



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 21, 2017 – 11:46 PM EDT

PDB ID : 5LJ5
EMDB ID: : EMD-4057
Title : Overall structure of the yeast spliceosome immediately after branching.
Authors : Galej, W.P.; Wilkinson, M.F.; Fica, S.M.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : unknown
Resolution : 3.80 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-20029824

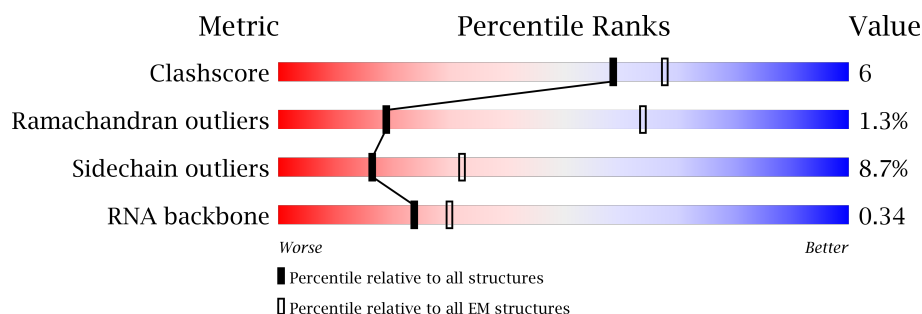
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.











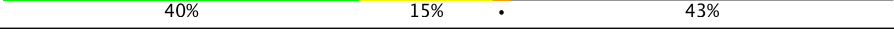

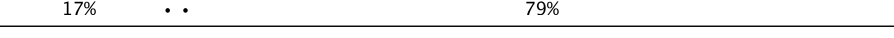
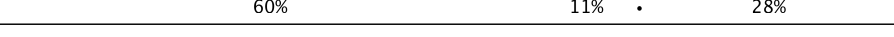

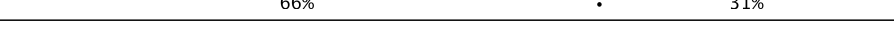


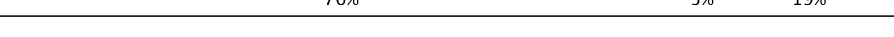

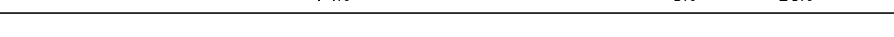






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	U	179	<div> <div>33%</div> <div>36%</div> <div>9%</div> <div>•</div> <div>21%</div> </div>
2	E	16	<div> <div>25%</div> <div>63%</div> <div>13%</div> </div>
3	I	76	<div> <div>22%</div> <div>20%</div> <div>•</div> <div>57%</div> </div>
4	Z	1175	<div> <div>9%</div> <div>5%</div> <div>85%</div> </div>
5	V	112	<div> <div>42%</div> <div>31%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>
6	A	2413	<div> <div>73%</div> <div>15%</div> <div>•</div> <div>10%</div> </div>
7	B	2163	<div> <div>77%</div> <div>•</div> <div>21%</div> </div>
8	D	278	<div> <div>34%</div> <div>7%</div> <div>59%</div> </div>






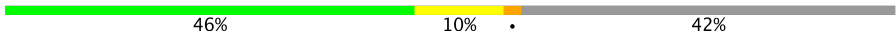






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Mol	Chain	Length	Quality of chain
9	F	179	
10	C	1008	
11	G	235	
12	H	591	
13	J	451	
14	K	379	
15	L	157	
16	M	339	
17	N	364	
18	O	590	
19	P	175	
20	R	135	
21	S	687	
22	T	859	
23	b	196	
23	k	196	
24	d	101	
24	n	101	
25	e	94	
25	p	94	
26	f	86	
26	q	86	
27	g	77	
27	r	77	
28	h	146	

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Mol	Chain	Length	Quality of chain
28	l	146	
29	j	110	
29	m	110	
30	W	238	
31	Y	111	
32	Q	1071	
33	t	503	
33	u	503	
33	v	503	
33	w	503	
34	s	175	
35	x	188	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	ZN	N	401	-	-	X	-
37	ZN	N	402	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 85476 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 U5 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 2 is a RNA chain called Exon 1 (5' exon) of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	16	Total	C	N	O	P	0	0
			346	155	66	109	16		

- Molecule 3 is a RNA chain called Intron of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	33	Total	C	N	O	P	0	0
			693	312	116	232	33		

- Molecule 4 is a RNA chain called U2 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	171	Total	C	N	O	P	0	0
			3610	1614	604	1221	171		

- Molecule 5 is a RNA chain called U6 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	97	Total	C	N	O	P	0	0
			2066	925	368	676	97		

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2168	Total	C	N	O	S	0	0
			16919	10835	2966	3060	58		

- Molecule 7 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1707	Total	C	N	O	1	0
			8462	5048	1707	1707		

- Molecule 8 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	114	Total	C	N	O	S	0	0
			912	577	165	162	8		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	46	Total	C	N	O	0	0
			321	203	61	57		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	882	Total	C	N	O	S	0	0
			6756	4393	1133	1203	27		

- Molecule 11 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			823	513	154	155	1		

- Molecule 12 is a protein called CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	399	Total	C	N	O	S	0	0
			2639	1657	468	506	8		

- Molecule 13 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	326	Total	C	N	O	S	0	0
			2556	1616	454	476	10		

- Molecule 14 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	163	Total	C	N	O	S	0	0
			1289	808	236	240	5		

- Molecule 15 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1270	797	238	225	10		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	252	Total	C	N	O	S	0	0
			2012	1277	354	370	11		

- Molecule 17 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	209	Total	C	N	O	S	0	0
			1658	1055	287	301	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	283	Total	C	N	O	S	0	0
			2068	1285	385	392	6		

- Molecule 19 is a protein called CWC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	36	Total	C	N	O	0	0
			275	176	53	46		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	97	Total	C	N	O	0	0
			544	325	106	113		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	464	Total	C	N	O	S	0	0
			3121	1949	581	584	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	592	Total	C	N	O	0	0
			2946	1762	592	592		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
23	k	80	Total	C	N	O		0	0
			396	236	80	80			

- Molecule 24 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
24	n	82	Total	C	N	O		0	0
			404	240	82	82			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
25	p	75	Total	C	N	O		0	0
			369	219	75	75			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
26	q	72	Total	C	N	O		0	0
			354	210	72	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	r	69	Total	C	N	O		0	0
			340	202	69	69			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
28	l	79	Total	C	N	O		0	0
			392	234	79	79			

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
29	m	94	Total	C	N	O		0	0
			467	279	94	94			

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	164	Total	C	N	O	0	0
			816	488	164	164		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 32 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Q	619	Total	C	N	O	0	0
			3066	1828	619	619		

- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
33	u	437	Total	C	N	O	0	0
			2166	1292	437	437		
33	v	426	Total	C	N	O	0	0
			2111	1259	426	426		
33	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 35 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	132	Total	C	N	O	0	0
			660	396	132	132		

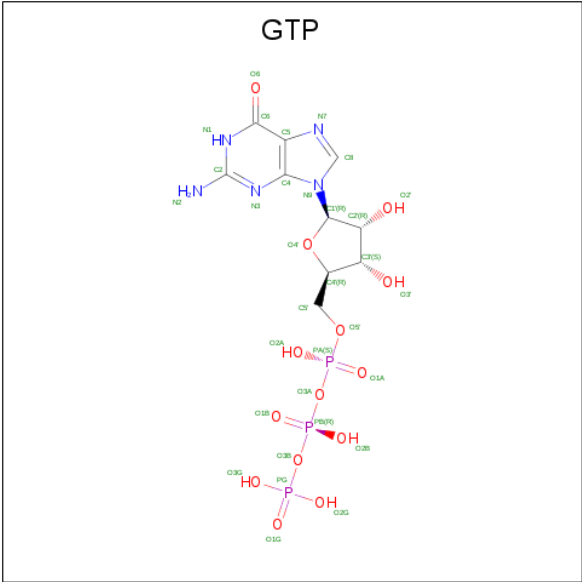
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	V	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

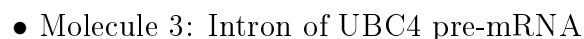
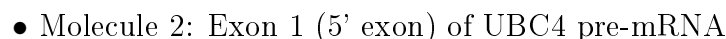
Mol	Chain	Residues	Atoms		AltConf
37	L	3	Total	Zn	0
			3	3	
37	D	1	Total	Zn	0
			1	1	
37	N	2	Total	Zn	0
			2	2	
37	M	1	Total	Zn	0
			1	1	

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



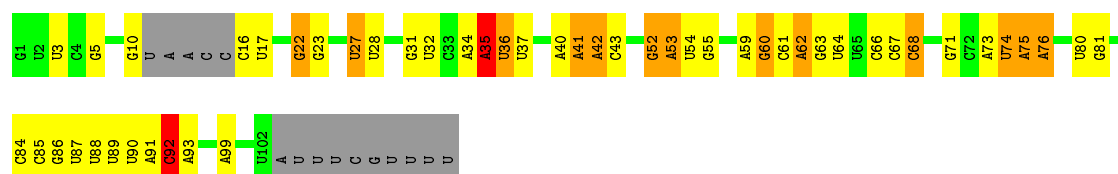
Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 1: U5 snRNA (small nuclear RNA)





- Chain V:  42% 31% 12% • 13%




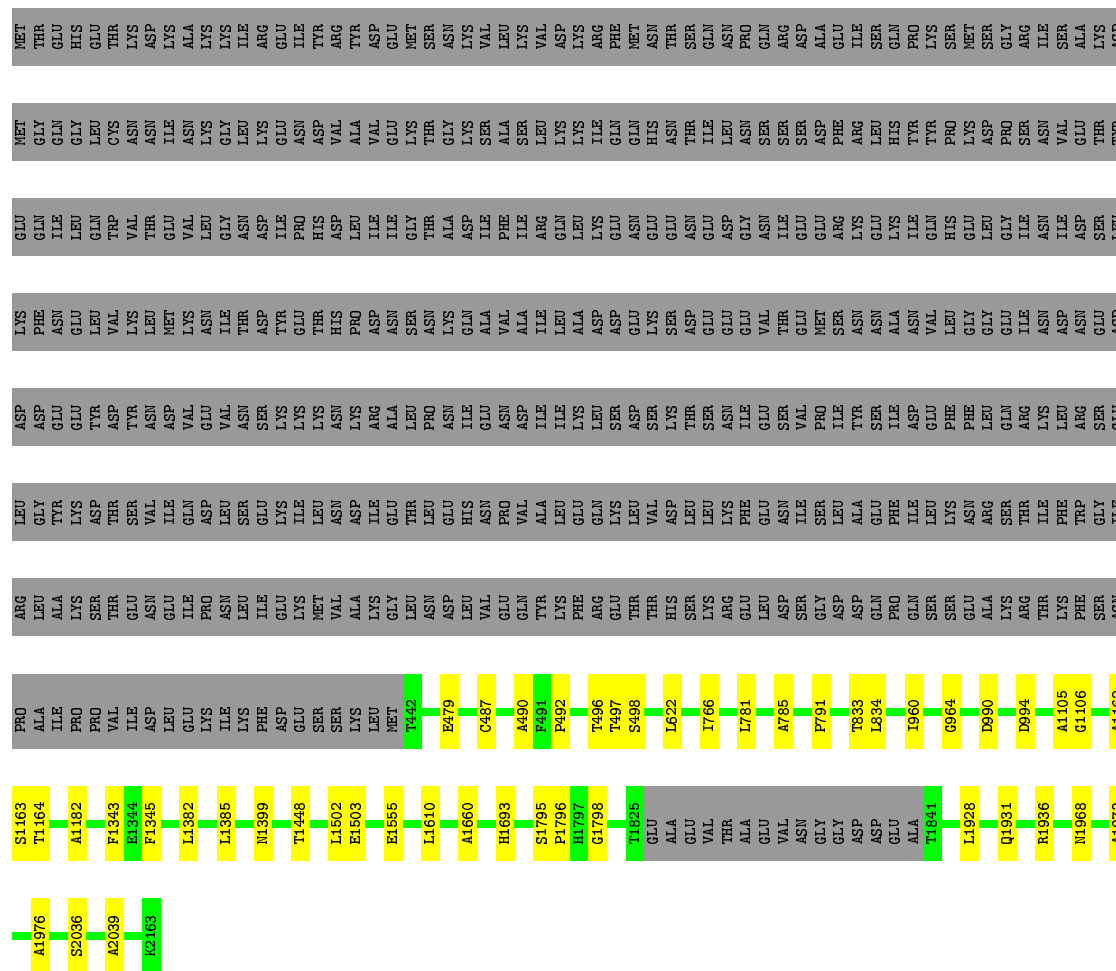
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Chain A:  73% 15% 10%

VAL	VAL	V1977	Q1737	Y1542	I1367	V1248	A1047	I882	A753	Q648	Y480	I370	K221	LYS	ILE
ALA	ALA	V1978	L1738	R1543	Q1368	V1249	V1048	K889	I753	L649	K493	R376	R225	ALA	ASN
SER	SER	W2048	D1742	V1546	M1369	Y1251	L1049	K893	I754	I656	L507	R376	R228	ALA	ALA
ASP	ASP	L2060	S1749	L1557	V1371	N1255	L1054	L912	I755	H659	L508	L390	F239	SER	GLU
GLU	GLU	E2078	V1752	T1560	L1373	L1258	T1064	L919	L756	I660	Y514	P395	P244	ASN	ILE
SER	SER	G2085	F1756	L1561	G1374	E1277	L1065	V922	K759	I663	S521	P395	P244	LEU	ASP
THR	THR	GLN	T1760	F1562	L1375	E1277	L1066	V922	I766	G665	Y522	V398	P244	ASP	THR
SER	SER	ASN	T1760	T1565	K1378	D1282	N1067	V922	I766	I666	Y522	V398	P244	LEU	THR
SER	SER	ILE	N1763	V1570	M1379	D1282	I1078	V922	I766	I666	Y522	V398	P244	LEU	THR
LYS	LYS	PRO	L1779	F1574	F1382	V1286	T1083	V922	I766	I666	Y522	V398	P244	LEU	THR
ALA	ALA	SER	K1795	K1589	F1383	V1286	A1084	V922	I766	I666	Y522	V398	P244	LEU	THR
VAL	VAL	VAL	P1796	L1590	V1387	L1302	V1088	V922	I766	I666	Y522	V398	P244	LEU	THR
ARG	ARG	ARG	S1801	A1593	K1392	I1309	V1089	V922	I766	I666	Y522	V398	P244	LEU	THR
GLN	GLN	GLN	M1802	L1598	E1393	K1310	V1098	V922	I766	I666	Y522	V398	P244	LEU	THR
LYS	LYS	LYS	R1803	L1599	L1394	R1315	M1098	V922	I766	I666	Y522	V398	P244	LEU	THR
MET	MET	MET	M1806	Q1600	L1397	I1316	M1099	V922	I766	I666	Y522	V398	P244	LEU	THR
ALA	ALA	ALA	M1806	T1601	L1397	R1317	M1099	V922	I766	I666	Y522	V398	P244	LEU	THR
GLU	GLU	GLU	L1815	P1602	T1400	S1323	L1103	V922	I766	I666	Y522	V398	P244	LEU	THR
LEU	LEU	LEU	R1820	R1604	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
GLU	GLU	GLU	L1823	L1609	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ASP	ASP	ASP	Q1824	V1610	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
LYS	LYS	LYS	Q1827	I1614	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
GLN	GLN	GLN	S1827	V1620	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ASN	ASN	ASN	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ASP	ASP	ASP	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
GLU	GLU	GLU	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ALA	ALA	ALA	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
GLU	GLU	GLU	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ALA	ALA	ALA	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ILE	ILE	ILE	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
ASP	ASP	ASP	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
VAL	VAL	VAL	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
PHE	PHE	PHE	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR
SER	SER	SER	S1827	V1621	T1400	G1324	L1113	V922	I766	I666	Y522	V398	P244	LEU	THR

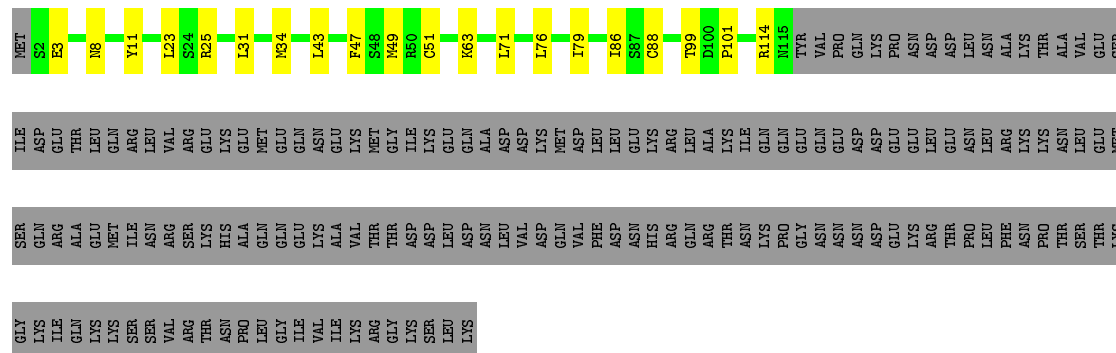
- Molecule 7: Pre-mRNA-splicing helicase BRR2

Chain B:  77% 21%



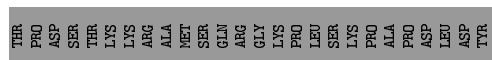
- Molecule 8: Protein CWC16

Chain D:  34% 7% 59%



- Molecule 9: Pre-mRNA-splicing factor CWC25

Chain F:  23% 74%



Chain C:  66% 20% • 13%

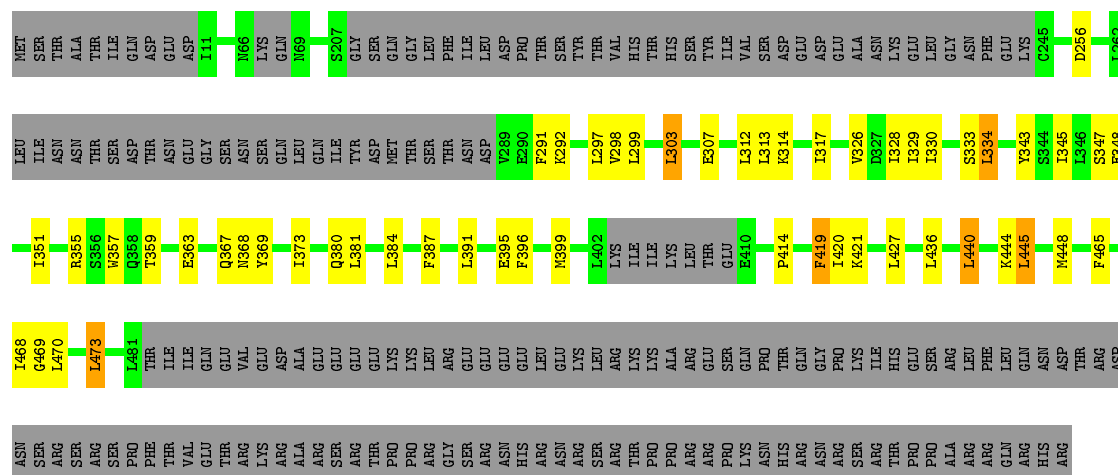


Chain G:  34% 6% 59%



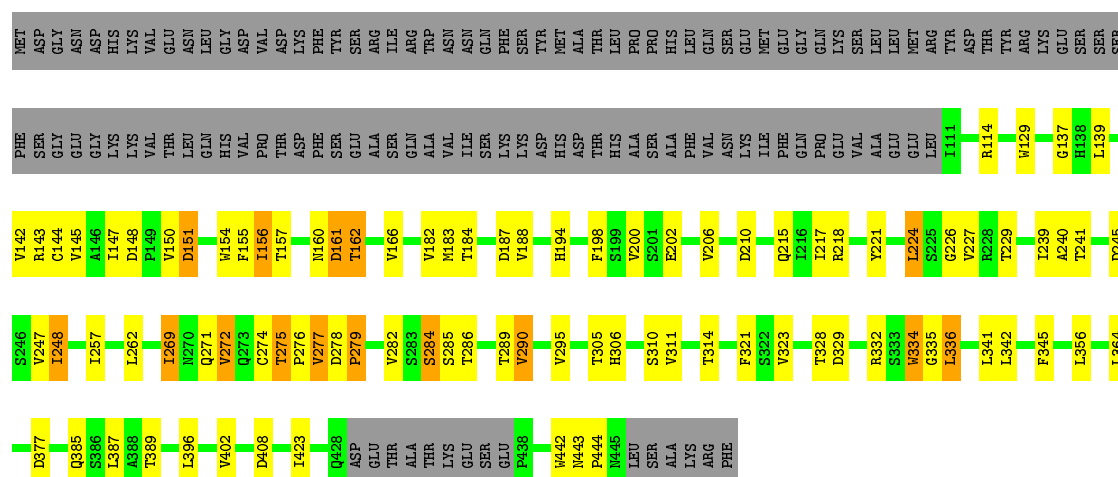
- Molecule 12: CWC22

Chain H: 58% 8% 32%



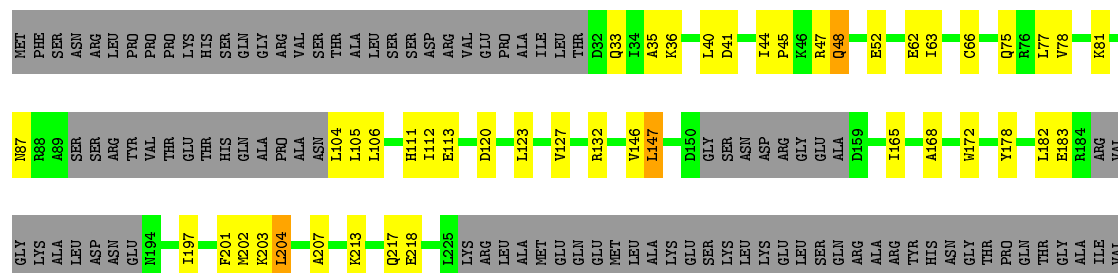
- Molecule 13: Pre-mRNA-splicing factor PRP46

Chain J:  52% 17% 0% 28%



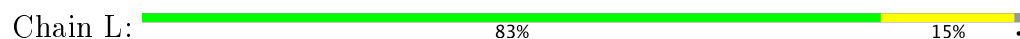
- Molecule 14: Pre-mRNA-processing protein 45

Chain K:  31% 11% . 57%

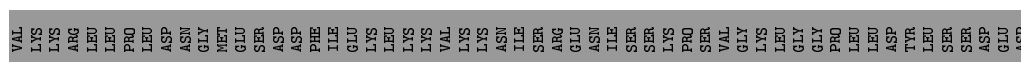
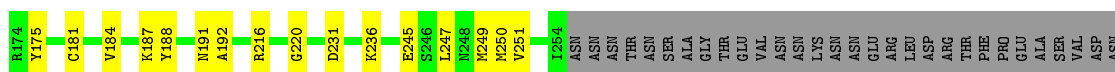




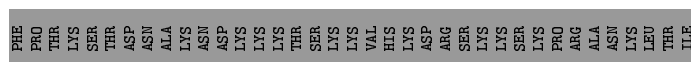
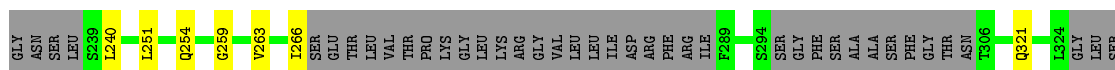
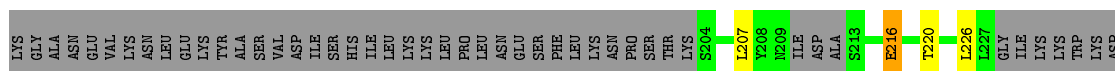
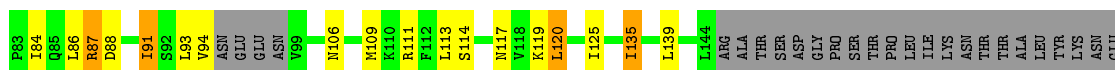
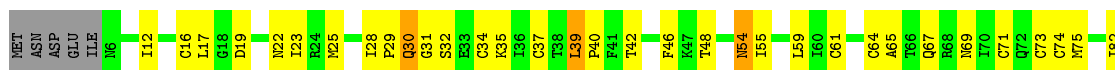
- Molecule 15: Pre-mRNA-splicing factor BUD31



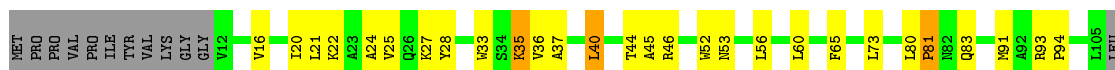
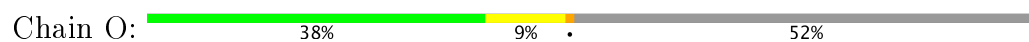
- Molecule 16: Pre-mRNA-splicing factor CWC2

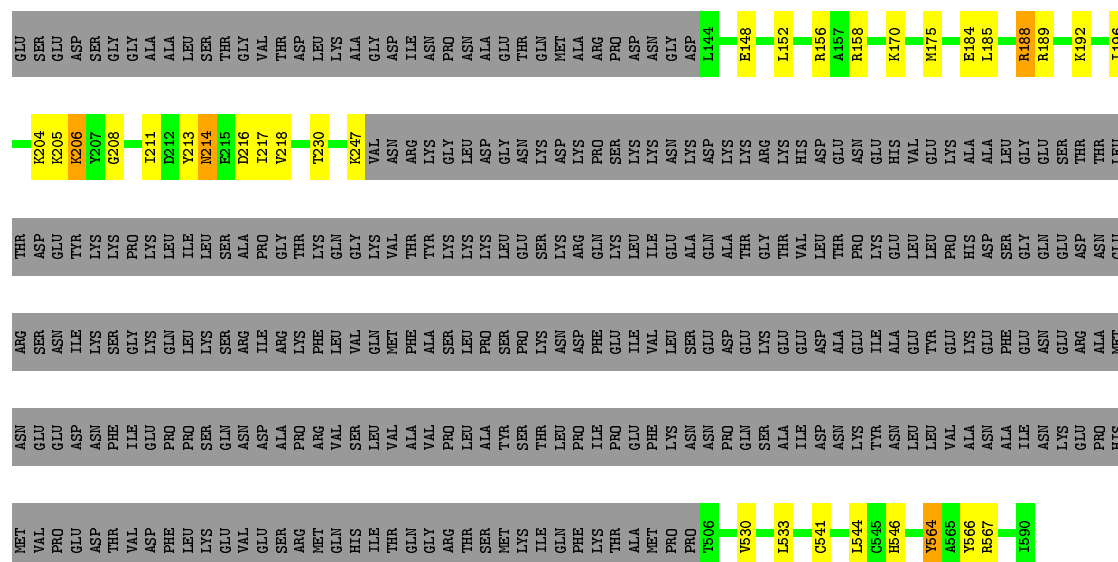


- Molecule 17: Pre-mRNA-splicing factor SLT11



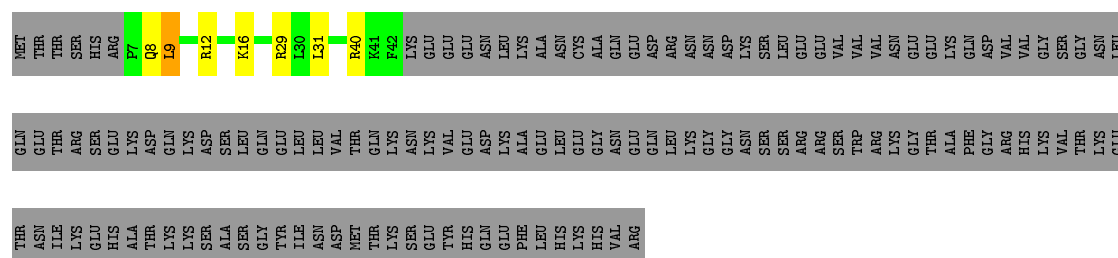
- Molecule 18: Pre-mRNA-splicing factor CEF1





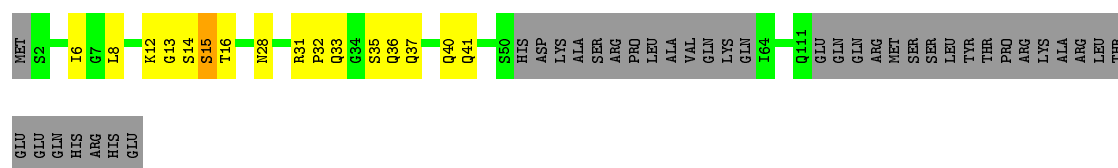
• Molecule 19: CWC15

Chain P: 17% 79%



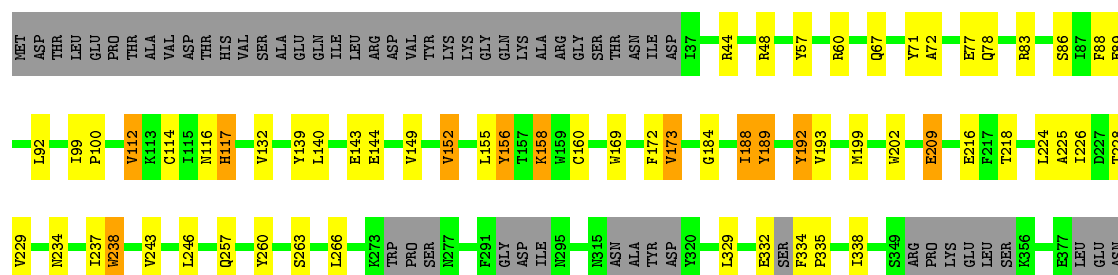
• Molecule 20: Pre-mRNA-splicing factor CWC21

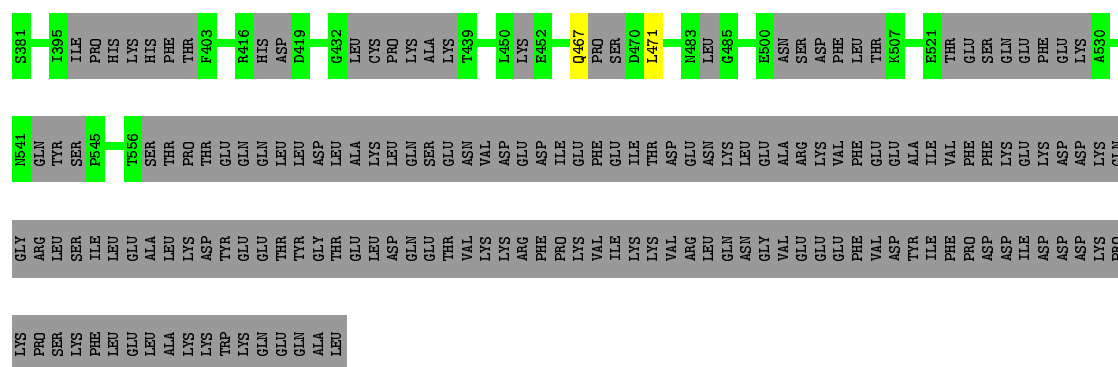
Chain R: 60% 11% 28%



• Molecule 21: Pre-mRNA-splicing factor CLF1

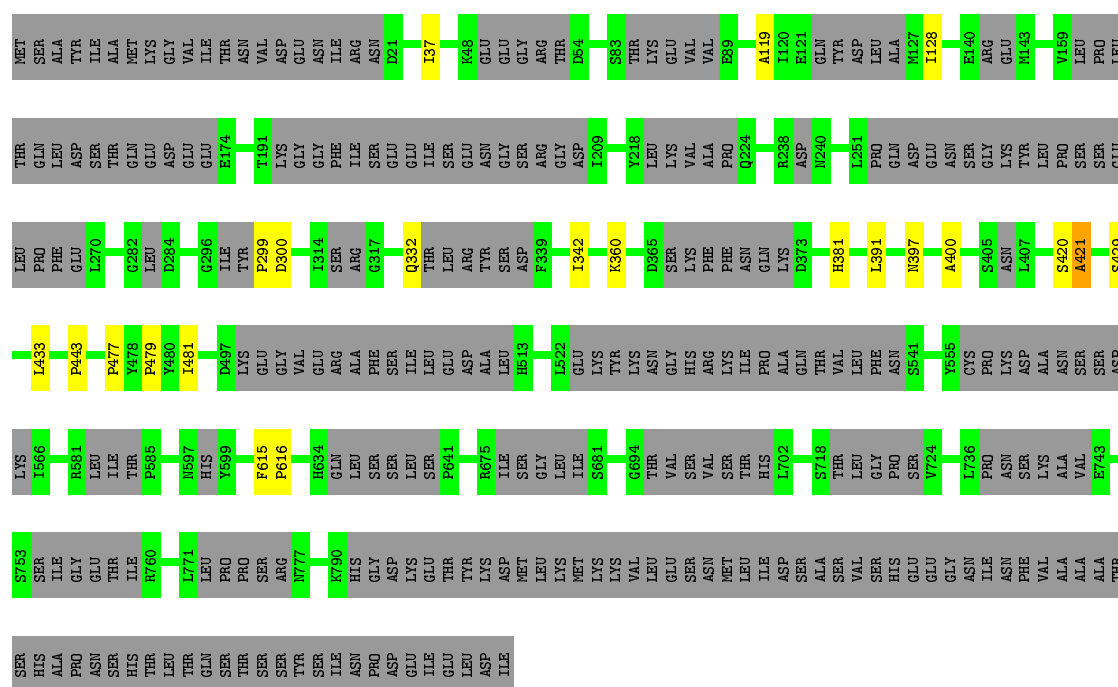
Chain S: 58% 8% 32%





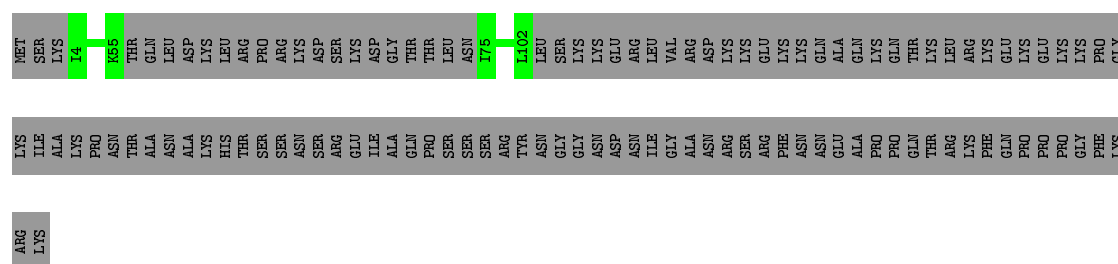
• Molecule 22: Pre-mRNA-splicing factor SYF1

Chain T: 66% 31%



• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain b: 41% 59%



• Molecule 23: Small nuclear ribonucleoprotein-associated protein B


[illegible][illegible]

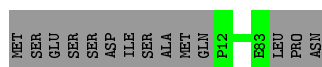
MET	THR	MET	N4	K85	LYS	ASN	SER	SER	ARG	PRO	MET	PRO	PRO	ILE	ARG	GLY	PRO	LYS	ARG	ARG
-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

MEI	SEN	ASN	LYS	VAL	THR	LYS	ALA	M10	G16	I17	F18	T25	S64	ALA	ASP	GLY	LYS	GLU	ASP	VAL	GLU	K73	K79	I80	L81	S92	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

MET SER ASN LYS VAL LYS THR LYS ALA M10 S64 ALA ASP GLY LYS GLU ASP VAL GLU K73 G74 S92 ALA ASP

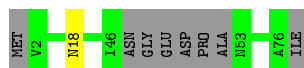
MET
SER
GLU
SER
SER
ASP
ILE
SER
ALA
MET
MET
GLN
P12
P15
T36
L79
E83
LEU
PRO
ASN

Chain q:  84% 16%



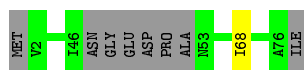
- Molecule 27: Small nuclear ribonucleoprotein G

Chain g: 88% 10%



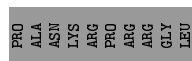
- Molecule 27: Small nuclear ribonucleoprotein G

Chain r: 88% 10%



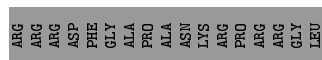
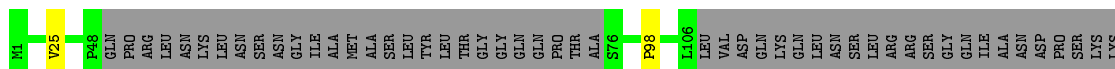
- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain h: 56% 44%



- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain l: 53% 46%



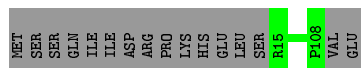
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain j: 83% 15%



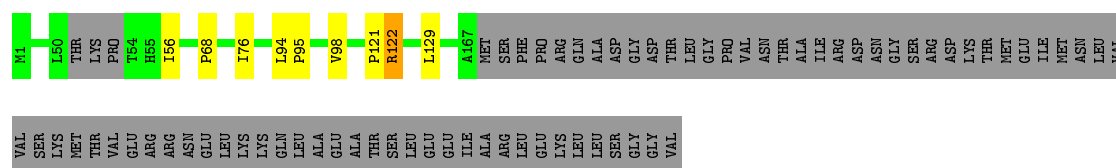
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain m: 85% 15%



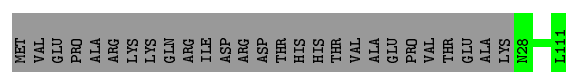
- Molecule 30: U2 small nuclear ribonucleoprotein A'

Chain W:



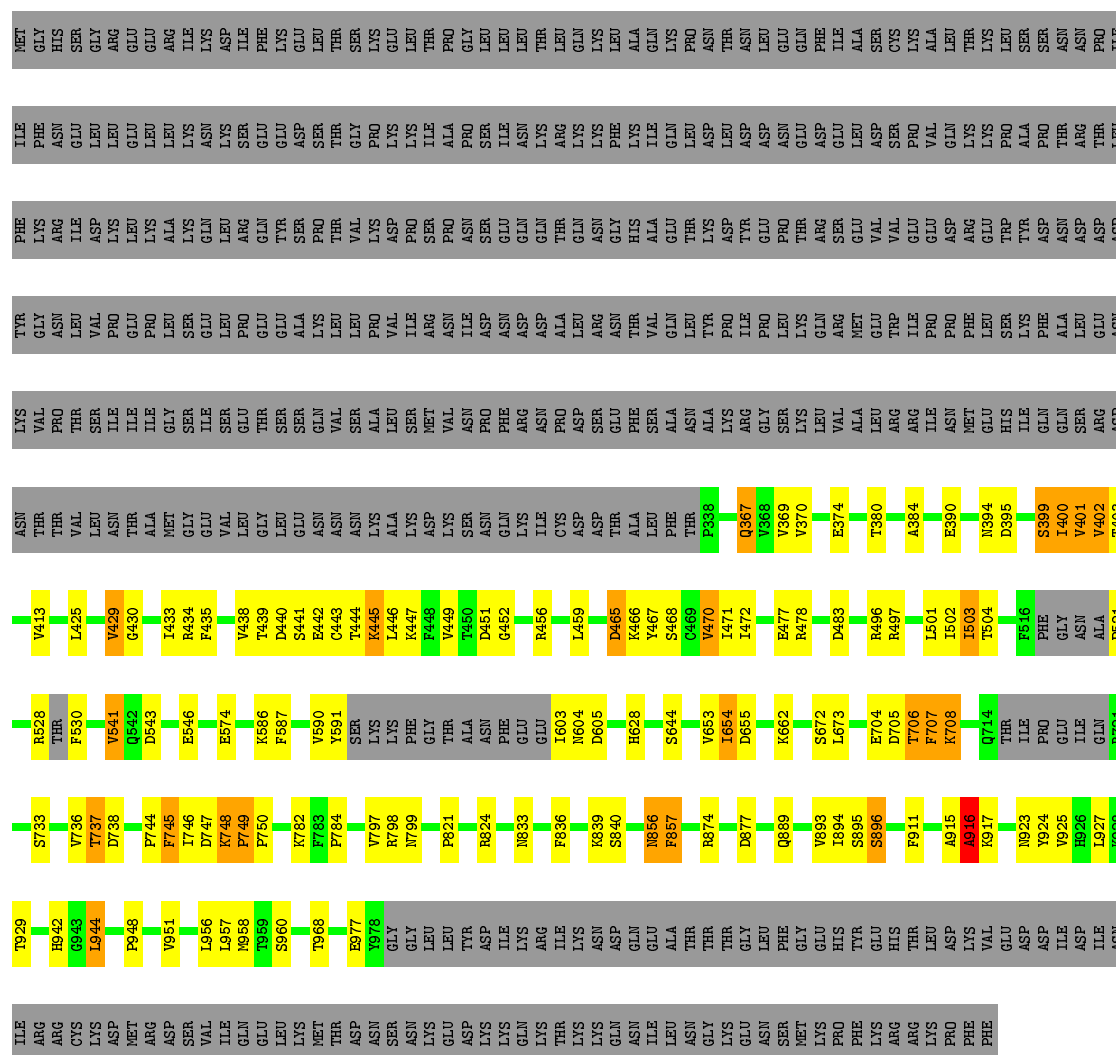
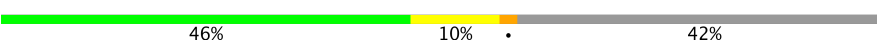
- Molecule 31: U2 small nuclear ribonucleoprotein B''

Chain Y:




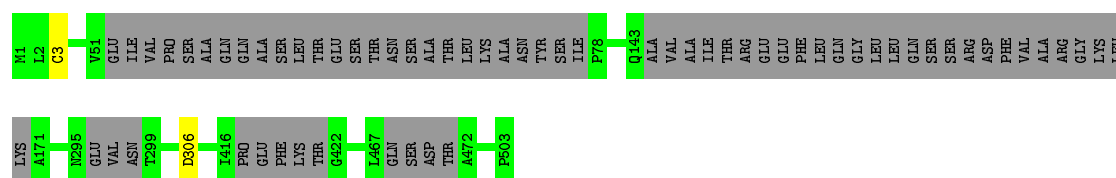
- Molecule 32: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

Chain Q:




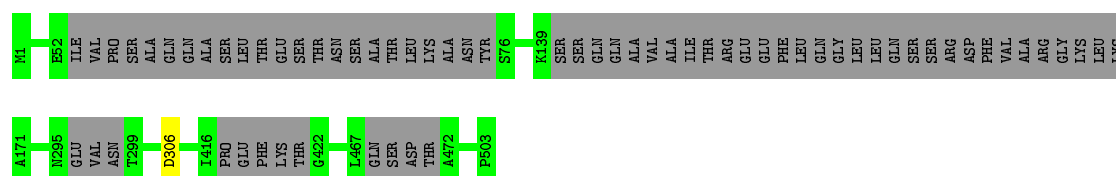
- Molecule 33: Pre-mRNA-processing factor 19

Chain t:  87% 13%




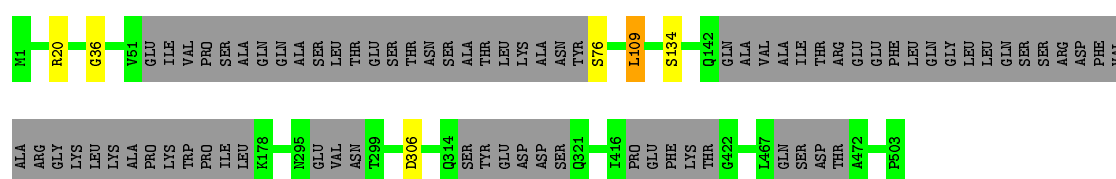
- Molecule 33: Pre-mRNA-processing factor 19

Chain u:  87% 13%




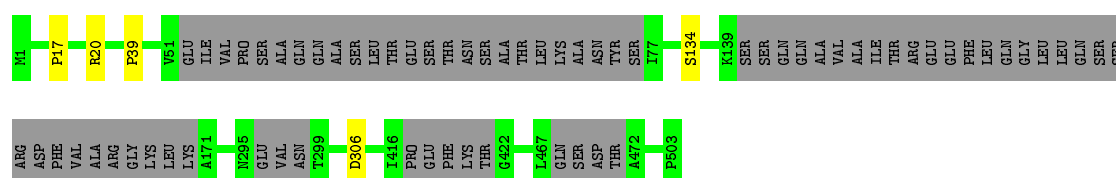
- Molecule 33: Pre-mRNA-processing factor 19

Chain v:  83% 15%



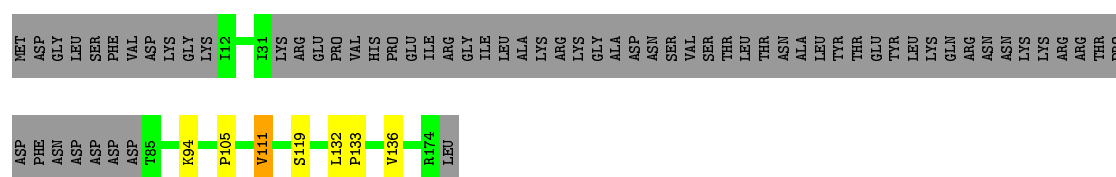
- Molecule 33: Pre-mRNA-processing factor 19

Chain w:  85% 14%



- Molecule 34: Pre-mRNA-splicing factor SNT309

Chain s:  59% 37%



- Molecule 35: unknown

Chain x:  70% 30%

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	15872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (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, 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 >2	RMSZ	# Z >2
1	U	0.31	0/3351	0.75	1/5213 (0.0%)
10	C	0.41	0/6902	0.73	0/9386
11	G	0.42	0/839	0.74	0/1126
12	H	0.43	0/2667	0.80	1/3630 (0.0%)
13	J	0.45	0/2613	0.74	0/3551
14	K	0.40	0/1308	0.72	0/1765
15	L	0.40	0/1294	0.75	0/1732
16	M	0.42	0/2058	0.70	0/2769
17	N	0.41	0/1680	0.76	0/2258
18	O	0.49	0/2091	0.86	2/2824 (0.1%)
19	P	0.43	0/282	0.69	0/380
2	E	0.36	0/388	0.69	0/603
20	R	0.40	0/545	0.77	0/748
21	S	0.44	0/3155	0.83	0/4298
22	T	0.38	0/2918	0.74	0/4032
23	b	0.34	0/636	0.59	0/856
23	k	0.28	0/394	0.50	0/546
24	d	0.36	0/634	0.62	1/859 (0.1%)
24	n	0.29	0/403	0.53	0/559
25	e	0.40	0/585	0.56	0/795
25	p	0.30	0/367	0.55	0/507
26	f	0.39	0/585	0.59	0/791
26	q	0.30	0/353	0.53	0/489
27	g	0.36	0/532	0.55	0/715
27	r	0.28	0/338	0.45	0/467
28	h	0.35	0/649	0.54	0/880
28	l	0.30	0/390	0.53	0/541
29	j	0.38	0/753	0.61	0/1013
29	m	0.31	0/466	0.54	0/649
3	I	0.28	0/772	0.71	0/1195
30	W	0.31	0/814	0.53	0/1134
31	Y	0.32	0/415	0.55	0/577

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
32	Q	0.51	0/3061	1.22	18/4260 (0.4%)
33	t	0.46	0/2165	0.67	1/3010 (0.0%)
33	u	0.50	0/2160	0.69	1/3003 (0.0%)
33	v	0.51	0/2104	0.74	4/2923 (0.1%)
33	w	0.47	0/2150	0.68	2/2989 (0.1%)
34	s	0.57	0/546	0.80	0/760
4	Z	0.26	0/4018	0.72	0/6233
5	V	0.32	0/2310	0.77	3/3594 (0.1%)
6	A	0.44	0/17321	0.75	0/23534
7	B	0.52	0/8463	0.72	0/11800
8	D	0.37	0/929	0.67	0/1243
9	F	0.42	0/325	0.74	0/442
All	All	0.43	0/86729	0.75	34/120679 (0.0%)

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
11	G	0	1
16	M	0	1
18	O	0	2
21	S	0	1
32	Q	0	45
33	t	0	1
33	v	0	1
33	w	0	1
34	s	0	2
6	A	0	2
All	All	0	57

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	384	ALA	CB-CA-C	8.22	122.43	110.10
1	U	39	U	C2'-C3'-O3'	8.13	127.38	109.50
32	Q	745	PHE	C-N-CA	7.85	141.32	121.70
32	Q	413	VAL	CB-CA-C	7.51	125.67	111.40
32	Q	745	PHE	O-C-N	-6.99	111.52	122.70

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
11	G	3	ARG	Peptide
16	M	231	ASP	Peptide
18	O	83	GLN	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	U	2999	0	1515	24	0
2	E	346	0	173	5	0
3	I	693	0	351	3	0
4	Z	3610	0	1831	10	0
5	V	2066	0	1042	23	0
6	A	16919	0	16184	233	0
7	B	8462	0	3706	27	0
8	D	912	0	936	11	0
9	F	321	0	282	3	0
10	C	6756	0	6801	117	0
11	G	823	0	808	10	0
12	H	2639	0	2073	25	0
13	J	2556	0	2551	54	0
14	K	1289	0	1309	17	0
15	L	1270	0	1294	12	0
16	M	2012	0	1968	32	0
17	N	1658	0	1712	59	0
18	O	2068	0	1853	39	0
19	P	275	0	283	4	0
20	R	544	0	345	17	0
21	S	3121	0	2399	55	0
22	T	2946	0	1252	11	0
23	b	631	0	670	0	0
23	k	396	0	169	0	0
24	d	625	0	647	0	0
24	n	404	0	180	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	e	575	0	597	0	0
25	p	369	0	152	0	0
26	f	573	0	572	0	0
26	q	354	0	153	0	0
27	g	529	0	557	0	0
27	r	340	0	152	0	0
28	h	644	0	686	0	0
28	l	392	0	165	0	0
29	j	741	0	778	0	0
29	m	467	0	199	0	0
30	W	816	0	341	1	0
31	Y	416	0	182	0	0
32	Q	3066	0	1345	52	0
33	t	2171	0	945	0	0
33	u	2166	0	942	0	0
33	v	2111	0	917	0	0
33	w	2156	0	938	0	0
34	s	548	0	219	0	0
35	x	660	0	142	0	0
36	E	1	0	0	0	0
36	V	1	0	0	0	0
37	D	1	0	0	1	0
37	L	3	0	0	0	0
37	M	1	0	0	0	0
37	N	2	0	0	5	0
38	C	32	0	12	0	0
All	All	85476	0	62328	741	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 6.

The worst 5 of 741 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)
32:Q:434:ARG:O	32:Q:874:ARG:HA	1.26	1.35
17:N:34:CYS:SG	17:N:37:CYS:SG	1.35	1.34
20:R:36:GLN:O	20:R:40:GLN:N	1.60	1.32
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
21:S:467:GLN:CA	21:S:471:LEU:HA	1.65	1.24

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	
6	A	2160/2413 (90%)	1997 (92%)	152 (7%)	11 (0%)	32	73
7	B	1704/2163 (79%)	1585 (93%)	111 (6%)	8 (0%)	32	73
8	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	10	50
9	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
10	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	12	53
11	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	17	60
12	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	18	61
13	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	4	36
14	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	28	70
15	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	14	56
16	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	15	58
17	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	12	53
18	O	277/590 (47%)	248 (90%)	24 (9%)	5 (2%)	10	50
19	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	5	41
20	R	93/135 (69%)	81 (87%)	11 (12%)	1 (1%)	17	60
21	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	32	73
22	T	536/859 (62%)	506 (94%)	21 (4%)	9 (2%)	11	51
23	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
23	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	6	43
24	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	14	56
24	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
25	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
25	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	13	54
26	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	13	54
26	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	12	53
28	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
28	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	6	43
29	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
29	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
30	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	2	30
31	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
32	Q	609/1071 (57%)	486 (80%)	73 (12%)	50 (8%)	1	17
33	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
33	u	425/503 (84%)	413 (97%)	12 (3%)	0	100	100
33	v	412/503 (82%)	403 (98%)	6 (2%)	3 (1%)	25	68
33	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	32	73
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	2	27
All	All	11527/16230 (71%)	10551 (92%)	821 (7%)	155 (1%)	19	56

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
7	B	766	ILE
12	H	414	PRO
16	M	127	ILE

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	
6	A	1701/2182 (78%)	1580 (93%)	121 (7%)	17	55
8	D	100/256 (39%)	91 (91%)	9 (9%)	11	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	26/163 (16%)	25 (96%)	1 (4%)	38	70
10	C	722/910 (79%)	659 (91%)	63 (9%)	12	46
11	G	89/216 (41%)	81 (91%)	8 (9%)	11	45
12	H	185/552 (34%)	164 (89%)	21 (11%)	7	34
13	J	283/397 (71%)	250 (88%)	33 (12%)	6	33
14	K	143/328 (44%)	115 (80%)	28 (20%)	1	12
15	L	138/141 (98%)	129 (94%)	9 (6%)	20	57
16	M	213/296 (72%)	189 (89%)	24 (11%)	7	34
17	N	194/332 (58%)	175 (90%)	19 (10%)	9	40
18	O	174/525 (33%)	152 (87%)	22 (13%)	5	29
19	P	26/152 (17%)	21 (81%)	5 (19%)	1	12
20	R	23/121 (19%)	19 (83%)	4 (17%)	2	17
21	S	208/633 (33%)	181 (87%)	27 (13%)	5	28
23	b	70/176 (40%)	70 (100%)	0	100	100
24	d	69/89 (78%)	66 (96%)	3 (4%)	33	68
25	e	65/83 (78%)	60 (92%)	5 (8%)	15	52
26	f	63/77 (82%)	61 (97%)	2 (3%)	44	74
27	g	58/66 (88%)	57 (98%)	1 (2%)	66	85
28	h	77/129 (60%)	77 (100%)	0	100	100
29	j	79/103 (77%)	76 (96%)	3 (4%)	38	70
All	All	4706/7927 (59%)	4298 (91%)	408 (9%)	16	46

5 of 408 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	C	851	LEU
13	J	161	ASP
21	S	144	GLU
10	C	965	ASP
12	H	334	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
10	C	608	GLN
13	J	273	GLN
26	f	24	ASN
10	C	837	GLN
14	K	33	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	66 (47%)	13 (9%)
2	E	15/16 (93%)	10 (66%)	2 (13%)
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	96/112 (85%)	35 (36%)	6 (6%)
All	All	442/1558 (28%)	184 (41%)	32 (7%)

5 of 184 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	18	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	-9	U
4	Z	20	G
5	V	74	U
4	Z	19	U
4	Z	32	G

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 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$
38	GTP	C	1101	-	27,34,34	0.99	2 (7%)	27,54,54	2.03	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C	1101	GTP	C5-C4	2.50	1.46	1.40
38	C	1101	GTP	C6-C5	3.25	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	1101	GTP	C6-C5-C4	-3.92	116.94	120.84
38	C	1101	GTP	N3-C2-N1	-3.42	122.47	127.46
38	C	1101	GTP	C5-C6-N1	-3.11	119.06	123.48
38	C	1101	GTP	C1'-N9-C4	-2.92	121.59	126.64
38	C	1101	GTP	C4-C5-N7	-2.52	106.97	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
35	x	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	54:UNK	C	55:UNK	N	111.76
1	x	110:UNK	C	111:UNK	N	53.94
1	x	36:UNK	C	37:UNK	N	49.39
1	x	87:UNK	C	88:UNK	N	31.03