



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 14, 2018 – 08:32 PM EDT

PDB ID : 5NRL
EMDB ID: : EMD-3683
Title : Structure of a pre-catalytic spliceosome
Authors : Plaschka, C.; Lin, P.-C.; Nagai, K.
Deposited on : 2017-04-24
Resolution : 7.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

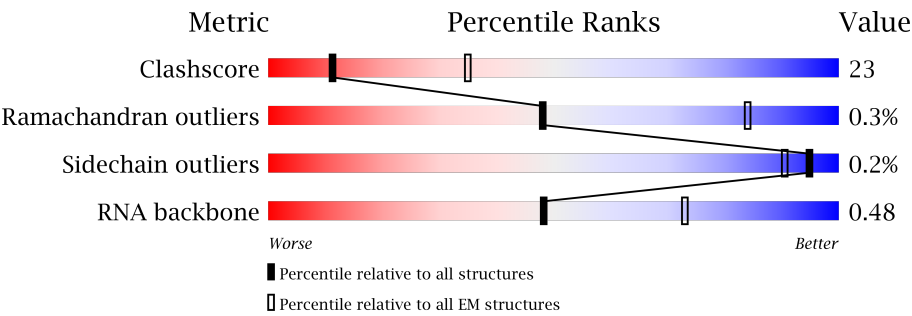
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

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 7.20 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.













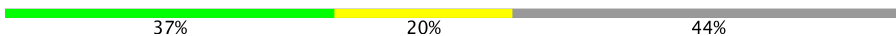
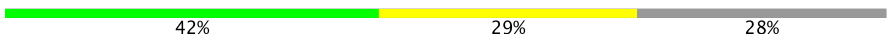











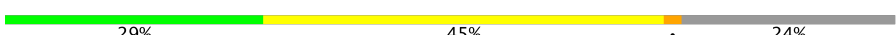

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	1175	<div><div>5% . .</div><div>87%</div></div>
2	3	89	<div><div>58%</div><div>28%</div><div>13%</div></div>
3	4	160	<div><div>16%</div><div>38%</div><div>17%</div><div>29%</div></div>
4	5	214	<div><div>15%</div><div>41%</div><div>23%</div><div>21%</div></div>
5	6	112	<div><div>29%</div><div>34%</div><div>22%</div><div>15%</div></div>
6	7	115	<div><div>50%</div><div>7%</div><div>43%</div></div>
7	8	109	<div><div>40%</div><div>18%</div><div>41%</div></div>
8	A	2413	<div><div>55%</div><div>37%</div><div>8%</div></div>

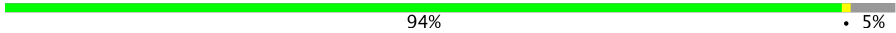














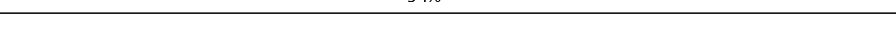
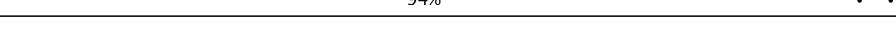


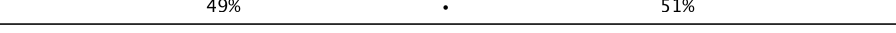





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Mol	Chain	Length	Quality of chain
9	B	2163	
10	C	1008	
11	D	143	
12	E	587	
13	F	494	
14	G	469	
15	H	465	
16	I	95	
17	J	899	
18	K	126	
19	L	194	
20	M	242	
21	N	291	
22	O	971	
23	P	1361	
24	Q	435	
25	R	213	
26	S	107	
27	T	530	
28	U	266	
29	V	280	
30	W	238	
31	X	111	
32	Y	111	
33	Z	85	

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Mol	Chain	Length	Quality of chain
34	a	95	 94% . 5%
35	b	196	 36% 64%
35	k	196	 36% 64%
35	s	196	 36% 64%
36	d	101	 82% 18%
36	n	101	 79% . 19%
36	v	101	 79% . 19%
37	e	94	 82% 18%
37	p	94	 81% . 18%
37	w	94	 81% . 18%
38	f	86	 84% 16%
38	q	86	 85% 15%
38	x	86	 85% 15%
39	g	77	 92% 8%
39	r	77	 94% . .
39	y	77	 94% . .
40	h	146	 55% 45%
40	l	146	 66% . 32%
40	t	146	 49% . 51%
41	i	110	 84% 16%
41	m	110	 84% 16%
41	u	110	 84% 16%
42	j	187	 40% 60%
43	o	93	 81% 19%
44	z	86	 86% 14%

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 118701 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
1	2	155	Total	C	N	O	P	0	0
			3275	1464	552	1104	155		

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	77	Total	C	N	O	S	0	0
			611	382	105	121	3		

- Molecule 3 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	114	Total	C	N	O	P	0	0
			2423	1084	419	806	114		

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	170	Total	C	N	O	P	0	0
			3615	1618	640	1188	169		

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	95	Total	C	N	O	P	0	0
			2019	904	355	665	95		

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	66	Total	C	N	O	S	0	0
			504	325	85	91	3		

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	64	Total	C	N	O	S	0	0
			498	320	86	90	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2216	Total	C	N	O	S	0	0
			18122	11661	3103	3294	64		

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1699	Total	C	N	O	S	1	0
			13607	8720	2269	2564	54		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	850	Total	C	N	O	S	0	0
			6784	4392	1129	1237	26		

- Molecule 11 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	142	Total	C	N	O	S	0	0
			1164	736	202	215	11		

- Molecule 12 is a protein called 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	124	Total	C	N	O	S	0	0
			825	501	153	170	1		

- Molecule 13 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	413	Total	C	N	O	S	0	0
			3238	2064	578	584	12		

- Molecule 14 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	372	Total	C	N	O	S	0	0
			2835	1786	523	512	14		

- Molecule 15 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	429	Total	C	N	O	S	0	0
			3396	2120	609	653	14		

- Molecule 16 is a RNA chain called Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	29	Total	C	N	O	P	0	0
			600	271	95	205	29		

- Molecule 17 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	800	Total	C	N	O	S	0	0
			6485	4151	1106	1201	27		

- Molecule 18 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	124	Total	C	N	O	S	0	0
			936	597	161	174	4		

- Molecule 19 is a protein called 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	109	Total	C	N	O	S	0	0
			882	570	150	159	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor 38.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	174	Total	C	N	O	S	0	0
			1407	915	236	249	7		

- Molecule 21 is a protein called Pre-mRNA-splicing factor SPP381.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	N	85	Total	C	N	O	0	0
			425	255	85	85		

- Molecule 22 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	833	Total	C	N	O	S	0	0
			6612	4258	1121	1192	41		

- Molecule 23 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	1186	Total	C	N	O	S	0	0
			9437	6034	1589	1763	51		

- Molecule 24 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	220	Total	C	N	O	S	0	0
			1786	1157	307	313	9		

- Molecule 25 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	173	Total	C	N	O	S	0	0
			1429	930	239	258	2		

- Molecule 26 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 27 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	462	Total	C	N	O	S	0	0
			3915	2487	677	735	16		

- Molecule 28 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	196	Total	C	N	O	S	0	0
			1488	933	258	291	6		

- Molecule 29 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	127	Total	C	N	O	S	0	0
			1084	689	193	196	6		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	170	Total	C	N	O	S	0	0
			1383	866	253	257	7		

- Molecule 31 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	X	30	Total	C	N	O	0	0
			150	90	30	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	84	Total	C	N	O	S	0	0
			683	439	119	122	3		

- Molecule 33 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	83	Total	C	N	O	S	0	0
			685	424	129	131	1		

- Molecule 34 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	90	Total	C	N	O	S	0	0
			735	469	124	139	3		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	70	Total	C	N	O	S	0	0
			563	360	98	102	3		
35	k	70	Total	C	N	O	S	0	0
			563	360	98	102	3		
35	s	70	Total	C	N	O	S	0	0
			563	360	98	102	3		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	83	Total	C	N	O	S	0	0
			641	408	111	120	2		
36	n	82	Total	C	N	O	S	0	0
			632	402	109	119	2		
36	v	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	77	Total	C	N	O	S	0	0
			602	396	95	108	3		
37	p	77	Total	C	N	O	S	0	0
			602	396	95	108	3		
37	w	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	72	Total	C	N	O	S	0	0
			578	371	101	105	1		
38	q	73	Total	C	N	O	S	0	0
			585	376	102	106	1		
38	x	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	71	Total	C	N	O	S	0	0
			549	345	96	106	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	75	Total	C	N	O	S	0	0
			577	363	100	112	2		
39	y	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	80	Total	C	N	O	S	0	0
			630	402	108	118	2		
40	l	99	Total	C	N	O	S	0	0
			751	475	137	137	2		
40	t	72	Total	C	N	O	S	0	0
			569	364	99	104	2		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	92	Total	C	N	O	S	0	0
			752	481	136	131	4		
41	m	92	Total	C	N	O	S	0	0
			752	481	136	131	4		
41	u	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

- Molecule 42 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	74	Total	C	N	O	S	0	0
			588	381	96	108	3		

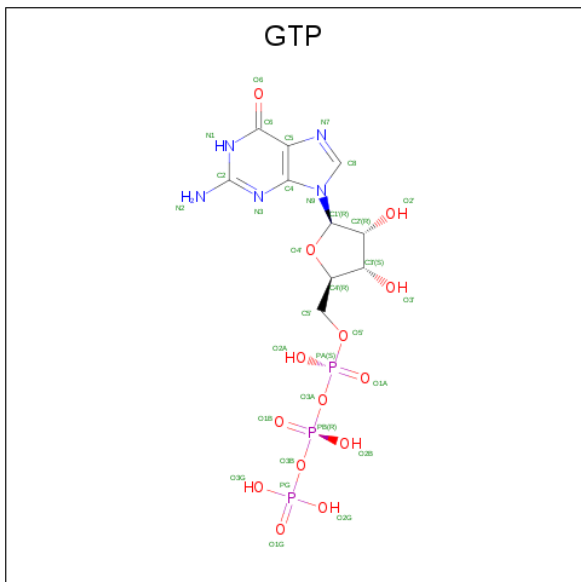
- Molecule 43 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	75	Total	C	N	O	S	0	0
			588	378	98	110	2		

- Molecule 44 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	74	Total	C	N	O	S	0	0
			577	364	95	116	2		

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

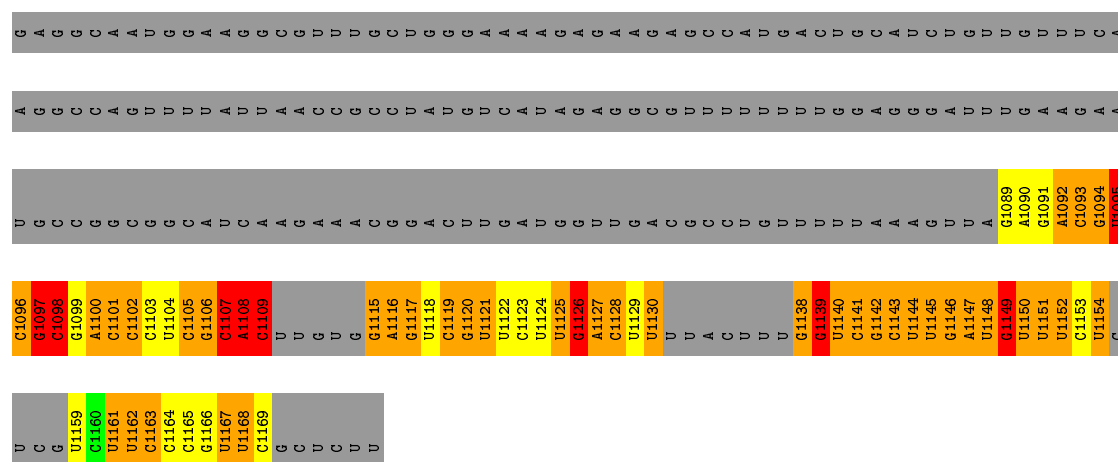
- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
46	T	2	Total Zn 2 2	0
46	L	1	Total Zn 1 1	0
46	S	3	Total Zn 3 3	0
46	U	1	Total Zn 1 1	0

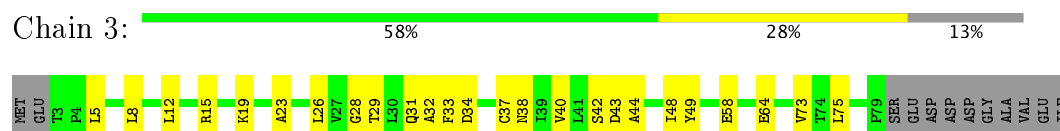
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- Molecule 1: U2 snRNA



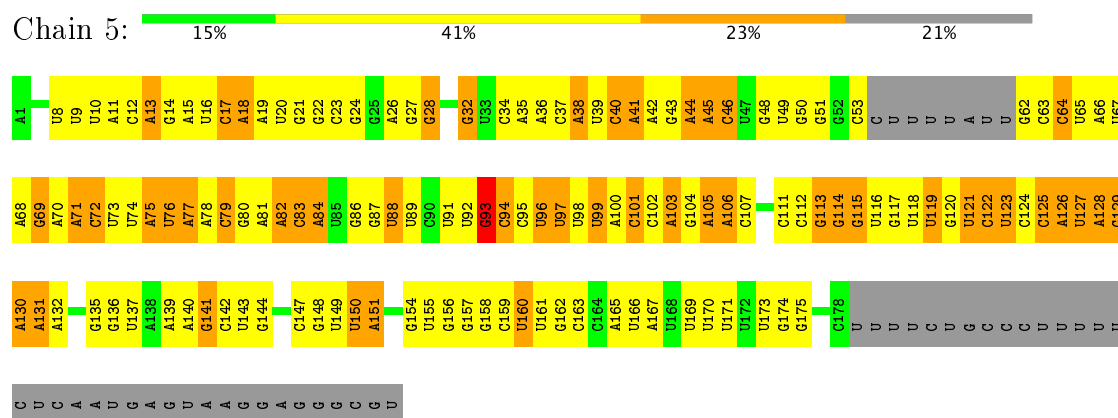
- Molecule 2: U6 snRNA-associated Sm-like protein LSm3



- Molecule 3: U4 snRNA

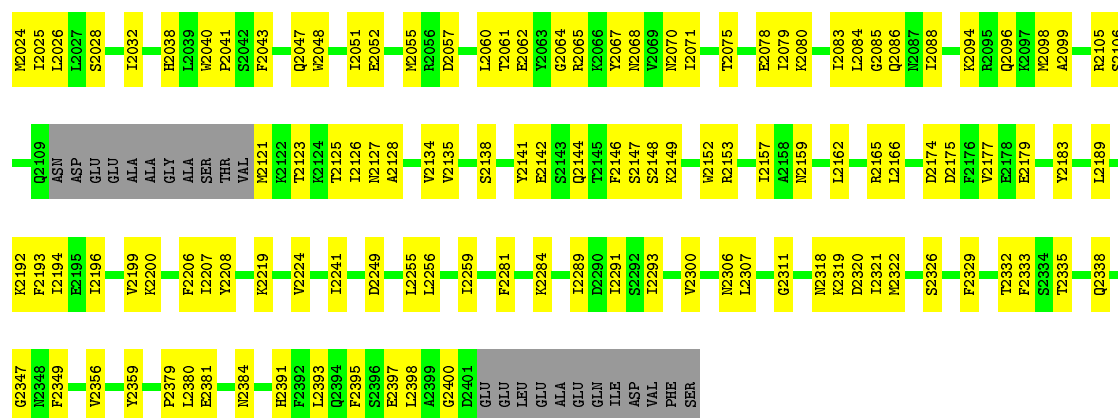


- Molecule 4: U5 snRNA



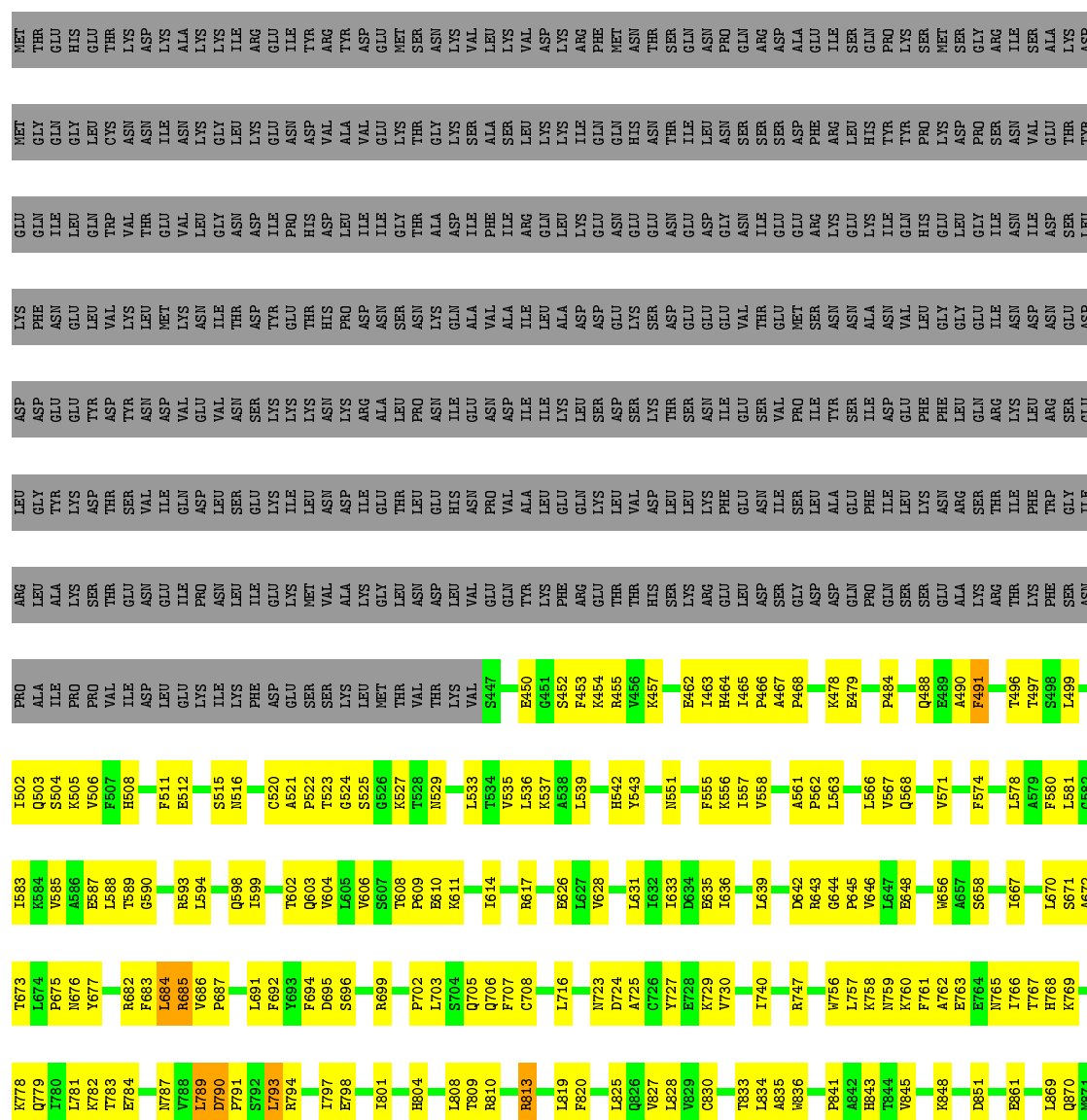
- Molecule 5: U6 snRNA



• Molecule 9: Pre-mRNA-splicing helicase BRR2

Chain B: 50% 28% 21%



R132	I133	G137	V138	I139	G140	F141	L142	H143	S144	G145	K146	T147	L148	M150	L153	V154	I155	D156	S157	K158	I161	P162	D163	K173	P174	L175	R176	Y177	L178	K182	Q183	D186	R187	N194	G195	S196	T197	C200	T201	D202	S207	R208	F212	L213	H218	V219	P230	N220	
GLU	GLY	ILE	SER	LEU	GLU	GLY	PRO	PHE	GLY	GLY	LYS	GLU	VAL	GLY	THR	GLY	ASN	GLN	THR	GLY	SER	PRO	GLN	THR	LEU	VAL	GLU	PRO	VAL	THR	GLU	ARG	LYS	GLN	GLY	THR	ASN	F106	T107	Q108	L109	K110	N112	R117	A127	H128	I129	V130	F131
MET	GLY	GLY	ASP	ASP	PHE	GLY	GLY	GLY	ASN	LEU	ILE	GLY	VAL	GLY	VAL	ASP	VAL	ASP	PRO	PHE	THR	ASP	THR	GLY	GLY	GLN	GLY	GLN	THR	THR	ASN	PHE	GLY	SER	GLY	ASN	THR	ILE	GLU	SER	ARG	GLN	LEU	THR	SER	LEU	LYS	LYS	

● Molecule 10: Pre-mRNA-splicing factor SNU114

Chain C:

49%

35%

16%

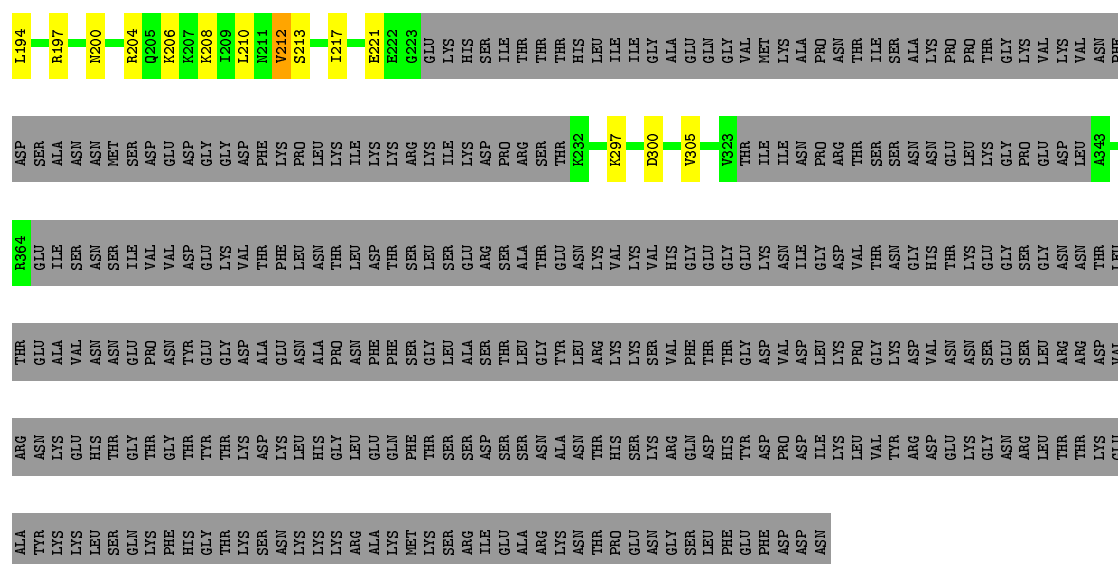
• Molecule 10: Pre-mRNA-splicing factor SNU114

Chain C: 49% 35% 16%

MET	GLU	GLY	ASP	ASP	LEU	PHE	ASP	GLU	PHE	GLY	ASN	LEU	ILE	GLY	VAL	ASP	ASP	PRO	PHE	ASP	SER	VAL	LEU	GLN	GLN	GLN	GLN	THR	THR	ASN	THR	PHE	GLU	GLY	SER	GLY	SER	GLY	ASN	ASN	ASN	ILE	GLU	GLU	SER	ARG	GLN	THR	SER	LEU	GLY	SER	LYS
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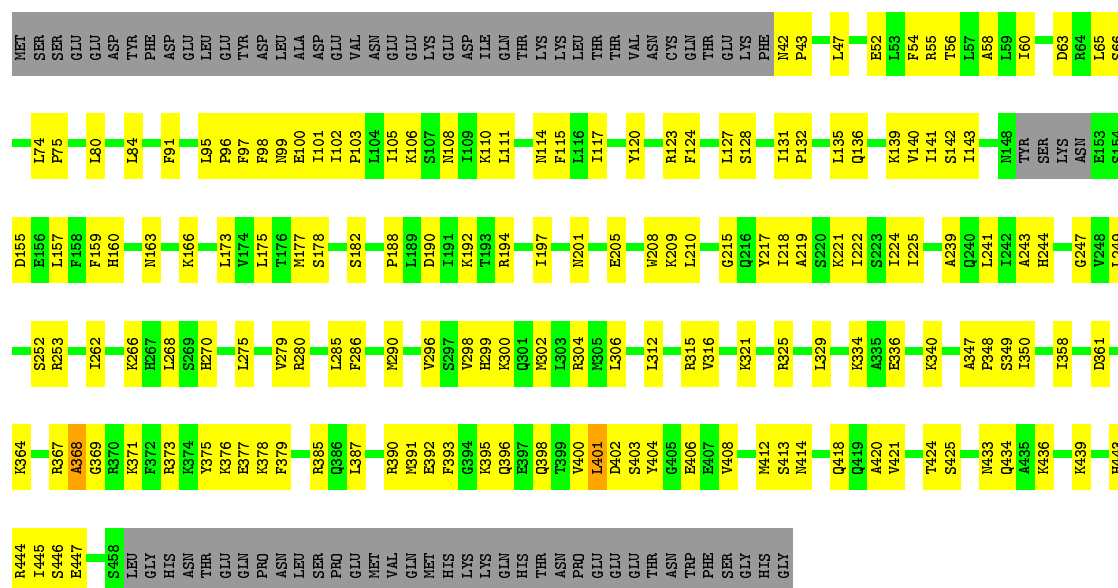
GLU	LEU	GLY	ILE	SER	LEU	GLU	HIS	PRO	TYR	GLY	LYS	GLU	VAL	GLU	VAL	VAL	ASP	MET	GLU	THR	LYS	ASN	THR	GLN	PRO	VAL	THR	GLU	ARG	THR	LYS	GLN	GLU	HIS	THR	T105	F106	T107	Q108	L109	K110	K111	N112	R117	A127	H128	I129	P130	E131
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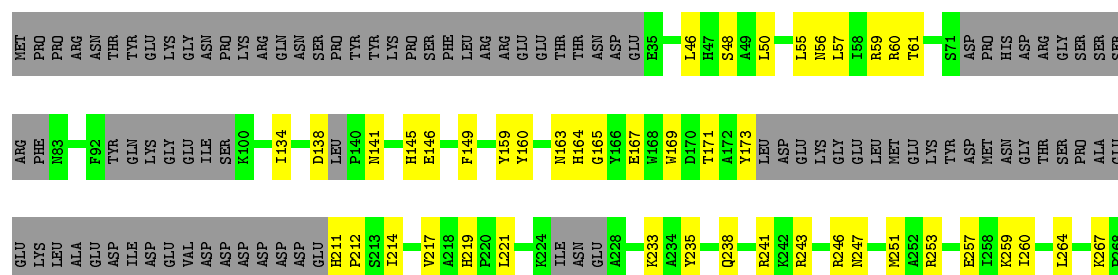
• Molecule 13: Pre-mRNA-processing factor 31

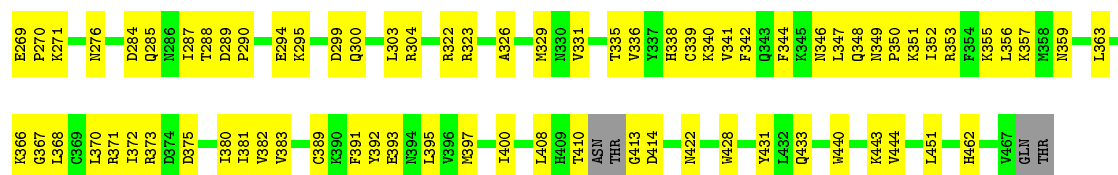
Chain F: 51% 32% 16%



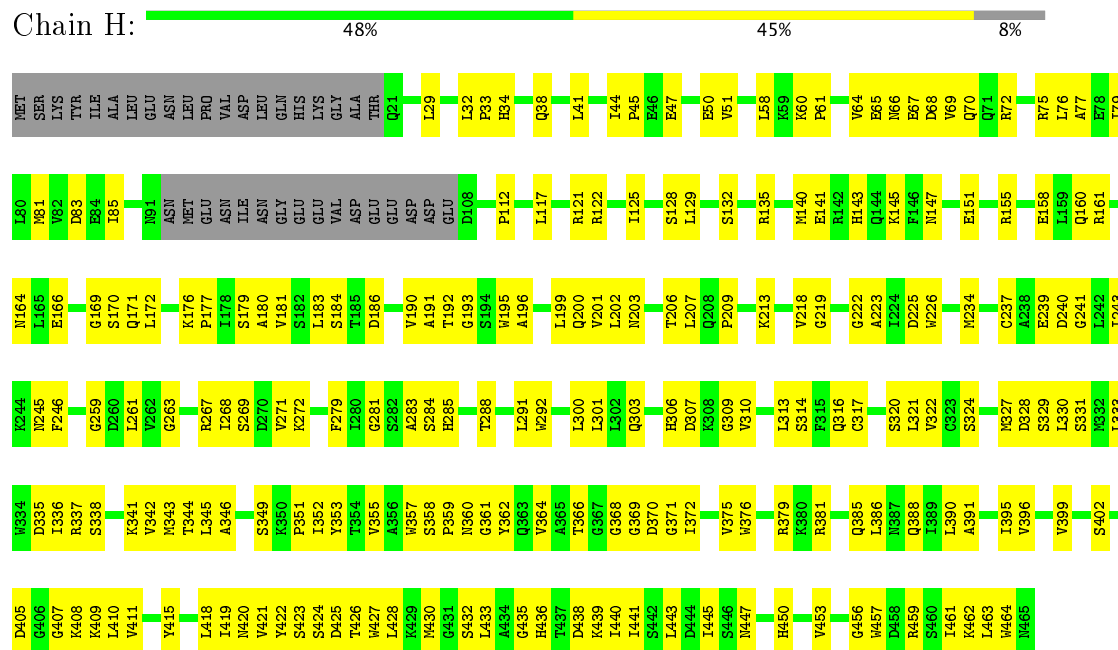
• Molecule 14: U4/U6 small nuclear ribonucleoprotein PRP3

Chain G: 54% 25% 21%

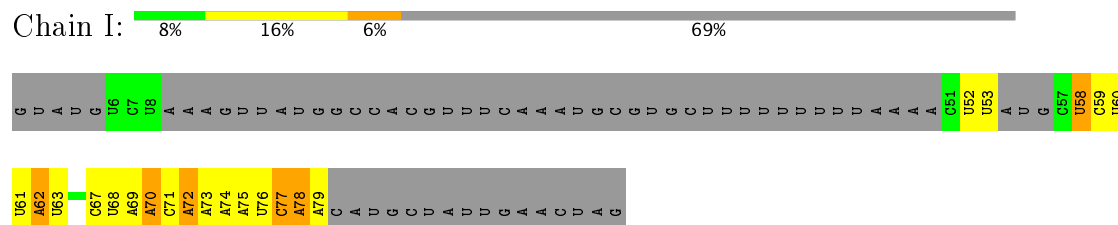




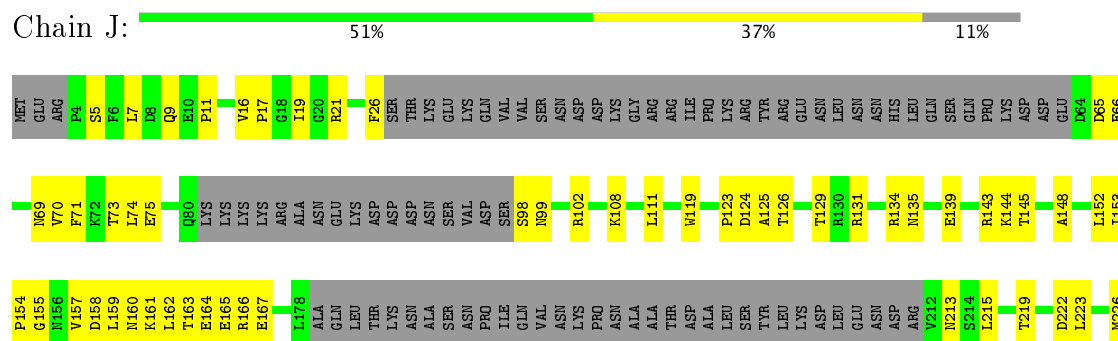
• Molecule 15: U4/U6 small nuclear ribonucleoprotein PRP4

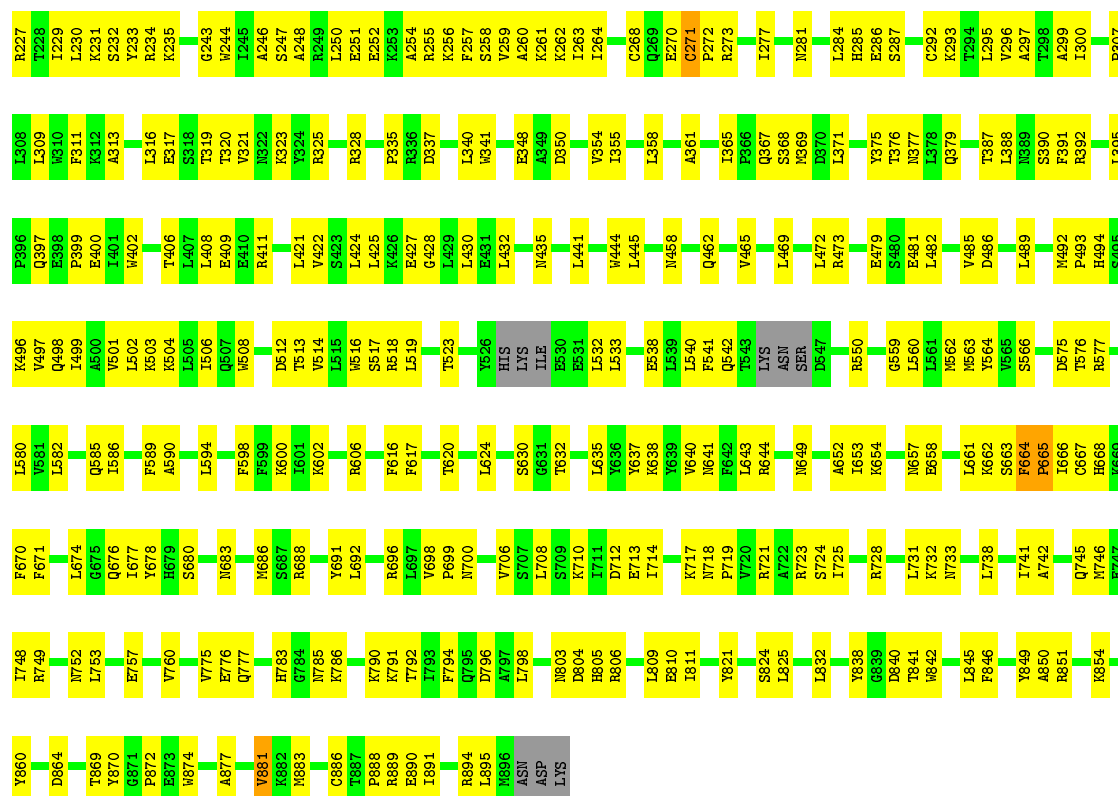


• Molecule 16: Yeast UBC4 gene for ubiquitin-conjugating enzyme



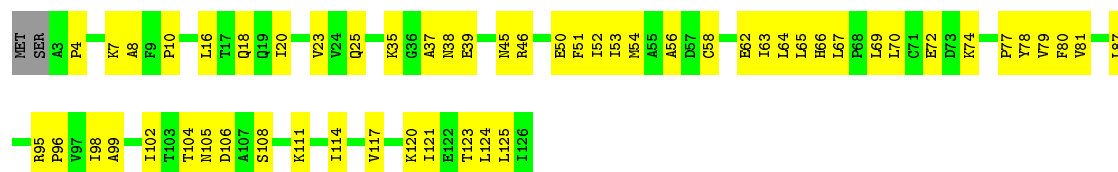
• Molecule 17: Pre-mRNA-splicing factor 6





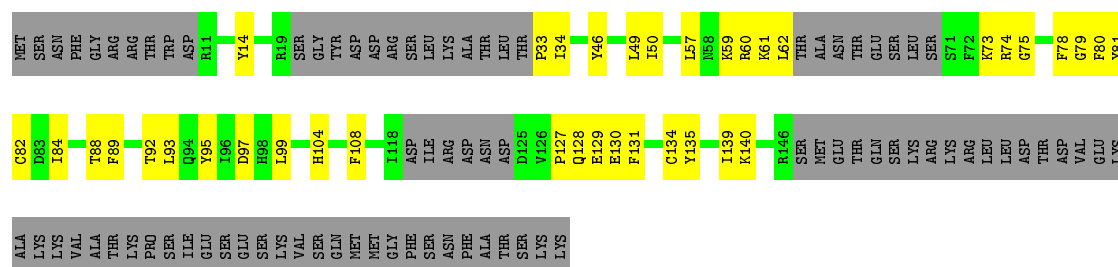
- Molecule 18: 13 kDa ribonucleoprotein-associated protein

Chain K: 55% 44%



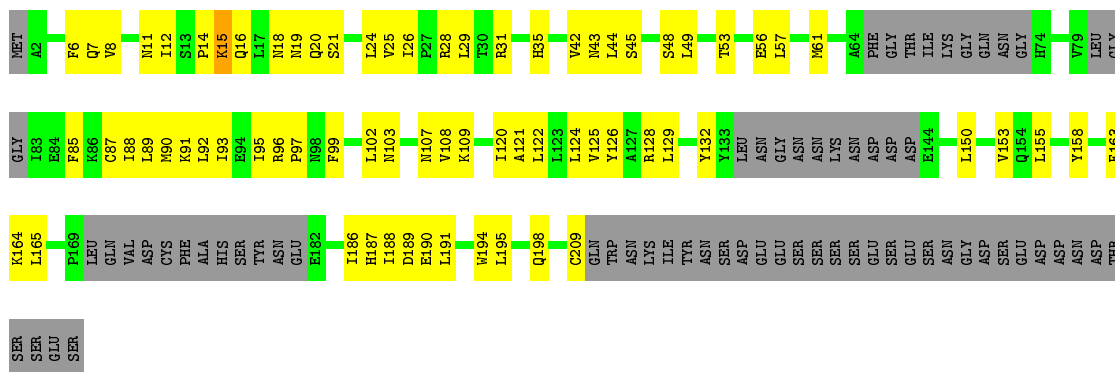
- Molecule 19: 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component

Chain L: 37% 20% 44%

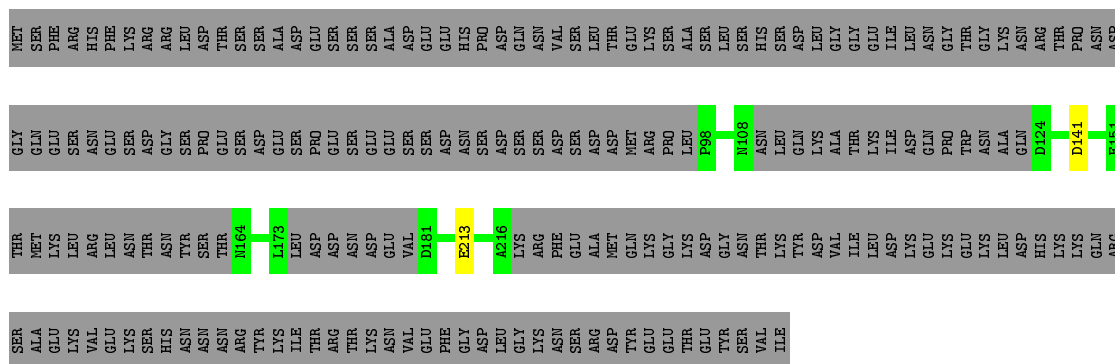


- Molecule 20: Pre-mRNA-splicing factor 38

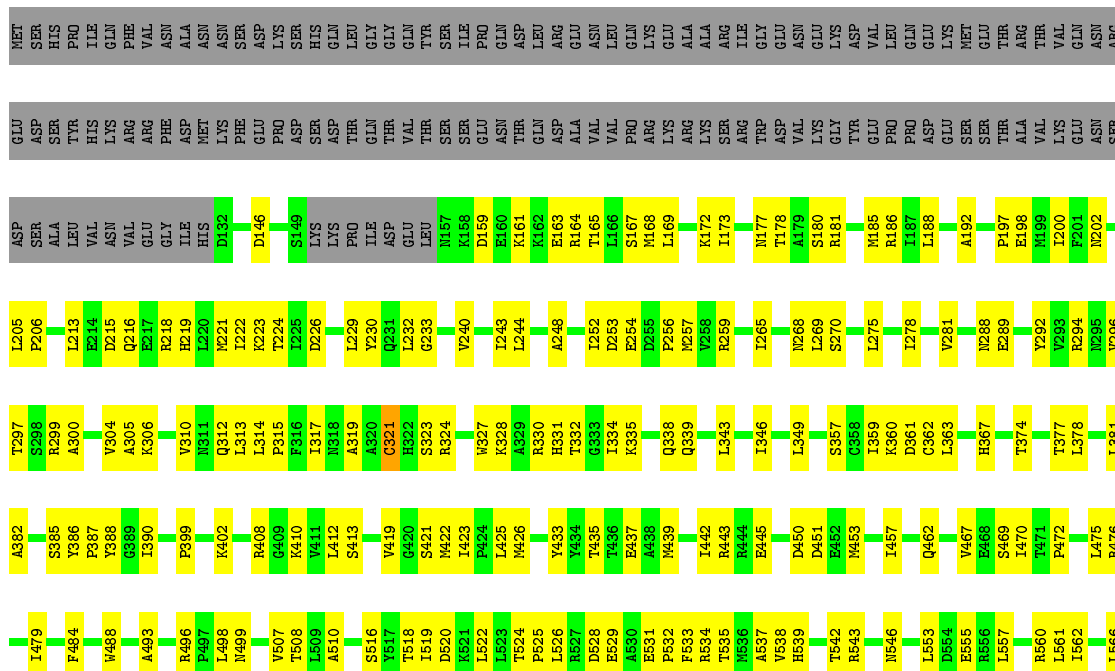
Chain M: 42% 29% 28%

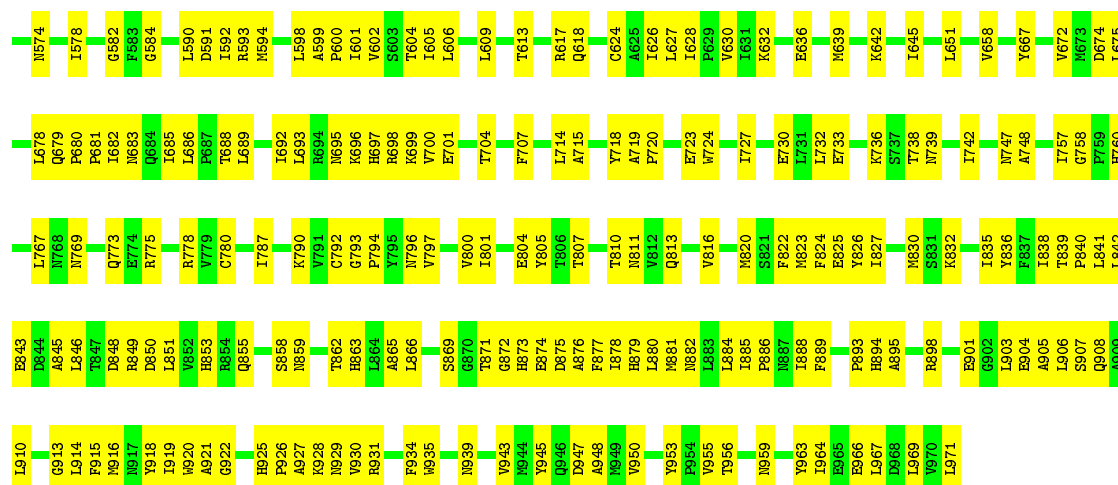


- Molecule 21: Pre-mRNA-splicing factor SPP381

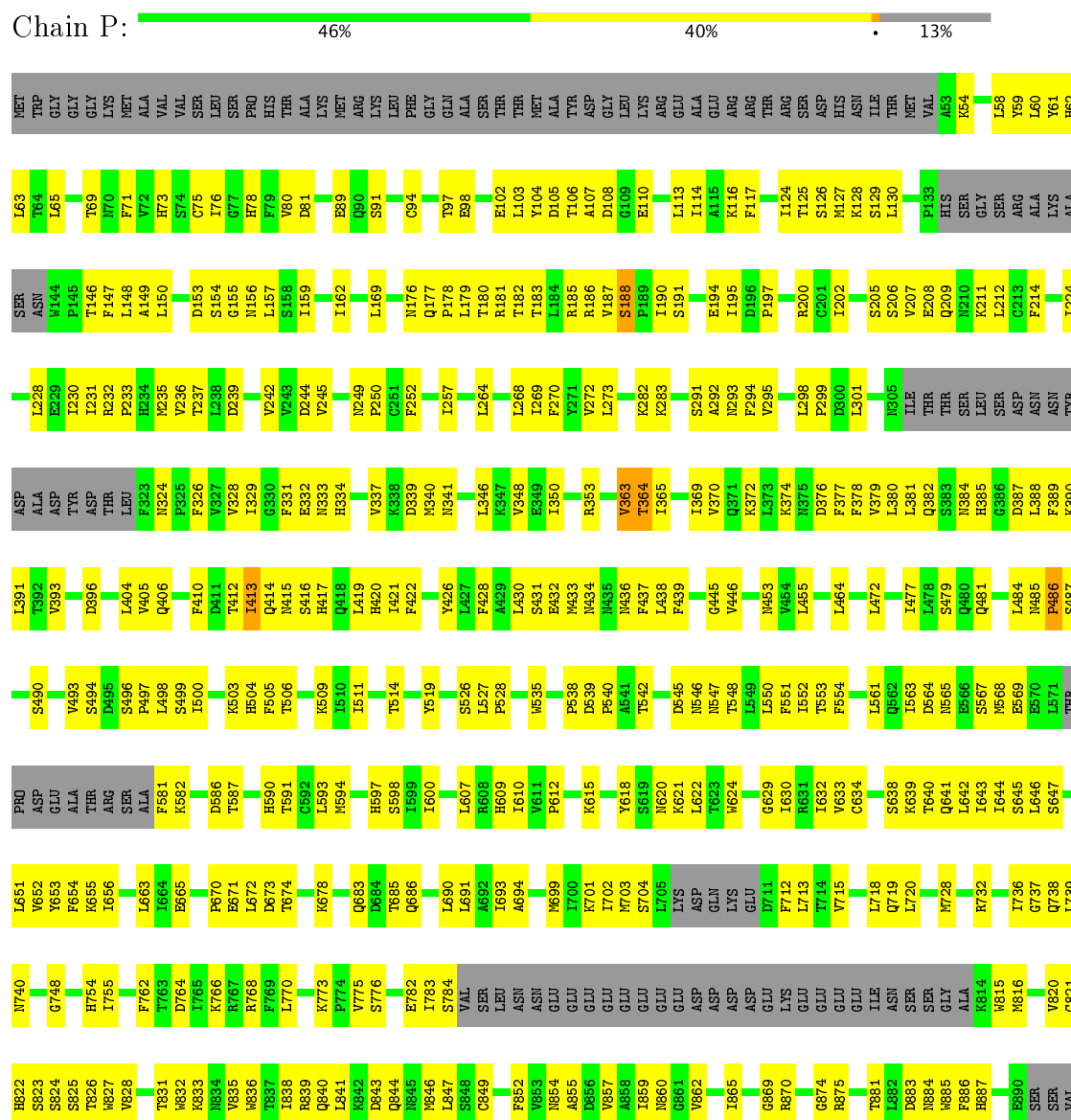


- Molecule 22: U2 snRNP component HSH155





- Molecule 23: Pre-mRNA-splicing factor RSE1



ASN	L974	K1056	G1223	S1298
LYS	D975	K1057	T1224	I1299
GLN	D976	Q1058	V1225	L1300
GLU	D977	L1059	G1226	G1301
ASN	D978	V1064	C1227	R1302
GLY	C979	T1065	F1228	Q1305
GLY	V980	T1066	I1229	E1306
GLY	S981	S1070	P1230	Y1307
ASP	S982	T1071	L1231	G1308
GLU	A983	T1072	L1232	R1309
SER	A984	K1073	S1233	Y1310
ASN	L994	K1077	K1234	Y1311
GLU	L995	Y1082	G1235	L1159
GLU	A998	E1083	E1236	S1160
ASP	R1002	R1084	V1237	M1161
GLU	L1003	L1085	F1238	G1162
MET	L1004	D1089	M1240	A1163
GLU	L1006	I1090	E1244	K1165
GLU	K1007	H1091	E1249	Y1166
MET	L1008	E1092	D1252	L1171
GLU	L1009	S1093	Y1177	P1178
W1018	W1011	L1096	H1179	T1180
R927	K1012	F1097	K1183	C1184
T928	K1014	I1098	G1184	K1263
T929	L1015	W1099	W1264	W1265
L930	S1016	D1100	ASN	ASN
P936	F1017	P1101	MET	MET
K937	D1018	A1102	ARG	ARG
S938	L1019	G1103	LYS	LYS
T939	L1021	N1104	GLU	GLU
L940	L1022	V1105	ASP	ASP
F941	H1023	H1106	GLU	GLU
D943	S1029	F1107	GLU	GLU
D944	P1030	P1108	SER	SER
H945	I1031	Y1109	GLY	GLY
S946	L1035	D1111	VAL	VAL
G947	K1036	T1112	VAL	VAL
Q950	F1037	S1113	VAL	VAL
C951	K1038	V1114	LEU	LEU
R952	L1041	K1115	GLY	GLY
T957	L1042	H1117	ARG	ARG
C961	M1045	K1122	GLY	GLY
L962	G1046	F1123	ILE	ILE
G965	S1047	L1124	ASP	ASP
T972	T1048	D1125	GLU	GLU
L973	L1049	T1128	VAL	VAL
	V1050	Y1129	ASP	ASP
	L1051	I1130	ILE	ILE
	A1132	T1218	GLY	GLY
	D1133	M1219	ASP	ASP
		G1220	GLY	GLY
		L1221	LEU	LEU
		E1294	HIS	HIS
		Q1222		

• Molecule 24: Cold sensitive U2 snRNA suppressor 1

Chain Q: 33% 17% 49%

MET	LYS	LEU	ASP	I294	ASP	LYS	ASP	I294	ASP
ALA	GLU	SER	GLU	S295	GLU	GLU	GLU	S295	GLU
ARG	PHE	ALA	PHE	W312	ARG	ALA	ALA	W312	ALA
LYS	LYS	ARG	LYS	M316	LYS	ARG	LYS	M316	LYS
SER	VAL	K125	VAL	T323	SER	VAL	SER	T323	SER
ARG	GLN	K128	GLN	G324	ARG	GLN	ARG	G324	ARG
LYS	GLN	K131	GLN	Y325	LYS	GLN	LYS	Y325	LYS
ASN	VAL	L134	VAL	K329	ASN	VAL	ASN	K329	ASN
ASN	GLN	K138	GLN	I330	ASN	GLN	ASN	I330	ASN
GLN	GLU	P144	GLU	A331	GLN	GLU	PHE	A331	PHE
ASN	ASN	Q145	ASN	W335	ASN	ASN	GLN	W335	GLN
LYS	ASP	Q146	LYS	D336	LYS	ASP	GLU	D336	GLU
ALA	THR	I147	ALA	I337	ALA	THR	ASP	I337	ASP
VAL	LYS	D153	VAL	D343	VAL	LYS	ILE	D343	ILE
VAL	ILE	L159	VAL	I349	VAL	ILE	SER	I349	SER
ASN	THR	L160	ASN	H353	THR	THR	VAL	H353	VAL
LYS	ASP	A161	LYS	K246	LYS	ASP	ALA	K246	ALA
GLU	GLY	S162	GLU	L247	GLY	GLY	GLU	L247	GLU
ILE	ASN	K167	ILE	H248	ASN	ASN	GLU	H248	GLU
ALA	ASN	M168	ALA	D249	ALA	ASN	LYS	D249	LYS
ALA	ALA	I170	ALA	V250	ALA	ALA	LEU	V250	LEU
MET	VAL	W176	MET	F251	MET	VAL	ARG	F251	ARG
ILE	VAL	P171	ILE	K253	ILE	VAL	ASN	P171	ASN
ASP	ILE	W172	ASP	P260	ASP	ILE	GLU	W172	GLU
ARG	VAL	P173	ARG	H261	ARG	VAL	GLU	P173	GLU
GLU	GLU	S174	GLU	D262	GLU	GLU	SER	S174	SER
LEU	LYS	H175	LEU	W176	LYS	LYS	GLU	H175	GLU
GLN	ASN	Q177	GLN	C265	GLN	ASN	LYS	Q177	LYS
VAL	VAL	L183	VAL	F266	VAL	VAL	GLN	L183	GLN
GLY	VAL	S184	GLY	G267	GLY	VAL	TYR	S184	TYR
LYS	ARG	L188	LYS	V269	LYS	ARG	VAL	L188	VAL
GLY	HIS	P193	GLY	Y271	GLY	HIS	LEU	P193	LEU
VAL	THR	F194	VAL	E272	VAL	THR	ALA	F194	ALA
ASN	ALA	E195	ASN	H273	ASN	ALA	ASP	E195	ASP
LYS	GLU	L196	LYS	N275	LYS	GLU	GLY	L196	GLY
GLY	GLU	L200	GLY	L276	GLY	GLU	LEU	L200	LEU
LYS	LEU	T203	LYS	F277	LYS	LEU	ASP	T203	ASP
THR	THR	P213	THR	T280	THR	THR	GLN	P213	GLN
ASN	ASN	G125	ASN	R284	ASN	ASN	ALA	G125	ALA
VAL	VAL	SER	VAL	D287	VAL	VAL	ALA	SER	ALA
ASP	ASP	GLY	ASP	H288	ASP	ASP	GLU	GLY	GLU
ALA	ILE	LEU	ALA	K289	ALA	ILE	ASN	LEU	ASN
LEU	GLY	ASP	LEU	R290	LEU	GLY	GLY	ASP	GLY
GLN	GLY	GLY	GLN	P291	GLN	GLY	ARG	GLY	ARG
GLU	GLU	GLU	GLU		GLU	GLU	GLY	GLU	GLY
HIS	HIS		HIS		HIS	HIS	ASP		ASP

• Molecule 25: Protein HSH49

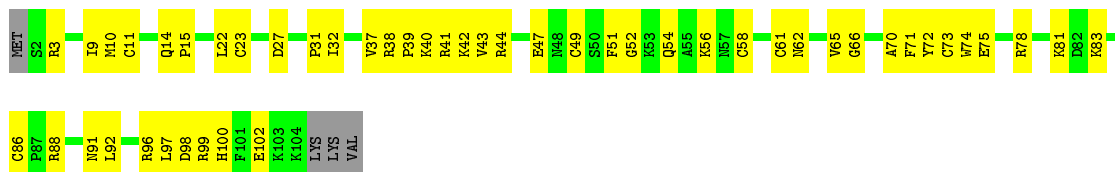
Chain R: 53% 29% 19%

MET	Y86	LYS	ASP	Y99	ASP	LYS	ASP	Y99	ASP
ASN	THR	ILE	ASN	T10	GLU	GLU	GLU	T10	GLU
TYR	SER	ASP	TYR	Y11	SER	ASP	ASP	Y11	SER
ALA	GLY	GLY	ALA	Y12	GLY	GLY	GLY	Y12	GLY
ASP	THR	THR	ASP	Y13	THR	THR	ASP	Y13	THR
SER	ASN	ASN	SER	I16	SER	ASN	SER	I16	SER
GLY	LEU	LEU	GLY	D17	GLY	LEU	GLY	D17	GLY
THR	PRO	PRO	THR	E27	THR	PRO	THR	E27	THR
ASP	ASN	ASN	ASP	Q31	ASP	ASN	ASP	Q31	ASP
ILE	ILE	ILE	ILE	P34	ILE	ILE	ILE	P34	ILE
SER	SER	SER	SER	V35	SER	SER	SER	V35	SER
LYS	GLU	GLU	LYS	L36	LYS	GLU	LYS	L36	LYS
ASP	THR	THR	ASP	R37	ASP	THR	ASP	R37	ASP
MET	Y40	LYS	MET	Y40	MET	LYS	MET	Y40	LYS
ILE	M114	LEU	ILE	P41	ILE	LEU	ILE	M114	LEU
LEU	A116	GLU	LEU	K42	LEU	GLU	LEU	A116	GLU
GLY	I119	ARG	GLY	V45	GLY	ARG	GLY	I119	ARG
ASN	I135	ASN	ASN	R361	ASN	ASN	ASN	I135	ASN
GLU	R336	GLU	GLU	A362	GLU	GLU	GLU	R336	GLU
SER	Y52	SER	SER	Y363	SER	SER	SER	Y52	SER
GLY	A53	GLY	GLY	F364	GLY	GLY	GLY	A53	GLY
LYS	F54	LYS	LYS	G365	LYS	LYS	LYS	F54	LYS
GLN	I55	GLN	GLN	A366	GLN	GLN	GLN	I55	GLN
TYR	E56	TYR	TYR	L367	TYR	TYR	TYR	E56	TYR
VAL	D60	VAL	VAL	S369	VAL	VAL	VAL	D60	VAL
LEU	G61	LEU	LEU	F370	LEU	LEU	LEU	G61	LEU
ALA	D62	ALA	ALA	F375	ALA	ALA	ALA	D62	ALA
ASN	A63	ASN	ASN	E376	ASN	ASN	ASN	A63	ASN
GLY	Q64	GLY	GLY	SER	GLY	GLY	GLY	Q64	GLY
ASP	Y65	ASP	ASP	LYS	ASP	ASP	ASP	Y65	ASP
GLY	A66	GLY	GLY	GLY	GLY	GLY	GLY	A66	GLY
THR	I69	THR	THR	ASP	THR	THR	THR	I69	THR
GLN	W70	GLN	GLN	THR	GLN	GLN	GLN	W70	GLN
ALA	L76	ALA	ALA	ALA	ALA	ALA	ALA	L76	ALA
ASN	R79	ASN	ASN	ALA	ASN	ASN	ASN	R79	ASN
GLU	L80	GLU	GLU	GLU	GLU	GLU	GLU	L80	GLU
ASN	I81	ASN	ASN	ASN	ASN	ASN	ASN	I81	ASN
GLY	K82	GLY	GLY	GLY	GLY	GLY	GLY	K82	GLY
ARG	M175	ARG	ARG	ARG	ARG	ARG	ARG	M175	ARG
GLY	R177	GLY	GLY	GLY	GLY	GLY	GLY	R177	GLY
GLU	I178	GLU	GLU	GLU	GLU	GLU	GLU	I178	GLU



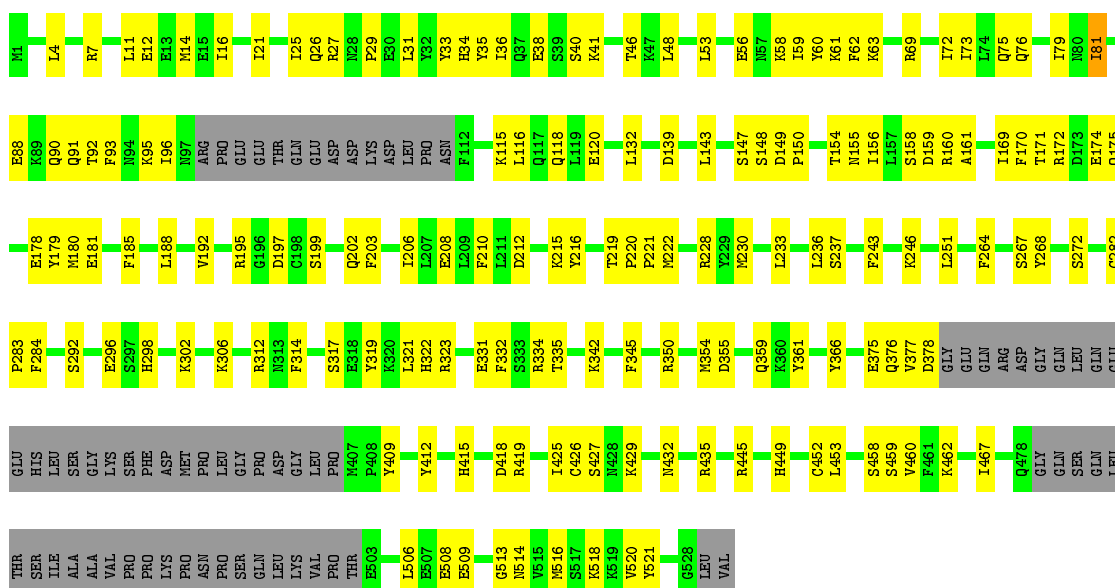
• Molecule 26: Pre-mRNA-splicing factor RDS3

Chain S: 50% 46%



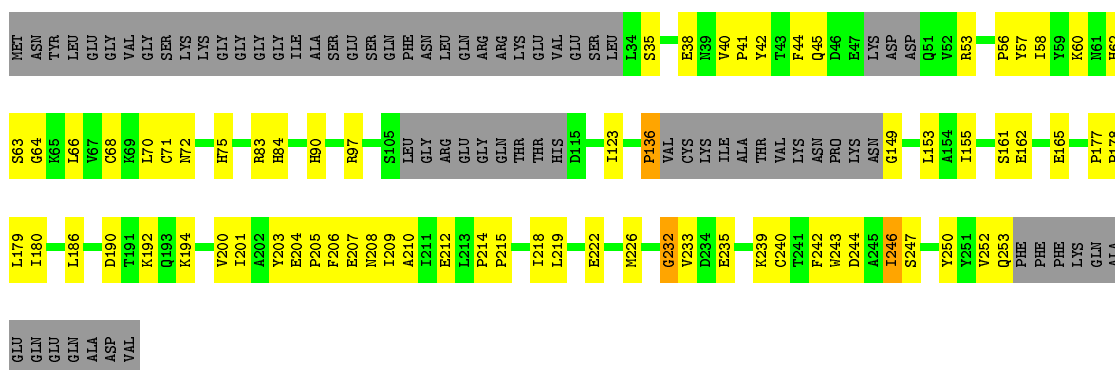
• Molecule 27: Pre-mRNA-splicing factor PRP9

Chain T: 57% 30% 13%



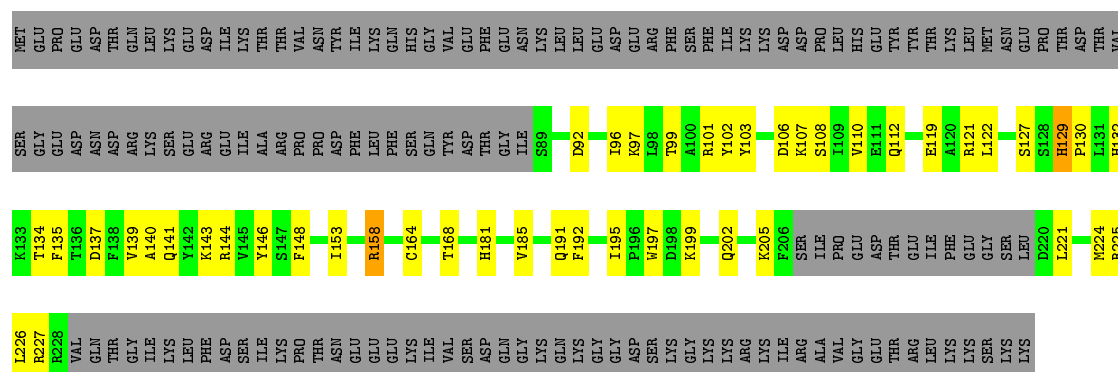
• Molecule 28: Pre-mRNA-splicing factor PRP11

Chain U: 47% 26% 26%



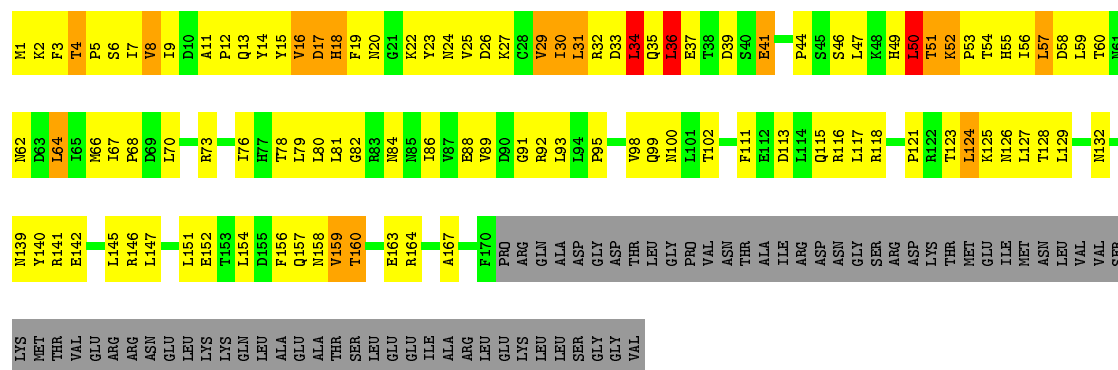
• Molecule 29: Pre-mRNA-splicing factor PRP21

Chain V:  29% 16% . 55%



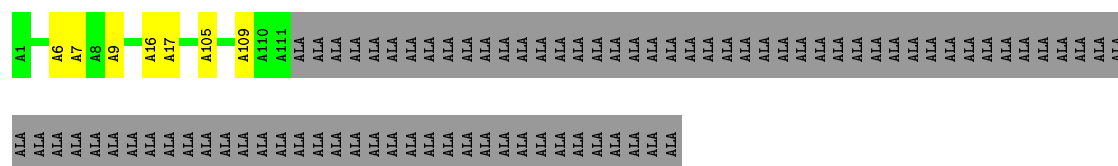
- Molecule 30: U2 small nuclear ribonucleoprotein A'

Chain W:  26% 38% 7% 29%



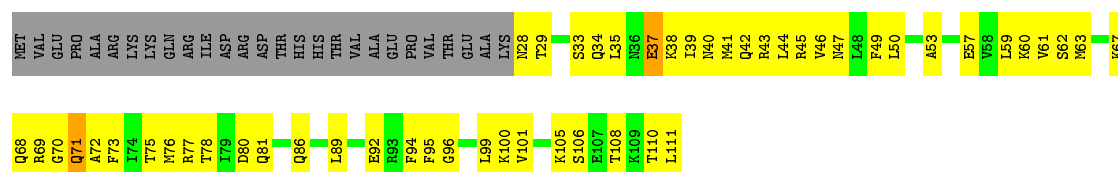
- Molecule 31: Unknown

Chain X:  21% 6% 73%



- Molecule 32: U2 small nuclear ribonucleoprotein B''

Chain Y: 29% 45% 1% 24%



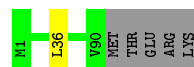
- Molecule 33: RDS3 complex subunit 10

Chain Z:  61% 36%



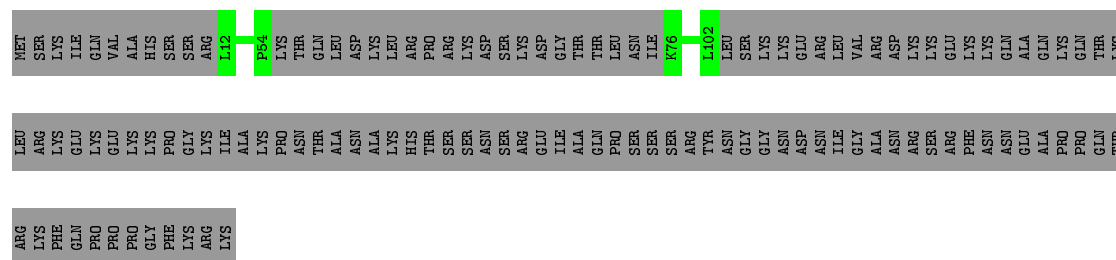
- Molecule 34: U6 snRNA-associated Sm-like protein LSm2

Chain a:  94% 5%



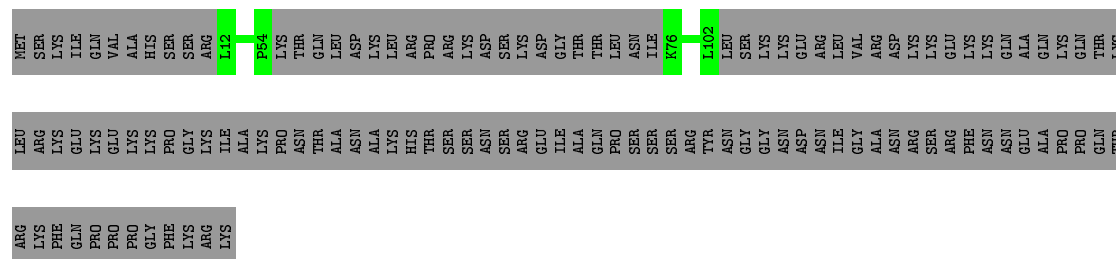
- Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain b:  36% 64%



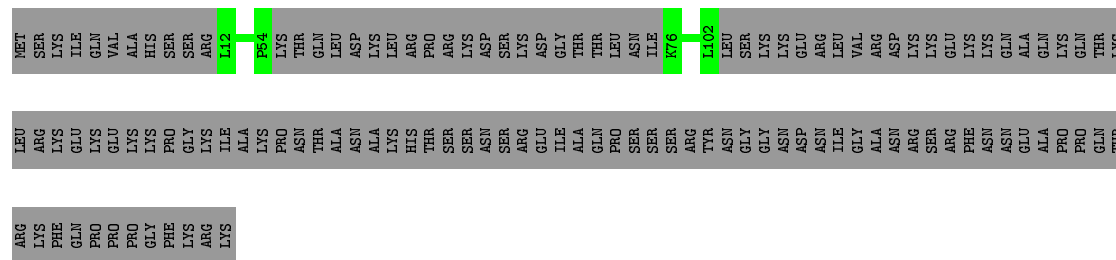
- Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain k:  36% 64%




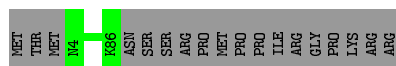
- Molecule 35: Small nuclear ribonucleoprotein-associated protein B

Chain s:  36% 64%




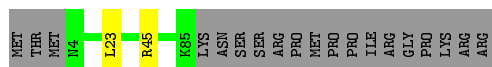
- Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain d:  82% 18%




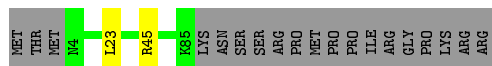
- Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain n:  79% 19%




- Molecule 36: Small nuclear ribonucleoprotein Sm D3

Chain v:  79% 19%




- Molecule 37: Small nuclear ribonucleoprotein E

Chain e:  82% 18%




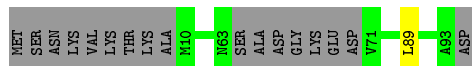
- Molecule 37: Small nuclear ribonucleoprotein E

Chain p:  81% 18%




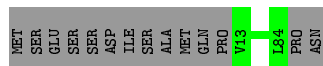
- Molecule 37: Small nuclear ribonucleoprotein E

Chain w:  81% 18%




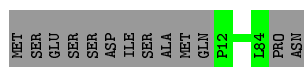
- Molecule 38: Small nuclear ribonucleoprotein F

Chain f:  84% 16%

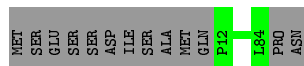
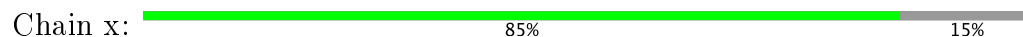


- Molecule 38: Small nuclear ribonucleoprotein F

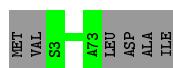
Chain q:  85% 15%



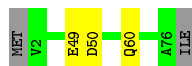
- Molecule 38: Small nuclear ribonucleoprotein F



- Molecule 39: Small nuclear ribonucleoprotein G



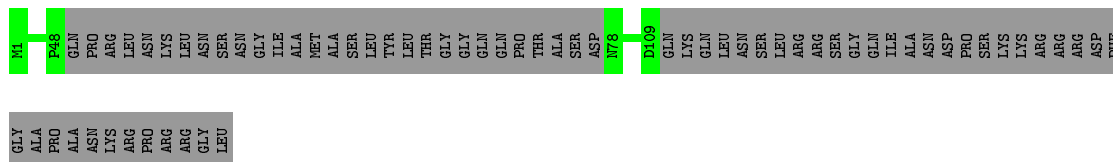
- Molecule 39: Small nuclear ribonucleoprotein G



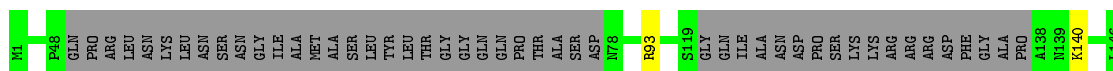
- Molecule 39: Small nuclear ribonucleoprotein G



- Molecule 40: Small nuclear ribonucleoprotein Sm D1

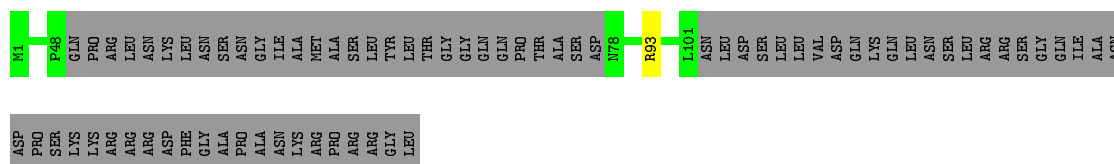


- Molecule 40: Small nuclear ribonucleoprotein Sm D1



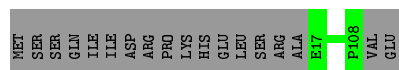
- Molecule 40: Small nuclear ribonucleoprotein Sm D1





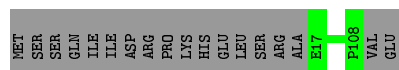
- Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain i: 84% 16%



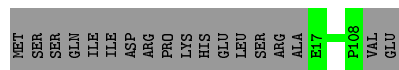
- Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain m: 84% 16%



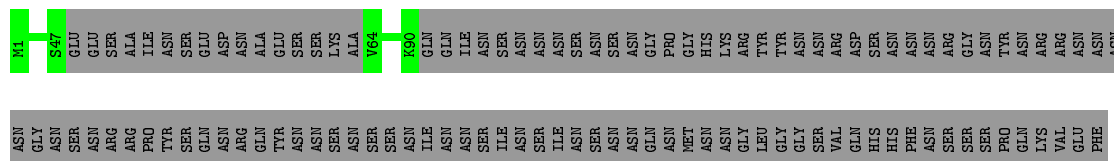
- Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain u: 84% 16%



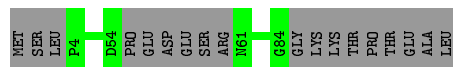
- Molecule 42: U6 snRNA-associated Sm-like protein LSm4

Chain j: 40% 60%



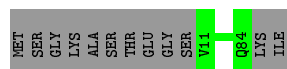
- Molecule 43: U6 snRNA-associated Sm-like protein LSm5

Chain o: 81% 19%



- Molecule 44: U6 snRNA-associated Sm-like protein LSm6

Chain z: 86% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9559	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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	5300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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, ZN, PSU

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 >2	RMSZ	# Z >2
1	2	1.35	52/3579 (1.5%)	1.69	123/5551 (2.2%)
10	C	0.32	0/6928	0.47	0/9377
11	D	0.28	0/1185	0.46	0/1596
12	E	0.24	0/822	0.40	0/1109
13	F	0.27	0/3292	0.45	1/4432 (0.0%)
14	G	0.29	0/2885	0.45	0/3882
15	H	0.27	0/3455	0.49	0/4663
16	I	0.28	0/665	0.82	0/1024
17	J	0.26	0/6613	0.43	0/8942
18	K	0.26	0/949	0.45	0/1292
19	L	0.25	0/899	0.44	0/1204
2	3	0.25	0/617	0.45	0/836
20	M	0.24	0/1430	0.44	0/1927
21	N	0.22	0/421	0.29	0/583
22	O	0.28	0/6745	0.45	0/9157
23	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
24	Q	0.27	0/1835	0.46	0/2480
25	R	0.26	0/1453	0.42	0/1954
26	S	0.29	0/827	0.46	0/1105
27	T	0.27	0/3992	0.41	0/5346
28	U	0.25	0/1511	0.41	1/2038 (0.0%)
29	V	0.24	0/1105	0.36	0/1475
3	4	0.45	4/2705 (0.1%)	0.95	10/4204 (0.2%)
30	W	0.42	0/1406	0.69	4/1905 (0.2%)
31	X	0.25	0/148	0.39	0/204
32	Y	0.30	0/692	0.54	0/923
33	Z	0.28	0/694	0.47	0/929
34	a	0.26	0/745	0.51	1/1005 (0.1%)
35	b	0.29	0/567	0.47	0/762
35	k	0.41	0/567	0.61	0/762
35	s	0.40	0/567	0.63	0/762
36	d	0.30	0/650	0.50	0/879

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
36	n	0.41	0/641	0.65	2/868 (0.2%)
36	v	0.43	0/641	0.65	2/868 (0.2%)
37	e	0.26	0/612	0.44	0/830
37	p	0.39	0/612	0.59	1/830 (0.1%)
37	w	0.40	0/612	0.61	1/830 (0.1%)
38	f	0.27	0/589	0.46	0/796
38	q	0.39	0/597	0.62	0/807
38	x	0.42	0/597	0.63	0/807
39	g	0.25	0/554	0.53	0/746
39	r	0.32	0/582	0.63	0/785
39	y	0.26	0/582	0.49	0/785
4	5	0.42	1/4039 (0.0%)	0.90	6/6284 (0.1%)
40	h	0.25	0/635	0.48	0/861
40	l	0.38	0/756	0.70	1/1023 (0.1%)
40	t	0.41	0/574	0.68	1/777 (0.1%)
41	i	0.25	0/764	0.44	0/1026
41	m	0.38	0/764	0.57	0/1026
41	u	0.40	0/764	0.57	0/1026
42	j	0.25	0/594	0.42	0/802
43	o	0.24	0/595	0.41	0/806
44	z	0.24	0/584	0.43	0/787
5	6	0.24	0/2253	0.83	3/3497 (0.1%)
6	7	0.24	0/505	0.44	0/675
7	8	0.24	0/501	0.45	0/673
8	A	0.29	0/18580	0.46	1/25189 (0.0%)
9	B	0.40	1/13905 (0.0%)	0.62	6/18852 (0.0%)
All	All	0.39	59/122004 (0.0%)	0.62	165/167605 (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	2	0	2
17	J	0	2
20	M	0	2
23	P	0	2
27	T	0	1
30	W	0	1
39	r	0	1
8	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	B	0	4
All	All	0	17

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1149	G	O3'-P	24.35	1.90	1.61
1	2	143	G	O3'-P	18.92	1.83	1.61
4	5	105	A	O3'-P	18.04	1.82	1.61
1	2	1161	U	O3'-P	-15.56	1.42	1.61
1	2	143	G	C3'-O3'	15.28	1.63	1.42

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40
1	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
1	2	1162	U	C5'-C4'-O4'	14.80	126.86	109.10
1	2	1147	A	C5'-C4'-C3'	-14.15	93.35	116.00
1	2	1092	A	C2'-C3'-O3'	14.11	140.53	109.50

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1109	C	Sidechain
1	2	141	A	Sidechain
8	A	1190	ASN	Peptide
8	A	1481	GLU	Peptide
9	B	684	LEU	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	2	3275	0	1663	200	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	611	0	620	14	0
3	4	2423	0	1216	138	0
4	5	3615	0	1829	155	0
5	6	2019	0	1022	97	0
6	7	504	0	557	4	0
7	8	498	0	533	15	0
8	A	18122	0	18041	931	0
9	B	13607	0	13606	682	0
10	C	6784	0	6967	283	0
11	D	1164	0	1152	59	0
12	E	825	0	657	38	0
13	F	3238	0	3345	146	0
14	G	2835	0	2608	111	0
15	H	3396	0	3364	190	0
16	I	600	0	310	30	0
17	J	6485	0	6515	311	0
18	K	936	0	987	49	0
19	L	882	0	844	60	0
20	M	1407	0	1416	79	0
21	N	425	0	183	3	0
22	O	6612	0	6823	302	0
23	P	9437	0	9532	470	0
24	Q	1786	0	1778	67	0
25	R	1429	0	1458	42	0
26	S	814	0	809	44	0
27	T	3915	0	3853	140	0
28	U	1488	0	1410	67	0
29	V	1084	0	1081	50	0
30	W	1383	0	1407	221	0
31	X	150	0	151	7	0
32	Y	683	0	715	89	0
33	Z	685	0	693	29	0
34	a	735	0	744	0	0
35	b	563	0	600	0	0
35	k	563	0	600	0	0
35	s	563	0	598	0	0
36	d	641	0	666	0	0
36	n	632	0	653	0	0
36	v	632	0	653	0	0
37	e	602	0	631	0	0
37	p	602	0	631	0	0
37	w	602	0	631	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	f	578	0	579	0	0
38	q	585	0	587	0	0
38	x	585	0	587	0	0
39	g	549	0	566	0	0
39	r	577	0	595	0	0
39	y	577	0	595	0	0
40	h	630	0	677	0	0
40	l	751	0	776	0	0
40	t	569	0	616	0	0
41	i	752	0	786	0	0
41	m	752	0	786	0	0
41	u	752	0	786	0	0
42	j	588	0	602	0	0
43	o	588	0	594	0	0
44	z	577	0	572	0	0
45	C	32	0	12	4	0
46	L	1	0	0	0	0
46	S	3	0	0	0	0
46	T	2	0	0	0	0
46	U	1	0	0	0	0
All	All	118701	0	113268	4465	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 23.

The worst 5 of 4465 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)
3:4:67:A:C2	9:B:716:LEU:HD21	1.32	1.63
8:A:2398:LEU:HD13	9:B:1060:LYS:CD	1.37	1.53
1:2:143:G:C3'	1:2:143:G:O3'	1.63	1.44
9:B:1070:ASP:OD2	12:E:208:LYS:CD	1.64	1.44
8:A:144:ASN:HB3	20:M:19:ASN:ND2	1.32	1.42

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	
2	3	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
6	7	62/115 (54%)	62 (100%)	0	0	100	100
7	8	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
8	A	2202/2413 (91%)	2095 (95%)	105 (5%)	2 (0%)	55	88
9	B	1694/2163 (78%)	1631 (96%)	60 (4%)	3 (0%)	51	84
10	C	838/1008 (83%)	785 (94%)	52 (6%)	1 (0%)	55	88
11	D	140/143 (98%)	126 (90%)	14 (10%)	0	100	100
12	E	114/587 (19%)	103 (90%)	9 (8%)	2 (2%)	10	49
13	F	409/494 (83%)	387 (95%)	21 (5%)	1 (0%)	51	84
14	G	358/469 (76%)	335 (94%)	23 (6%)	0	100	100
15	H	425/465 (91%)	398 (94%)	27 (6%)	0	100	100
17	J	788/899 (88%)	722 (92%)	61 (8%)	5 (1%)	28	71
18	K	122/126 (97%)	121 (99%)	1 (1%)	0	100	100
19	L	101/194 (52%)	94 (93%)	7 (7%)	0	100	100
20	M	164/242 (68%)	141 (86%)	23 (14%)	0	100	100
21	N	77/291 (26%)	76 (99%)	1 (1%)	0	100	100
22	O	829/971 (85%)	789 (95%)	40 (5%)	0	100	100
23	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	28	71
24	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	32	74
25	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
26	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
27	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
28	U	188/266 (71%)	159 (85%)	28 (15%)	1 (0%)	32	74
29	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
30	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	X	26/111 (23%)	26 (100%)	0	0	100	100
32	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	15	57
33	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	15	57
34	a	88/95 (93%)	81 (92%)	7 (8%)	0	100	100
35	b	66/196 (34%)	61 (92%)	5 (8%)	0	100	100
35	k	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
35	s	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
36	d	81/101 (80%)	79 (98%)	2 (2%)	0	100	100
36	n	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
36	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
37	e	73/94 (78%)	71 (97%)	2 (3%)	0	100	100
37	p	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
37	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
38	f	70/86 (81%)	67 (96%)	3 (4%)	0	100	100
38	q	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
38	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
39	g	69/77 (90%)	63 (91%)	6 (9%)	0	100	100
39	r	73/77 (95%)	66 (90%)	5 (7%)	2 (3%)	6	40
39	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	3	30
40	h	76/146 (52%)	75 (99%)	1 (1%)	0	100	100
40	l	93/146 (64%)	89 (96%)	3 (3%)	1 (1%)	17	60
40	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
41	i	90/110 (82%)	90 (100%)	0	0	100	100
41	m	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
41	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
42	j	70/187 (37%)	67 (96%)	3 (4%)	0	100	100
43	o	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
44	z	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
All	All	13125/17406 (75%)	12318 (94%)	765 (6%)	42 (0%)	48	81

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	881	VAL
23	P	1299	ILE
24	Q	368	ILE
30	W	34	LEU
30	W	52	LYS

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	
2	3	71/81 (88%)	71 (100%)	0	100	100
6	7	56/103 (54%)	56 (100%)	0	100	100
7	8	56/99 (57%)	56 (100%)	0	100	100
8	A	1982/2182 (91%)	1982 (100%)	0	100	100
9	B	1525/1955 (78%)	1523 (100%)	2 (0%)	94	97
10	C	761/910 (84%)	761 (100%)	0	100	100
11	D	131/132 (99%)	131 (100%)	0	100	100
12	E	60/534 (11%)	60 (100%)	0	100	100
13	F	354/445 (80%)	354 (100%)	0	100	100
14	G	267/436 (61%)	267 (100%)	0	100	100
15	H	377/410 (92%)	377 (100%)	0	100	100
17	J	708/813 (87%)	708 (100%)	0	100	100
18	K	102/104 (98%)	102 (100%)	0	100	100
19	L	92/179 (51%)	92 (100%)	0	100	100
20	M	154/224 (69%)	154 (100%)	0	100	100
22	O	739/867 (85%)	738 (100%)	1 (0%)	94	97
23	P	1093/1244 (88%)	1093 (100%)	0	100	100
24	Q	192/391 (49%)	192 (100%)	0	100	100
25	R	154/189 (82%)	154 (100%)	0	100	100
26	S	93/97 (96%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	T	429/492 (87%)	424 (99%)	5 (1%)	75	88
28	U	158/236 (67%)	157 (99%)	1 (1%)	89	94
29	V	118/259 (46%)	116 (98%)	2 (2%)	66	84
30	W	161/219 (74%)	151 (94%)	10 (6%)	21	54
32	Y	76/100 (76%)	75 (99%)	1 (1%)	73	87
33	Z	75/77 (97%)	75 (100%)	0	100	100
34	a	85/91 (93%)	85 (100%)	0	100	100
35	b	64/176 (36%)	64 (100%)	0	100	100
35	k	64/176 (36%)	64 (100%)	0	100	100
35	s	64/176 (36%)	64 (100%)	0	100	100
36	d	72/89 (81%)	72 (100%)	0	100	100
36	n	71/89 (80%)	71 (100%)	0	100	100
36	v	71/89 (80%)	71 (100%)	0	100	100
37	e	69/83 (83%)	69 (100%)	0	100	100
37	p	69/83 (83%)	69 (100%)	0	100	100
37	w	69/83 (83%)	69 (100%)	0	100	100
38	f	64/77 (83%)	64 (100%)	0	100	100
38	q	65/77 (84%)	65 (100%)	0	100	100
38	x	65/77 (84%)	65 (100%)	0	100	100
39	g	61/66 (92%)	61 (100%)	0	100	100
39	r	64/66 (97%)	64 (100%)	0	100	100
39	y	64/66 (97%)	64 (100%)	0	100	100
40	h	75/129 (58%)	75 (100%)	0	100	100
40	l	81/129 (63%)	81 (100%)	0	100	100
40	t	67/129 (52%)	67 (100%)	0	100	100
41	i	85/103 (82%)	85 (100%)	0	100	100
41	m	85/103 (82%)	85 (100%)	0	100	100
41	u	85/103 (82%)	85 (100%)	0	100	100
42	j	64/172 (37%)	64 (100%)	0	100	100
43	o	66/84 (79%)	66 (100%)	0	100	100
44	z	66/75 (88%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11739/15369 (76%)	11717 (100%)	22 (0%)	95 97

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	V	129	HIS
30	W	8	VAL
30	W	160	THR
29	V	158	ARG
30	W	4	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 193 such sidechains are listed below:

Mol	Chain	Res	Type
15	H	160	GLN
20	M	19	ASN
41	m	52	HIS
15	H	203	ASN
17	J	379	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	147/1175 (12%)	47 (31%)	25 (17%)
16	I	26/95 (27%)	8 (30%)	2 (7%)
3	4	110/160 (68%)	33 (30%)	6 (5%)
4	5	166/214 (77%)	61 (36%)	8 (4%)
5	6	91/112 (81%)	33 (36%)	8 (8%)
All	All	540/1756 (30%)	182 (33%)	49 (9%)

5 of 182 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	33	U
1	2	41	C
1	2	46	C
1	2	47	U
1	2	66	A

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1142	G
3	4	39	C
5	6	83	A
1	2	1145	U
3	4	91	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	PSU	2	35	1,16	16,21,22	1.08	1 (6%)	20,30,33	3.45	6 (30%)
1	PSU	2	42	1,16	16,21,22	1.12	2 (12%)	20,30,33	3.57	6 (30%)
1	PSU	2	44	1,16	16,21,22	1.08	1 (6%)	20,30,33	3.58	7 (35%)

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
1	PSU	2	35	1,16	-	0/7/25/26	0/2/2/2
1	PSU	2	42	1,16	-	0/7/25/26	0/2/2/2
1	PSU	2	44	1,16	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	42	PSU	C5-C1'	-2.10	1.50	1.52
1	2	44	PSU	C4-N3	2.72	1.38	1.33
1	2	35	PSU	C4-N3	2.72	1.38	1.33
1	2	42	PSU	C4-N3	2.77	1.38	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	2	44	PSU	N1-C2-N3	-11.70	119.98	128.40
1	2	35	PSU	N1-C2-N3	-11.56	120.08	128.40
1	2	42	PSU	N1-C2-N3	-11.48	120.14	128.40
1	2	44	PSU	C5-C4-N3	-7.33	119.41	125.43
1	2	42	PSU	C5-C4-N3	-6.80	119.85	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	35	PSU	1	0
1	2	42	PSU	2	0
1	2	44	PSU	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	GTP	C	1101	-	27,34,34	0.91	1 (3%)	27,54,54	1.57	4 (14%)

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
45	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1101	GTP	C6-N1	2.65	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1101	GTP	N3-C2-N1	-4.97	120.20	127.46
45	C	1101	GTP	C5-C6-N1	-2.50	119.93	123.48
45	C	1101	GTP	C6-N1-C2	2.47	119.61	116.06
45	C	1101	GTP	C2-N3-C4	4.39	120.29	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	1101	GTP	4	0

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
1	2	3
4	5	3
31	X	1
12	E	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	236:SER	C	297:LYS	N	126.30
1	X	19:ALA	C	101:ALA	N	56.70
1	5	72:C	O3'	73:U	P	3.93
1	5	42:A	O3'	43:G	P	3.10
1	2	1149:G	O3'	1150:U	P	1.90