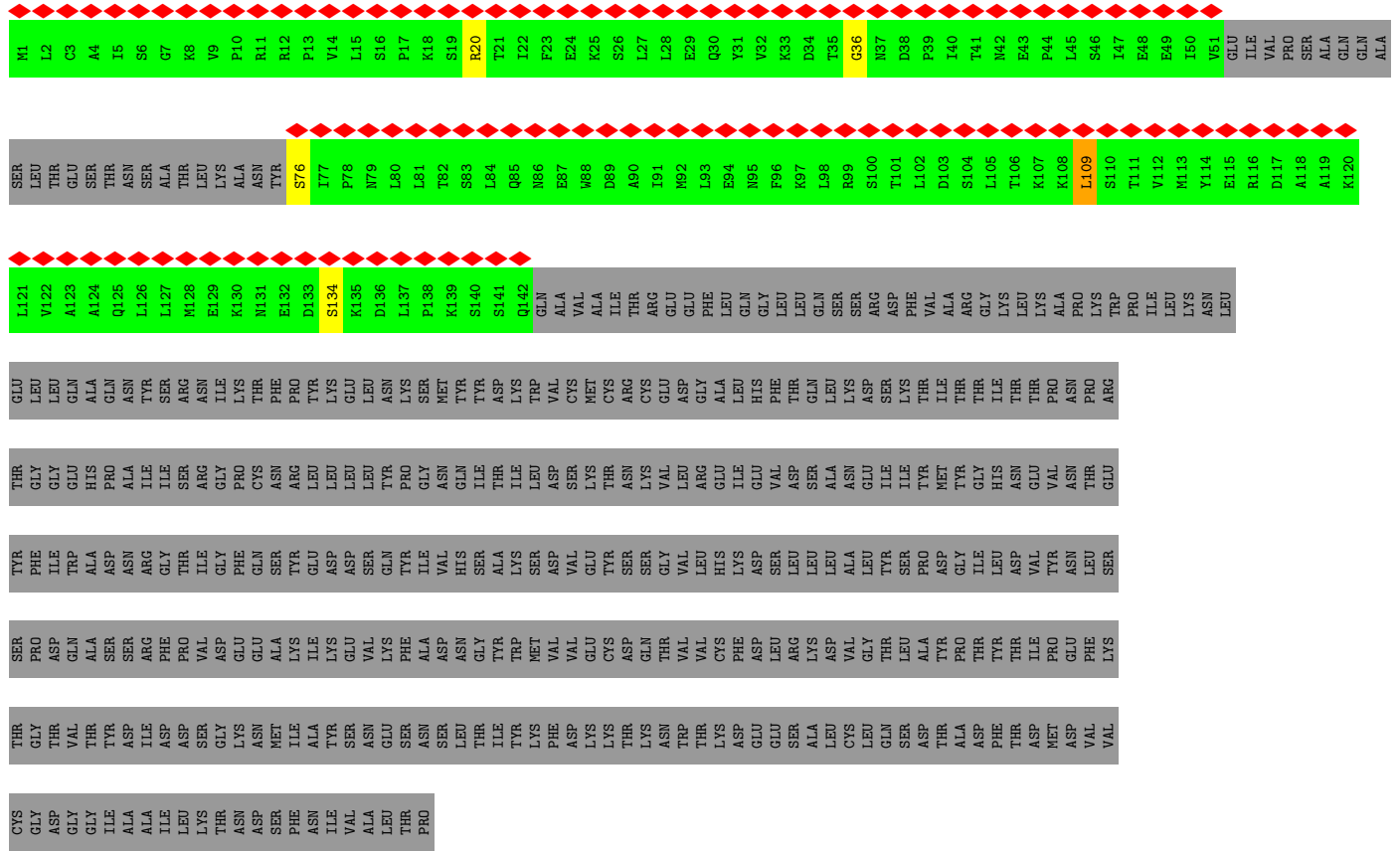




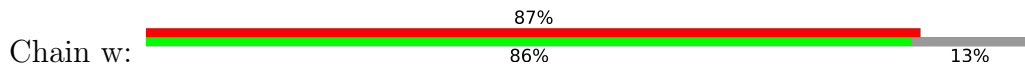
• Molecule 35: Pre-mRNA-processing factor Prp19

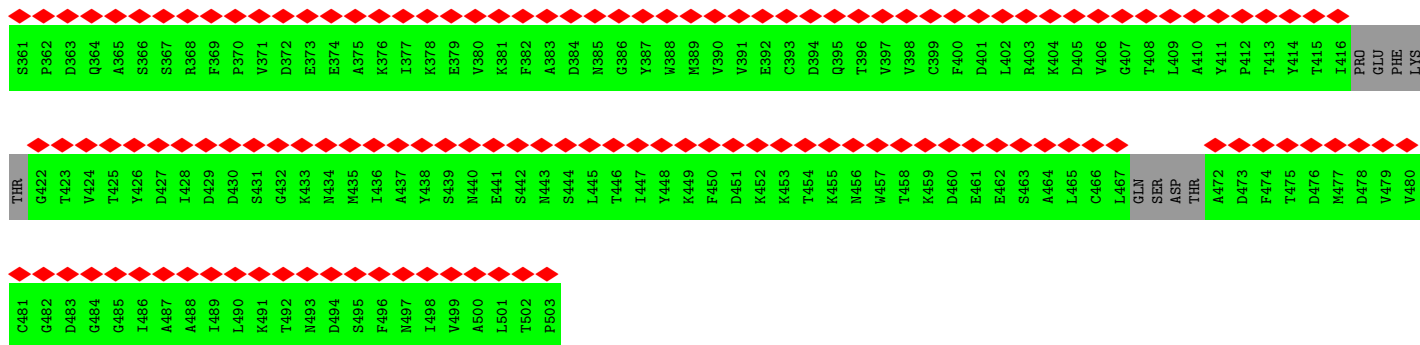


• Molecule 35: Pre-mRNA-processing factor Prp19

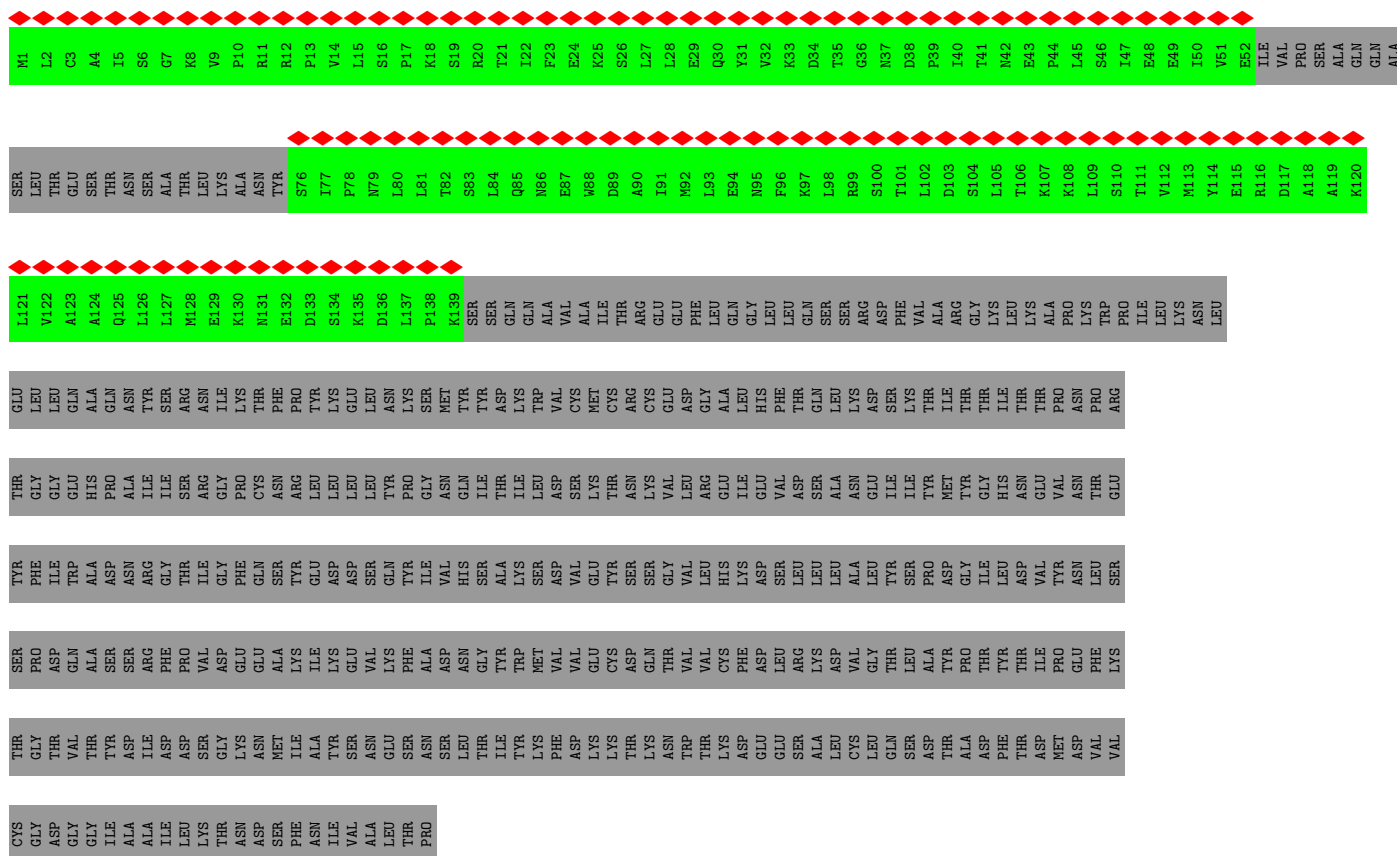


• Molecule 35: Pre-mRNA-processing factor Prp19

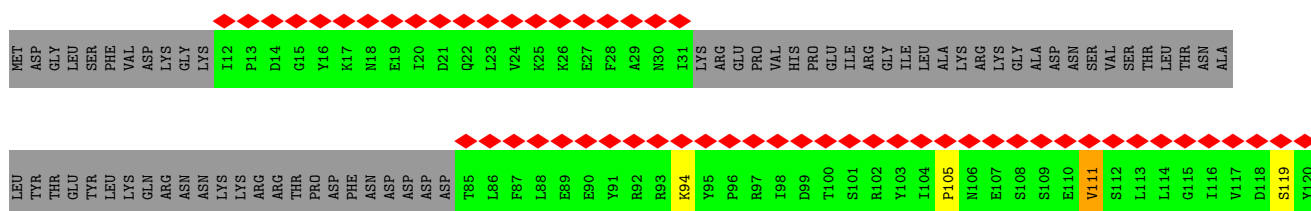




● Molecule 35: Pre-mRNA-processing factor Prp19



● Molecule 36: Pre-mRNA-splicing factor SNT309



L121	K122	H123	Q124	E125	I126	V127	L128	D129	T130	L131	L132	P133	Q134	T135	V136	S137	N138	Q139	W140	R141	I142	N143	N144	D145	Y146	I147	R148	Q149	T150	C151	T152	I153	V154	E155	E156	M157	N158	I159	Q160	Q161	R162	K163	Q164	I165	N166	D167	L168	E169	I170	Y171	R172	K173	R174	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.0	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	0.404	Depositor
Minimum map value	-0.197	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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, MG, GTP, IHP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.50	1/3167 (0.0%)	0.92	8/4911 (0.2%)
2	5	0.88	0/2422	1.16	21/3762 (0.6%)
3	6	0.89	0/2427	1.13	15/3778 (0.4%)
4	e	0.82	4/787 (0.5%)	1.48	17/1219 (1.4%)
5	i	0.59	0/1379	1.10	3/2131 (0.1%)
6	A	0.52	0/16570	0.68	8/22456 (0.0%)
7	B	0.49	0/7331	0.70	8/9926 (0.1%)
8	D	0.56	1/2889 (0.0%)	0.71	2/3924 (0.1%)
9	E	0.44	0/1517	0.63	0/2043
10	F	0.43	0/1598	0.67	2/2151 (0.1%)
11	G	0.47	0/2094	0.62	2/2815 (0.1%)
12	H	0.41	0/584	0.76	1/781 (0.1%)
13	I	0.49	0/1307	0.59	0/1748
14	K	0.35	0/552	0.56	0/746
15	L	0.38	0/3406	0.63	1/4592 (0.0%)
16	M	0.37	0/2678	0.61	1/3619 (0.0%)
17	N	0.39	0/1354	0.59	0/1838
18	O	0.36	0/1967	0.62	2/2624 (0.1%)
19	P	0.29	0/3918	0.48	2/5386 (0.0%)
20	R	0.39	0/817	0.57	1/1083 (0.1%)
21	S	0.46	0/1978	0.63	1/2655 (0.0%)
22	T	0.45	0/3411	0.55	1/4632 (0.0%)
23	U	0.27	0/3625	0.45	0/4963
26	a	0.36	0/753	0.57	0/1013
26	q	0.38	0/738	0.61	0/995
27	b	0.41	0/585	0.57	0/791
27	m	0.40	0/585	0.61	0/791
28	c	0.42	0/585	0.61	0/795
28	l	0.40	0/585	0.56	0/795
29	d	0.50	0/532	0.61	0/715
29	n	0.36	0/529	0.50	0/711
30	f	0.36	0/636	0.63	0/856

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	k	0.35	0/614	0.57	0/826
31	g	0.35	0/634	0.56	0/859
31	o	0.37	0/607	0.53	0/820
32	h	0.38	0/649	0.54	0/880
32	p	0.40	0/623	0.65	0/844
33	r	0.33	0/415	0.55	0/577
34	s	0.31	0/814	0.53	0/1134
35	u	0.47	0/2150	0.68	2/2989 (0.1%)
35	v	0.59	0/586	0.89	3/816 (0.4%)
35	w	0.47	0/2165	0.71	3/3010 (0.1%)
35	x	0.58	0/576	0.79	0/802
36	y	0.58	0/546	0.80	0/760
All	All	0.49	6/83685 (0.0%)	0.72	104/115562 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	A	0	6
7	B	0	9
8	D	0	2
9	E	0	3
10	F	0	1
11	G	0	2
15	L	0	1
18	O	0	1
30	k	0	1
35	u	0	1
35	v	0	1
35	w	0	2
36	y	0	2
All	All	0	32

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	9	U	C1'-N1	7.04	1.59	1.48
4	e	-13	U	C1'-N1	6.81	1.58	1.48
4	e	-11	U	C1'-N1	6.04	1.57	1.48
4	e	-2	A	N9-C4	-6.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	227	VAL	CB-CG1	-5.37	1.41	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	954	LEU	CA-CB-CG	9.20	136.46	115.30
4	e	11	U	C2-N1-C1'	9.14	128.67	117.70
4	e	11	U	N1-C2-O2	8.22	128.55	122.80
35	w	134	SER	CA-C-O	-7.91	103.49	120.10
4	e	2	U	N1-C2-O2	7.86	128.30	122.80

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	405	ASN	Peptide
6	A	542	HIS	Peptide
6	A	774	ILE	Peptide
6	A	775	ARG	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
6	A	1954/2413 (81%)	1813 (93%)	126 (6%)	15 (1%)	19 51
7	B	889/1008 (88%)	830 (93%)	55 (6%)	4 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	357/451 (79%)	329 (92%)	28 (8%)	0	100	100
9	E	176/379 (46%)	164 (93%)	11 (6%)	1 (1%)	25	57
10	F	193/364 (53%)	173 (90%)	19 (10%)	1 (0%)	29	61
11	G	253/339 (75%)	229 (90%)	23 (9%)	1 (0%)	34	66
12	H	64/175 (37%)	55 (86%)	8 (12%)	1 (2%)	9	36
13	I	154/157 (98%)	140 (91%)	14 (9%)	0	100	100
14	K	76/135 (56%)	72 (95%)	4 (5%)	0	100	100
15	L	406/577 (70%)	380 (94%)	26 (6%)	0	100	100
16	M	320/455 (70%)	302 (94%)	18 (6%)	0	100	100
17	N	163/251 (65%)	157 (96%)	6 (4%)	0	100	100
18	O	215/382 (56%)	196 (91%)	19 (9%)	0	100	100
19	P	645/1145 (56%)	610 (95%)	35 (5%)	0	100	100
20	R	97/215 (45%)	94 (97%)	3 (3%)	0	100	100
21	S	234/590 (40%)	223 (95%)	11 (5%)	0	100	100
22	T	451/687 (66%)	442 (98%)	9 (2%)	0	100	100
23	U	587/859 (68%)	555 (94%)	30 (5%)	2 (0%)	41	71
26	a	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
26	q	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
27	b	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	m	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	c	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
28	l	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	11	38
29	d	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
29	n	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
30	f	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
30	k	74/196 (38%)	66 (89%)	7 (10%)	1 (1%)	11	38
31	g	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
31	o	74/101 (73%)	70 (95%)	4 (5%)	0	100	100
32	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
32	p	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	5	26
33	r	82/111 (74%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	s	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	2	14
35	u	423/503 (84%)	413 (98%)	8 (2%)	2 (0%)	29	61
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	5	27
35	w	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
35	x	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
36	y	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	11
All	All	9709/14738 (66%)	9051 (93%)	610 (6%)	48 (0%)	32	61

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	1905	LEU
12	H	9	LEU
23	U	37	ILE
34	s	76	ILE
36	y	94	LYS

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	
6	A	1778/2182 (82%)	1741 (98%)	37 (2%)	53	75
7	B	809/910 (89%)	797 (98%)	12 (2%)	65	81
8	D	313/397 (79%)	307 (98%)	6 (2%)	57	77
9	E	168/328 (51%)	166 (99%)	2 (1%)	71	83
10	F	183/332 (55%)	183 (100%)	0	100	100
11	G	219/296 (74%)	216 (99%)	3 (1%)	67	82
12	H	58/151 (38%)	53 (91%)	5 (9%)	10	35
13	I	140/141 (99%)	139 (99%)	1 (1%)	84	90
14	K	44/121 (36%)	43 (98%)	1 (2%)	50	73
15	L	379/538 (70%)	377 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	M	288/413 (70%)	283 (98%)	5 (2%)	60	78
17	N	144/225 (64%)	143 (99%)	1 (1%)	84	90
18	O	210/346 (61%)	208 (99%)	2 (1%)	76	86
19	P	178/1029 (17%)	176 (99%)	2 (1%)	73	85
20	R	90/193 (47%)	89 (99%)	1 (1%)	73	85
21	S	208/525 (40%)	207 (100%)	1 (0%)	88	93
22	T	248/633 (39%)	244 (98%)	4 (2%)	62	79
23	U	131/786 (17%)	126 (96%)	5 (4%)	33	62
26	a	79/103 (77%)	79 (100%)	0	100	100
26	q	77/103 (75%)	74 (96%)	3 (4%)	32	62
27	b	63/77 (82%)	63 (100%)	0	100	100
27	m	63/77 (82%)	61 (97%)	2 (3%)	39	67
28	c	65/83 (78%)	63 (97%)	2 (3%)	40	67
28	l	65/83 (78%)	60 (92%)	5 (8%)	13	38
29	d	58/66 (88%)	57 (98%)	1 (2%)	60	78
29	n	57/66 (86%)	56 (98%)	1 (2%)	59	78
30	f	70/176 (40%)	70 (100%)	0	100	100
30	k	67/176 (38%)	66 (98%)	1 (2%)	65	81
31	g	69/89 (78%)	69 (100%)	0	100	100
31	o	67/89 (75%)	64 (96%)	3 (4%)	27	58
32	h	77/129 (60%)	76 (99%)	1 (1%)	69	82
32	p	73/129 (57%)	63 (86%)	10 (14%)	3	16
All	All	6538/10992 (60%)	6419 (98%)	119 (2%)	61	78

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	G	44	ASN
32	p	43	VAL
16	M	339	MET
32	p	25	VAL
26	q	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
17	N	177	ASN
22	T	210	ASN
18	O	39	ASN
19	P	1107	GLN
29	n	53	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	127/1175 (10%)	44 (34%)	4 (3%)
2	5	100/214 (46%)	25 (25%)	2 (2%)
3	6	101/112 (90%)	28 (27%)	3 (2%)
4	e	33/34 (97%)	19 (57%)	0
5	i	54/59 (91%)	18 (33%)	0
All	All	415/1594 (26%)	134 (32%)	9 (2%)

5 of 134 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	11	U
1	2	16	U
1	2	17	U
1	2	18	U

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	6	56	A
3	6	64	U
1	2	1145	U
2	5	78	A
2	5	81	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

Of 14 ligands modelled in this entry, 12 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
38	IHP	A	3001	-	36,36,36	0.87	0	54,60,60	1.55	8 (14%)
39	GTP	B	2001	37	26,34,34	1.41	3 (11%)	32,54,54	1.84	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	IHP	A	3001	-	-	7/30/54/54	0/1/1/1
39	GTP	B	2001	37	-	5/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	2001	GTP	C5-C6	-4.67	1.37	1.47
39	B	2001	GTP	C5-C4	-2.39	1.37	1.43
39	B	2001	GTP	O4'-C4'	-2.13	1.40	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B	2001	GTP	PB-O3B-PG	-5.88	112.65	132.83
39	B	2001	GTP	C5-C6-N1	3.84	120.73	113.95
38	A	3001	IHP	C4-C3-C2	3.67	118.45	110.41
38	A	3001	IHP	C5-C6-C1	3.64	118.38	110.41
38	A	3001	IHP	C5-C4-C3	3.48	118.02	110.41

There are no chirality outliers.

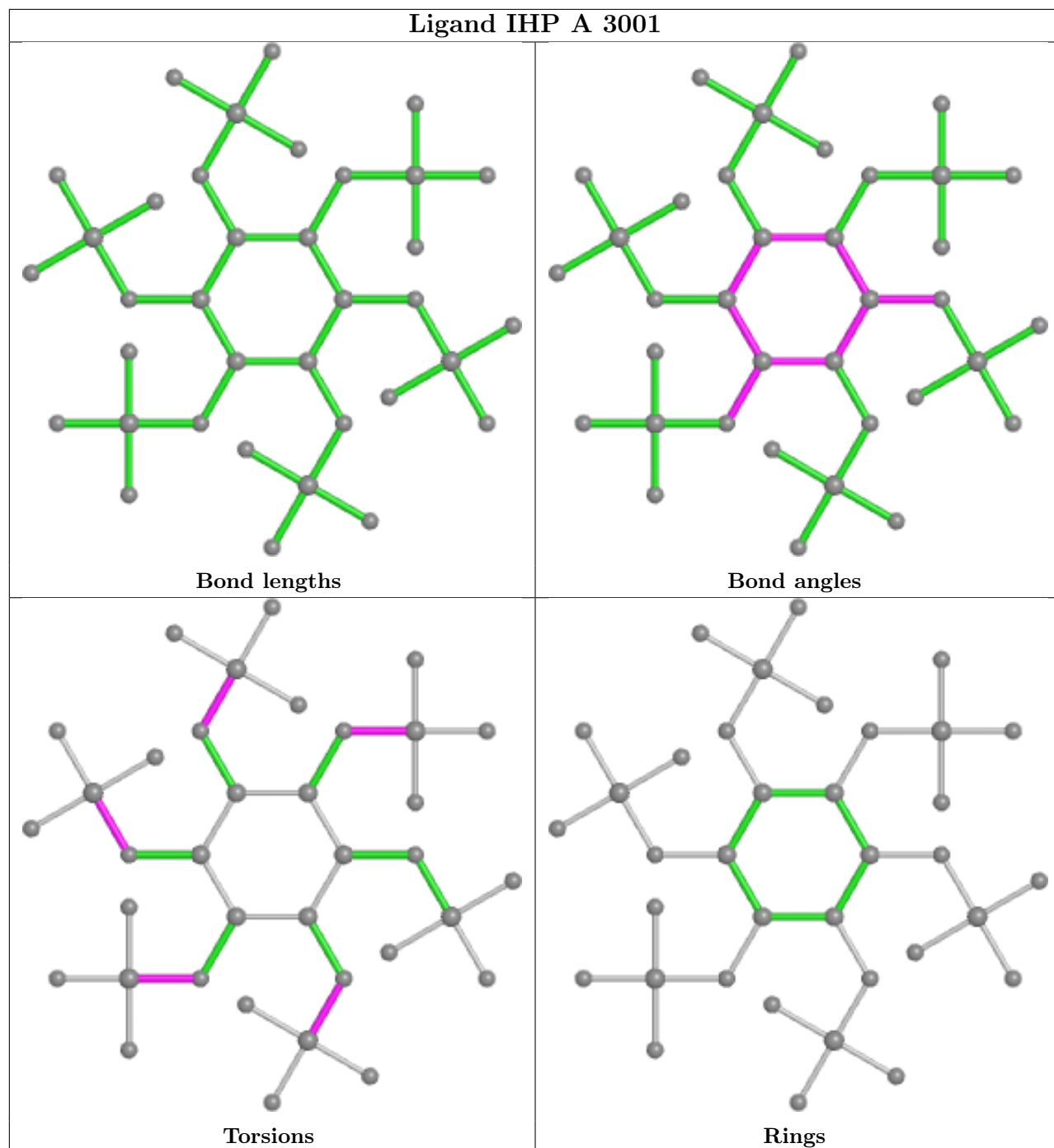
5 of 12 torsion outliers are listed below:

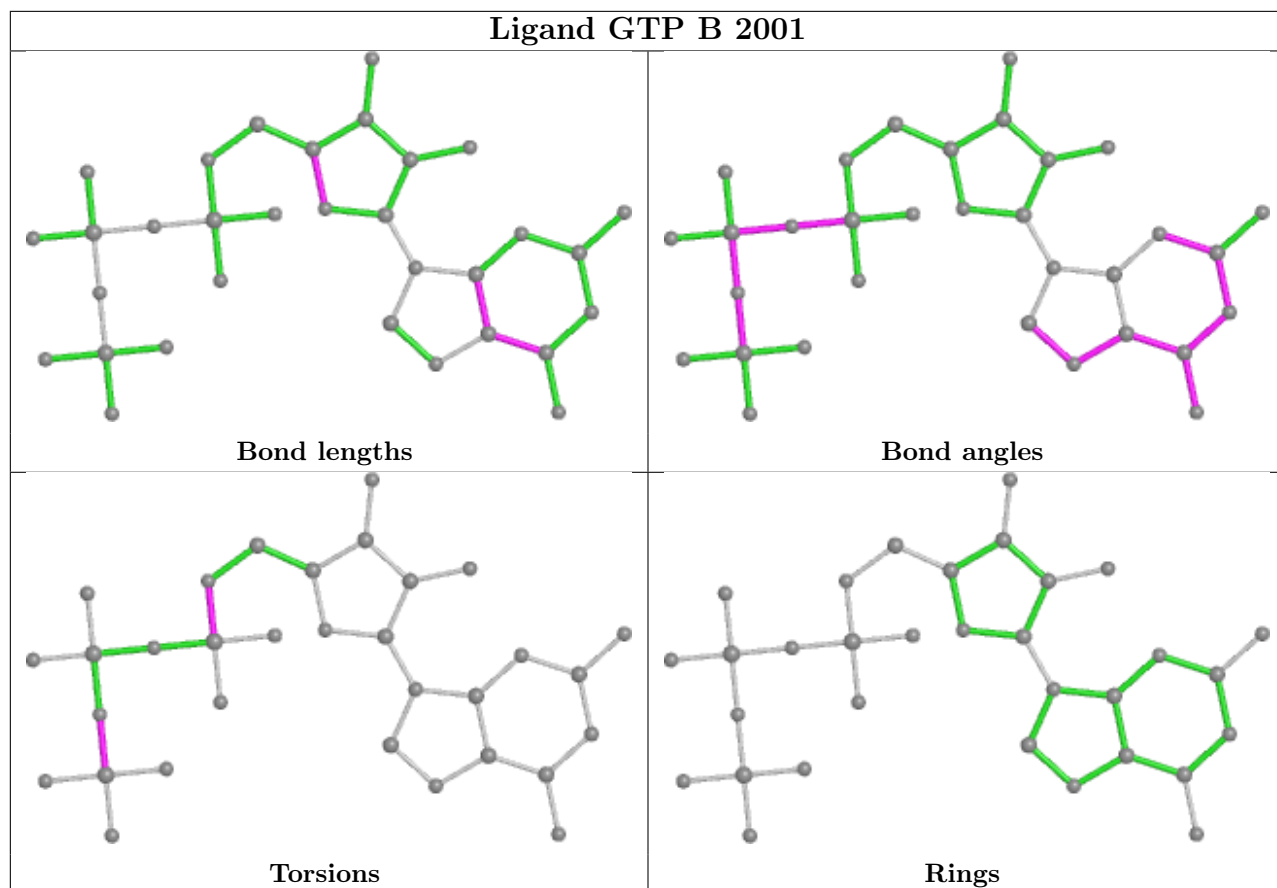
Mol	Chain	Res	Type	Atoms
38	A	3001	IHP	C1-O11-P1-O21
38	A	3001	IHP	C2-O12-P2-O22
38	A	3001	IHP	C3-O13-P3-O23
38	A	3001	IHP	C4-O14-P4-O34
38	A	3001	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	i	4
24	X	4

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	15:U	O3'	501:A	P	58.05
1	X	3370:UNK	C	3389:UNK	N	35.33
1	X	1031:UNK	C	2287:UNK	N	34.77
1	X	125:UNK	C	1001:UNK	N	25.13
1	X	2322:UNK	C	3364:UNK	N	19.85

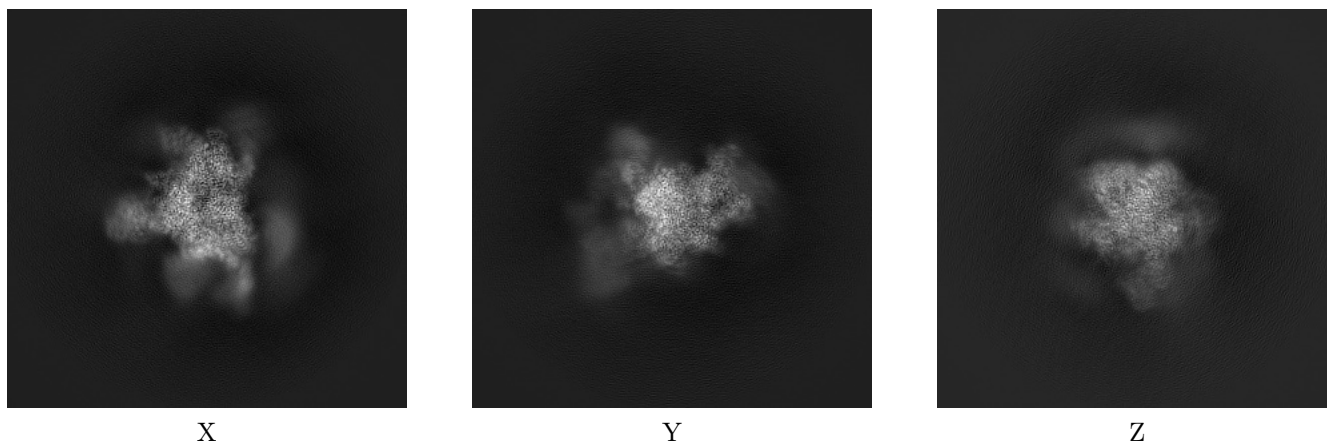
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7109. 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 [i](#)

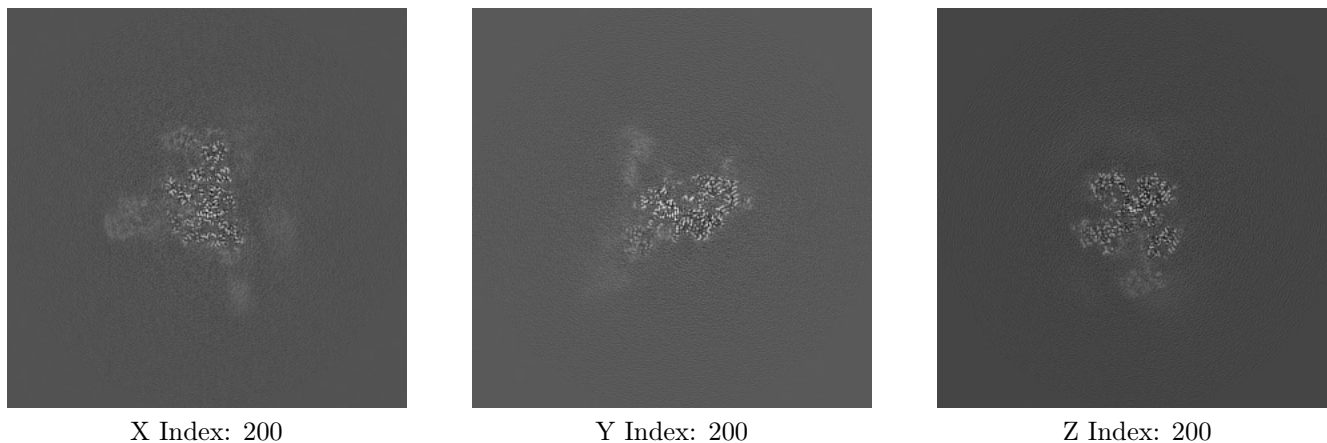
6.1.1 Primary map



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

6.2 Central slices [i](#)

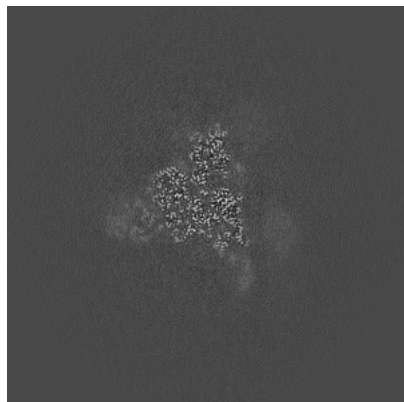
6.2.1 Primary map



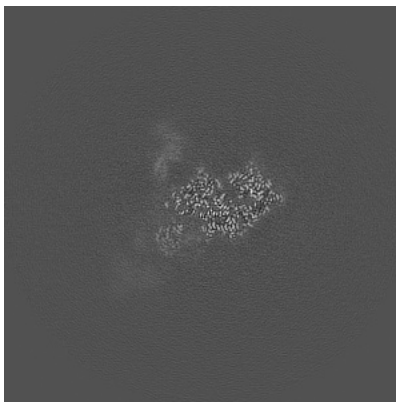
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

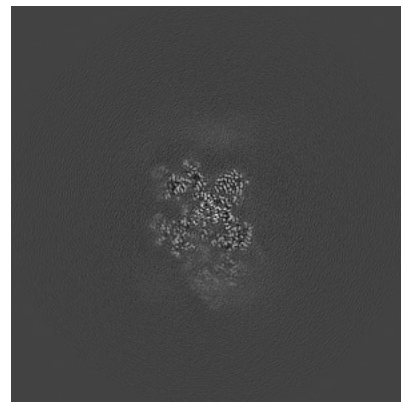
6.3.1 Primary map



X Index: 212



Y Index: 204



Z Index: 191

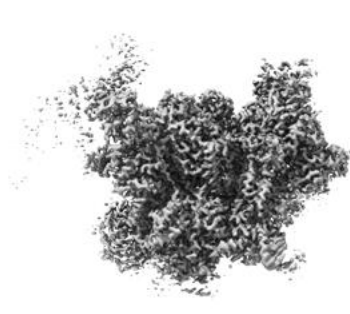
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

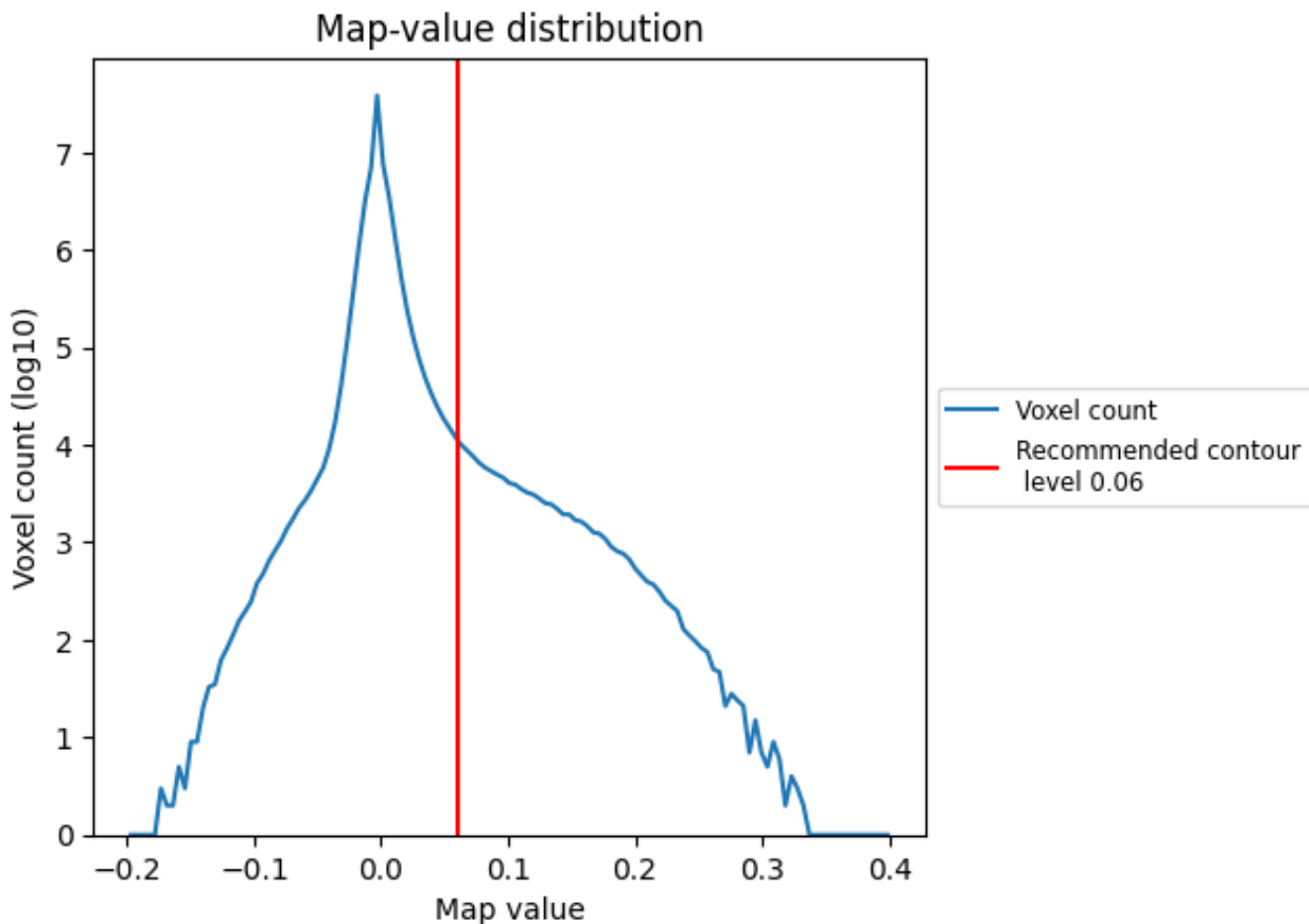
6.5 Mask visualisation

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

7 Map analysis [i](#)

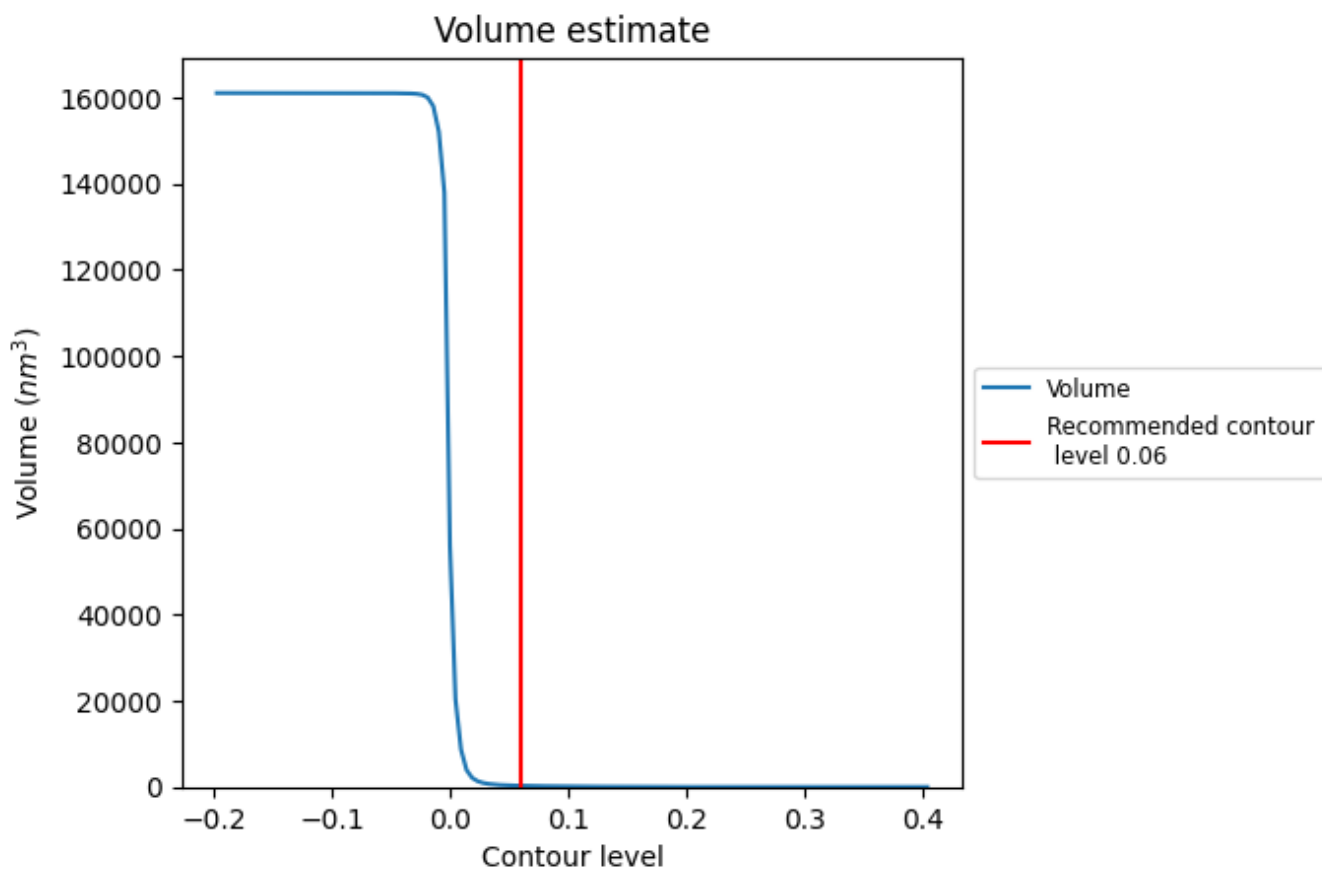
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

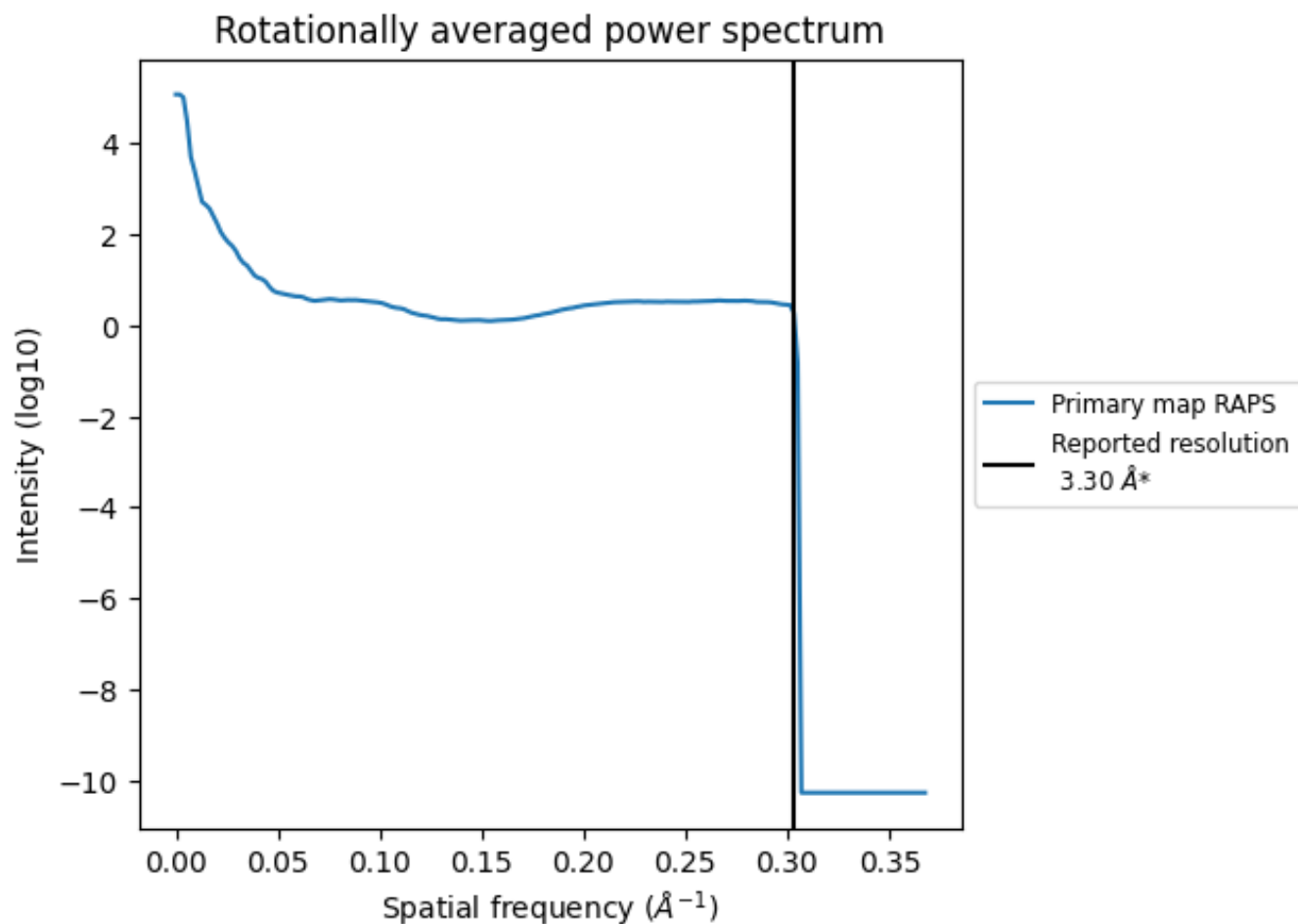
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 272 nm³; this corresponds to an approximate mass of 246 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 0.303 Å⁻¹

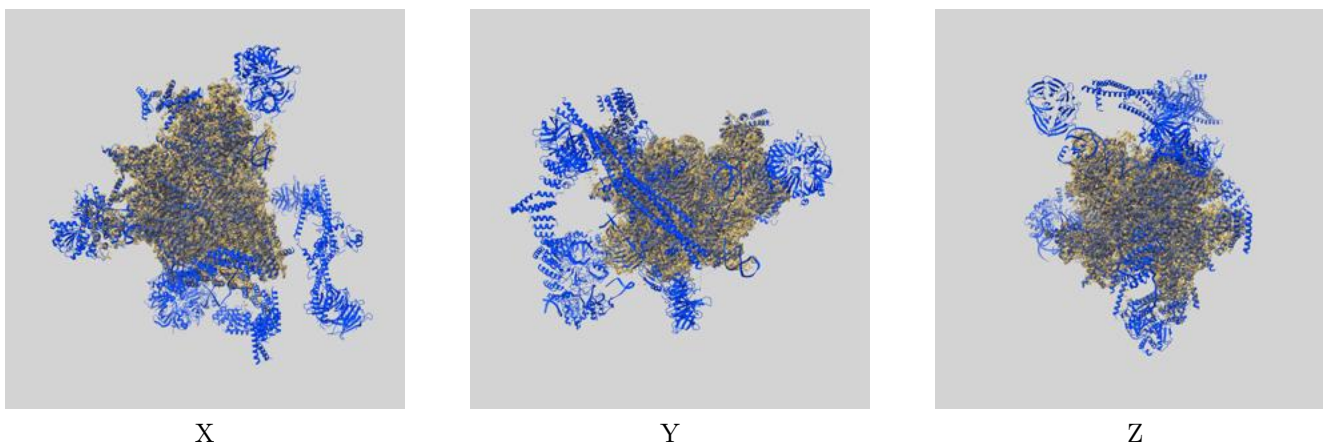
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

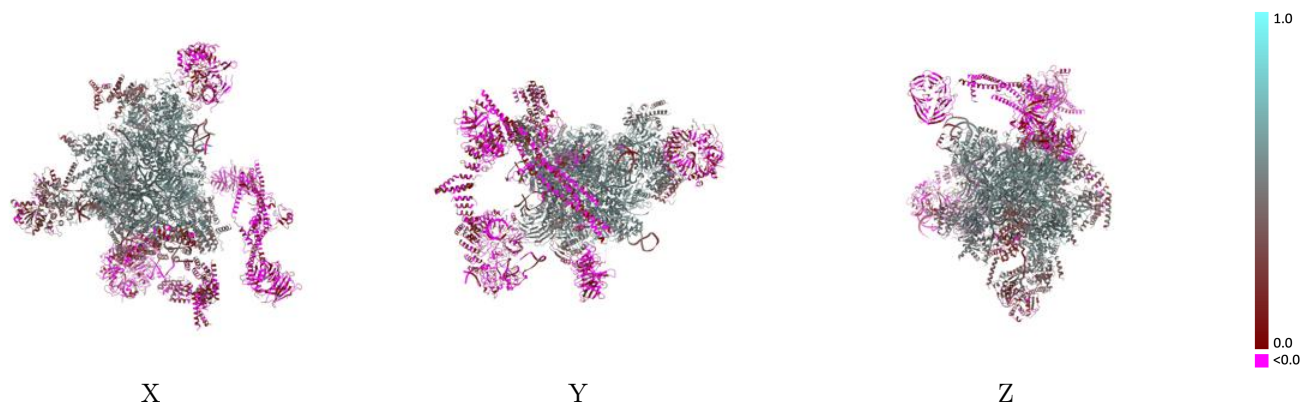
This section contains information regarding the fit between EMDB map EMD-7109 and PDB model 6BK8. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



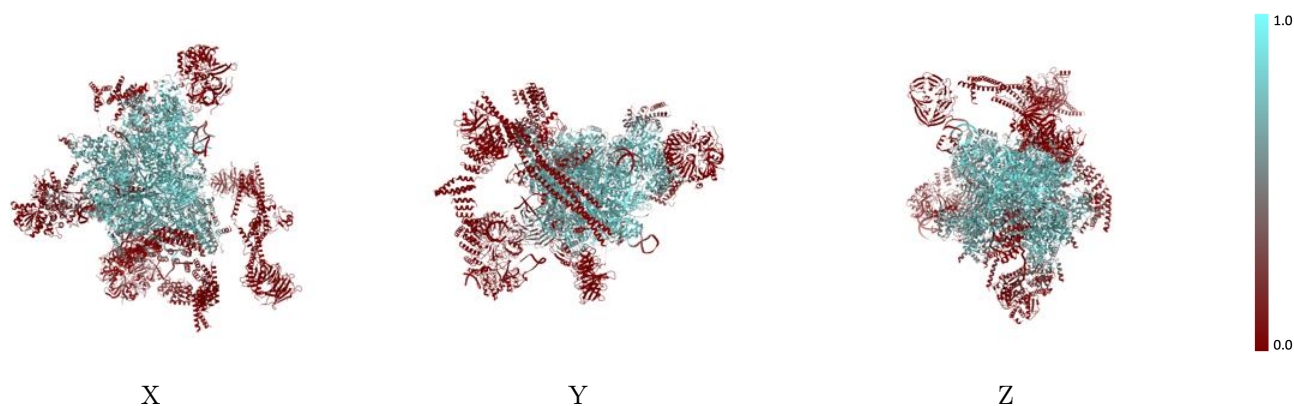
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



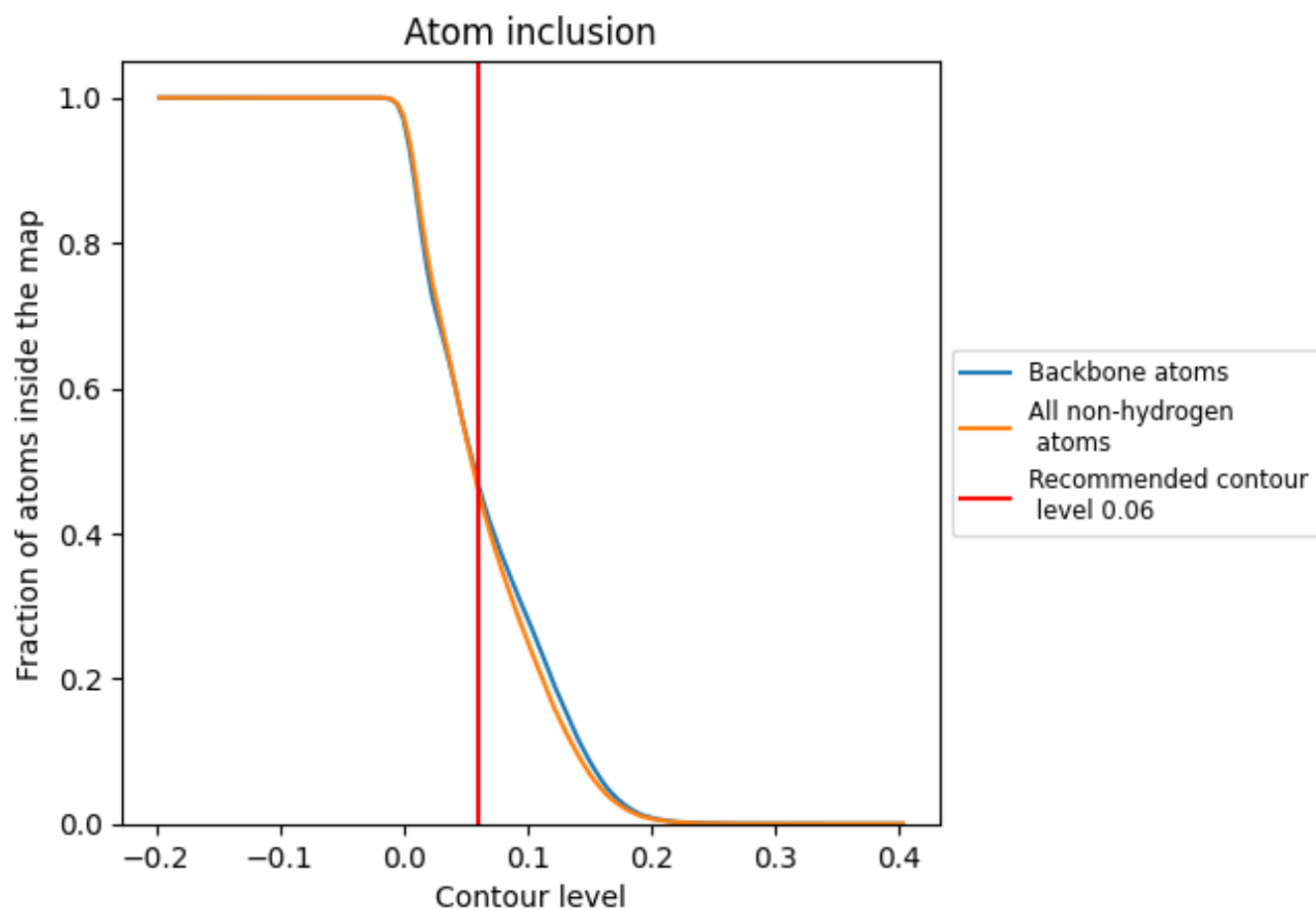
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 46% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4632	 0.3800
2	 0.2015	 0.1350
5	 0.7193	 0.4800
6	 0.7544	 0.5110
A	 0.7657	 0.5480
B	 0.7221	 0.5340
D	 0.7989	 0.5590
E	 0.6658	 0.5200
F	 0.5405	 0.4790
G	 0.6927	 0.5240
H	 0.5263	 0.5260
I	 0.7560	 0.5480
K	 0.3796	 0.4500
L	 0.4029	 0.3920
M	 0.5041	 0.5000
N	 0.5580	 0.4770
O	 0.4718	 0.4870
P	 0.1572	 0.3460
R	 0.5997	 0.5230
S	 0.7018	 0.5300
T	 0.5065	 0.4260
U	 0.0772	 0.2040
X	 0.4055	 0.4340
Y	 0.3375	 0.3790
a	 0.0000	 0.0440
b	 0.0000	 0.0190
c	 0.0000	 0.0250
d	 0.0000	 0.0920
e	 0.4158	 0.4330
f	 0.0000	 0.0780
g	 0.0000	 0.1650
h	 0.0000	 0.0050
i	 0.4262	 0.3650
k	 0.0000	 0.0040
l	 0.0000	 0.0130



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Chain	Atom inclusion	Q-score
m	0.0000	0.0240
n	0.0000	0.0090
o	0.0000	0.0240
p	0.0000	0.0100
q	0.0000	0.0120
r	0.0000	0.0330
s	0.0000	0.0040
u	0.0000	-0.0080
v	0.0000	-0.0290
w	0.0000	-0.0040
x	0.0000	-0.0220
y	0.0000	-0.0290