



wwPDB EM Map/Model Validation Report ⓘ

Sep 12, 2016 – 01:29 PM EDT

PDB ID : 5LJ3
EMDB ID: : EMD-4055
Title : Structure of the core 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 : 2016-07-17
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

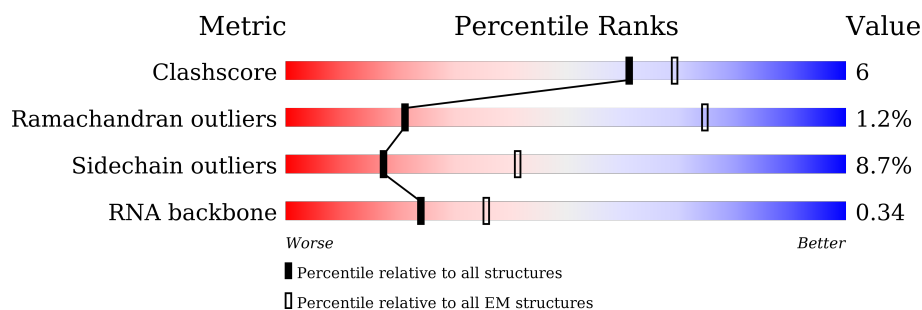
1 Overall quality at a glance

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.










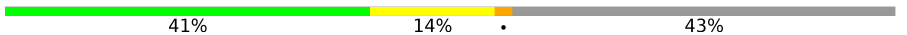

















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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>44%</div> <div>30%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>
6	A	2413	<div> <div>63%</div> <div>15%</div> <div>•</div> <div>20%</div> </div>
7	D	278	<div> <div>34%</div> <div>7%</div> <div>59%</div> </div>
8	F	179	<div> <div>23%</div> <div>•</div> <div>74%</div> </div>

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

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Mol	Chain	Length	Quality of chain
28	j	110	 83% 15%
28	m	110	 85% 15%
29	W	238	 65% 31%
30	Y	111	 76% 24%
31	x	132	 100%

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
33	ZN	N	401	-	-	X	-
33	ZN	N	402	-	-	X	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 63161 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	1922	Total	C	N	O	S	0	0
			15704	10112	2720	2814	58		

- Molecule 7 is a protein called Protein CWC16.

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

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC25.

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

- Molecule 9 is a protein called Pre-mRNA-splicing factor SNU114.

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

- Molecule 10 is a protein called ISY1.

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

- Molecule 11 is a protein called CWC22.

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

- Molecule 12 is a protein called PRP46.

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

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor BUD31.

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

- Molecule 15 is a protein called CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	252	Total	C	N	O	S	0	0
			2010	1275	354	370	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor SLT11.

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

- Molecule 17 is a protein called CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	198	Total	C	N	O	S	0	0
			1645	1032	300	307	6		

- Molecule 18 is a protein called CWC15.

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

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	97	Total	C	N	O	0	0
			550	328	109	113		

- Molecule 20 is a protein called CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	464	Total	C	N	O	S	0	0
			3120	1948	581	584	7		

- Molecule 21 is a protein called SYF1.

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

- Molecule 22 is a protein called Small nuclear ribonucleoprotein-associated protein B.

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

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

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

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

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

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

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

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

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

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

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

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

- Molecule 31 is a protein called unknown.

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

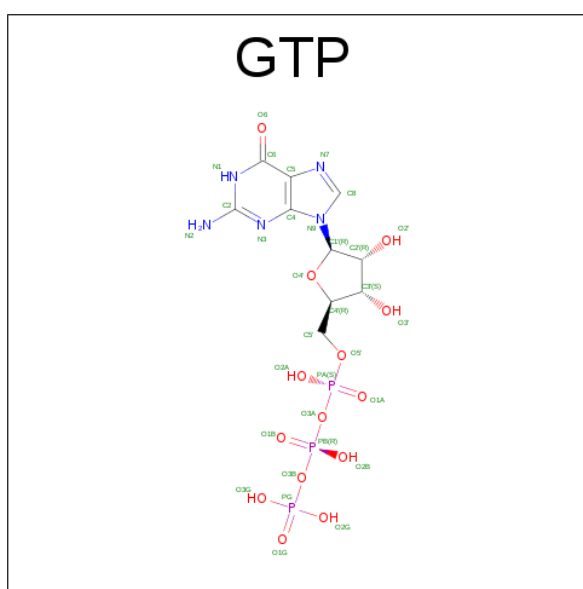
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

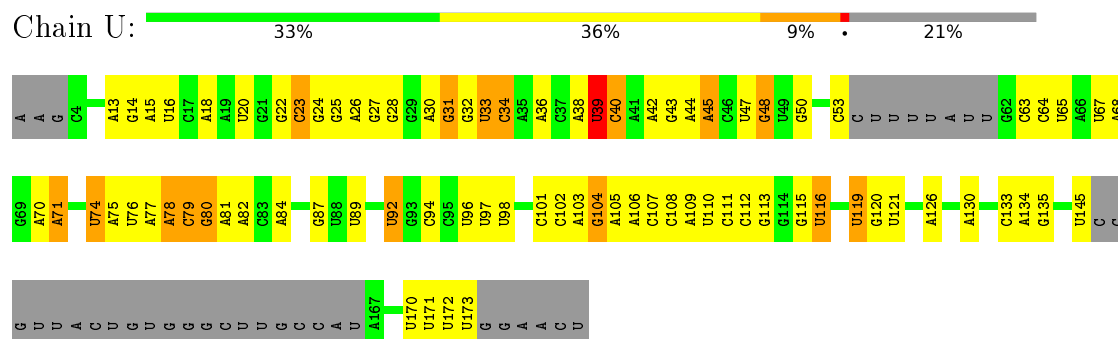
- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

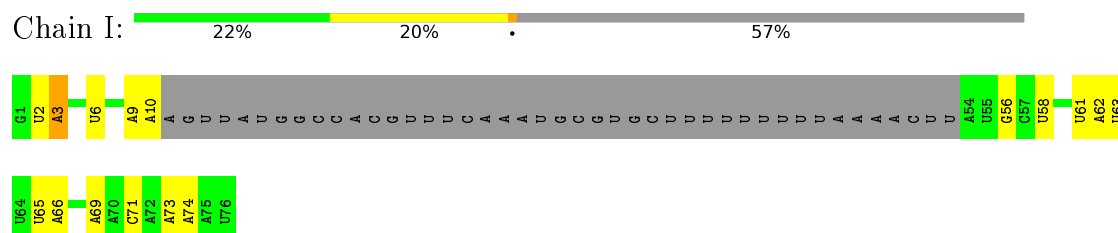
- Molecule 1: U5 snRNA (small nuclear RNA)



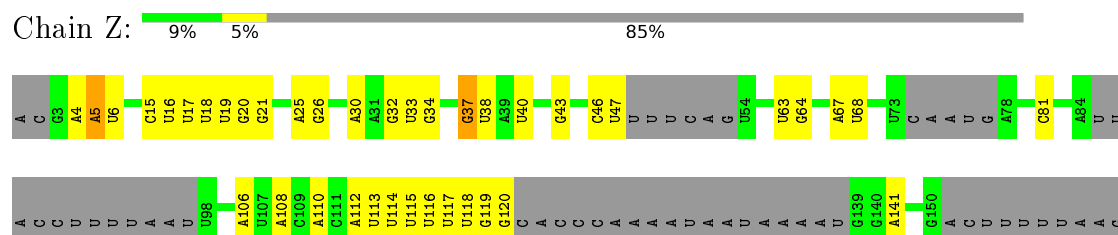
- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA

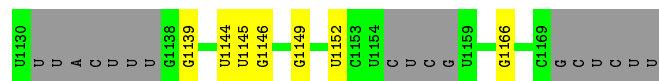


- Molecule 3: Intron of UBC4 pre-mRNA



- Molecule 4: U2 snRNA (small nuclear RNA)





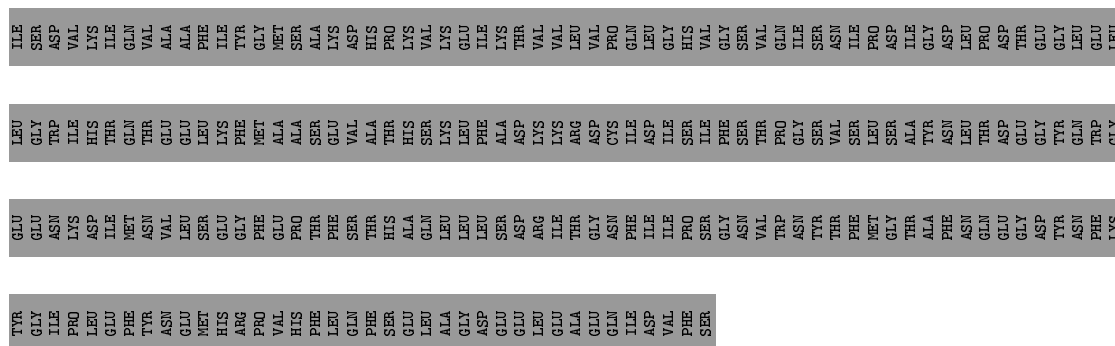
- Chain V: 44% 30% 12% 1% 13%



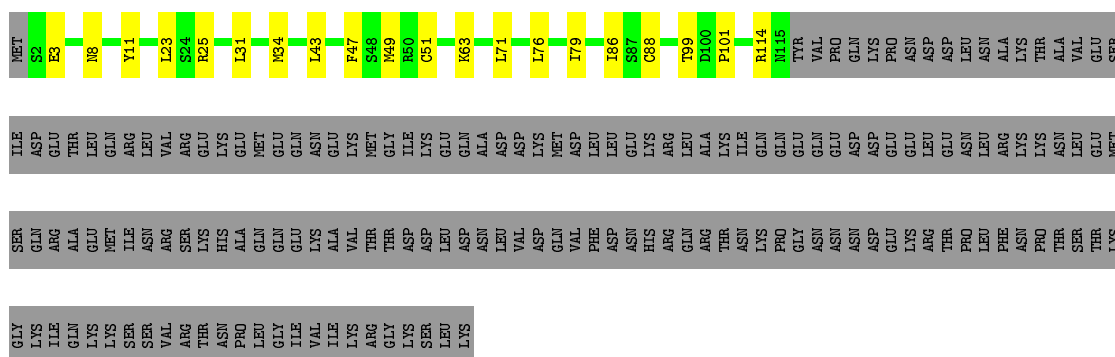
- 


Device Type	Percentage
Smartphones	63%
Tablets	15%
Other mobile devices	20%

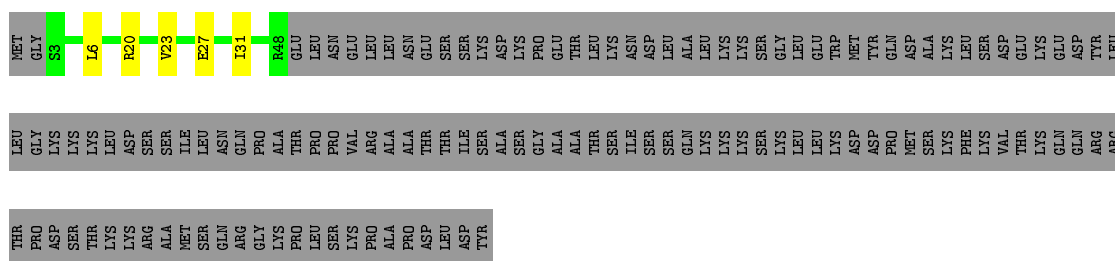


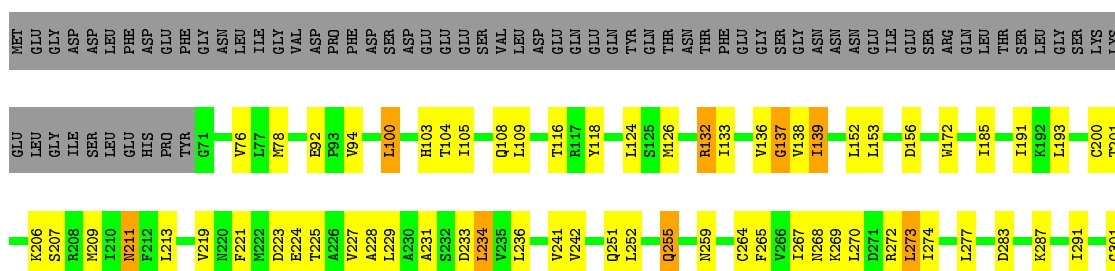
- Molecule 7: Protein CWC16

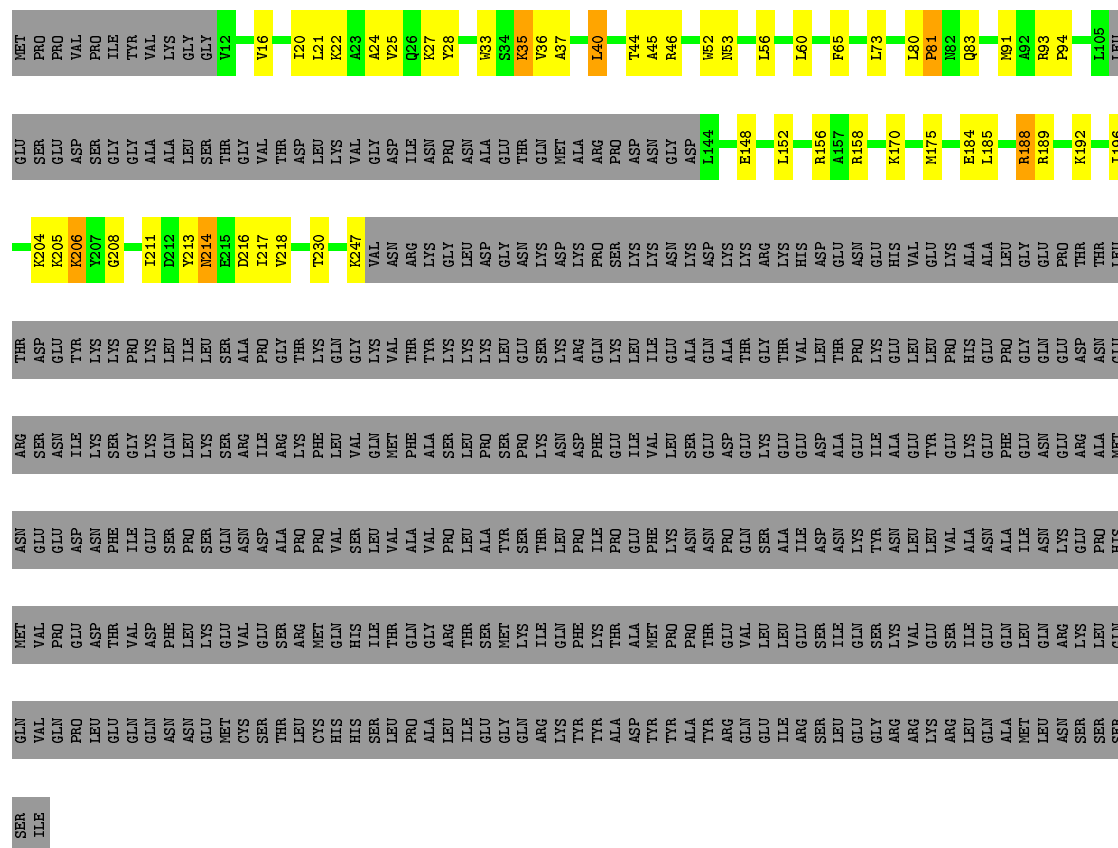


- Molecule 8: Pre-mRNA-splicing factor CWC25



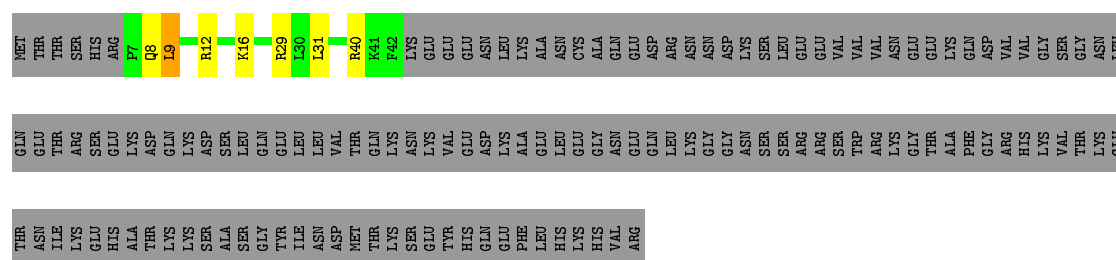
- Molecule 9: Pre-mRNA-splicing factor SNU114





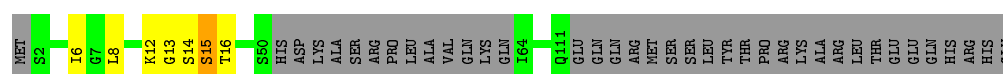
- Molecule 18: CWC15

Chain P:  17% .. 79%



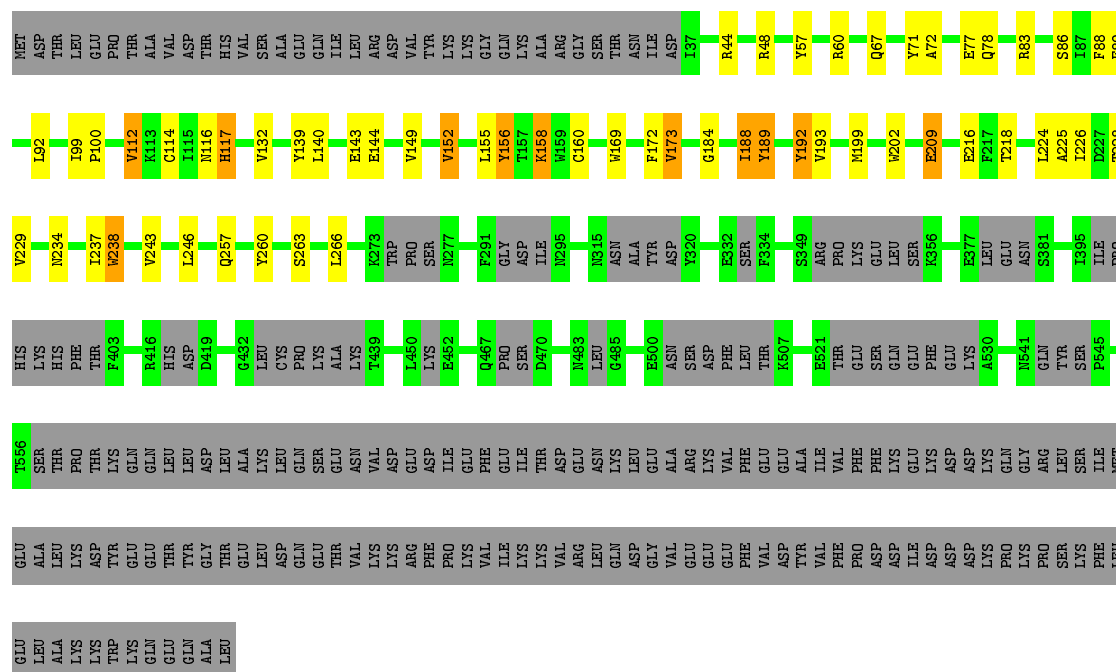
- Molecule 19: Pre-mRNA-splicing factor CWC21

Chain R: 67% . . 28%



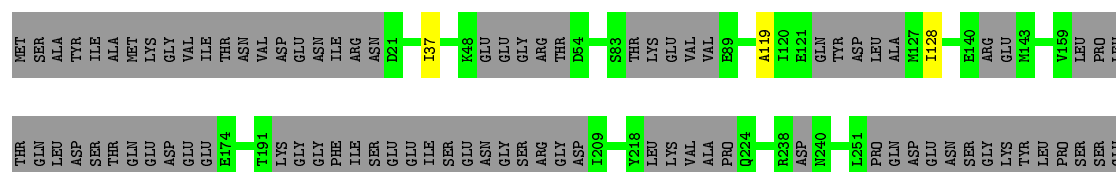
- Molecule 20: CLF1

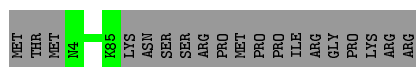
Chain S:  59% 7% 32%



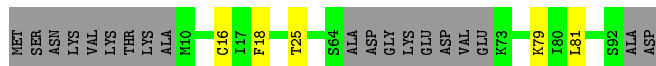
- Molecule 21: SYF1

Chain T:  67% . 31%

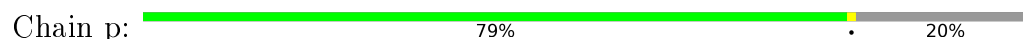




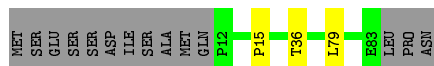
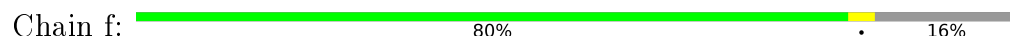
- Molecule 24: Small nuclear ribonucleoprotein E



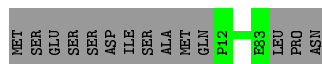
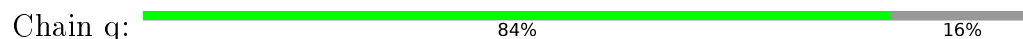
- Molecule 24: Small nuclear ribonucleoprotein E



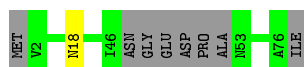
- Molecule 25: Small nuclear ribonucleoprotein F



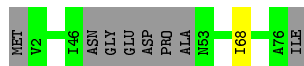
- Molecule 25: Small nuclear ribonucleoprotein F



- Molecule 26: Small nuclear ribonucleoprotein G



- Molecule 26: Small nuclear ribonucleoprotein G



- Molecule 27: Small nuclear ribonucleoprotein Sm D1



PRO
ALA
ASN
LYS
ARG
PRO
ARG
ARG
GLY
LEU


- Molecule 27: Small nuclear ribonucleoprotein Sm D1

Chain l:  53% 46%

H1 V25 P48 PRQ ARG LEU ASN LYS LEU ASN SER ASN ILE MET ALA SER LEU TYR THR GLY GLN GLN PRO THR ALA S76 P98 L106 LEU VAL ASP GLN LYS GLN LEU ASN SER LEU ARG ARG SER GLY ILE ALA ASN ASP PRO SER LYS


ARG
ARG
ASP
PHE
GLY
ALA
PRO
ALA
ALA
LYS
LYS
ARG
PRO
ARG
ARG
GLY
LEU

- Molecule 28: Small nuclear ribonucleoprotein Sm D2

Chain j:  83% 15%

MET
SER
SER
GLN
ILE
ILE
ASP
ARG
PRO
LYS
HIS
GLU
LEU
SER
R15 F24 R49 R82 P108 VAL GLU

- Molecule 28: Small nuclear ribonucleoprotein Sm D2

Chain m:  85% 15%

MET
SER
SER
GLN
ILE
ILE
ASP
ARG
PRO
LYS
HIS
GLU
LEU
SER
R15 P108 VAL GLU


- Molecule 29: U2 small nuclear ribonucleoprotein A'

Chain W:  65% 31%

H1 L50 THR LYS PRO T64 H55 I56 P68 I76 I94 P95 V98 P121 R122 L129 A167 MET SER PHE PRO ARG GLN ALA ASP GLY THR LEU GLY PRO VAL ASN THR THR ILE ARG ASP ASN GLY SER ARG ASP LYS THR MET GLU ILE MET ASN LEU VAL

VAL
SER
LYS
MET
THR
VAL
GLU
ARG
ARG
ASN
GLU
LEU
LYS
GLN
LEU
ALA
ALA
THR
SER
LEU
GLU
GLU
ILE
ALA
ARG
LEU
GLU
LYS
LEU
LEU
SER
GLY
GLY
VAL

- Molecule 30: U2 small nuclear ribonucleoprotein B''

Chain Y:  76% 24%

MET
VAL
GLU
PRO
ALA
ARG
LYS
LYS
GLN
ARG
ILE
ASP
ASP
THR
HIS
HIS
THR
VAL
ALA
GLU
PRO
VAL
THR
GLU
ALA
LYS
N28 L111

- Molecule 31: unknown

Chain x:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	93106	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	81000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	G	0.42	0/839	0.74	0/1126
11	H	0.43	0/2667	0.80	1/3630 (0.0%)
12	J	0.45	0/2613	0.74	0/3551
13	K	0.40	0/1308	0.72	0/1765
14	L	0.40	0/1294	0.75	0/1732
15	M	0.42	0/2056	0.70	0/2766
16	N	0.41	0/1680	0.76	0/2258
17	O	0.43	0/1669	0.81	0/2236
18	P	0.43	0/282	0.69	0/380
19	R	0.40	0/550	0.76	0/752
2	E	0.36	0/388	0.69	0/603
20	S	0.44	0/3154	0.83	0/4297
21	T	0.38	0/2916	0.74	0/4026
22	b	0.34	0/636	0.59	0/856
22	k	0.28	0/394	0.50	0/546
23	d	0.36	0/634	0.62	1/859 (0.1%)
23	n	0.29	0/403	0.53	0/559
24	e	0.40	0/585	0.56	0/795
24	p	0.30	0/367	0.55	0/507
25	f	0.39	0/585	0.59	0/791
25	q	0.30	0/353	0.53	0/489
26	g	0.36	0/532	0.55	0/715
26	r	0.28	0/338	0.45	0/467
27	h	0.35	0/649	0.54	0/880
27	l	0.30	0/390	0.53	0/541
28	j	0.38	0/753	0.61	0/1013
28	m	0.31	0/466	0.54	0/649
29	W	0.31	0/814	0.53	0/1134
3	I	0.28	0/772	0.71	0/1195
30	Y	0.32	0/415	0.55	0/577
4	Z	0.26	0/4018	0.72	0/6233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
5	V	0.31	0/2309	0.76	2/3590 (0.1%)
6	A	0.43	0/16107	0.75	0/21845
7	D	0.37	0/929	0.67	0/1243
8	F	0.42	0/325	0.74	0/442
9	C	0.41	0/6902	0.73	0/9386
All	All	0.39	0/64443	0.73	5/89647 (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
10	G	0	1
15	M	0	1
17	O	0	1
20	S	0	1
6	A	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	39	U	C2'-C3'-O3'	8.13	127.38	109.50
5	V	35	A	C5'-C4'-O4'	6.92	117.40	109.10
11	H	440	LEU	CA-CB-CG	6.54	130.33	115.30
23	d	81	ALA	C-N-CD	-6.46	106.39	120.60
5	V	35	A	O4'-C4'-C3'	5.43	110.44	106.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
10	G	3	ARG	Peptide
15	M	231	ASP	Peptide
17	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	1043	21	0
6	A	15704	0	15649	227	0
7	D	912	0	936	11	0
8	F	321	0	282	3	0
9	C	6756	0	6801	117	0
10	G	823	0	808	10	0
11	H	2639	0	2073	25	0
12	J	2556	0	2551	54	0
13	K	1289	0	1309	17	0
14	L	1270	0	1294	12	0
15	M	2010	0	1964	20	0
16	N	1658	0	1713	49	0
17	O	1645	0	1672	32	0
18	P	275	0	283	4	0
19	R	550	0	356	2	0
20	S	3120	0	2397	39	0
21	T	2946	0	1250	6	0
22	b	631	0	670	0	0
22	k	396	0	169	0	0
23	d	625	0	647	0	0
23	n	404	0	180	0	0
24	e	575	0	597	0	0
24	p	369	0	152	0	0
25	f	573	0	572	0	0
25	q	354	0	153	0	0
26	g	529	0	557	0	0
26	r	340	0	152	0	0
27	h	644	0	686	0	0
27	l	392	0	165	0	0
28	j	741	0	778	0	0
28	m	467	0	199	0	0
29	W	816	0	341	1	0
30	Y	416	0	182	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	x	660	0	142	0	0
32	E	1	0	0	0	0
32	V	1	0	0	0	0
33	D	1	0	0	1	0
33	L	3	0	0	0	0
33	M	1	0	0	0	0
33	N	2	0	0	4	0
34	C	32	0	12	0	0
All	All	63161	0	52605	611	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 611 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)
16:N:34:CYS:SG	16:N:37:CYS:SG	1.40	1.39
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
16:N:16:CYS:SG	16:N:73:CYS:HB2	1.85	1.16
21:T:360:LYS:CB	21:T:381:HIS:CB	2.36	1.03
16:N:61:CYS:SG	33:N:401:ZN:ZN	1.54	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	A	1916/2413 (79%)	1762 (92%)	143 (8%)	11 (1%)	30 74
7	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	11 55
8	F	44/179 (25%)	41 (93%)	3 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	13	59
10	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	17	65
11	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	19	66
12	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	4	40
13	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	30	74
14	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	15	61
15	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	16	63
16	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	13	59
17	O	194/590 (33%)	173 (89%)	17 (9%)	4 (2%)	9	53
18	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	6	46
19	R	91/135 (67%)	80 (88%)	10 (11%)	1 (1%)	17	65
20	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	34	77
21	T	532/859 (62%)	504 (95%)	20 (4%)	8 (2%)	13	59
22	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
22	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	7	48
23	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	15	61
23	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
24	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
24	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	14	59
25	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	14	59
25	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
26	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
26	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	13	59
27	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
27	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	6	48
28	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
28	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
29	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	3	31
30	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
All	All	7089/10809 (66%)	6428 (91%)	577 (8%)	84 (1%)	21	63

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
11	H	414	PRO
15	M	127	ILE
16	N	120	LEU

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%)	18	59
7	D	100/256 (39%)	91 (91%)	9 (9%)	12	49
8	F	26/163 (16%)	25 (96%)	1 (4%)	40	76
9	C	722/910 (79%)	659 (91%)	63 (9%)	13	50
10	G	89/216 (41%)	81 (91%)	8 (9%)	12	49
11	H	185/552 (34%)	164 (89%)	21 (11%)	7	37
12	J	283/398 (71%)	250 (88%)	33 (12%)	7	36
13	K	143/328 (44%)	115 (80%)	28 (20%)	1	13
14	L	138/141 (98%)	129 (94%)	9 (6%)	21	62
15	M	212/295 (72%)	188 (89%)	24 (11%)	7	38
16	N	194/332 (58%)	175 (90%)	19 (10%)	10	44
17	O	174/526 (33%)	152 (87%)	22 (13%)	5	32
18	P	26/152 (17%)	21 (81%)	5 (19%)	2	13
19	R	24/121 (20%)	20 (83%)	4 (17%)	3	20
20	S	208/633 (33%)	181 (87%)	27 (13%)	5	32
22	b	70/176 (40%)	70 (100%)	0	100	100
23	d	69/89 (78%)	66 (96%)	3 (4%)	35	74
24	e	65/83 (78%)	60 (92%)	5 (8%)	16	56
25	f	63/77 (82%)	61 (97%)	2 (3%)	46	79
26	g	58/66 (88%)	57 (98%)	1 (2%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	h	77/129 (60%)	77 (100%)	0	100	100
28	j	79/103 (77%)	76 (96%)	3 (4%)	40	76
All	All	4706/7928 (59%)	4298 (91%)	408 (9%)	17	50

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

Mol	Chain	Res	Type
9	C	851	LEU
12	J	161	ASP
20	S	144	GLU
9	C	965	ASP
11	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
9	C	608	GLN
12	J	273	GLN
25	f	24	ASN
9	C	837	GLN
13	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	95/112 (84%)	34 (35%)	5 (5%)
All	All	441/1558 (28%)	183 (41%)	31 (7%)

5 of 183 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

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Mol	Chain	Res	Type
1	U	18	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	-9	U
4	Z	20	G
5	V	60	G
4	Z	16	U
4	Z	32	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
34	GTP	C	1101	-	26,34,34	1.00	2 (7%)	29,54,54	1.91	5 (17%)

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
34	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)
34	C	1101	GTP	C5-C4	2.50	1.46	1.40
34	C	1101	GTP	C6-C5	3.09	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	C1'-N9-C4	-4.67	121.59	126.81
34	C	1101	GTP	N3-C2-N1	-3.74	122.47	127.56
34	C	1101	GTP	C6-C5-C4	-3.43	116.94	120.86
34	C	1101	GTP	C5-C6-N1	-3.42	119.06	123.52
34	C	1101	GTP	C6-N1-C2	4.91	121.63	115.88

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
31	x	4
21	T	2
19	R	1
5	V	1

The worst 5 of 8 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
1	T	419:LYS	C	420:SER	N	5.13