wwPDB EM Validation Summary Report (i)

Sep 18, 2021 – 08:04 am BST

PDB ID	:	7OQE
EMDB ID	:	EMD-13033
Title	:	Saccharomyces cerevisiae spliceosomal pre-A complex (delta BS-A ACT1)
Authors	:	Zhang, Z.; Rigo, N.; Dybkov, O.; Fourmann, J.; Will, C.L.; Kumar, V.; Urlaub, H.; Stark, H.; Luehrmann, R.
Deposited on	:	2021-06-03
Resolution	:	5.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

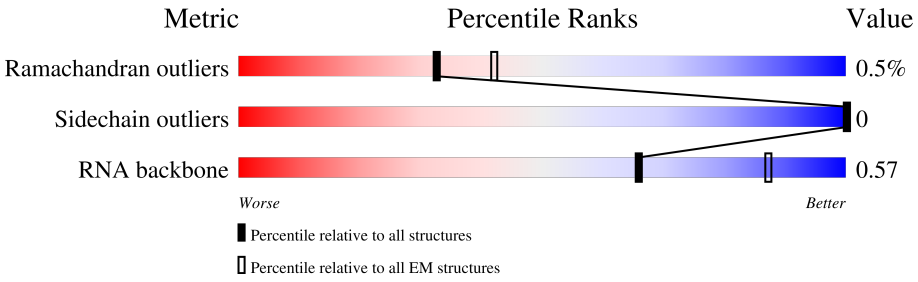
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 5.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	F	523	51% 49%
2	I	373	19% • • 77%
3	E	544	100%
4	J	620	17% 83%
5	1	568	75% 23% • •
6	G	492	49% 51%
7	A	298	44% 56%
8	C	231	84% 16%
9	b	196	62% 38%

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Mol	Chain	Length	Quality of chain
9	s	196	33% 67%
10	d	101	92% 8%
10	v	101	81% 19%
11	e	94	81% 18%
11	w	94	82% 18%
12	f	86	85% 15%
12	x	86	85% 15%
13	g	77	91% 6%
13	y	77	94%
14	h	146	73% 27%
14	t	146	49% 51%
15	i	110	90% 10%
15	u	110	84% 16%
16	H	261	74% 26%
17	D	629	92% 8%
18	B	300	62% 38%
19	K	583	69% 30%
20	O	971	80% 16%
21	U	282	66% 33%
22	V	280	36% 63%
23	T	530	87% 13%
24	S	107	86% 14%
25	Q	436	50% 50%
26	P	1361	86% 13%
27	R	213	81% 19%

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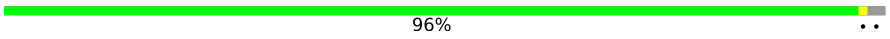
Mol	Chain	Length	Quality of chain
28	Z	85	
29	W	238	
30	Y	111	
31	p	849	
32	2	1175	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 56606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	267	Total 1335	C 801	N 267	O 267	0	0

- Molecule 2 is a RNA chain called ACT1 pre-mRNA (delta BS-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	86	Total 1327	C 575	N 111	O 555	P 86	0	0

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	544	Total 2732	C 1644	N 544	O 544	0	0

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	105	Total 529	C 319	N 105	O 105	0	0

- Molecule 5 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	558	Total 11822	C 5287	N 2003	O 3974	P 558	0	0

- Molecule 6 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	239	Total 1202	C 724	N 239	O 239	0	0

- Molecule 7 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	A	132	Total 668	C 404	N 132	O 132	0	0

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	195	Total 985	C 595	N 195	O 195	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	b	121	Total 607	C 365	N 121	O 121	0	0
9	s	65	Total 323	C 193	N 65	O 65	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	93	Total 473	C 287	N 93	O 93	0	0
10	v	82	Total 412	C 248	N 82	O 82	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	77	Total 389	C 235	N 77	O 77	0	0
11	w	77	Total 389	C 235	N 77	O 77	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	73	Total 365	C 219	N 73	O 73	0	0
12	x	73	Total 365	C 219	N 73	O 73	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	72	Total	C	N	O	0	0
			356	212	72	72		
13	y	75	Total	C	N	O	0	0
			373	223	75	75		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	h	107	Total	C	N	O	0	0
			535	321	107	107		
14	t	72	Total	C	N	O	0	0
			363	219	72	72		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	i	99	Total	C	N	O	0	0
			501	303	99	99		
15	u	92	Total	C	N	O	0	0
			463	279	92	92		

- Molecule 16 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	192	Total	C	N	O	0	0
			960	576	192	192		

- Molecule 17 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	D	576	Total	C	N	O	0	0
			2892	1740	576	576		

- Molecule 18 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	B	186	Total	C	N	O	0	0
			940	568	186	186		

- Molecule 19 is a protein called Pre-mRNA-processing protein PRP40.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	K	406	Total	C	N	O	0	0
			2042	1230	406	406		

- Molecule 20 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	O	812	Total	C	N	O	0	0
			4108	2484	812	812		

- Molecule 21 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	188	Total	C	N	O	0	0
			943	567	188	188		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	121	UNK	-	insertion	UNP Q07350
U	122	UNK	-	insertion	UNP Q07350
U	123	UNK	-	insertion	UNP Q07350
U	124	UNK	-	insertion	UNP Q07350
U	125	UNK	-	insertion	UNP Q07350
U	126	UNK	-	insertion	UNP Q07350
U	127	UNK	-	insertion	UNP Q07350
U	128	UNK	-	insertion	UNP Q07350
U	129	UNK	-	insertion	UNP Q07350
U	130	UNK	-	insertion	UNP Q07350
U	131	UNK	-	insertion	UNP Q07350
U	132	UNK	-	insertion	UNP Q07350
U	133	UNK	-	insertion	UNP Q07350
U	134	UNK	-	insertion	UNP Q07350
U	135	UNK	-	insertion	UNP Q07350
U	136	UNK	-	insertion	UNP Q07350

- Molecule 22 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 23 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	462	Total	C	N	O	0	0
			2318	1394	462	462		

- Molecule 24 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	S	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 25 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	220	Total	C	N	O	0	0
			1122	682	220	220		

- Molecule 26 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	P	1186	Total	C	N	O	0	0
			5972	3600	1186	1186		

- Molecule 27 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	R	173	Total	C	N	O	0	0
			868	522	173	173		

- Molecule 28 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	83	Total	C	N	O	0	0
			412	246	83	83		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	170	Total	C	N	O	0	0
			862	522	170	170		

- 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
			418	250	84	84		

- Molecule 31 is a protein called Pre-mRNA-processing ATP-dependent RNA helicase PRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	p	444	Total	C	N	O	5	0
			2239	1351	444	444		

- Molecule 32 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2	143	Total	C	N	O	P	0	0
			3021	1351	511	1017	142		

3 Residue-property plots (i)

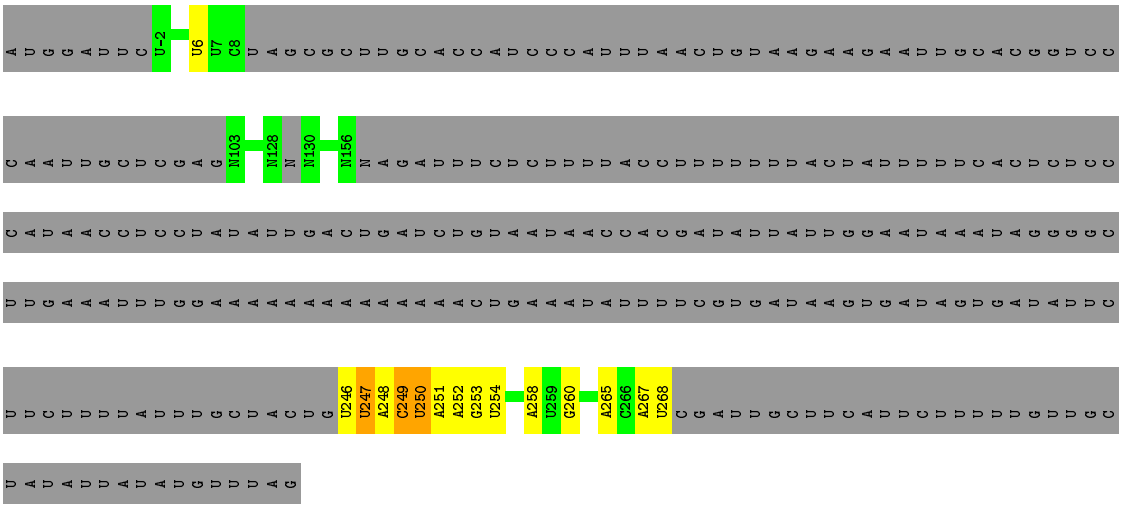
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Protein NAM8

Chain F:

- Molecule 2: ACT1 pre-mRNA (delta BS-A)

Chain I:



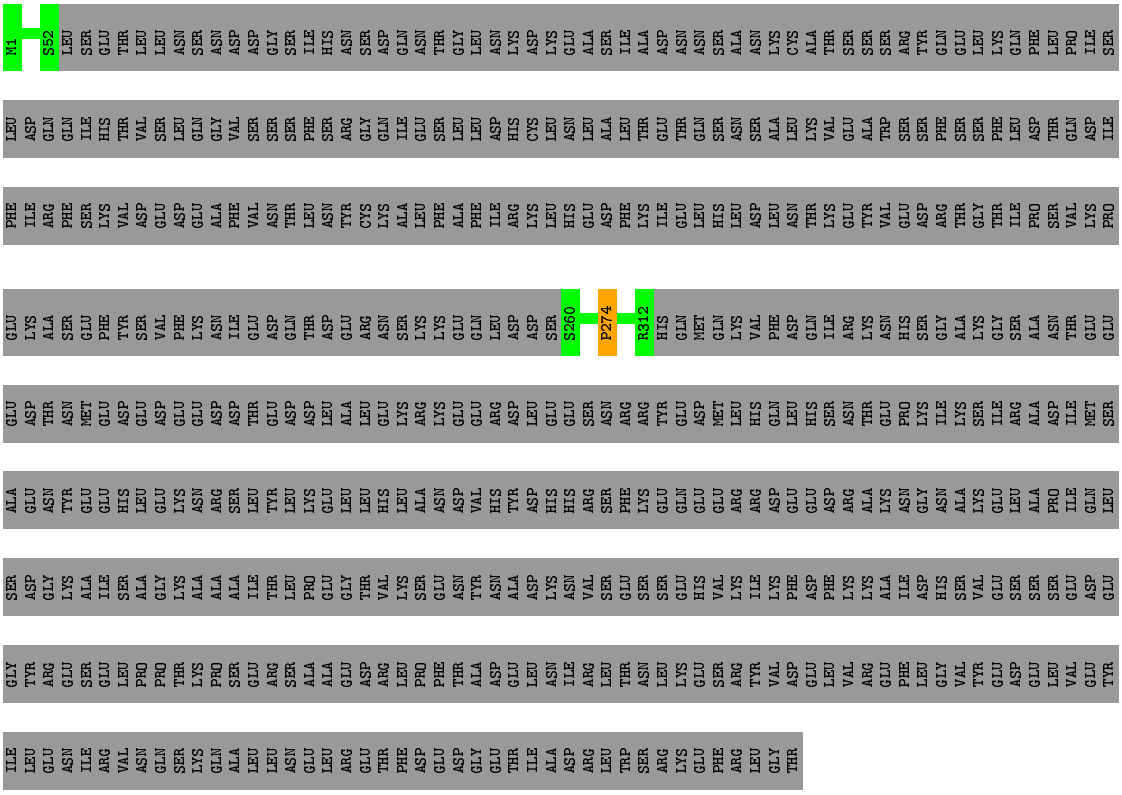
- Molecule 3: U1 small nuclear ribonucleoprotein component PRP42

Chain E:

There are no outlier residues recorded for this chain.

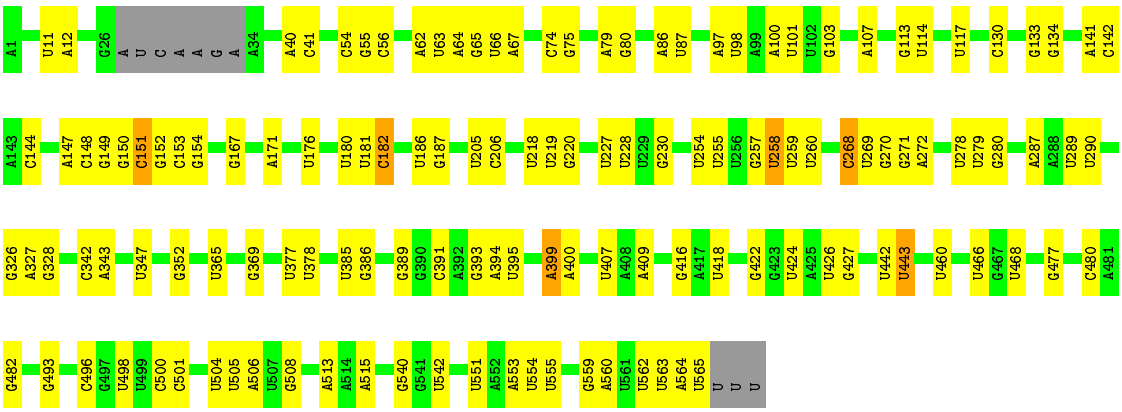
• Molecule 4: U1 small nuclear ribonucleoprotein component SNU71

Chain J:



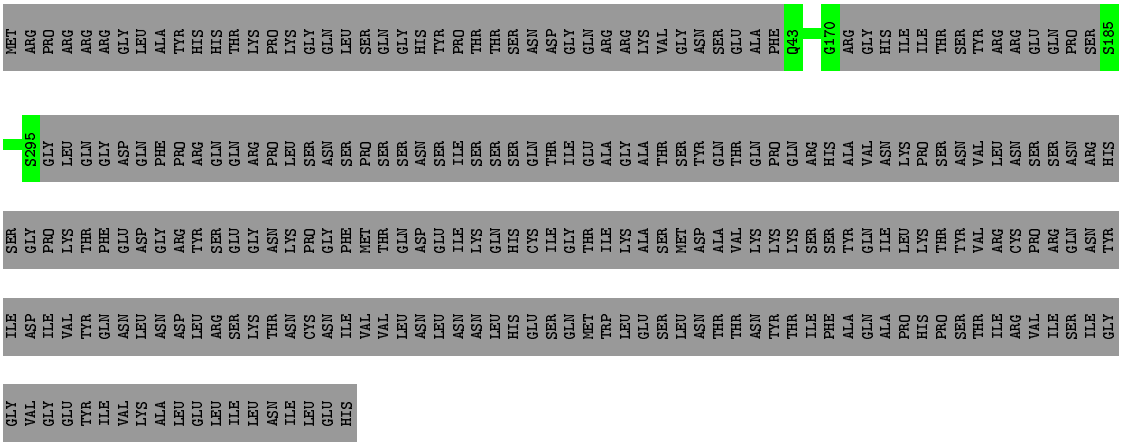
• Molecule 5: U1 snRNA

Chain 1:



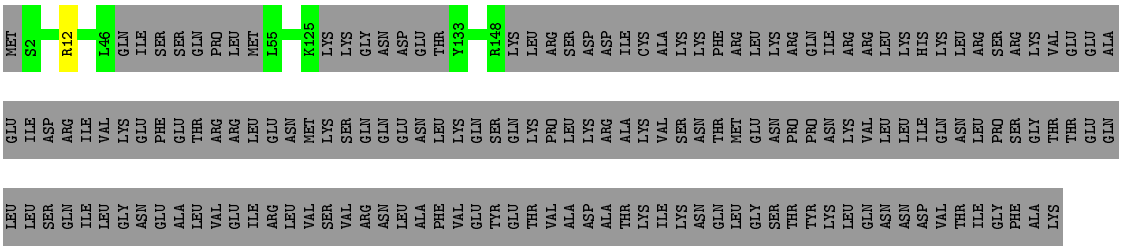
• Molecule 6: 56 kDa U1 small nuclear ribonucleoprotein component

Chain G:



• Molecule 7: U1 small nuclear ribonucleoprotein A

Chain A:

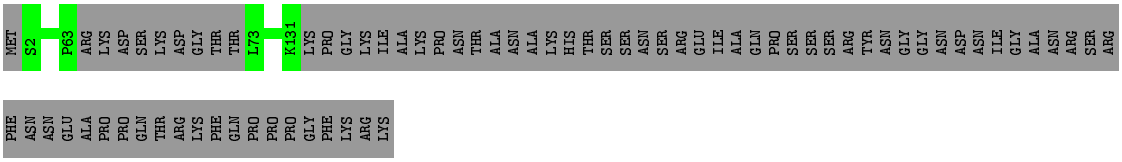


• Molecule 8: U1 small nuclear ribonucleoprotein C

Chain C:

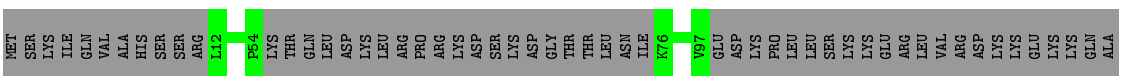
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B

Chain b:



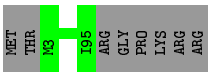
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B

Chain s:



• Molecule 10: Small nuclear ribonucleoprotein Sm D3

Chain d:

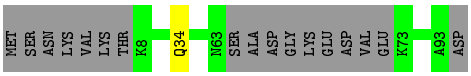


• Molecule 10: Small nuclear ribonucleoprotein Sm D3

Chain v:

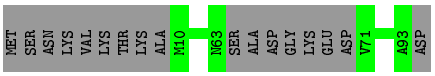
• Molecule 11: Small nuclear ribonucleoprotein E

Chain e:



• Molecule 11: Small nuclear ribonucleoprotein E

Chain w:



• Molecule 12: Small nuclear ribonucleoprotein F

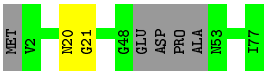
Chain f:

• Molecule 12: Small nuclear ribonucleoprotein F

Chain x:

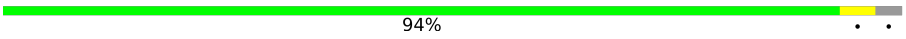
• Molecule 13: Small nuclear ribonucleoprotein G

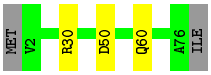
Chain g:



• Molecule 13: Small nuclear ribonucleoprotein G

Chain y:



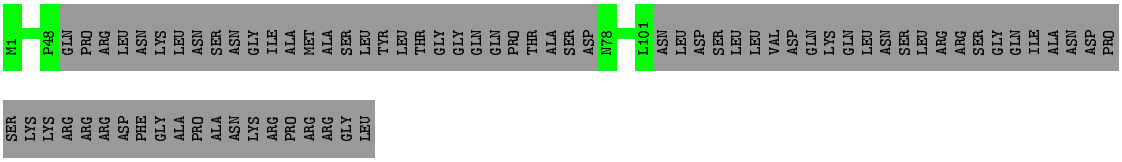


• Molecule 14: Small nuclear ribonucleoprotein Sm D1

Chain h:

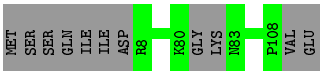
• Molecule 14: Small nuclear ribonucleoprotein Sm D1

Chain t:



• Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain i:

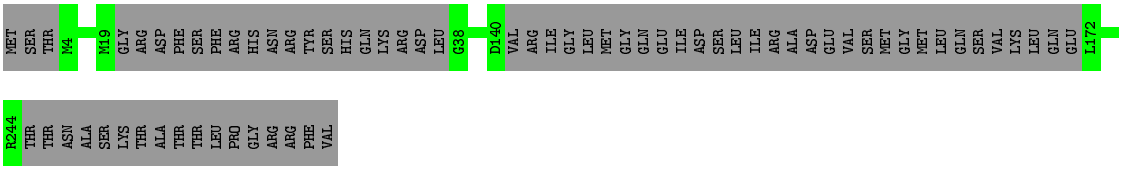


• Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain u:

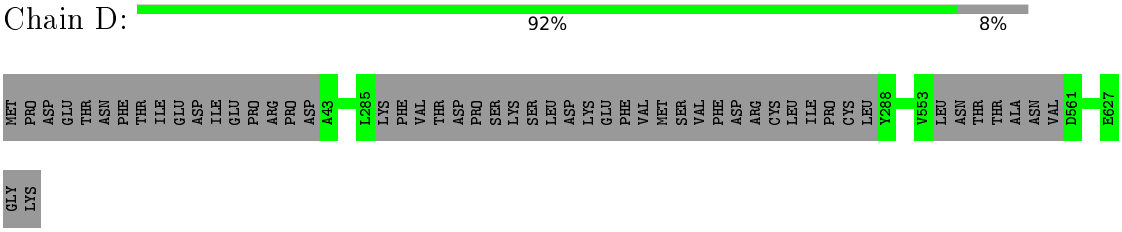
• Molecule 16: Protein LUC7

Chain H:



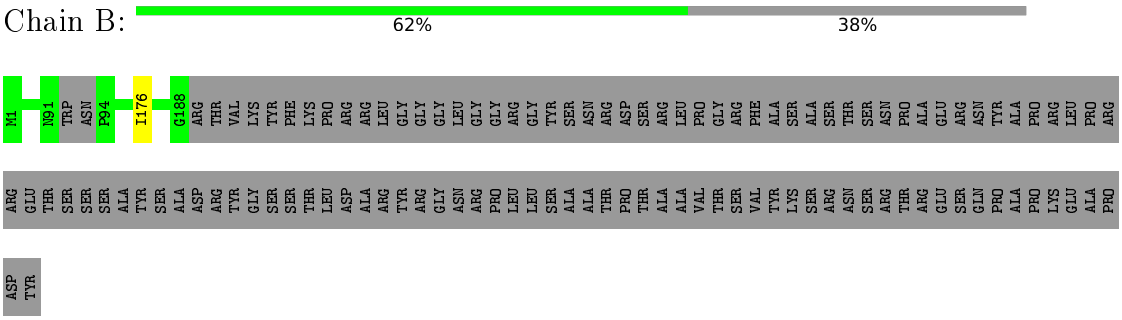
• Molecule 17: Pre-mRNA-processing factor 39

Chain D:



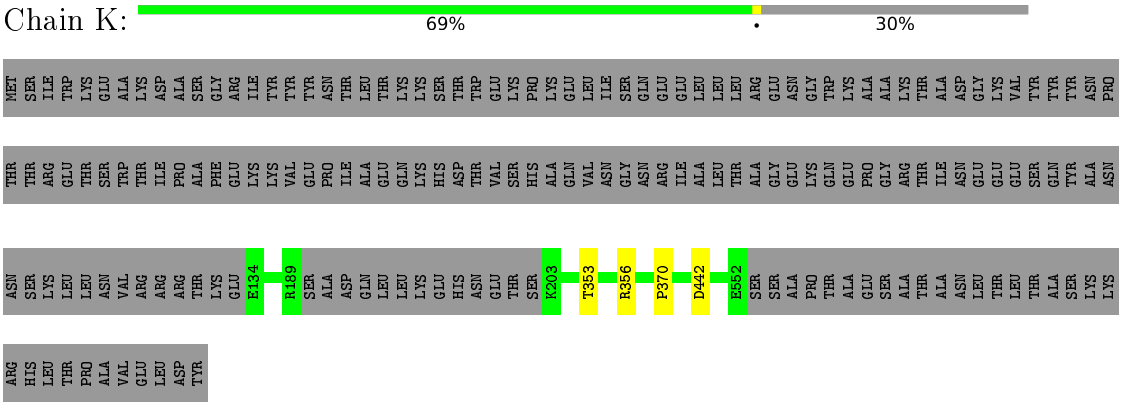
• Molecule 18: U1 small nuclear ribonucleoprotein 70 kDa homolog

Chain B:



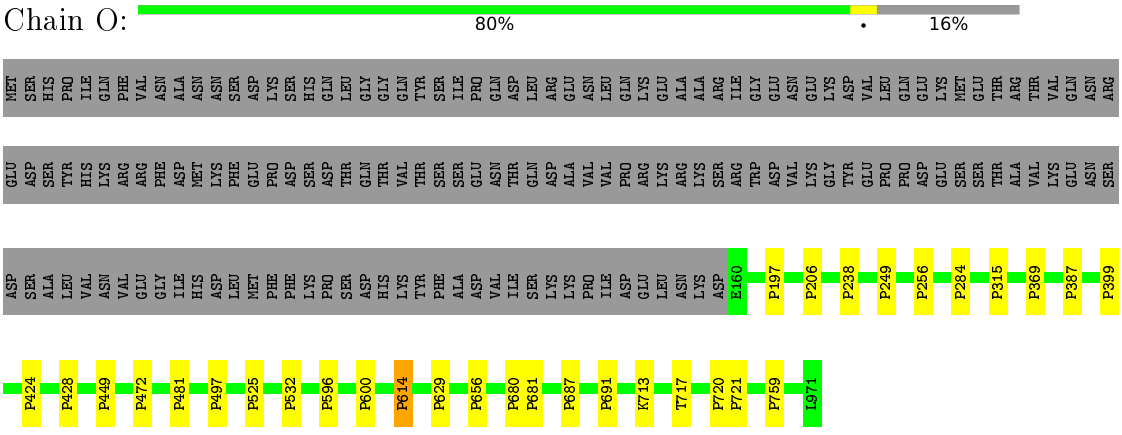
• Molecule 19: Pre-mRNA-processing protein PRP40

Chain K:



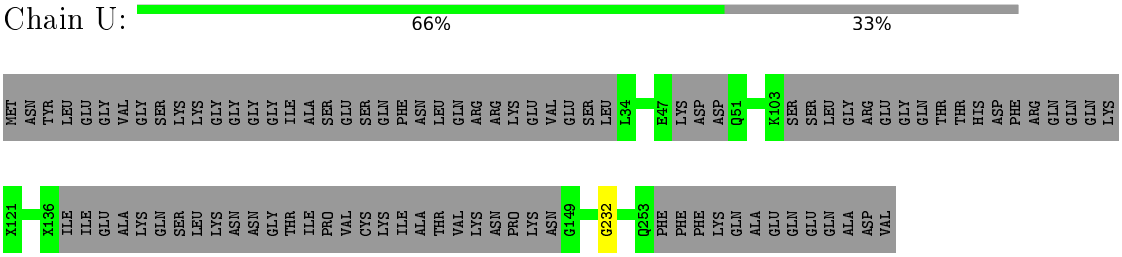
• Molecule 20: U2 snRNP component HSH155

Chain O:



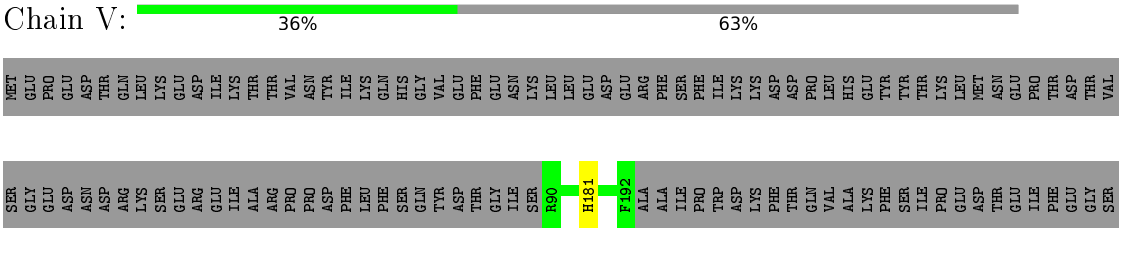
- Molecule 21: Pre-mRNA-splicing factor PRP11

Chain U:



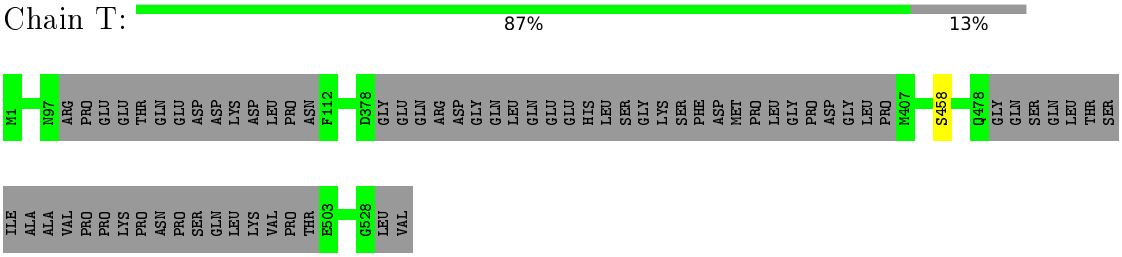
- Molecule 22: Pre-mRNA-splicing factor PRP21

Chain V:



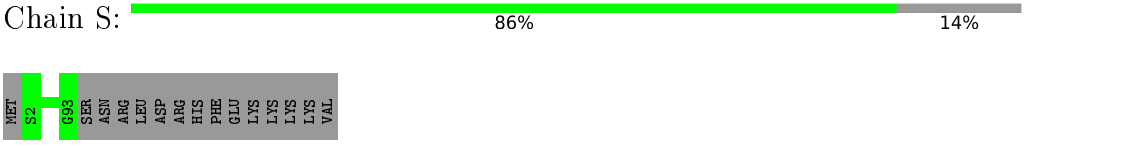
- Molecule 23: Pre-mRNA-splicing factor PRP9

Chain T:



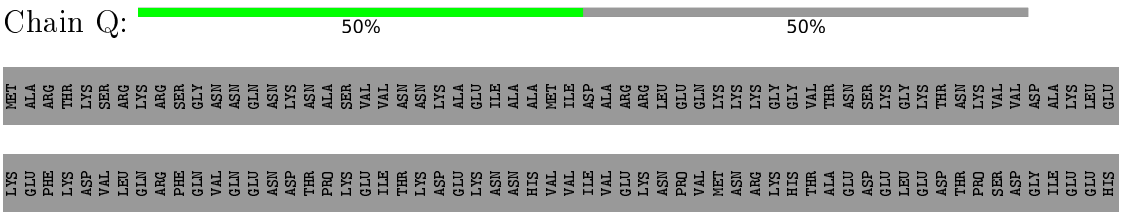
- Molecule 24: Pre-mRNA-splicing factor RDS3

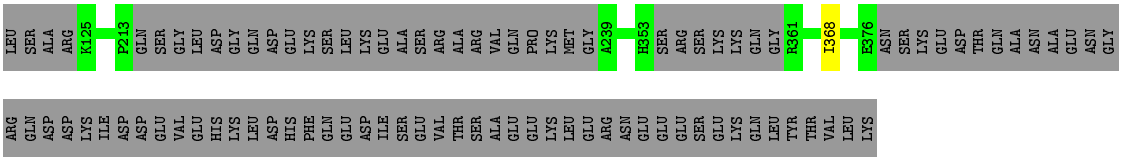
Chain S:



- Molecule 25: Cold sensitive U2 snRNA suppressor 1

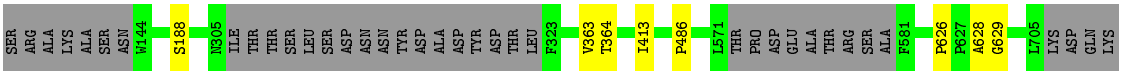
Chain Q:





• Molecule 26: Pre-mRNA-splicing factor RSE1

Chain P:

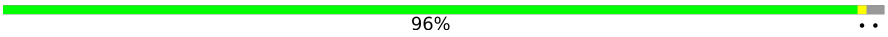


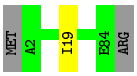
• Molecule 27: Protein HSH49

Chain R:

• Molecule 28: RDS3 complex subunit 10

Chain Z:





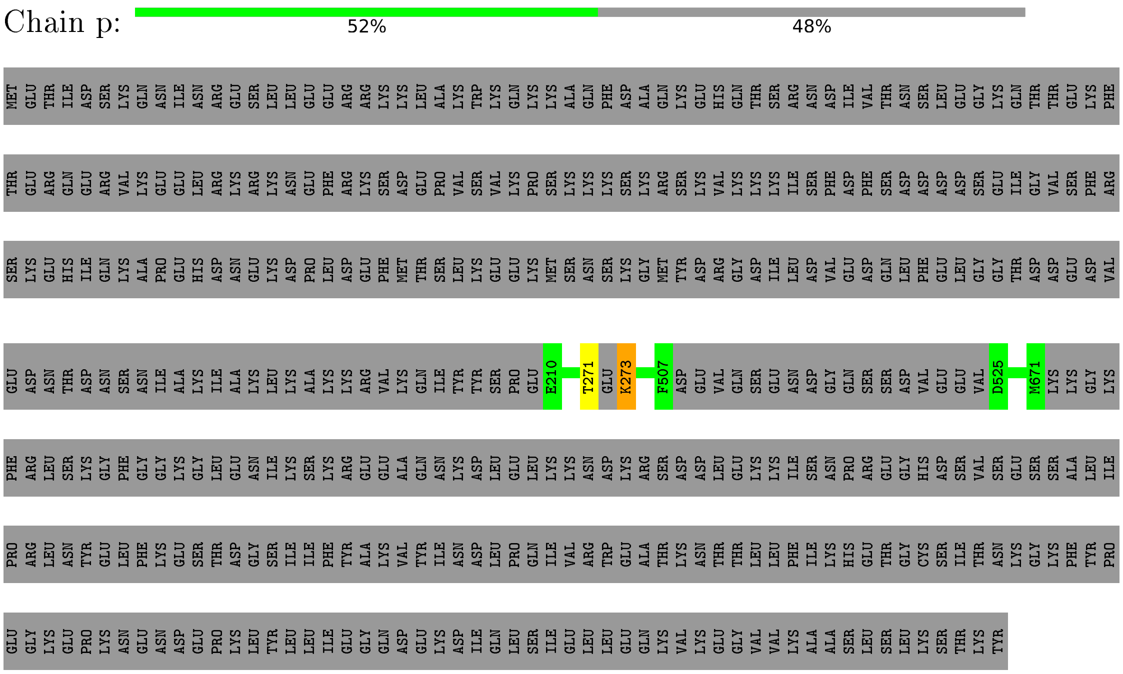
• Molecule 29: U2 small nuclear ribonucleoprotein A'

Chain W:

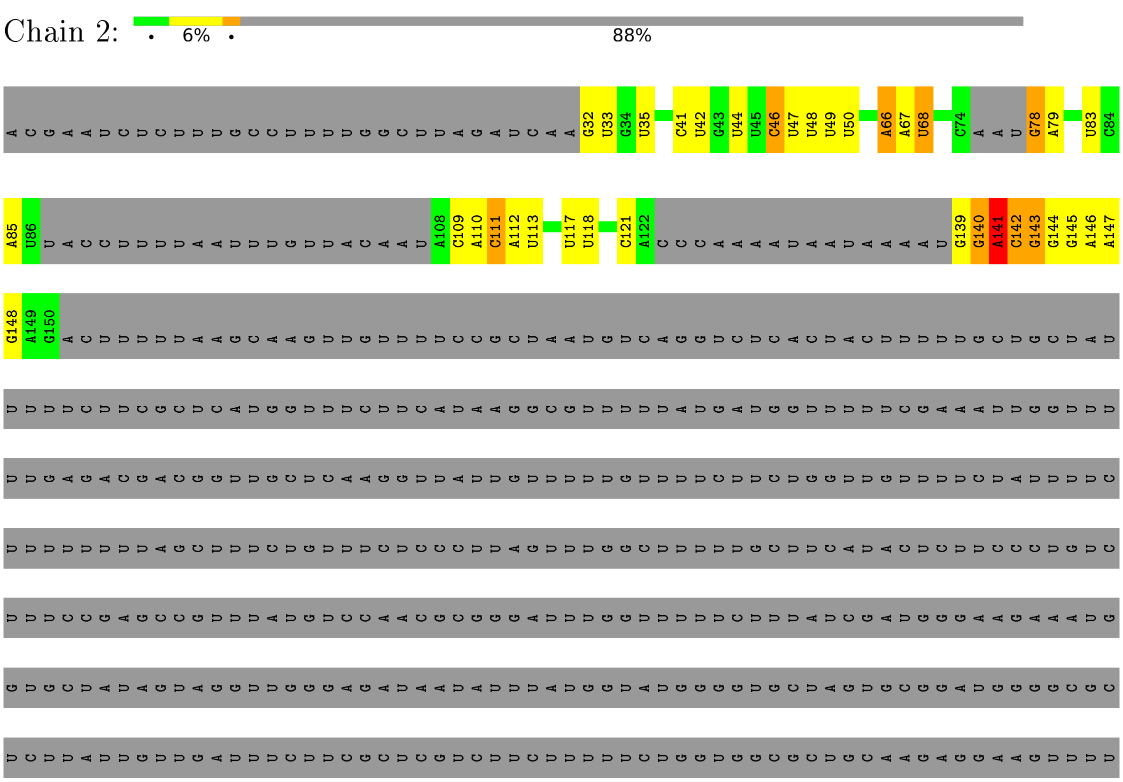
• Molecule 30: U2 small nuclear ribonucleoprotein B"

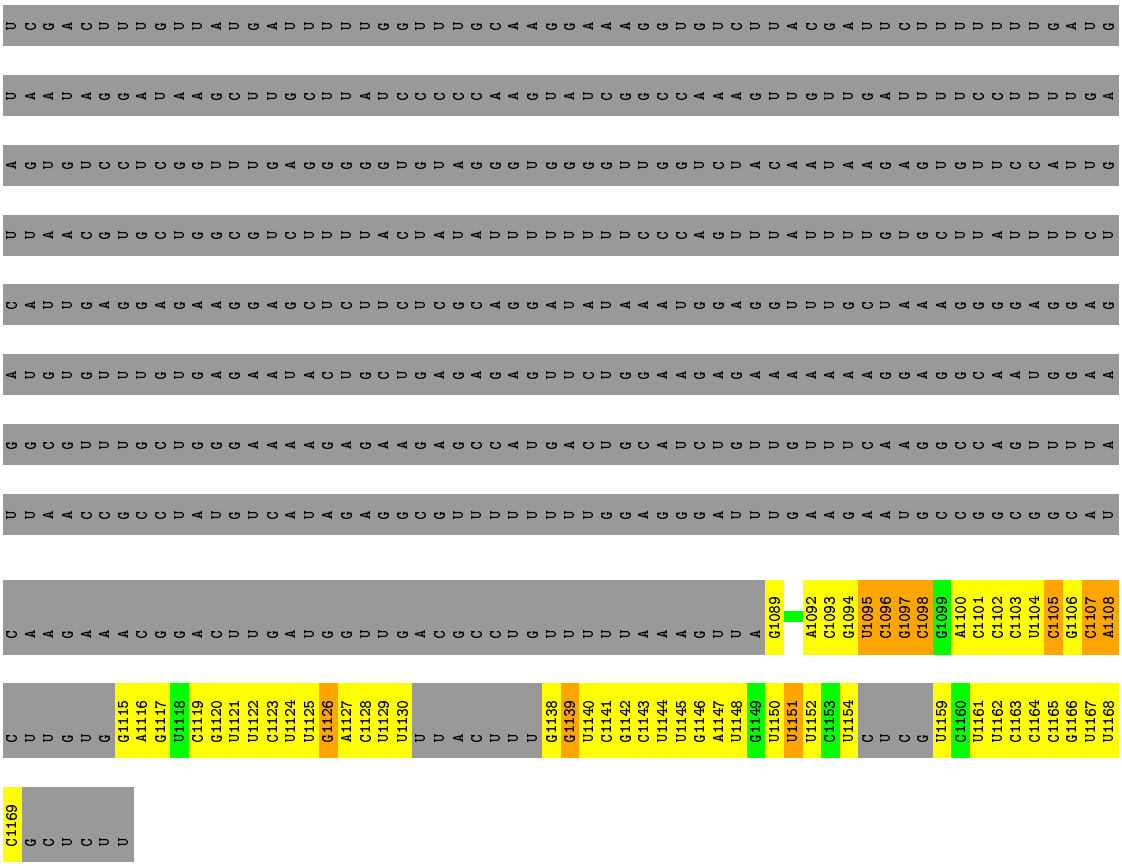
Chain Y:

• Molecule 31: Pre-mRNA-processing ATP-dependent RNA helicase PRP5



• Molecule 32: U2 snRNA




G1089
A1092
C1093
G1094
U1095
C1096
G1097
C1098
G1099
A1100
C1101
C1102
C1103
U1104
C1105
G1106
C1107
A1108
G1115
A1116
G1117
U1118
C1119
G1120
U1121
U1122
C1123
U1124
U1125
G1126
A1127
C1128
U1129
U1130
G1138
G1139
U1140
C1141
G1142
C1143
U1144
U1145
G1146
A1147
U1148
G1149
U1150
U1151
U1152
C1153
U1154
U1159
C1160
U1161
U1162
C1163
C1164
C1165
G1166
U1167
U1168
C1169

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217460	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 ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	F	0.26	0/1342	0.50	0/1868
2	I	0.60	6/768 (0.8%)	0.89	1/1189 (0.1%)
3	E	0.24	0/2743	0.45	0/3841
4	J	0.26	0/530	0.50	1/740 (0.1%)
5	1	0.30	0/13201	1.01	30/20553 (0.1%)
6	G	0.25	0/1208	0.49	0/1689
7	A	0.24	0/671	0.51	0/937
8	C	0.25	0/992	0.48	0/1390
9	b	0.25	0/608	0.51	0/848
9	s	0.30	0/322	0.57	0/446
10	d	0.27	0/479	0.52	0/671
10	v	0.29	0/415	0.54	0/579
11	e	0.24	0/392	0.57	0/546
11	w	0.29	0/392	0.54	0/546
12	f	0.26	0/367	0.54	0/510
12	x	0.31	0/367	0.58	0/510
13	g	0.25	0/355	0.56	0/491
13	y	0.26	0/374	0.50	0/520
14	h	0.24	0/535	0.48	0/743
14	t	0.33	0/364	0.55	0/507
15	i	0.24	0/503	0.52	0/703
15	u	0.32	0/465	0.53	0/650
16	H	0.23	0/962	0.37	0/1340
17	D	0.24	0/2901	0.41	0/4059
18	B	0.24	0/947	0.43	0/1325
19	K	0.52	0/2050	0.94	0/2870
20	O	0.42	0/4149	0.77	30/5819 (0.5%)
21	U	0.22	0/867	0.43	0/1208
22	V	0.38	0/515	0.43	0/719
23	T	0.27	0/2324	0.44	0/3248
24	S	0.27	0/463	0.49	0/645
25	Q	0.27	0/1137	0.47	0/1593
26	P	0.29	1/6009 (0.0%)	0.54	0/8407
27	R	0.28	0/869	0.46	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	Z	0.26	0/412	0.41	0/573
29	W	0.31	0/869	0.60	0/1219
30	Y	0.27	0/418	0.49	0/582
31	p	0.55	1/2269 (0.0%)	0.66	3/3172 (0.1%)
32	2	4.64	44/3363 (1.3%)	2.45	107/5218 (2.1%)
All	All	1.16	52/57917 (0.1%)	0.92	172/83683 (0.2%)

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
7	A	0	1
13	g	0	1
18	B	0	1
23	T	0	1
26	P	0	2
29	W	0	1
32	2	0	2
All	All	0	9

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	35	U	C1'-N1	151.33	3.75	1.48
32	2	42	U	C1'-N1	150.94	3.75	1.48
32	2	44	U	C1'-N1	149.92	3.73	1.48
31	p	271	THR	C-N	20.19	1.80	1.34
32	2	1161	U	O3'-P	-15.61	1.42	1.61

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	44	U	C6-N1-C1'	-74.43	17.00	121.20
32	2	42	U	C6-N1-C1'	-73.72	17.99	121.20
32	2	35	U	C6-N1-C1'	-73.60	18.16	121.20
32	2	44	U	O4'-C1'-N1	-27.50	86.20	108.20
32	2	42	U	O4'-C1'-N1	-21.03	91.37	108.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	12	ARG	Peptide
18	B	176	ILE	Peptide
26	P	1013	ASP	Peptide
23	T	458	SER	Peptide
13	g	20	ASN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	259/523 (50%)	251 (97%)	8 (3%)	0	100	100
3	E	542/544 (100%)	521 (96%)	21 (4%)	0	100	100
4	J	101/620 (16%)	92 (91%)	8 (8%)	1 (1%)	15	54
6	G	235/492 (48%)	222 (94%)	13 (6%)	0	100	100
7	A	126/298 (42%)	116 (92%)	10 (8%)	0	100	100
8	C	193/231 (84%)	183 (95%)	10 (5%)	0	100	100
9	b	117/196 (60%)	110 (94%)	7 (6%)	0	100	100
9	s	61/196 (31%)	58 (95%)	3 (5%)	0	100	100
10	d	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
10	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
11	e	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	11	46
11	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
12	f	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
12	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
13	g	68/77 (88%)	62 (91%)	5 (7%)	1 (2%)	10	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	3 22
14	h	101/146 (69%)	98 (97%)	3 (3%)	0	100 100
14	t	68/146 (47%)	67 (98%)	1 (2%)	0	100 100
15	i	95/110 (86%)	91 (96%)	4 (4%)	0	100 100
15	u	90/110 (82%)	89 (99%)	1 (1%)	0	100 100
16	H	186/261 (71%)	180 (97%)	6 (3%)	0	100 100
17	D	570/629 (91%)	554 (97%)	16 (3%)	0	100 100
18	B	182/300 (61%)	169 (93%)	13 (7%)	0	100 100
19	K	402/583 (69%)	379 (94%)	19 (5%)	4 (1%)	15 54
20	O	810/971 (83%)	772 (95%)	35 (4%)	3 (0%)	34 72
21	U	166/282 (59%)	141 (85%)	24 (14%)	1 (1%)	25 65
22	V	101/280 (36%)	90 (89%)	10 (10%)	1 (1%)	15 54
23	T	454/530 (86%)	414 (91%)	40 (9%)	0	100 100
24	S	90/107 (84%)	79 (88%)	11 (12%)	0	100 100
25	Q	214/436 (49%)	202 (94%)	11 (5%)	1 (0%)	29 69
26	P	1170/1361 (86%)	1055 (90%)	105 (9%)	10 (1%)	17 56
27	R	165/213 (78%)	161 (98%)	3 (2%)	1 (1%)	25 65
28	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13 50
29	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1 16
30	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	13 50
31	p	445/849 (52%)	431 (97%)	13 (3%)	1 (0%)	47 81
All	All	7874/11564 (68%)	7373 (94%)	460 (6%)	41 (0%)	32 69

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	Q	368	ILE
26	P	1299	ILE
29	W	34	LEU
29	W	52	LYS
13	y	50	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	11/451 (2%)	11 (100%)	0	100	100
3	E	12/519 (2%)	12 (100%)	0	100	100
4	J	3/568 (0%)	3 (100%)	0	100	100
6	G	8/448 (2%)	8 (100%)	0	100	100
7	A	6/273 (2%)	6 (100%)	0	100	100
8	C	8/214 (4%)	8 (100%)	0	100	100
9	b	3/176 (2%)	3 (100%)	0	100	100
9	s	1/176 (1%)	1 (100%)	0	100	100
10	d	7/89 (8%)	7 (100%)	0	100	100
10	v	4/89 (4%)	4 (100%)	0	100	100
11	e	5/83 (6%)	5 (100%)	0	100	100
11	w	5/83 (6%)	5 (100%)	0	100	100
12	f	3/77 (4%)	3 (100%)	0	100	100
12	x	3/77 (4%)	3 (100%)	0	100	100
13	g	1/66 (2%)	1 (100%)	0	100	100
13	y	2/66 (3%)	2 (100%)	0	100	100
14	h	3/129 (2%)	3 (100%)	0	100	100
14	t	3/129 (2%)	3 (100%)	0	100	100
15	i	4/103 (4%)	4 (100%)	0	100	100
15	u	3/103 (3%)	3 (100%)	0	100	100
16	H	5/234 (2%)	5 (100%)	0	100	100
17	D	12/603 (2%)	12 (100%)	0	100	100
18	B	9/265 (3%)	9 (100%)	0	100	100
19	K	10/538 (2%)	10 (100%)	0	100	100
20	O	42/867 (5%)	42 (100%)	0	100	100
21	U	7/236 (3%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	V	1/259 (0%)	1 (100%)	0	100	100
23	T	10/492 (2%)	10 (100%)	0	100	100
24	S	4/97 (4%)	4 (100%)	0	100	100
25	Q	18/392 (5%)	18 (100%)	0	100	100
26	P	45/1244 (4%)	45 (100%)	0	100	100
27	R	5/189 (3%)	5 (100%)	0	100	100
28	Z	1/77 (1%)	1 (100%)	0	100	100
29	W	8/219 (4%)	8 (100%)	0	100	100
30	Y	1/100 (1%)	1 (100%)	0	100	100
31	p	17/768 (2%)	17 (100%)	0	100	100
All	All	290/10499 (3%)	290 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	31/373 (8%)	11 (35%)	0
32	2	138/1175 (11%)	53 (38%)	27 (19%)
5	1	556/568 (97%)	118 (21%)	9 (1%)
All	All	725/2116 (34%)	182 (25%)	36 (4%)

5 of 182 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	247	U
2	I	248	A
2	I	249	C
2	I	250	U
2	I	251	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	2	1124	U

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Mol	Chain	Res	Type
32	2	1150	U
32	2	1125	U
32	2	1142	G
32	2	67	A

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.