



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 11:37 AM JST

PDB ID : 5ZWO
EMDB ID : EMD-6974
Title : Cryo-EM structure of the yeast B complex at average resolution of 3.9 angstrom
Authors : Bai, R.; Wan, R.; Yan, C.; Shi, Y.
Deposited on : 2018-05-16
Resolution : 3.90 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

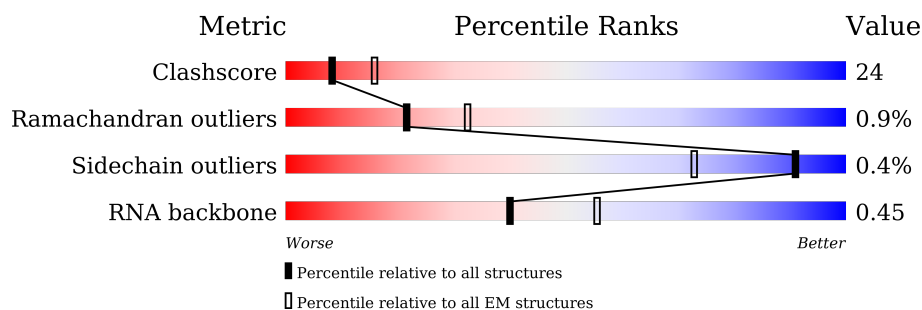
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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






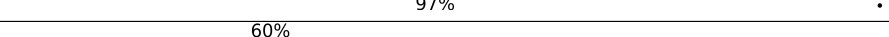



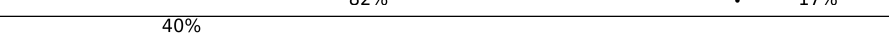


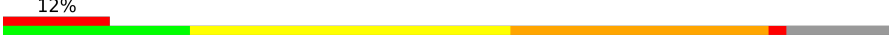
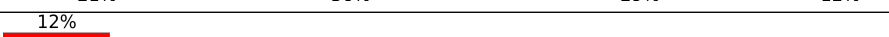













Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	2413	
2	K	465	
3	L	494	
4	N	899	
5	J	469	
6	E	143	
7	M	126	

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Mol	Chain	Length	Quality of chain
8	C	1008	
9	z	109	
10	q	95	
11	r	89	
12	x	86	
13	t	93	
14	y	115	
15	s	187	
16	F	112	
17	B	214	
18	O	587	
19	S	101	
19	d	101	
19	l	101	
20	P	196	
20	a	196	
20	h	196	
21	Q	146	
21	b	146	
21	m	146	
22	R	110	
22	c	110	
22	n	110	
23	T	94	
23	e	94	

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Mol	Chain	Length	Quality of chain
23	i	94	
24	U	86	
24	f	86	
24	j	86	
25	V	77	
25	g	77	
25	k	77	
26	I	161	
27	D	2163	
28	G	60	
29	1	971	
30	2	436	
31	3	1361	
32	4	213	
33	5	107	
34	6	85	
35	X	148	
36	Y	266	
37	Z	204	
38	H	1175	
39	o	238	
40	p	111	
41	u	530	
42	w	280	
43	v	266	

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Mol	Chain	Length	Quality of chain
44	W	194	<div><div><div>16%</div><div>44%</div><div>8%</div><div>48%</div></div></div>
45	0	242	<div><div><div>21%</div><div>66%</div><div>31%</div></div></div>
46	9	291	<div><div><div>16%</div><div>22%</div><div>78%</div></div></div>

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 91261 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
1	A	2172	Total	C	N	O	S	0	0
			17092	10927	2976	3131	58		

- Molecule 2 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	429	Total	C	N	O	S	0	0
			3375	2101	610	650	14		

- Molecule 3 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	416	Total	C	N	O	S	0	0
			3171	2001	573	585	12		

- Molecule 4 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	725	Total	C	N	O	S	0	0
			4882	3036	902	930	14		

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	308	Total	C	N	O	S	0	0
			2467	1557	451	445	14		

- Molecule 6 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	138	Total	C	N	O	S	0	0
			1135	719	195	210	11		

- Molecule 7 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	126	Total	C	N	O	S	0	0
			950	605	163	177	5		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	843	Total	C	N	O	S	0	0
			6732	4350	1119	1235	28		

- Molecule 9 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	z	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 10 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	q	92	Total	C	N	O	0	0
			368	184	92	92		

- Molecule 11 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	r	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	x	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	t	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	y	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	s	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 16 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	99	Total	C	N	O	P	0	0
			2043	913	341	690	99		

- Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	175	Total	C	N	O	P	0	0
			3677	1644	634	1225	174		

- Molecule 18 is a protein called 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	75	Total	C	N	O	S	0	0
			568	347	103	117	1		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	d	79	Total	C	N	O	0	0
			316	158	79	79		
19	S	82	Total	C	N	O	0	0
			404	240	82	82		
19	l	76	Total	C	N	O	0	0
			375	223	76	76		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	a	73	Total	C	N	O	0	0
			292	146	73	73		

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	P	70	Total	C	N	O	0	0
			346	206	70	70		
20	h	76	Total	C	N	O	0	0
			376	224	76	76		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	b	77	Total	C	N	O	0	0
			308	154	77	77		
21	Q	99	Total	C	N	O	0	0
			491	293	99	99		
21	m	82	Total	C	N	O	0	0
			407	243	82	82		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	c	90	Total	C	N	O	0	0
			360	180	90	90		
22	R	92	Total	C	N	O	0	0
			457	273	92	92		
22	n	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	e	72	Total	C	N	O	0	0
			288	144	72	72		
23	T	77	Total	C	N	O	0	0
			379	225	77	77		
23	i	75	Total	C	N	O	0	0
			369	219	75	75		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	f	70	Total	C	N	O	0	0
			280	140	70	70		
24	U	73	Total	C	N	O	0	0
			359	213	73	73		

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Mol	Chain	Residues	Atoms				AltConf	Trace
24	j	70	Total	C	N	O	0	0
			344	204	70	70		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	g	70	Total	C	N	O	0	0
			280	140	70	70		
25	V	75	Total	C	N	O	0	0
			369	219	75	75		
25	k	69	Total	C	N	O	0	0
			340	202	69	69		

- Molecule 26 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	110	Total	C	N	O	P	0	0
			2334	1044	399	781	110		

- Molecule 27 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	D	1699	Total	C	N	O	1	0
			8422	5024	1699	1699		

- Molecule 28 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	60	Total	C	N	O	P	0	0
			1264	571	217	416	60		

- Molecule 29 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	1	816	Total	C	N	O	0	0
			4044	2412	816	816		

- Molecule 30 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	2	211	Total	C	N	O	0	0
			1042	620	211	211		

- Molecule 31 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	3	1180	Total	C	N	O	0	0
			5852	3492	1180	1180		

- Molecule 32 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4	174	Total	C	N	O	0	0
			862	514	174	174		

- Molecule 33 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	5	103	Total	C	N	O	0	0
			507	301	103	103		

- Molecule 34 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	6	84	Total	C	N	O	0	0
			415	247	84	84		

- Molecule 35 is a protein called U2 snRNP component IST3.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	X	128	Total	C	N	O	0	0
			631	375	128	128		

- Molecule 36 is a protein called Pre-mRNA-splicing factor CWC26.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Y	89	Total	C	N	O	0	0
			439	261	89	89		

- Molecule 37 is a protein called Pre-mRNA leakage protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	Z	22	Total	C	N	O	0	0
			109	65	22	22		

- Molecule 38 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	H	150	Total	C	N	O	P	0	0
			3169	1416	531	1072	150		

- Molecule 39 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	o	135	Total	C	N	O	0	0
			673	403	135	135		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	73	Total	C	N	O	0	0
			361	215	73	73		

- Molecule 41 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	u	462	Total	C	N	O	0	0
			2298	1374	462	462		

- Molecule 42 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	w	127	Total	C	N	O	0	0
			633	379	127	127		

- Molecule 43 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	v	174	Total	C	N	O	0	0
			859	511	174	174		

- Molecule 44 is a protein called 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	W	100	Total	C	N	O	0	0
			497	297	100	100		

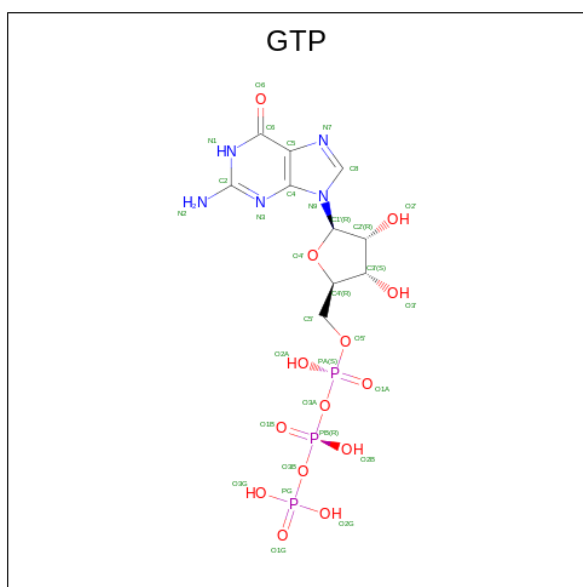
- Molecule 45 is a protein called Pre-mRNA-splicing factor 38.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	0	167	Total	C	N	O	0	0
			830	496	167	167		

- Molecule 46 is a protein called Pre-mRNA-splicing factor SPP381.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	9	64	Total	C	N	O	0	0
			320	192	64	64		

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



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

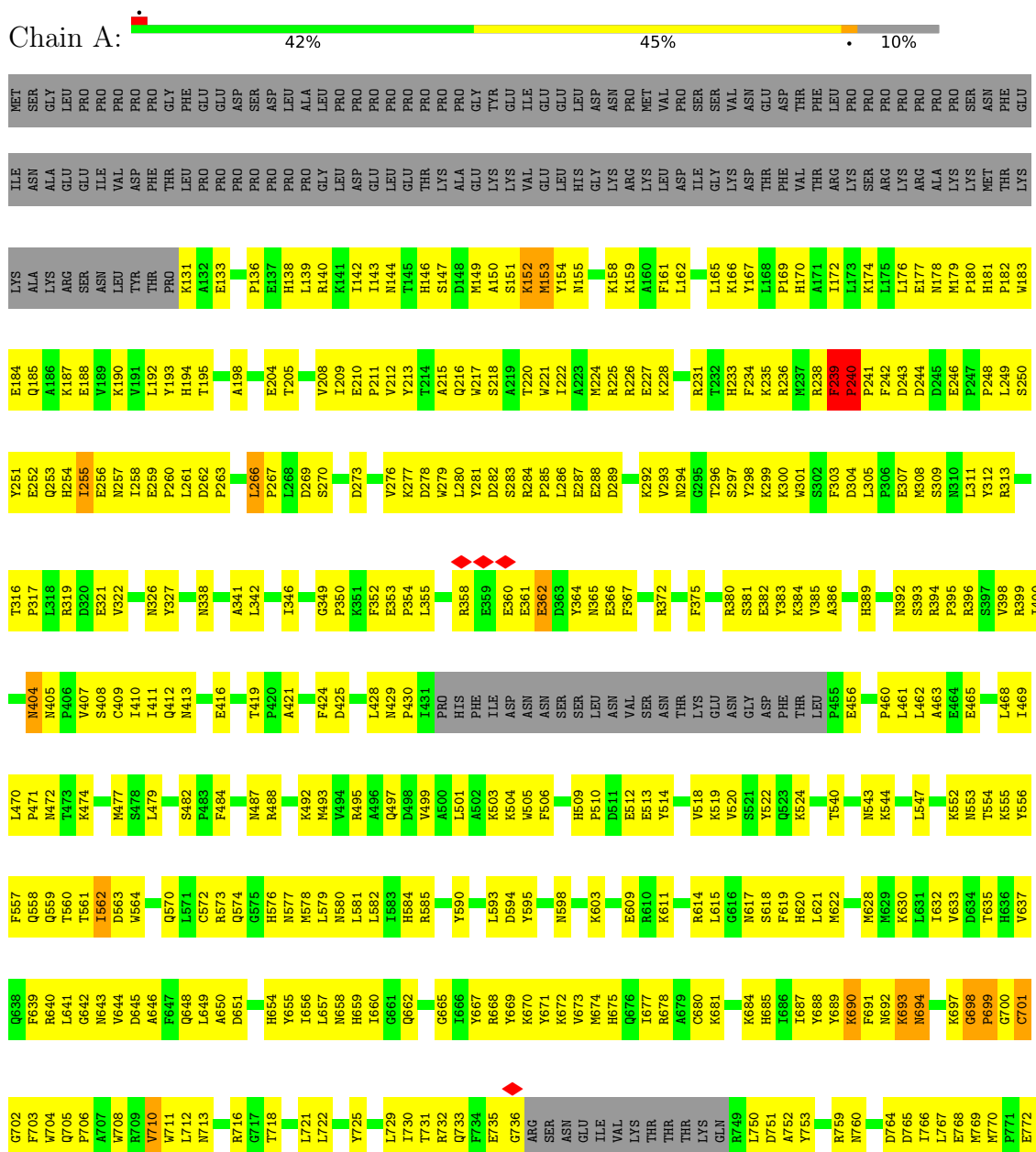
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

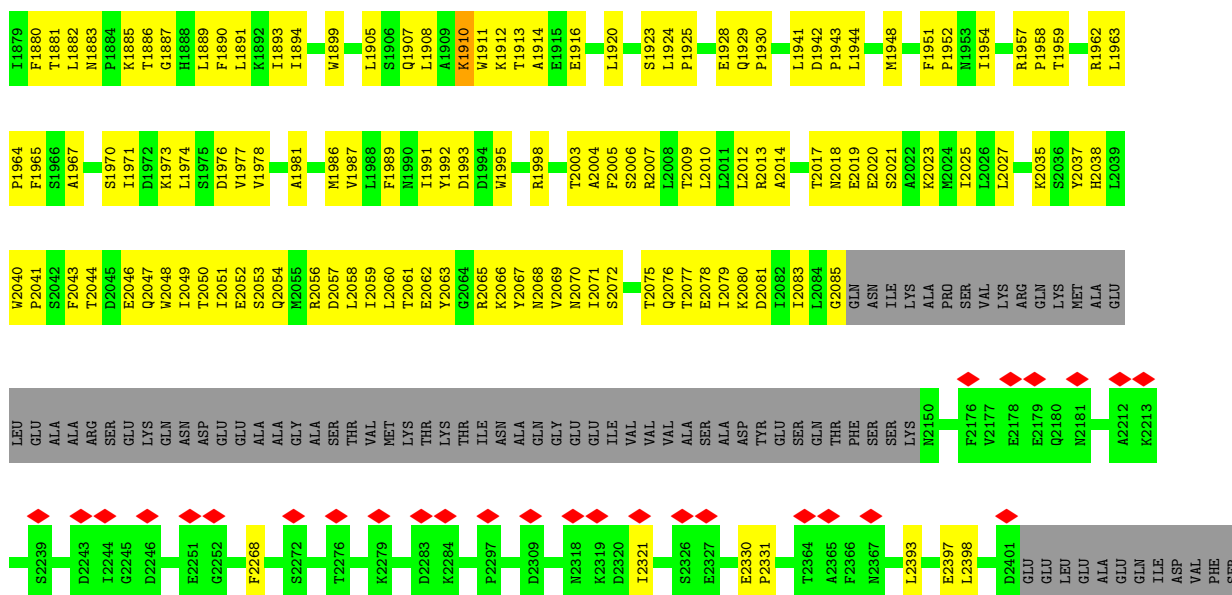
3 Residue-property plots

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

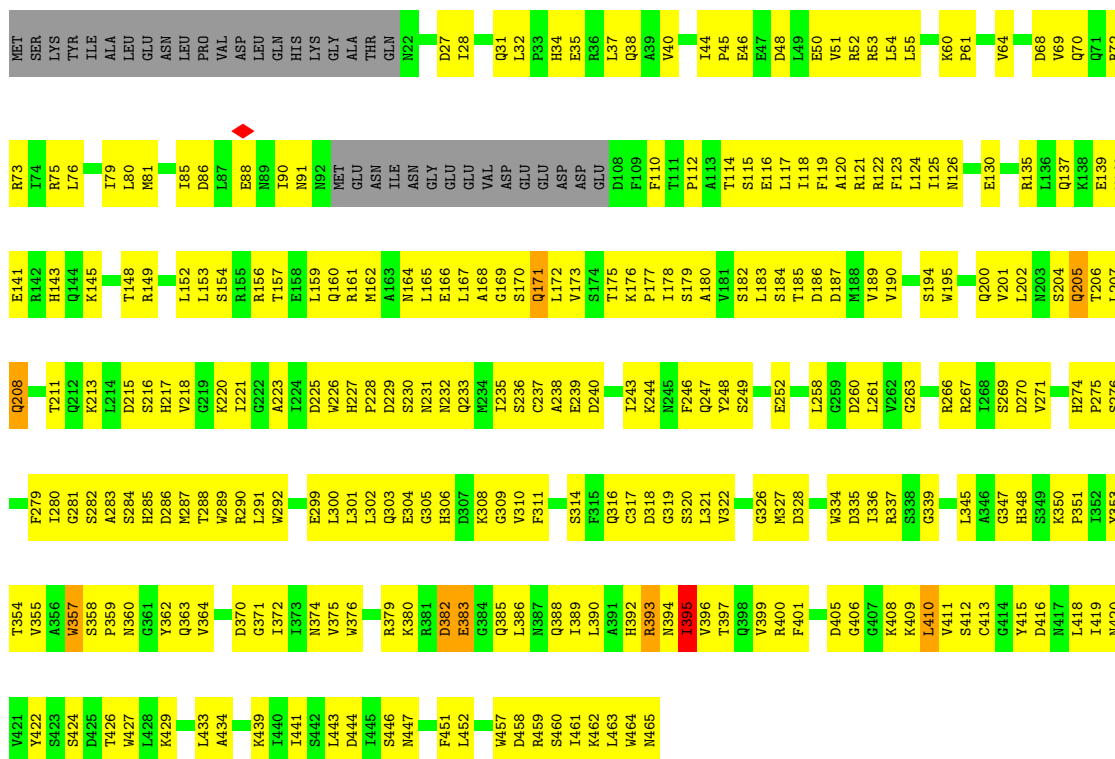






• Molecule 2: U4/U6 small nuclear ribonucleoprotein PRP4

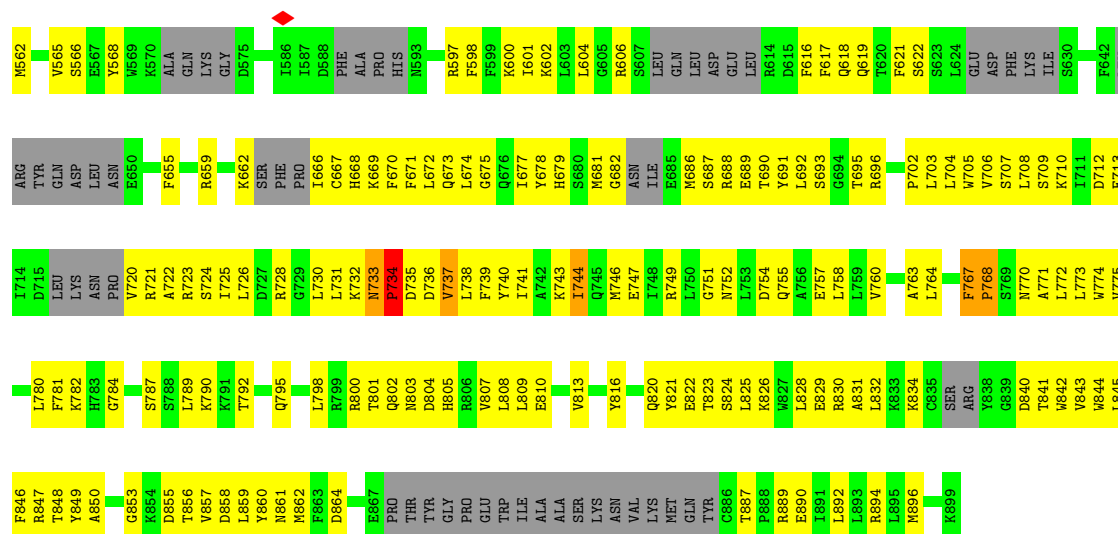
Chain K: 35% 55% 8%



• Molecule 3: Pre-mRNA-processing factor 31

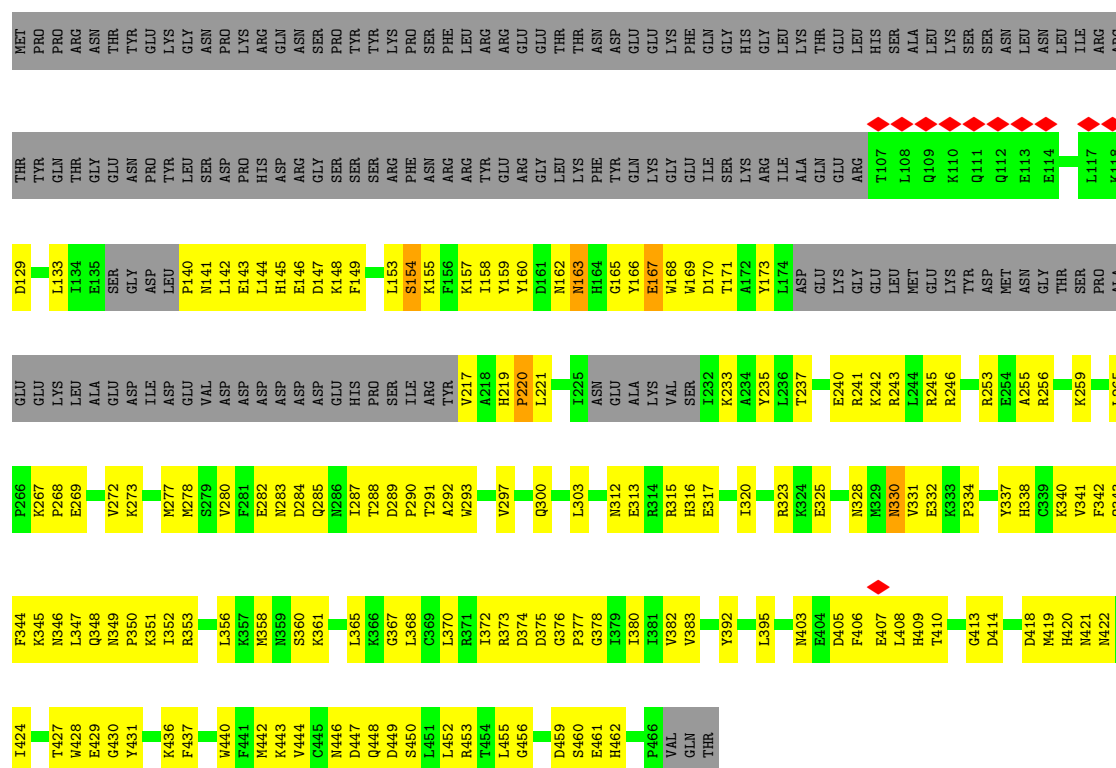
Chain L: 41% 43% 16%





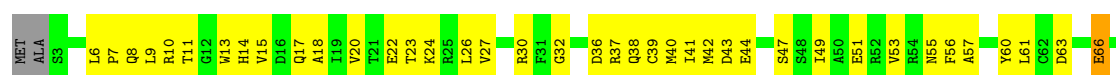
- Molecule 5: U4/U6 small nuclear ribonucleoprotein PRP3

Chain J: 32% 32% 34%



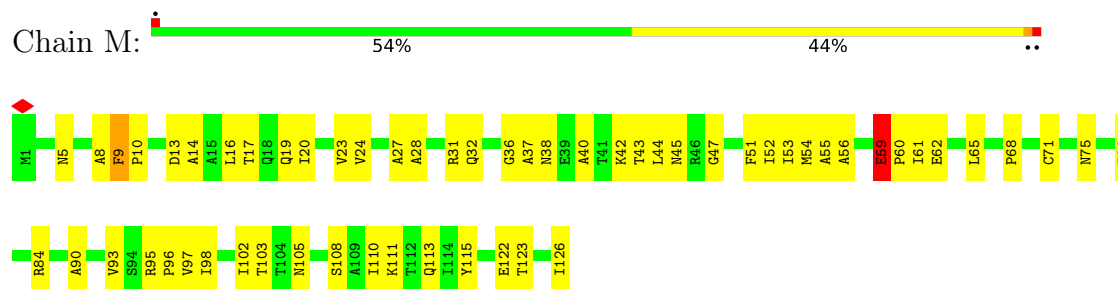
- Molecule 6: Spliceosomal protein DIB1

Chain E: 38% 58%



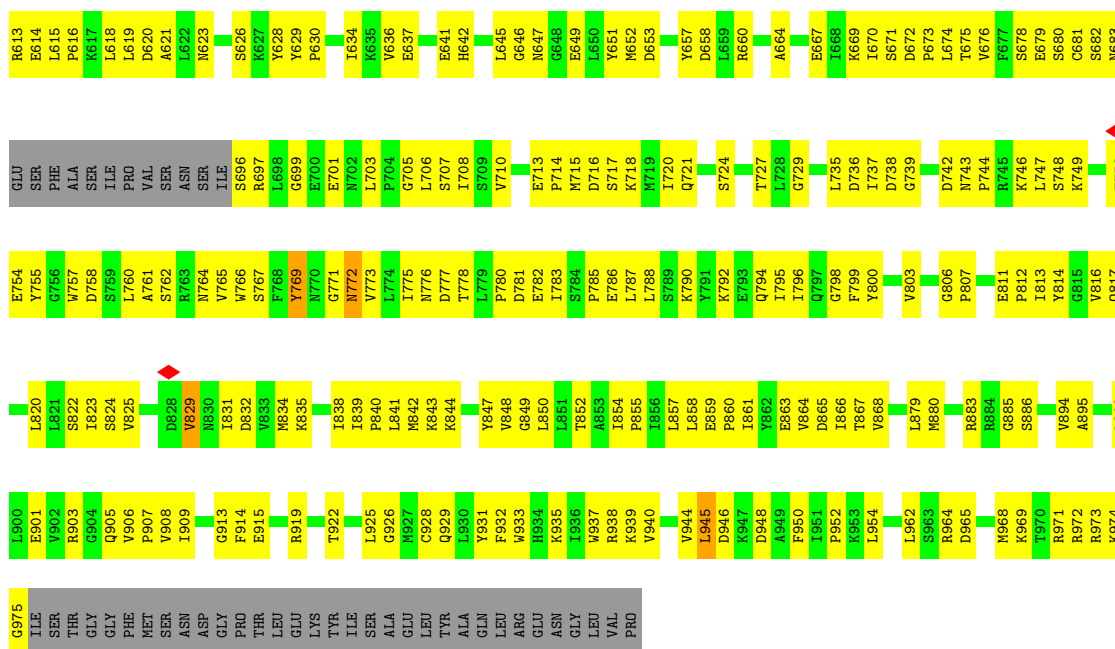


• Molecule 7: 13 kDa ribonucleoprotein-associated protein



• Molecule 8: Pre-mRNA-splicing factor SNU114

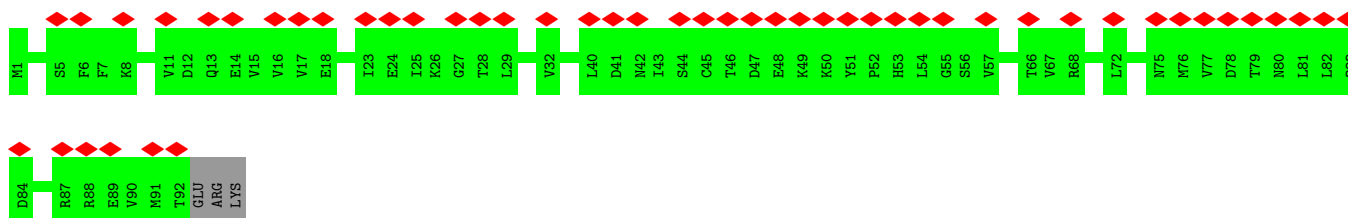




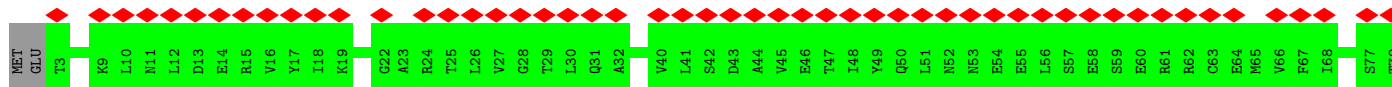
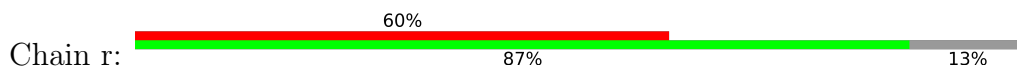
• Molecule 9: U6 snRNA-associated Sm-like protein LSm8

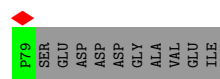


• Molecule 10: U6 snRNA-associated Sm-like protein LSm2

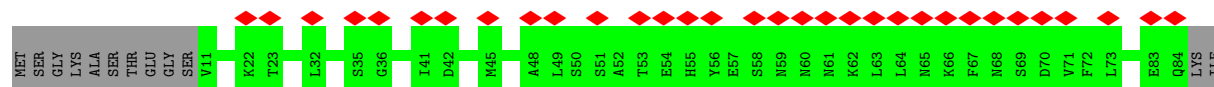
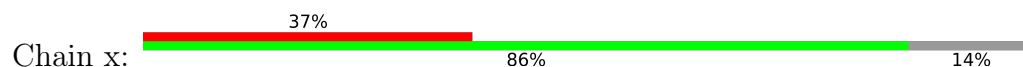


• Molecule 11: U6 snRNA-associated Sm-like protein LSm3

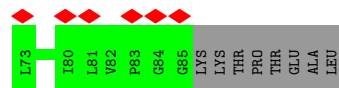
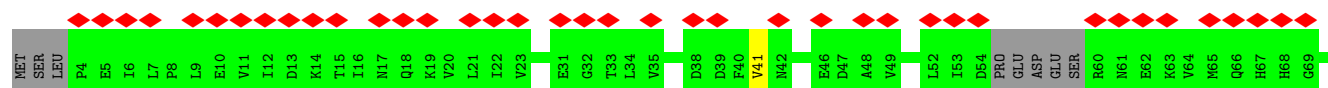
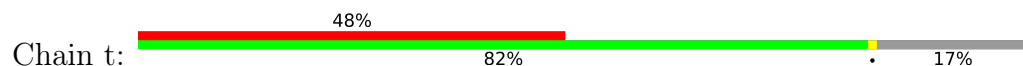




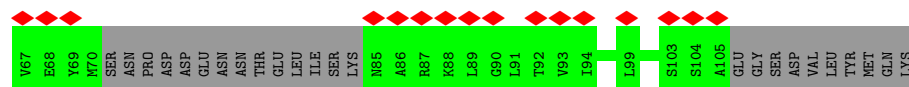
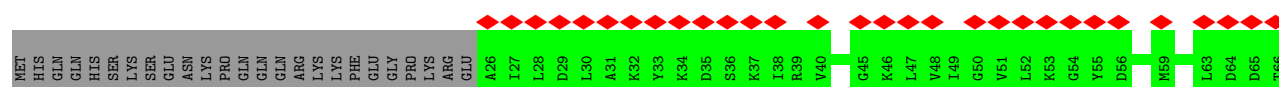
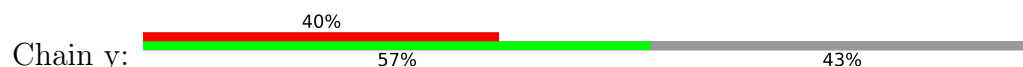
- Molecule 12: U6 snRNA-associated Sm-like protein LSm6



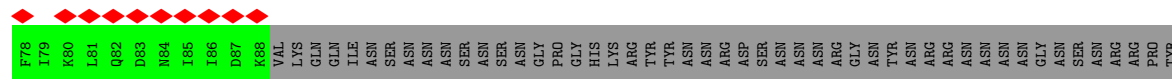
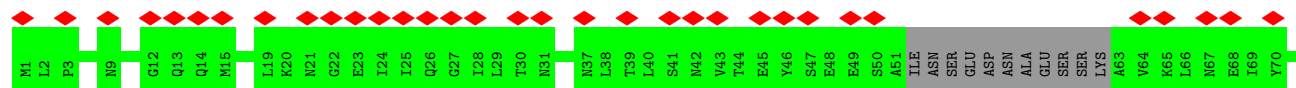
- Molecule 13: U6 snRNA-associated Sm-like protein LSm5



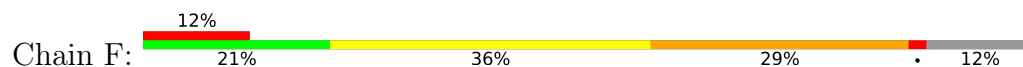
- Molecule 14: U6 snRNA-associated Sm-like protein LSm7

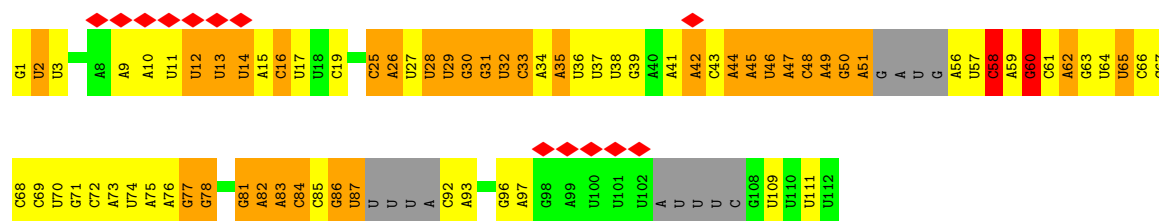


- Molecule 15: U6 snRNA-associated Sm-like protein LSm4

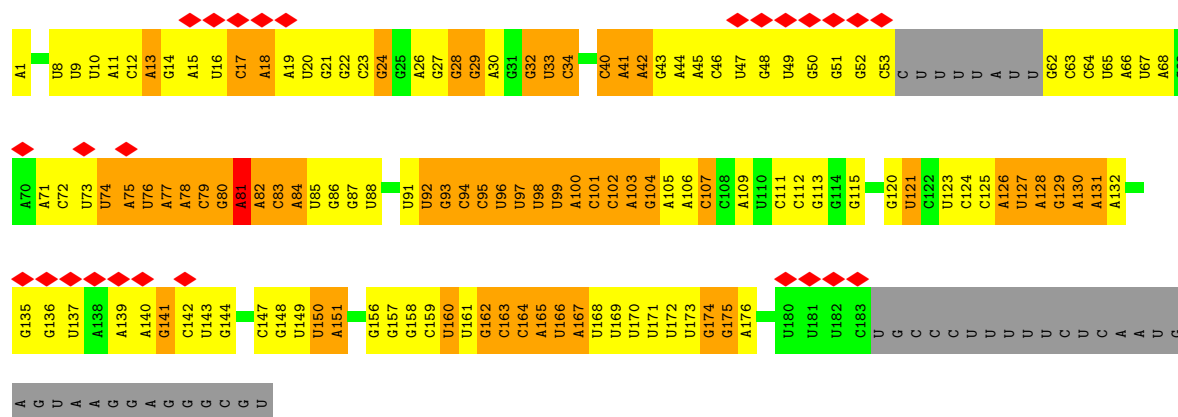
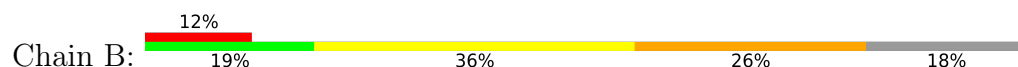


- Molecule 16: U6 snRNA

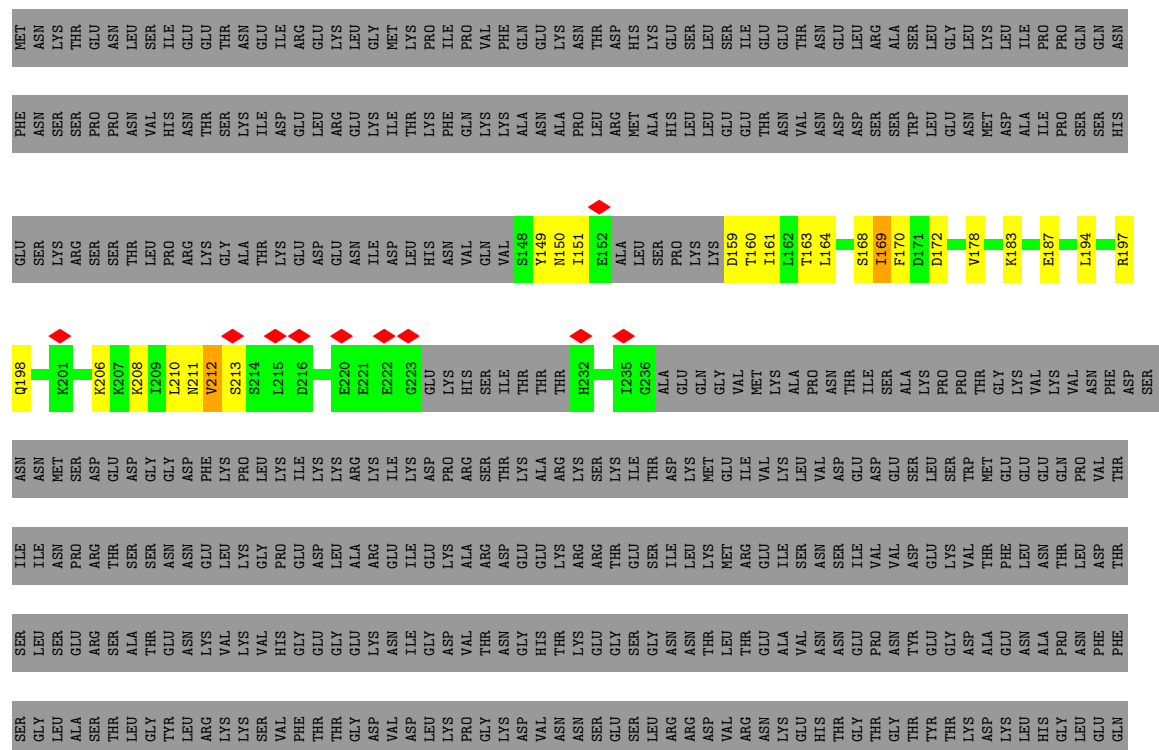




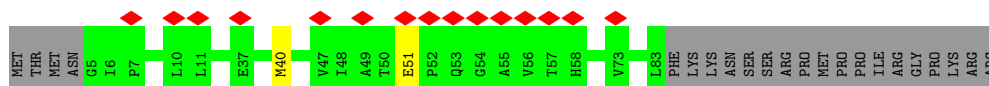
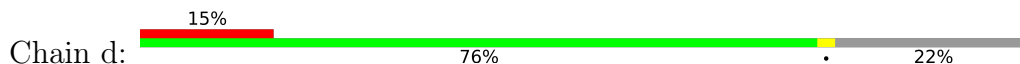
• Molecule 17: U5 snRNA



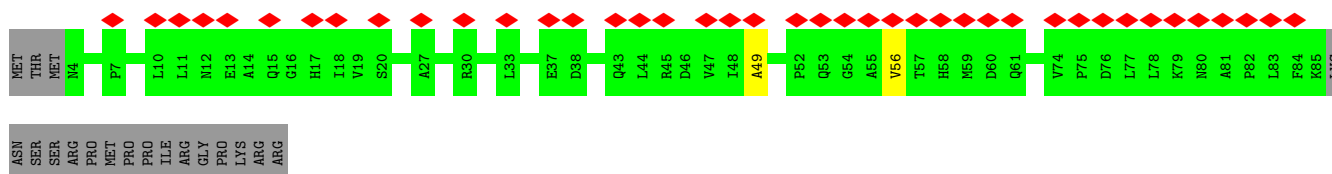
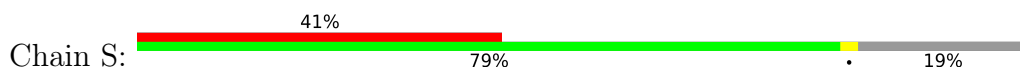
• Molecule 18: 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component



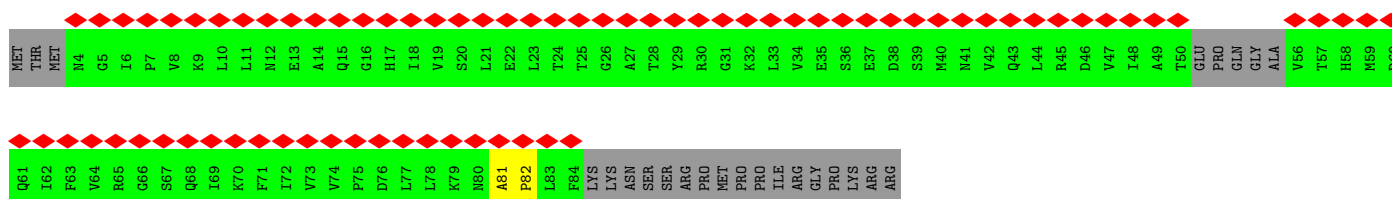
- Molecule 19: Small nuclear ribonucleoprotein Sm D3



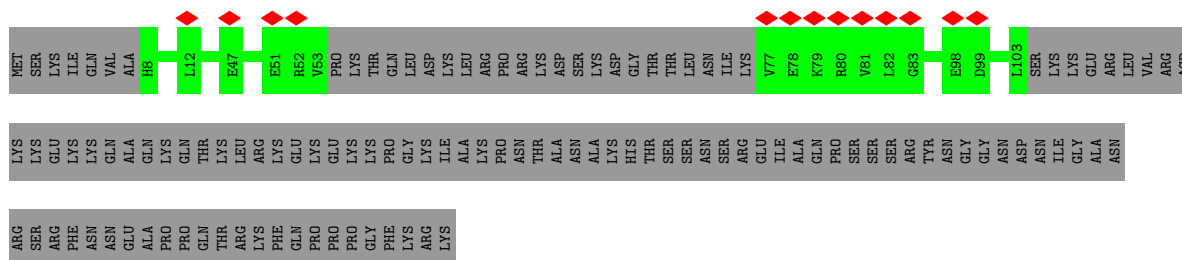
- Molecule 19: Small nuclear ribonucleoprotein Sm D3



- Molecule 19: Small nuclear ribonucleoprotein Sm D3

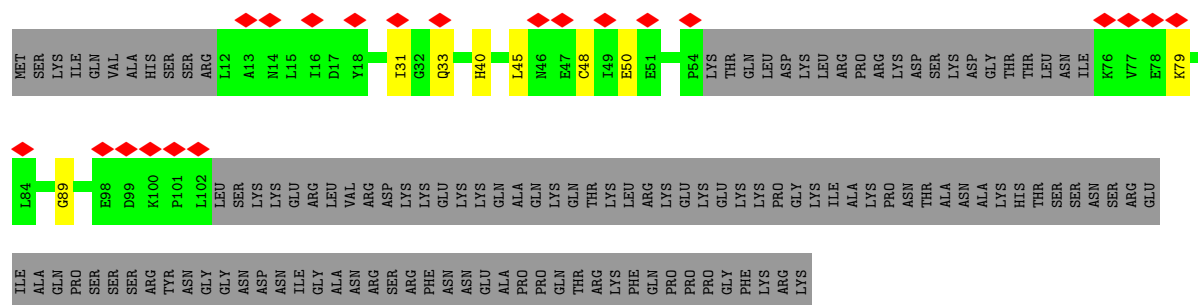


- Molecule 20: Small nuclear ribonucleoprotein-associated protein B

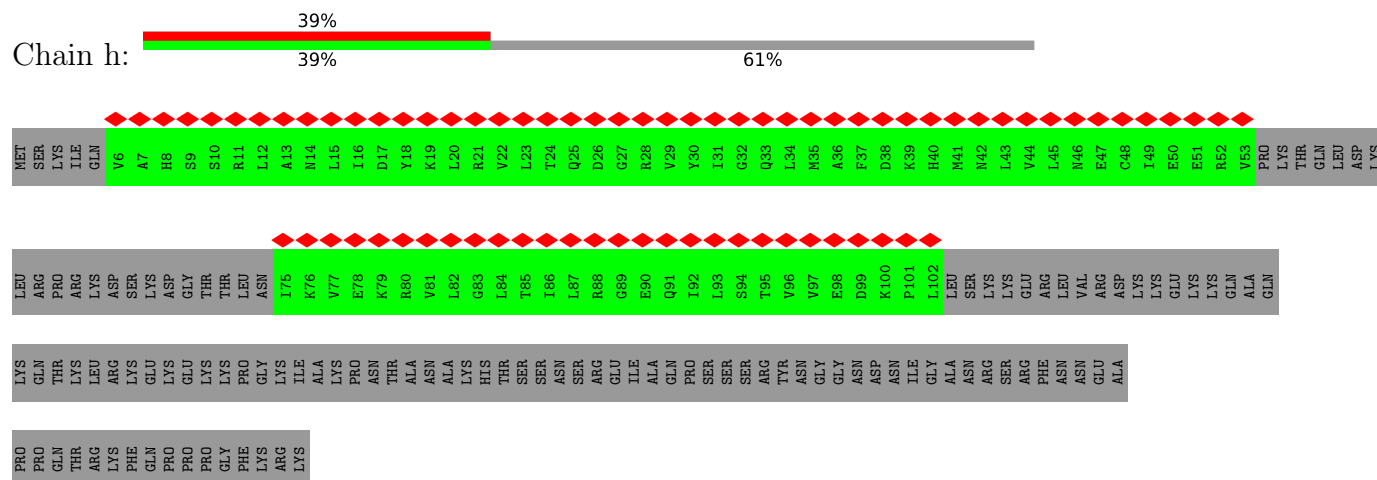


- Molecule 20: Small nuclear ribonucleoprotein-associated protein B

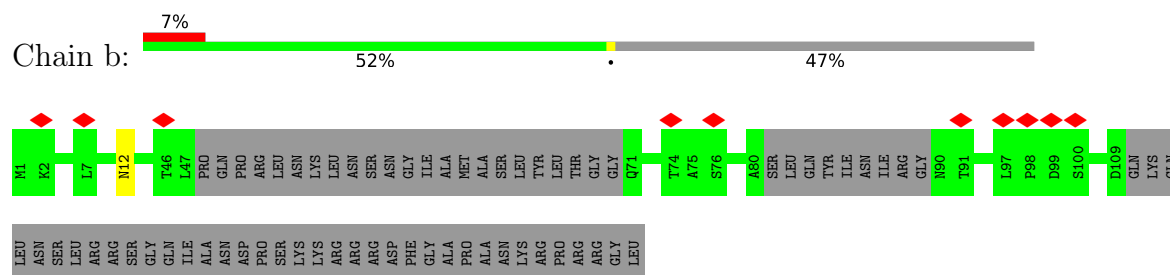




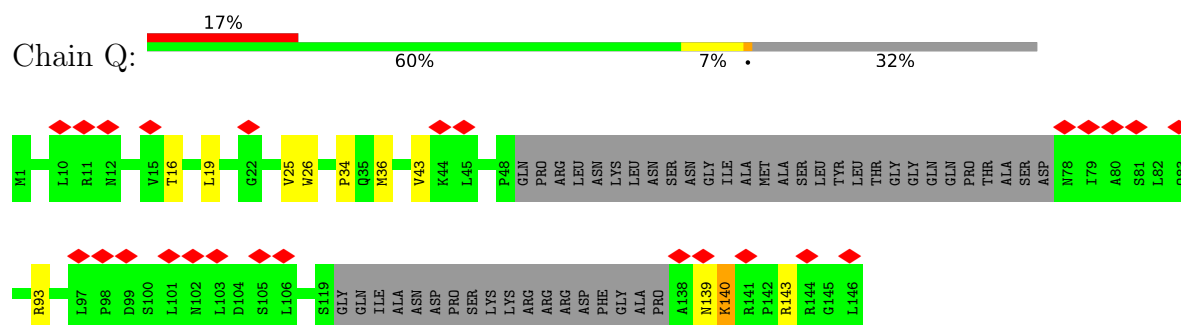
- Molecule 20: Small nuclear ribonucleoprotein-associated protein B



- Molecule 21: Small nuclear ribonucleoprotein Sm D1

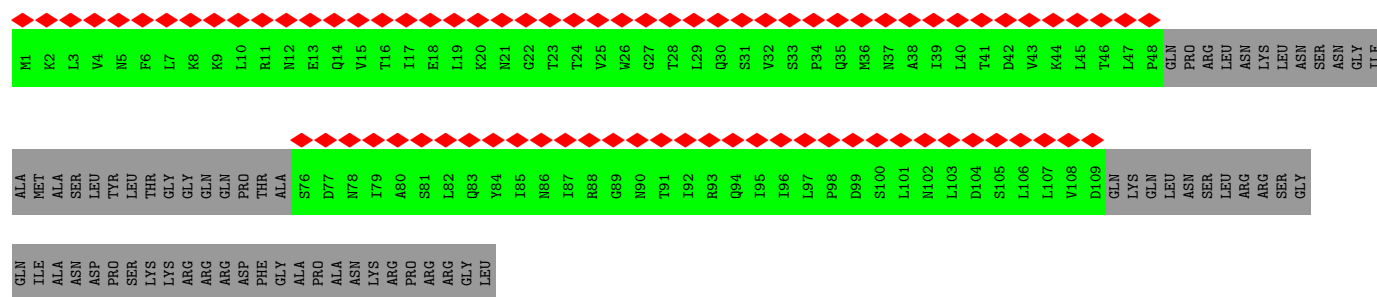


- Molecule 21: Small nuclear ribonucleoprotein Sm D1

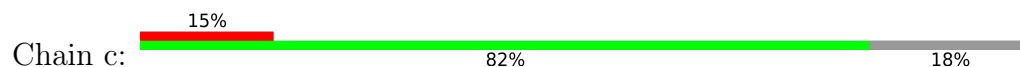


- Molecule 21: Small nuclear ribonucleoprotein Sm D1

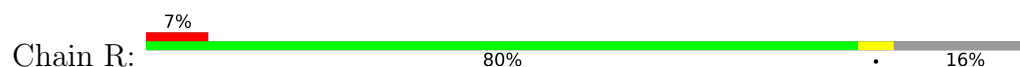




• Molecule 22: Small nuclear ribonucleoprotein Sm D2



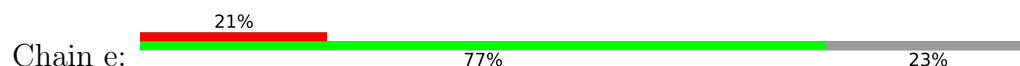
• Molecule 22: Small nuclear ribonucleoprotein Sm D2



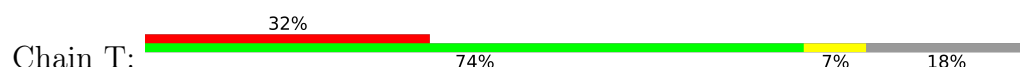
• Molecule 22: Small nuclear ribonucleoprotein Sm D2



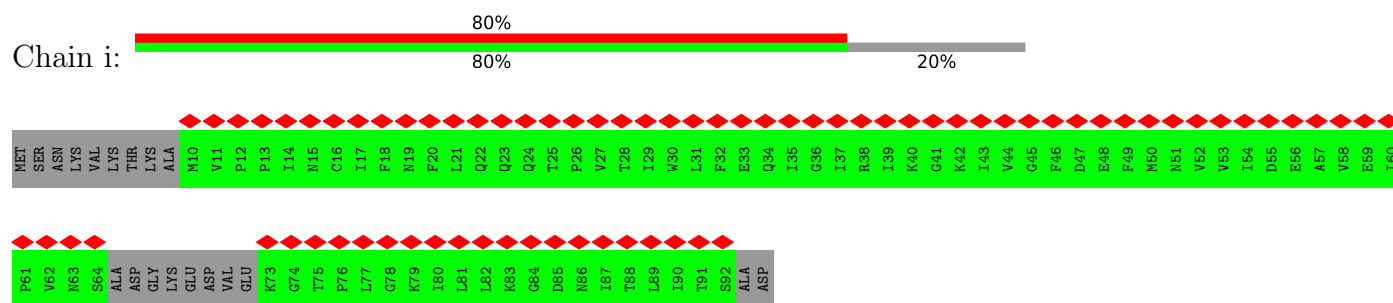
• Molecule 23: Small nuclear ribonucleoprotein E



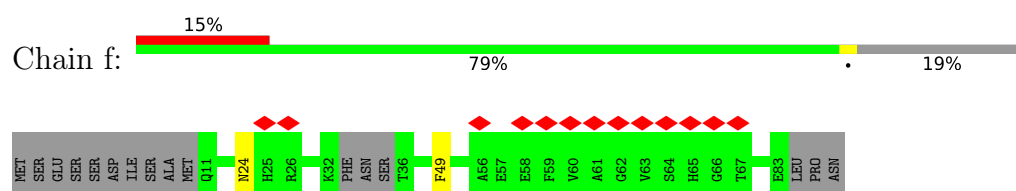
• Molecule 23: Small nuclear ribonucleoprotein E



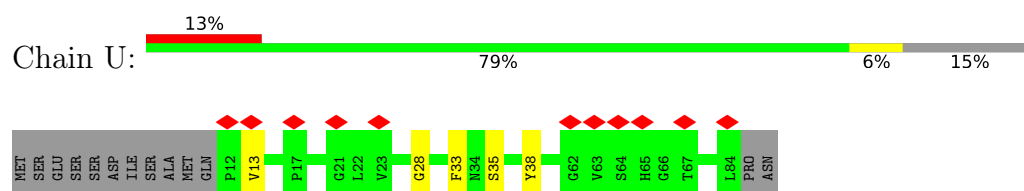
- Molecule 23: Small nuclear ribonucleoprotein E



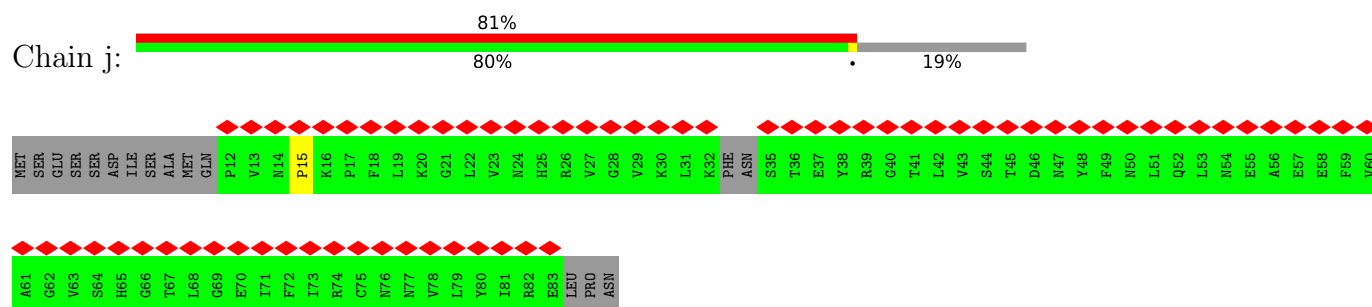
- Molecule 24: Small nuclear ribonucleoprotein F



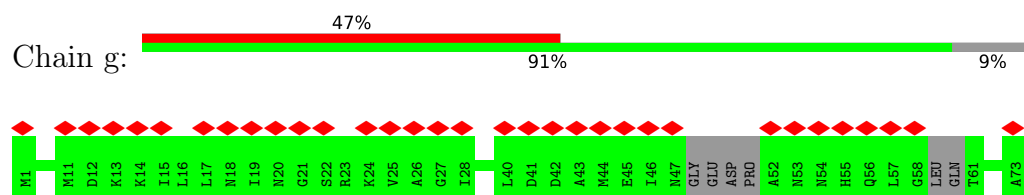
- Molecule 24: Small nuclear ribonucleoprotein F



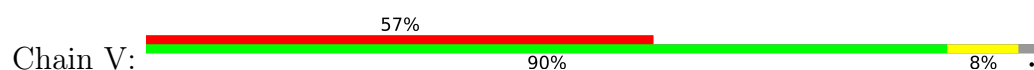
- Molecule 24: Small nuclear ribonucleoprotein F

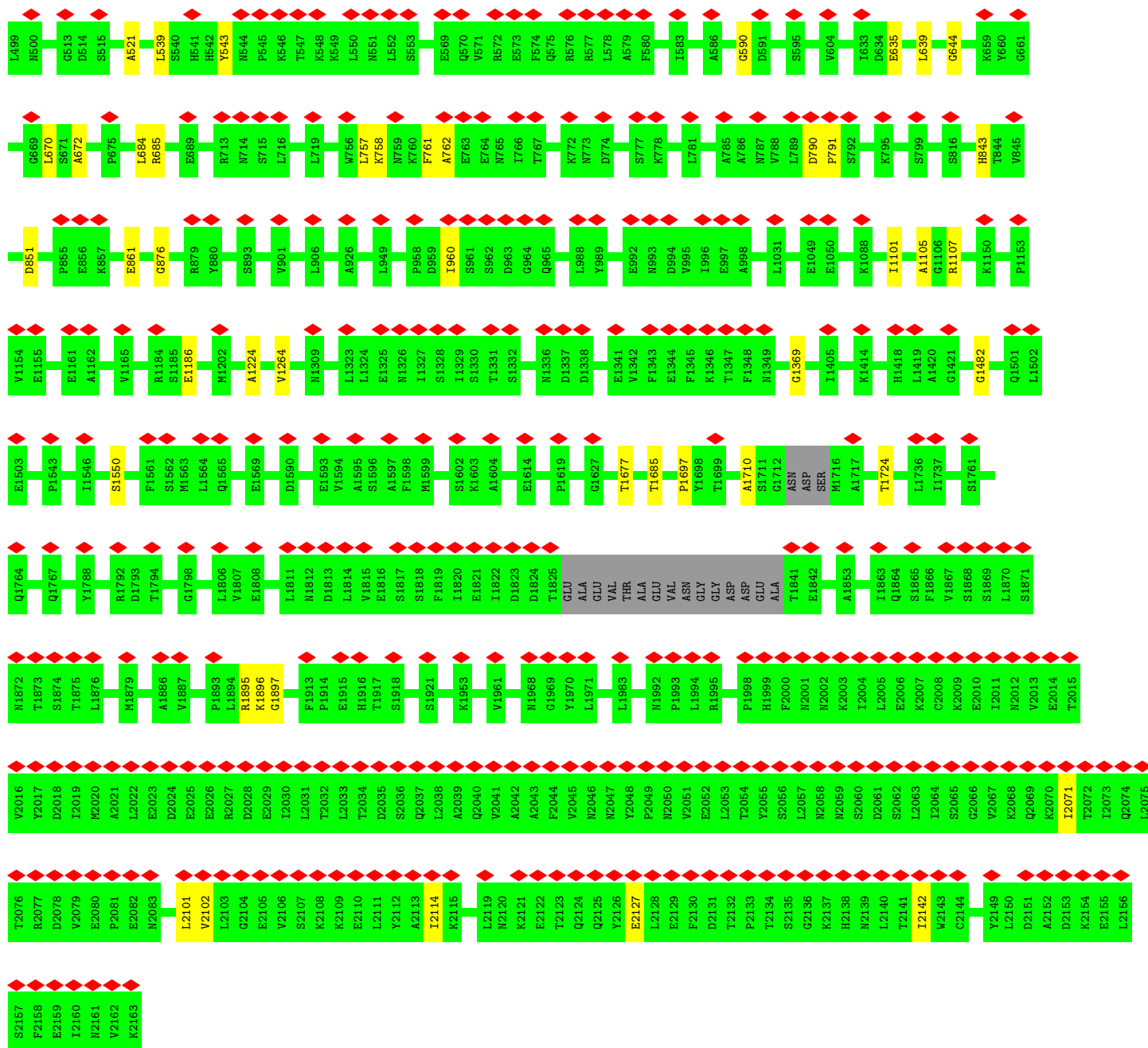


- Molecule 25: Small nuclear ribonucleoprotein G

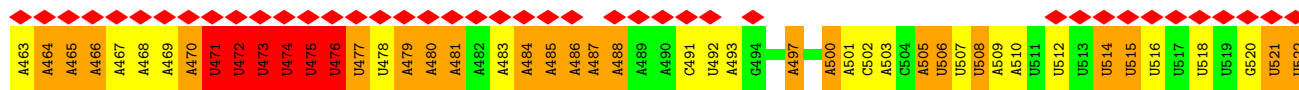
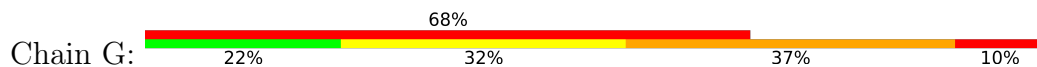


- Molecule 25: Small nuclear ribonucleoprotein G

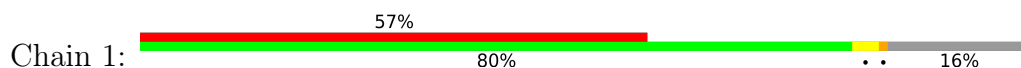




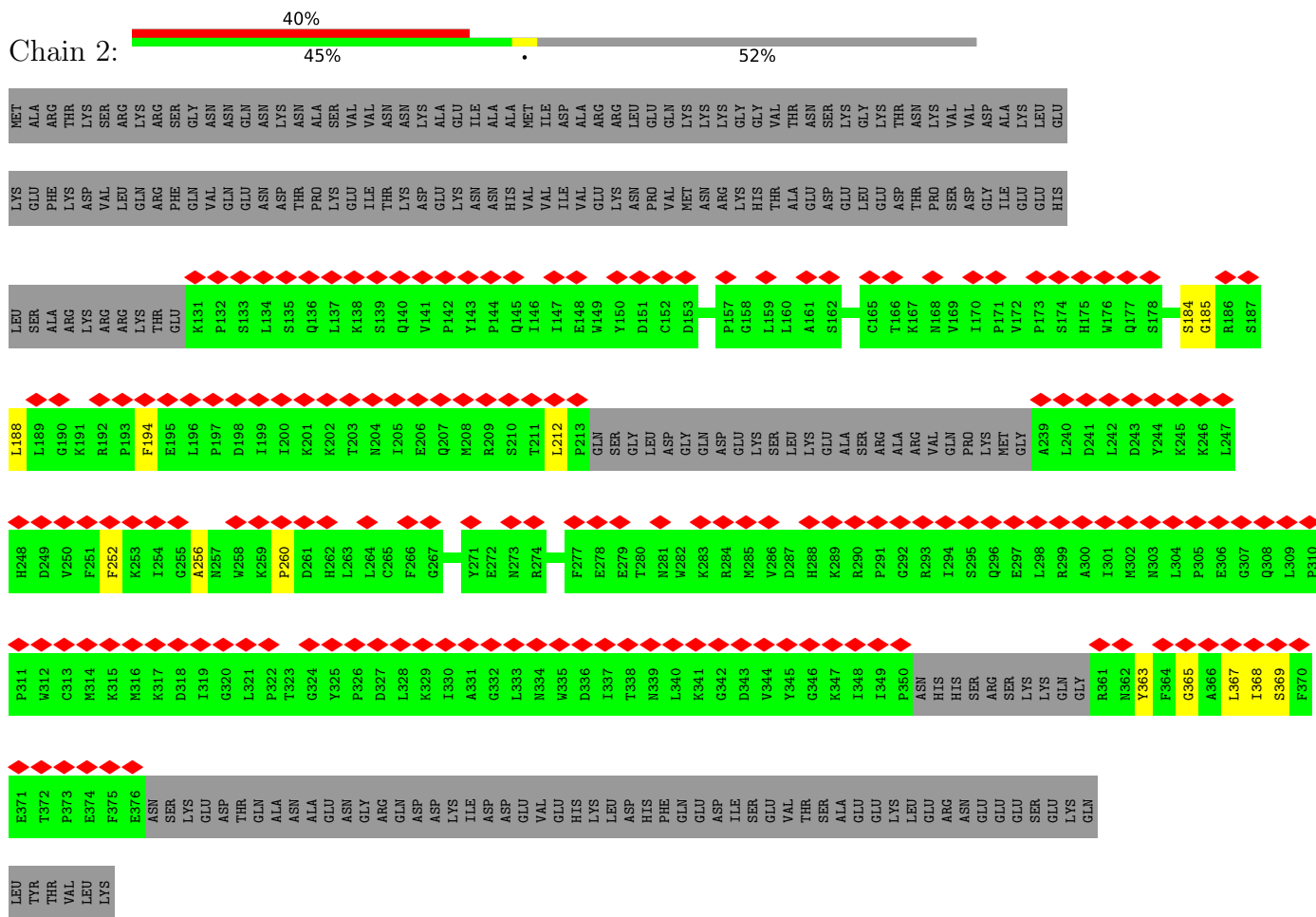
- Molecule 28: Pre-mRNA



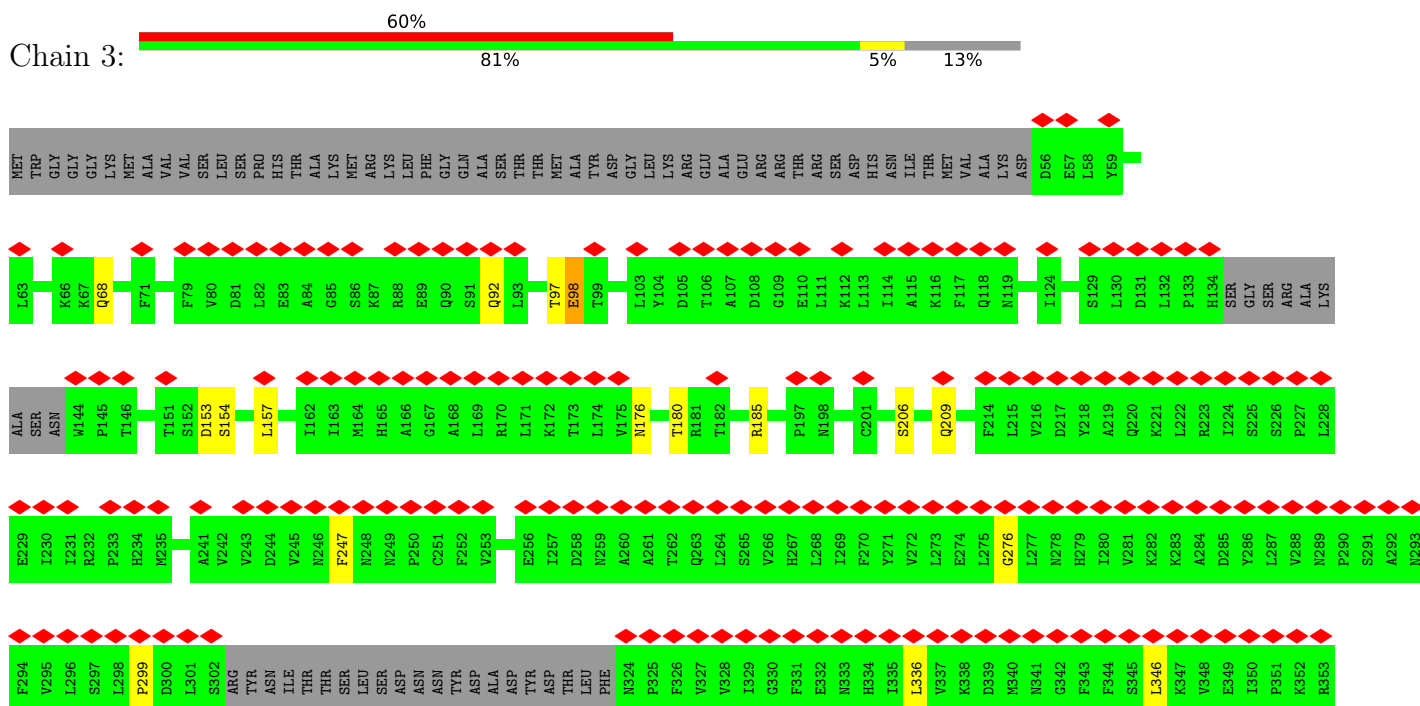
- Molecule 29: U2 snRNP component HSH155



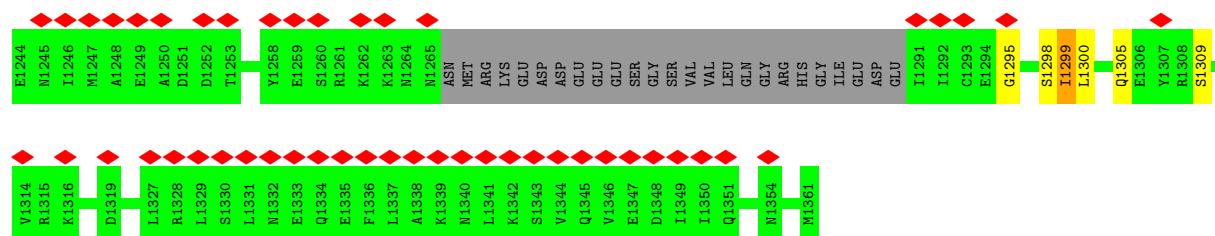
- Molecule 30: Cold sensitive U2 snRNA suppressor 1



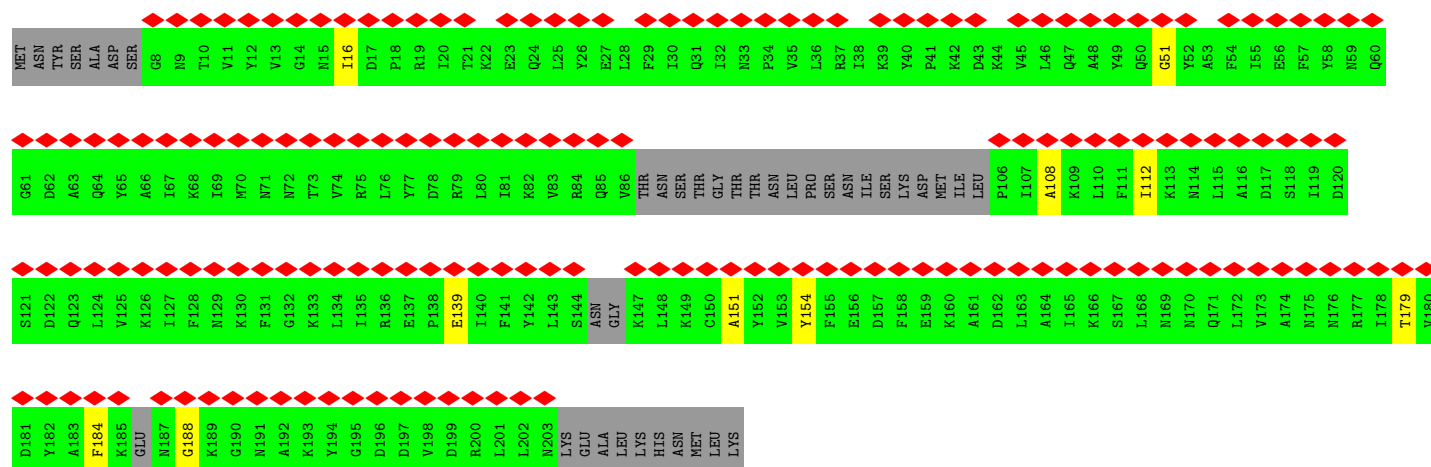
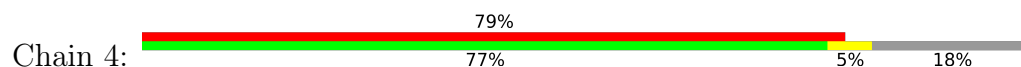
- Molecule 31: Pre-mRNA-splicing factor RSE1



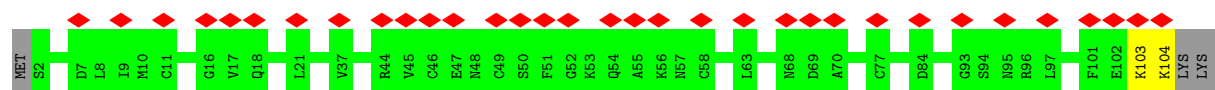




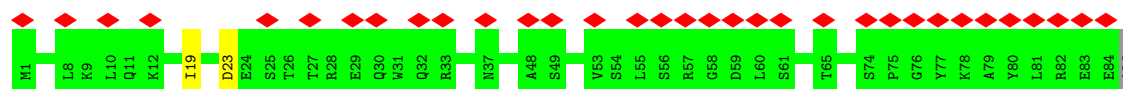
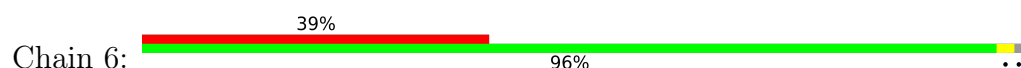
• Molecule 32: Protein HSH49



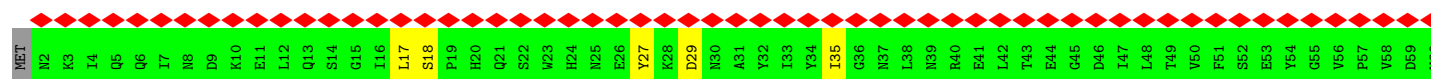
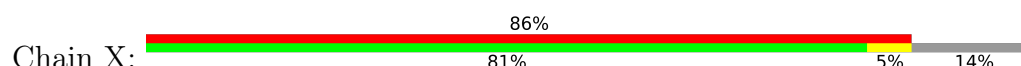
• Molecule 33: Pre-mRNA-splicing factor RDS3

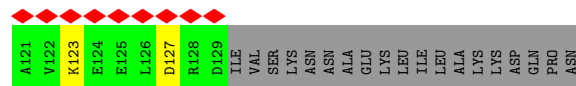
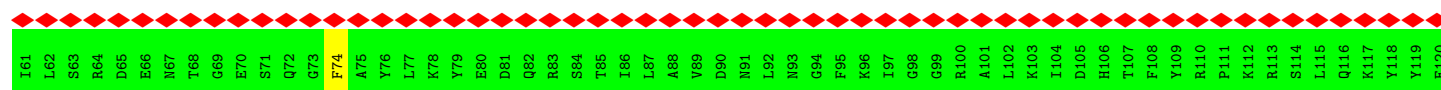


• Molecule 34: RDS3 complex subunit 10

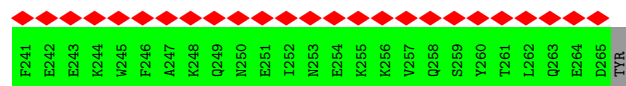
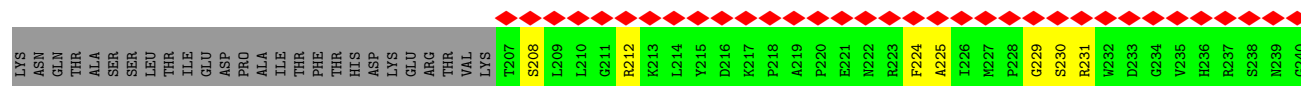
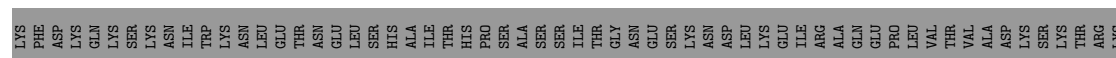


• Molecule 35: U2 snRNP component IST3

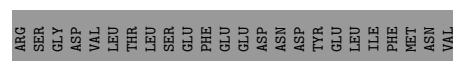
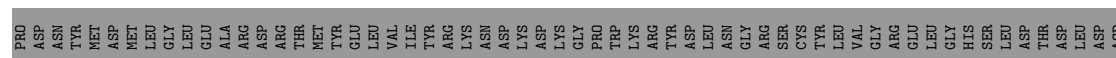
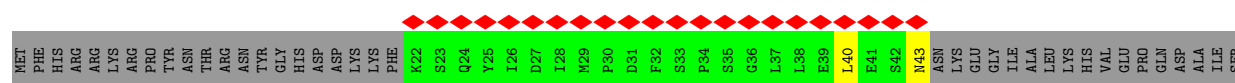




• Molecule 36: Pre-mRNA-splicing factor CWC26

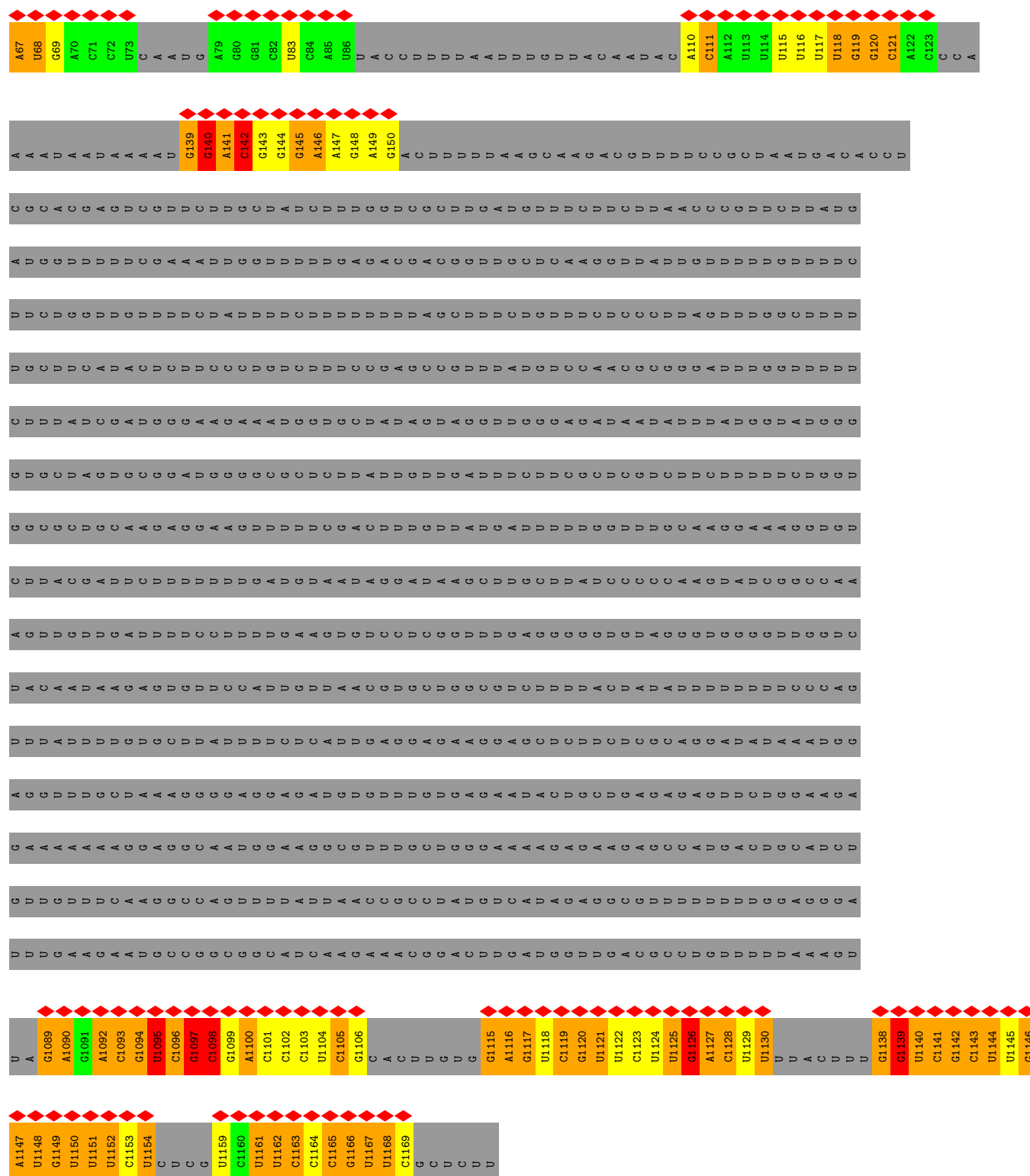


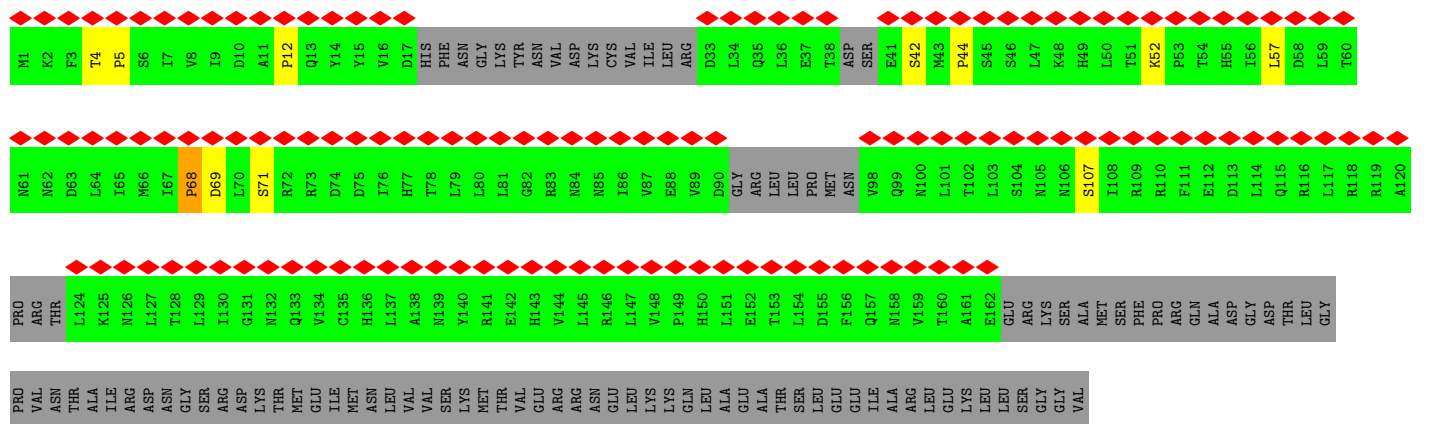
• Molecule 37: Pre-mRNA leakage protein 1



• Molecule 38: U2 snRNA



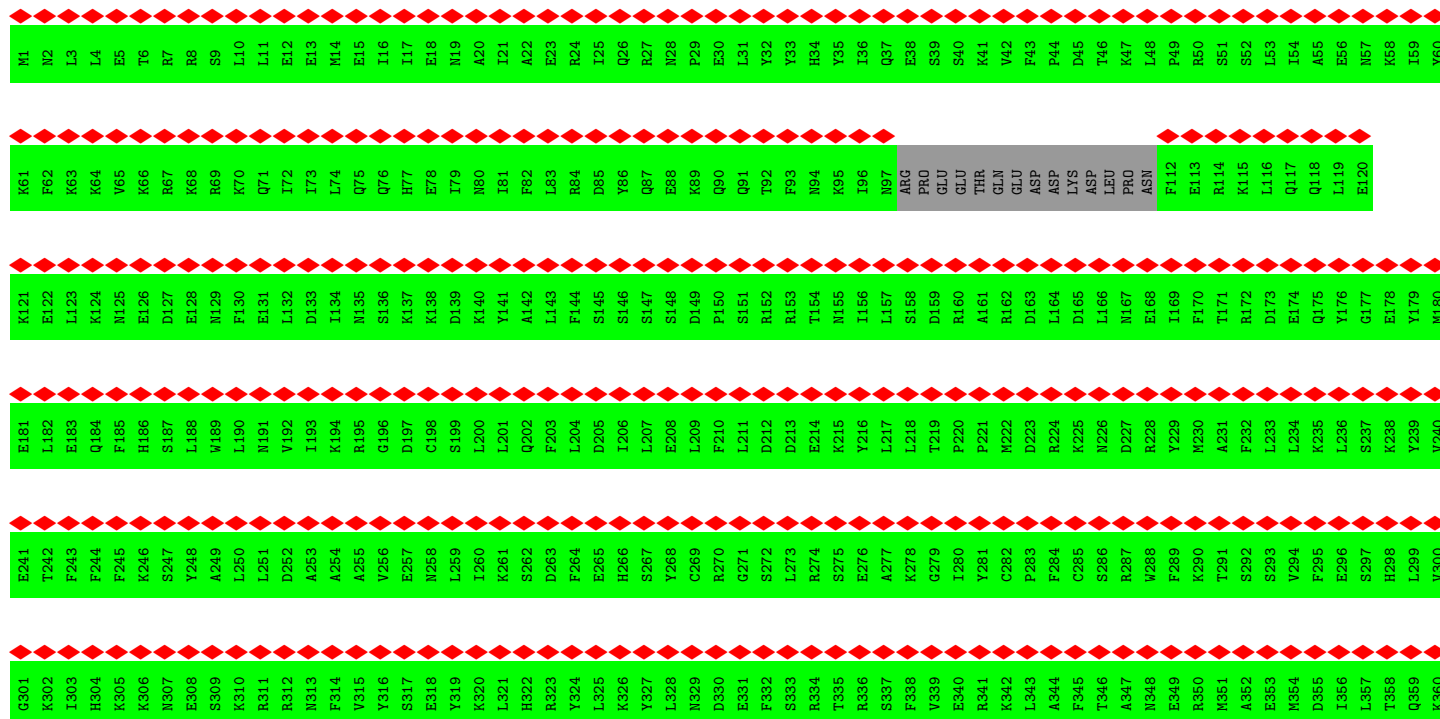
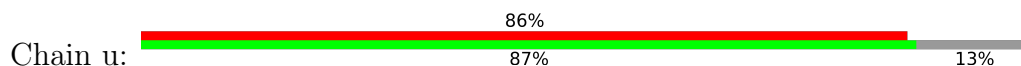




• Molecule 40: U2 small nuclear ribonucleoprotein B



• Molecule 41: Pre-mRNA-splicing factor PRP9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	342588	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.249	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.78	12/17497 (0.1%)	0.73	18/23758 (0.1%)
2	K	0.60	0/3431	0.73	3/4631 (0.1%)
3	L	0.65	0/3219	0.71	1/4332 (0.0%)
4	N	0.44	0/4922	0.56	0/6683
5	J	0.50	0/2513	0.59	0/3374
6	E	0.72	0/1156	0.69	0/1557
7	M	0.80	0/963	0.78	0/1310
8	C	0.55	1/6874 (0.0%)	0.66	1/9305 (0.0%)
9	z	0.53	0/259	0.64	0/322
10	q	0.40	0/367	0.57	0/457
11	r	0.43	0/307	0.58	0/382
12	x	0.40	0/295	0.56	0/367
13	t	0.38	0/306	0.58	0/379
14	y	0.37	0/262	0.60	0/324
15	s	0.36	0/306	0.59	0/379
16	F	0.77	1/2277 (0.0%)	0.89	3/3534 (0.1%)
17	B	0.39	0/4106	0.78	2/6391 (0.0%)
18	O	0.58	0/567	0.65	0/757
19	S	0.27	0/403	0.53	0/559
19	d	0.46	0/315	0.52	0/392
19	l	0.42	0/373	0.70	0/516
20	P	0.28	0/344	0.54	0/476
20	a	0.42	0/290	0.47	0/359
20	h	0.36	0/374	0.57	0/518
21	Q	0.29	0/488	0.59	0/676
21	b	0.39	0/305	0.50	0/376
21	m	0.43	0/405	0.59	0/562
22	R	0.28	0/456	0.53	0/635
22	c	0.38	0/358	0.49	0/444
22	n	0.45	0/322	0.71	2/448 (0.4%)
23	T	0.28	0/377	0.55	0/521
23	e	0.40	0/285	0.48	0/351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	i	0.43	0/367	0.61	0/507
24	U	0.29	0/358	0.58	0/496
24	f	0.42	0/278	0.46	0/344
24	j	0.42	0/342	0.63	0/472
25	V	0.28	0/368	0.61	0/510
25	g	0.38	0/277	0.49	0/341
25	k	0.38	0/338	0.61	0/467
26	I	1.17	9/2604 (0.3%)	1.25	19/4046 (0.5%)
27	D	0.29	0/8422	0.56	0/11741
28	G	0.61	7/1414 (0.5%)	0.83	0/2195
29	1	0.77	1/4043 (0.0%)	0.78	2/5637 (0.0%)
30	2	0.75	0/1039	0.78	0/1442
31	3	0.92	1/5844 (0.0%)	0.88	3/8140 (0.0%)
32	4	0.49	0/858	0.58	0/1190
33	5	0.91	0/506	0.79	0/702
34	6	0.97	0/414	0.84	0/575
35	X	0.47	0/630	0.60	0/875
36	Y	0.50	0/437	0.66	0/605
37	Z	0.47	0/108	0.55	0/149
38	H	1.06	30/3526 (0.9%)	1.42	76/5468 (1.4%)
39	o	0.76	1/668 (0.1%)	1.60	9/926 (1.0%)
40	p	0.63	0/359	1.32	1/497 (0.2%)
41	u	0.31	0/2294	0.45	0/3198
42	w	0.21	0/631	0.37	0/879
43	v	0.50	0/856	0.57	0/1187
44	W	0.24	0/494	0.46	0/685
45	0	0.24	0/825	0.44	0/1144
46	9	0.23	0/318	0.28	0/442
All	All	0.66	63/93340 (0.1%)	0.77	140/129935 (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	10
2	K	0	6
3	L	0	3
4	N	0	4
5	J	0	3
7	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	C	0	6
19	l	0	2
22	n	0	2
25	V	0	1
25	k	0	1
27	D	0	4
29	1	0	2
30	2	0	3
31	3	0	15
41	u	0	1
45	0	0	2
All	All	0	67

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	H	1161	U	O3'-P	-15.67	1.42	1.61
38	H	1092	A	O3'-P	-14.82	1.43	1.61
38	H	1116	A	O3'-P	-11.49	1.47	1.61
38	H	1163	C	O5'-C5'	9.10	1.59	1.44
38	H	1116	A	C3'-O3'	-9.03	1.29	1.42

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	81	A	P-O3'-C3'	-15.08	101.61	119.70
38	H	1162	U	C5'-C4'-O4'	14.88	126.96	109.10
38	H	1093	C	P-O5'-C5'	14.75	144.50	120.90
38	H	1147	A	C5'-C4'-C3'	-14.15	93.36	116.00
38	H	1092	A	C2'-C3'-O3'	14.10	140.51	109.50

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1050	LEU	Peptide
1	A	239	PHE	Peptide
1	A	240	PRO	Peptide
1	A	255	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17092	0	16374	1323	0
2	K	3375	0	3343	293	0
3	L	3171	0	3140	204	0
4	N	4882	0	3988	259	0
5	J	2467	0	2365	181	0
6	E	1135	0	1120	91	0
7	M	950	0	1004	56	0
8	C	6732	0	6904	495	0
9	z	260	0	72	0	0
10	q	368	0	99	0	0
11	r	308	0	80	0	0
12	x	296	0	83	0	0
13	t	308	0	85	0	0
14	y	264	0	76	0	0
15	s	308	0	85	0	0
16	F	2043	0	1033	275	0
17	B	3677	0	1859	272	0
18	O	568	0	537	56	0
19	S	404	0	180	1	0
19	d	316	0	86	0	0
19	l	375	0	164	0	0
20	P	346	0	146	4	0
20	a	292	0	78	0	0
20	h	376	0	162	0	0
21	Q	491	0	207	6	0
21	b	308	0	78	0	0
21	m	407	0	171	0	0
22	R	457	0	192	2	0
22	c	360	0	89	0	0
22	n	323	0	136	0	0
23	T	379	0	159	6	0
23	e	288	0	74	0	0
23	i	369	0	152	0	0
24	U	359	0	155	3	0
24	f	280	0	77	0	0
24	j	344	0	148	0	0
25	V	369	0	168	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	g	280	0	79	0	0
25	k	340	0	152	0	0
26	I	2334	0	1173	184	0
27	D	8422	0	3689	23	0
28	G	1264	0	636	69	0
29	1	4044	0	1793	21	0
30	2	1042	0	435	4	0
31	3	5852	0	2487	30	0
32	4	862	0	384	5	0
33	5	507	0	215	1	0
34	6	415	0	183	1	0
35	X	631	0	276	3	0
36	Y	439	0	194	5	0
37	Z	109	0	42	1	0
38	H	3169	0	1608	155	0
39	o	673	0	276	0	0
40	p	361	0	159	0	0
41	u	2298	0	979	0	0
42	w	633	0	273	0	0
43	v	859	0	364	0	0
44	W	497	0	204	11	0
45	0	830	0	341	6	0
46	9	320	0	141	0	0
47	C	32	0	12	7	0
48	C	1	0	0	0	0
All	All	91261	0	60964	3655	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 3655 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1861:THR:CG2	18:O:161:ILE:HG12	1.34	1.56
1:A:1652:HIS:HE1	16:F:48:C:C6	1.21	1.53
5:J:350:PRO:CB	16:F:83:A:C8	1.94	1.51
1:A:1652:HIS:CE1	16:F:48:C:C6	1.95	1.50
5:J:350:PRO:HB2	16:F:83:A:C8	1.00	1.50

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	2164/2413 (90%)	1843 (85%)	298 (14%)	23 (1%)	14	51
2	K	425/465 (91%)	354 (83%)	68 (16%)	3 (1%)	22	60
3	L	410/494 (83%)	349 (85%)	55 (13%)	6 (2%)	10	45
4	N	675/899 (75%)	558 (83%)	109 (16%)	8 (1%)	13	49
5	J	300/469 (64%)	260 (87%)	36 (12%)	4 (1%)	12	48
6	E	136/143 (95%)	116 (85%)	19 (14%)	1 (1%)	22	60
7	M	124/126 (98%)	108 (87%)	15 (12%)	1 (1%)	19	57
8	C	837/1008 (83%)	727 (87%)	102 (12%)	8 (1%)	15	52
9	z	63/109 (58%)	61 (97%)	2 (3%)	0	100	100
10	q	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
11	r	75/89 (84%)	71 (95%)	4 (5%)	0	100	100
12	x	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
13	t	73/93 (78%)	68 (93%)	4 (6%)	1 (1%)	11	46
14	y	62/115 (54%)	62 (100%)	0	0	100	100
15	s	73/187 (39%)	72 (99%)	1 (1%)	0	100	100
18	O	69/587 (12%)	65 (94%)	2 (3%)	2 (3%)	4	33
19	S	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
19	d	77/101 (76%)	71 (92%)	4 (5%)	2 (3%)	5	35
19	l	72/101 (71%)	63 (88%)	8 (11%)	1 (1%)	11	46
20	P	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
20	a	69/196 (35%)	63 (91%)	6 (9%)	0	100	100
20	h	72/196 (37%)	65 (90%)	7 (10%)	0	100	100
21	Q	93/146 (64%)	89 (96%)	3 (3%)	1 (1%)	14	51
21	b	71/146 (49%)	66 (93%)	4 (6%)	1 (1%)	11	46
21	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	R	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
22	c	86/110 (78%)	81 (94%)	5 (6%)	0	100	100
22	n	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	9	44
23	T	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
23	e	66/94 (70%)	61 (92%)	5 (8%)	0	100	100
23	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
24	U	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
24	f	66/86 (77%)	60 (91%)	4 (6%)	2 (3%)	4	33
24	j	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	45
25	V	73/77 (95%)	66 (90%)	5 (7%)	2 (3%)	5	35
25	g	64/77 (83%)	56 (88%)	8 (12%)	0	100	100
25	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	D	1694/2163 (78%)	1631 (96%)	60 (4%)	3 (0%)	47	79
29	1	814/971 (84%)	770 (95%)	32 (4%)	12 (2%)	10	45
30	2	205/436 (47%)	192 (94%)	10 (5%)	3 (2%)	10	45
31	3	1164/1361 (86%)	1039 (89%)	107 (9%)	18 (2%)	10	45
32	4	166/213 (78%)	166 (100%)	0	0	100	100
33	5	101/107 (94%)	87 (86%)	14 (14%)	0	100	100
34	6	82/85 (96%)	77 (94%)	4 (5%)	1 (1%)	13	49
35	X	126/148 (85%)	117 (93%)	7 (6%)	2 (2%)	9	44
36	Y	85/266 (32%)	80 (94%)	3 (4%)	2 (2%)	6	37
37	Z	20/204 (10%)	14 (70%)	6 (30%)	0	100	100
39	o	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	9	44
40	p	69/111 (62%)	67 (97%)	2 (3%)	0	100	100
41	u	454/530 (86%)	417 (92%)	35 (8%)	2 (0%)	34	71
42	w	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
43	v	168/266 (63%)	142 (84%)	23 (14%)	3 (2%)	8	42
44	W	94/194 (48%)	87 (93%)	7 (7%)	0	100	100
45	0	157/242 (65%)	135 (86%)	22 (14%)	0	100	100
46	9	60/291 (21%)	59 (98%)	1 (2%)	0	100	100
All	All	12887/17914 (72%)	11601 (90%)	1170 (9%)	116 (1%)	21	54

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	PRO
2	K	171	GLN
2	K	395	ILE
3	L	328	VAL
4	N	735	ASP

5.3.2 Protein sidechains ⓘ

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	1743/2182 (80%)	1729 (99%)	14 (1%)	81	89
2	K	373/410 (91%)	373 (100%)	0	100	100
3	L	327/445 (74%)	327 (100%)	0	100	100
4	N	361/813 (44%)	361 (100%)	0	100	100
5	J	252/436 (58%)	252 (100%)	0	100	100
6	E	128/132 (97%)	128 (100%)	0	100	100
7	M	104/104 (100%)	104 (100%)	0	100	100
8	C	757/910 (83%)	753 (100%)	4 (0%)	88	93
18	O	57/534 (11%)	57 (100%)	0	100	100
All	All	4102/5966 (69%)	4084 (100%)	18 (0%)	91	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	190	SER
8	C	945	LEU
8	C	769	TYR
1	A	701	CYS
1	A	1910	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	433	GLN
8	C	817	GLN
6	E	14	HIS
8	C	218	HIS
1	A	1635	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	F	95/112 (84%)	44 (46%)	3 (3%)
17	B	173/214 (80%)	66 (38%)	14 (8%)
26	I	106/161 (65%)	44 (41%)	6 (5%)
28	G	59/60 (98%)	39 (66%)	7 (11%)
38	H	142/1175 (12%)	54 (38%)	23 (16%)
All	All	575/1722 (33%)	247 (42%)	53 (9%)

5 of 247 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	F	2	U
16	F	12	U
16	F	13	U
16	F	14	U
16	F	17	U

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	G	514	U
38	H	1097	G
38	H	1142	G
28	G	515	U
38	H	117	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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
47	GTP	C	1500	48	26,34,34	1.50	4 (15%)	32,54,54	2.11	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
47	GTP	C	1500	48	-	7/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	C	1500	GTP	C5-C6	-4.99	1.37	1.47
47	C	1500	GTP	C5-C4	-2.32	1.37	1.43
47	C	1500	GTP	C2'-C1'	-2.26	1.50	1.53
47	C	1500	GTP	O4'-C4'	-2.12	1.40	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	C	1500	GTP	PB-O3B-PG	-7.36	107.56	132.83
47	C	1500	GTP	PA-O3A-PB	-5.25	114.81	132.83
47	C	1500	GTP	C2-N1-C6	-3.09	119.40	125.10
47	C	1500	GTP	C5-C6-N1	2.93	119.12	113.95
47	C	1500	GTP	C8-N7-C5	2.87	108.46	102.99

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

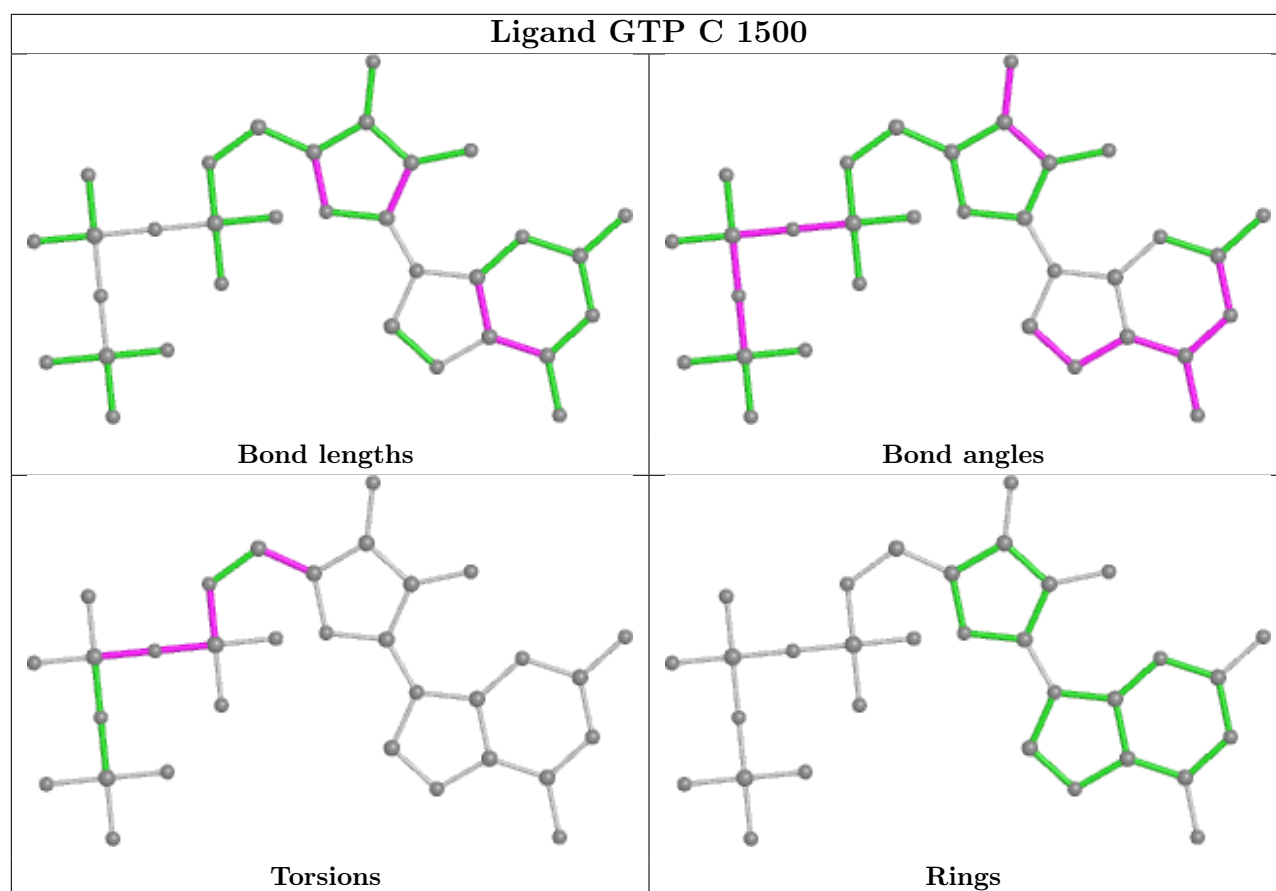
Mol	Chain	Res	Type	Atoms
47	C	1500	GTP	PB-O3A-PA-O5'
47	C	1500	GTP	C5'-O5'-PA-O1A
47	C	1500	GTP	C5'-O5'-PA-O2A
47	C	1500	GTP	C3'-C4'-C5'-O5'
47	C	1500	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	C	1500	GTP	7	0

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](#)

There are no chain breaks in this entry.

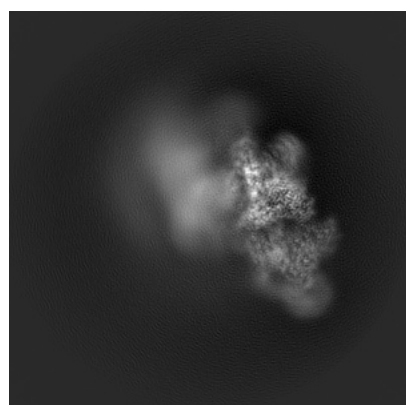
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6974. These allow visual inspection of the internal detail of the map and identification of artifacts.

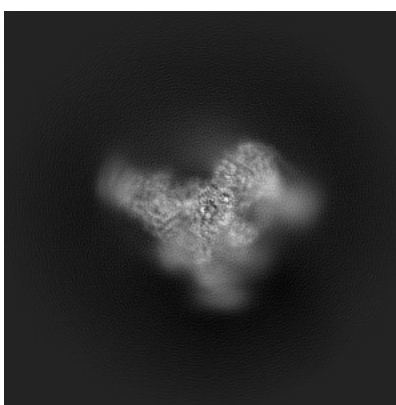
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

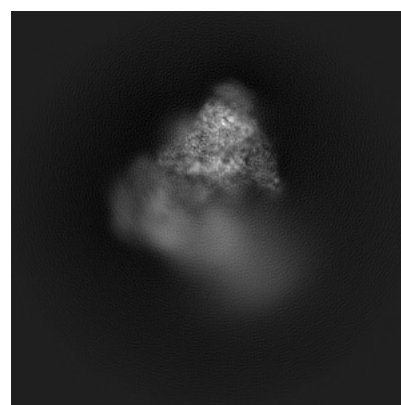
6.1.1 Primary map



X



Y

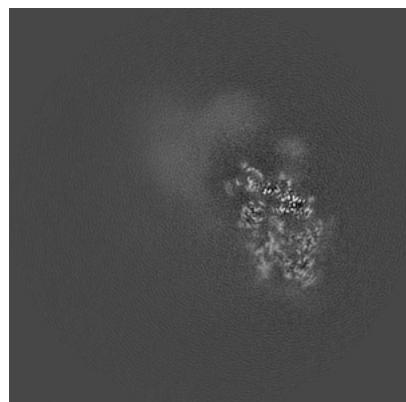


Z

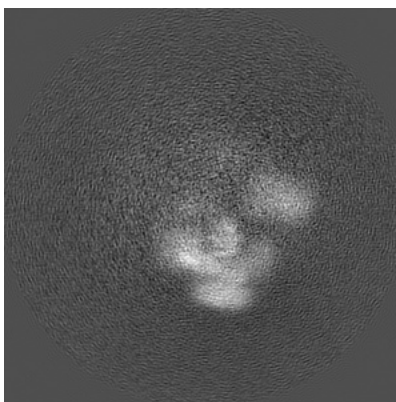
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

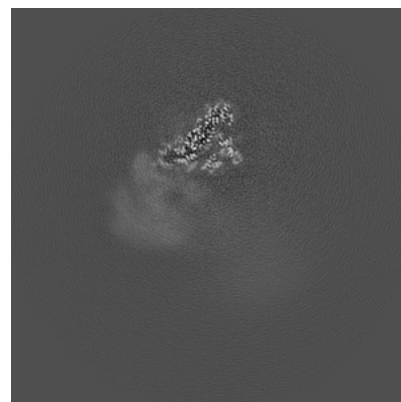
6.2.1 Primary map



X Index: 200



Y Index: 200

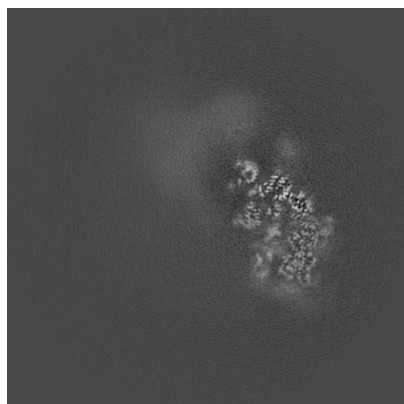


Z Index: 200

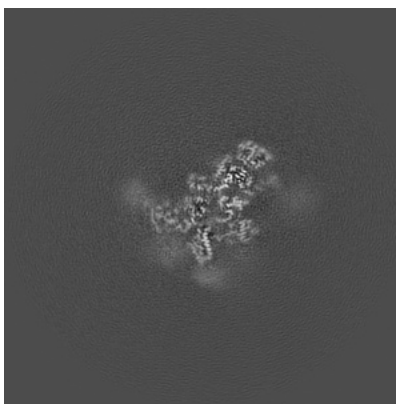
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

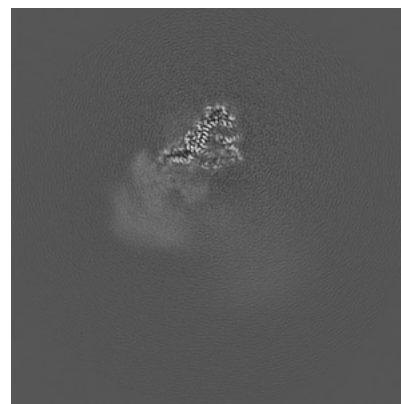
6.3.1 Primary map



X Index: 206



Y Index: 247



Z Index: 202

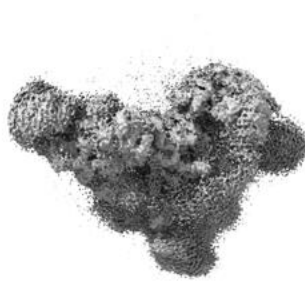
The images above show the largest variance slices of the map in three orthogonal directions.

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

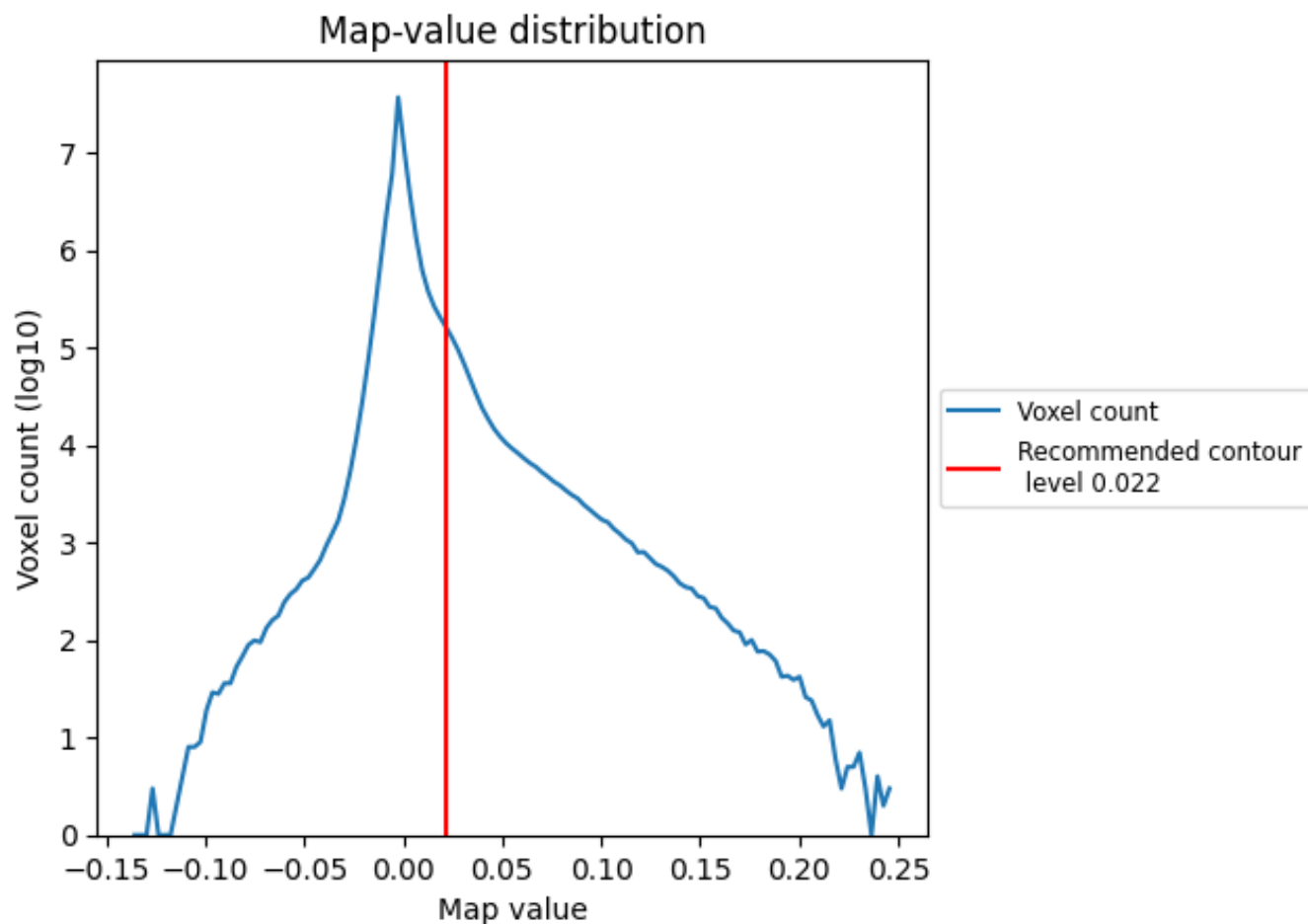
6.5 Mask visualisation

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

7 Map analysis [i](#)

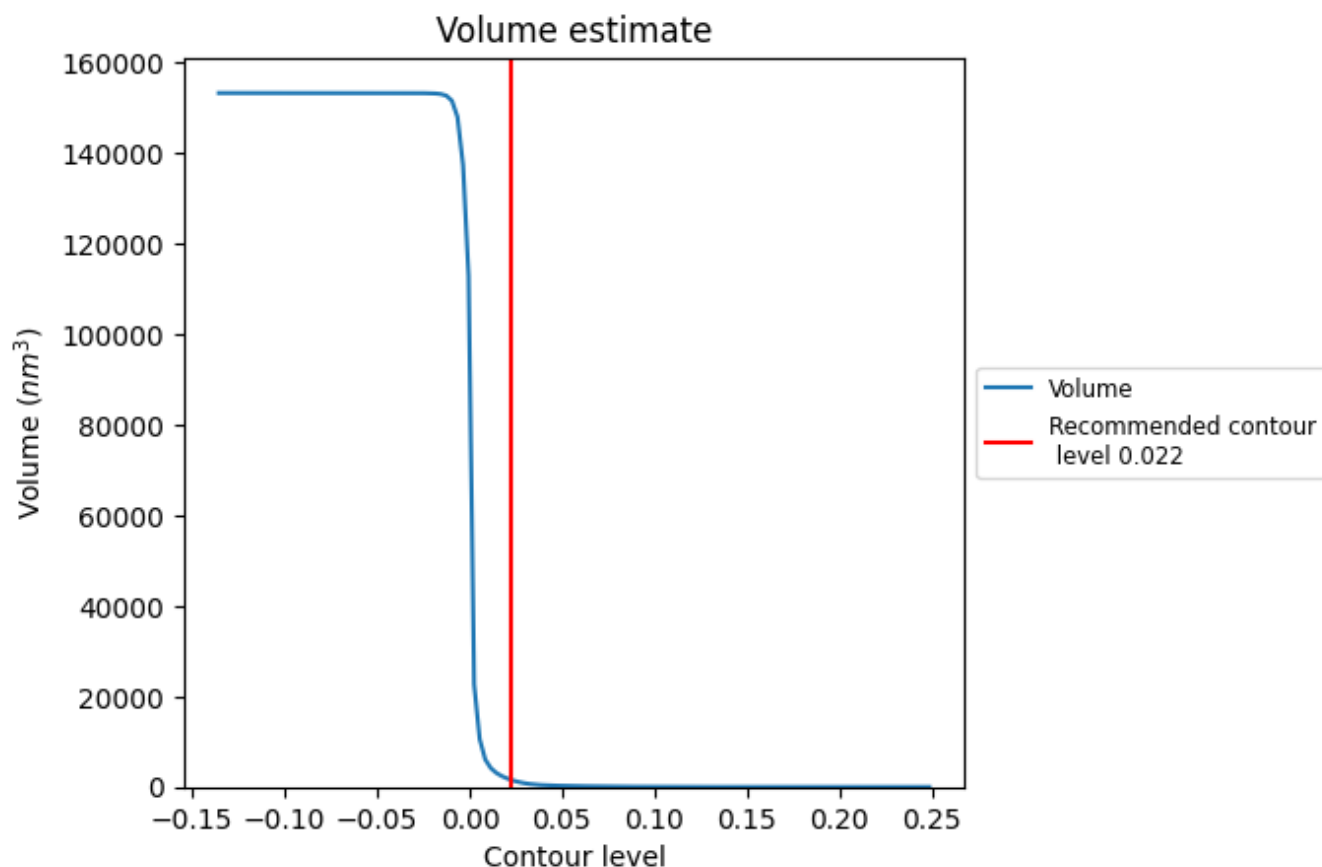
This section contains the results of statistical analysis of the map.

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.

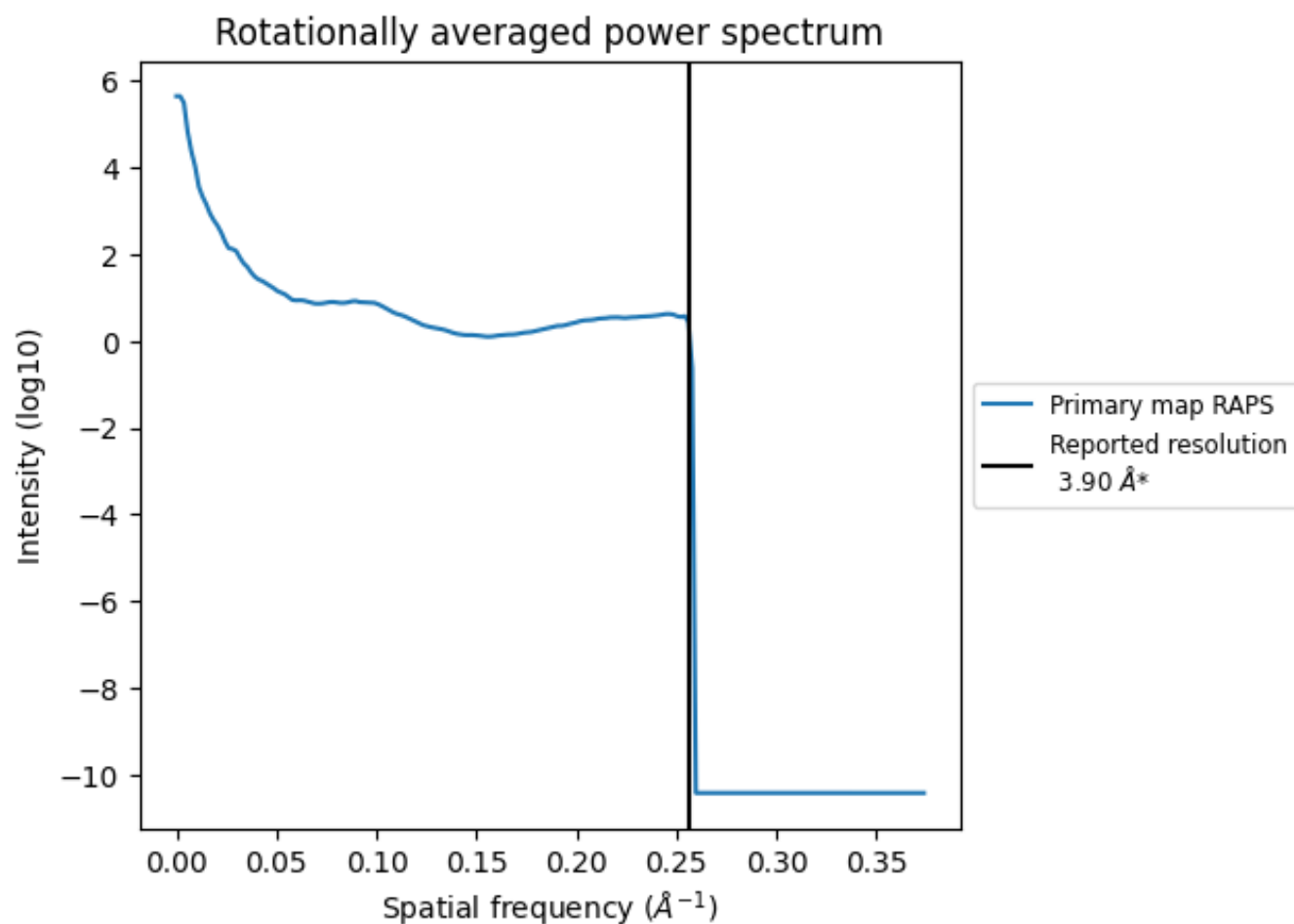
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1643 nm³; this corresponds to an approximate mass of 1484 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

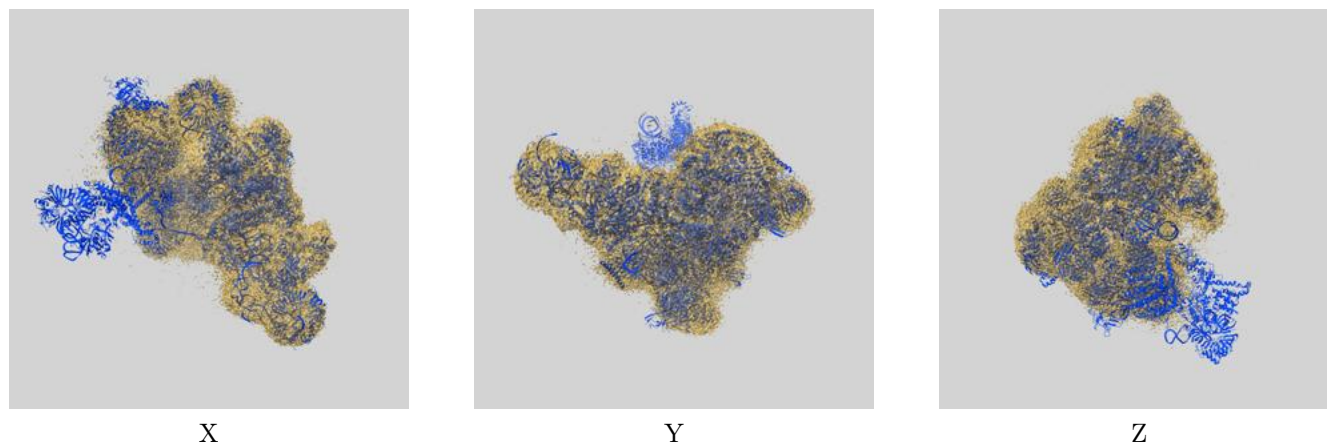
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

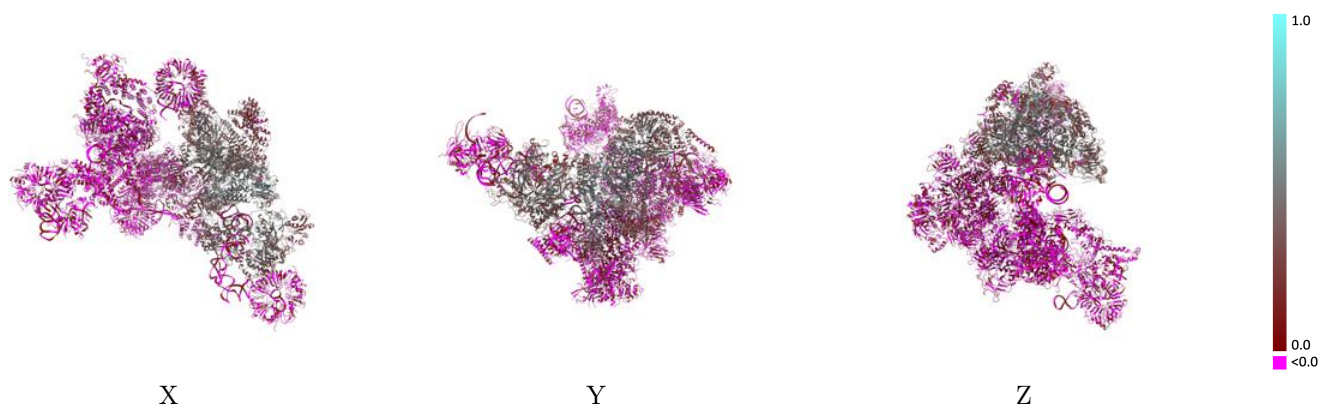
This section contains information regarding the fit between EMDB map EMD-6974 and PDB model 5ZWO. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



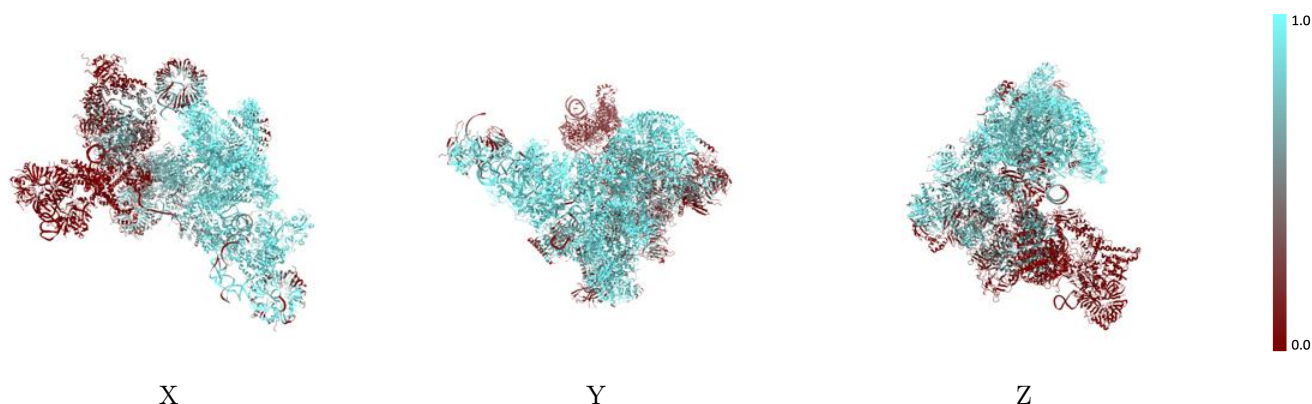
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



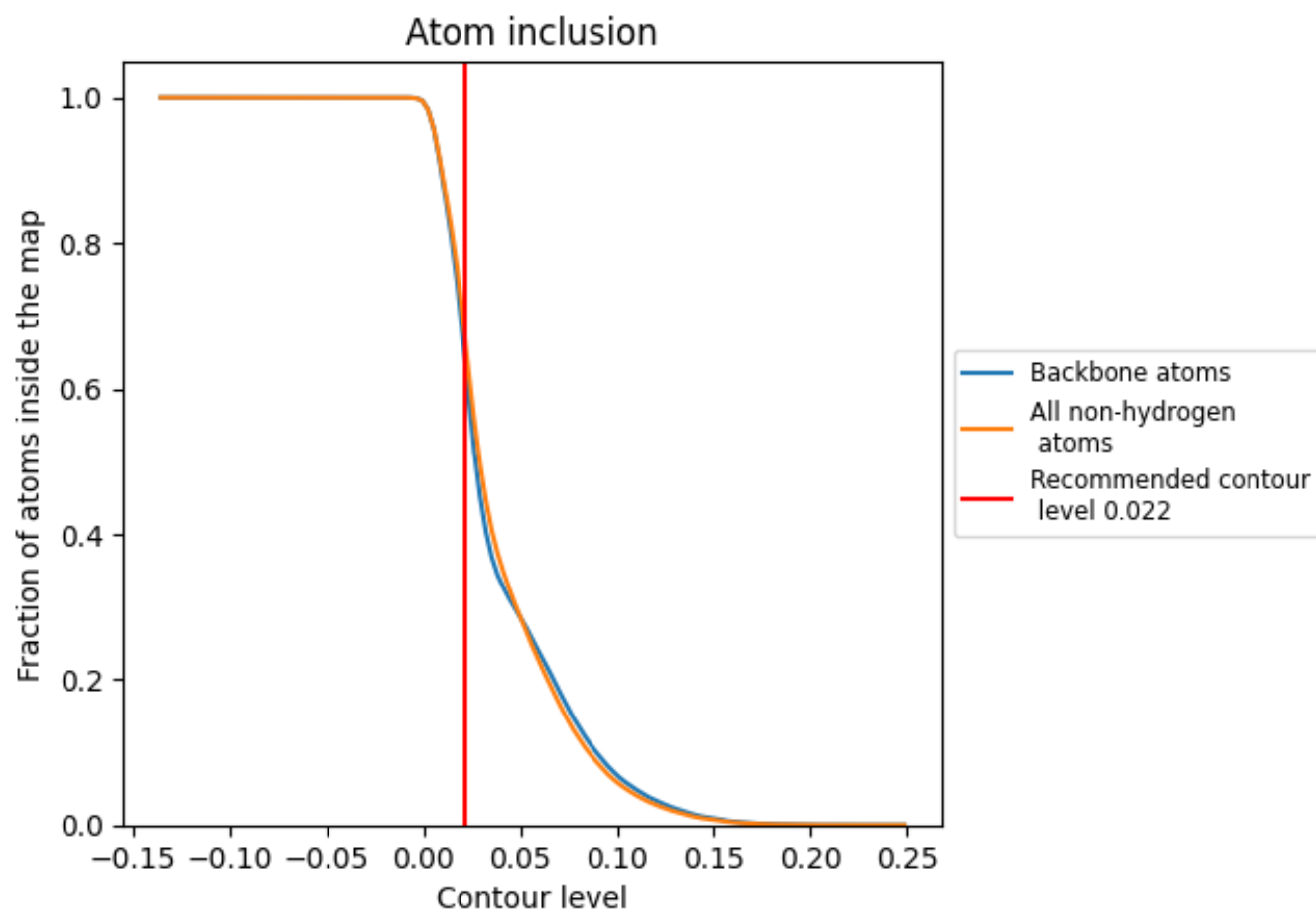
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 66% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6623	 0.1910
0	 0.6446	 0.0150
1	 0.3484	 0.0000
2	 0.2217	 0.0270
3	 0.3134	 -0.0030
4	 0.0696	 -0.0010
5	 0.6371	 -0.0140
6	 0.5566	 0.0050
9	 0.3156	 0.0410
A	 0.9460	 0.3990
B	 0.7987	 0.1080
C	 0.9413	 0.3770
D	 0.7403	 0.0420
E	 0.9334	 0.4360
F	 0.7885	 0.1650
G	 0.3078	 0.0070
H	 0.1278	 0.0120
I	 0.9666	 0.2600
J	 0.9200	 0.3510
K	 0.9365	 0.3910
L	 0.9433	 0.4200
M	 0.9563	 0.4810
N	 0.8601	 0.3180
O	 0.6499	 0.1870
P	 0.6965	 0.0150
Q	 0.7251	 0.0060
R	 0.8775	 0.0420
S	 0.5000	 0.0060
T	 0.5541	 0.0130
U	 0.8189	 0.0140
V	 0.4444	 0.0190
W	 0.6519	 0.0170
X	 0.0063	 0.0000
Y	 0.0000	 -0.0170
Z	 0.0000	 0.0380



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Chain	Atom inclusion	Q-score
a	 0.7671	 0.0500
b	 0.7825	 0.0160
c	 0.7583	 0.0350
d	 0.7278	 0.0790
e	 0.7014	 0.0630
f	 0.7286	 -0.0160
g	 0.4071	 -0.0160
h	 0.0000	 -0.0320
i	 0.0000	 0.0350
j	 0.0000	 -0.0450
k	 0.0000	 -0.0280
l	 0.0000	 0.0300
m	 0.0025	 0.0080
n	 0.0000	 0.0290
o	 0.0000	 -0.0170
p	 0.0000	 -0.0010
q	 0.3723	 0.0020
r	 0.2370	 -0.0630
s	 0.3604	 -0.0040
t	 0.3409	 -0.0020
u	 0.0187	 0.0050
v	 0.1059	 0.0160
w	 0.0047	 -0.0040
x	 0.4730	 0.0370
y	 0.2803	 0.0050
z	 0.5077	 0.0170