Full wwPDB EM Validation 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 Full wwPDB EM Validation 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 (i)) were used in the production of this report:

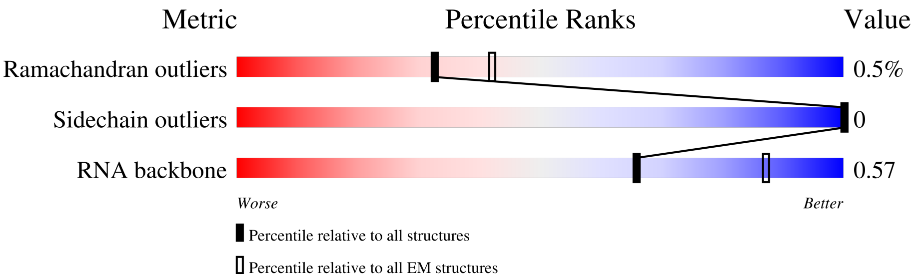
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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%

Continued on next page...

Continued from previous page...

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%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	Z	85	96% • •
29	W	238	66% 5% 29%
30	Y	111	75% • 24%
31	p	849	52% 48%
32	2	1175	• 6% • 88%

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
			Total	C	N	O		
1	F	267	1335	801	267	267	0	0

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

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

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

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

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

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

- Molecule 5 is a RNA chain called U1 snRNA.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	G	239	1202	724	239	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 356	C 212	N 72	O 72	0	0
13	y	75	Total 373	C 223	N 75	O 75	0	0

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

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

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

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

- Molecule 16 is a protein called Protein LUC7.

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O		
22	V	103	515	309	103	103	0	0

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Protein HSH49.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	Y	84	418	250	84	84	0	0

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

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

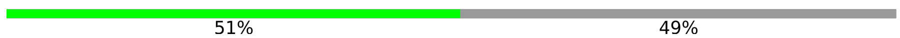
- Molecule 32 is a RNA chain called U2 snRNA.

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

3 Residue-property plots

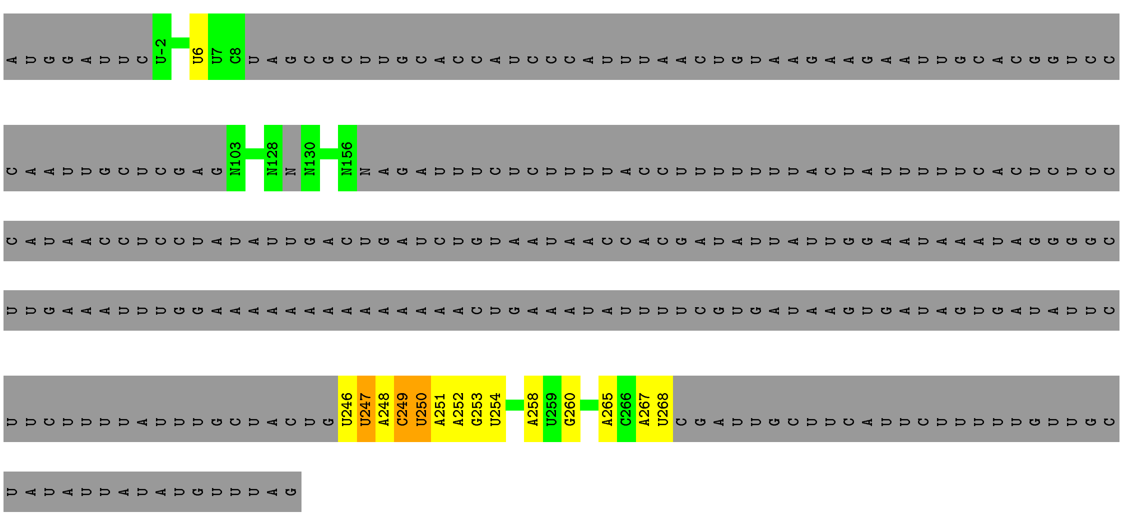
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

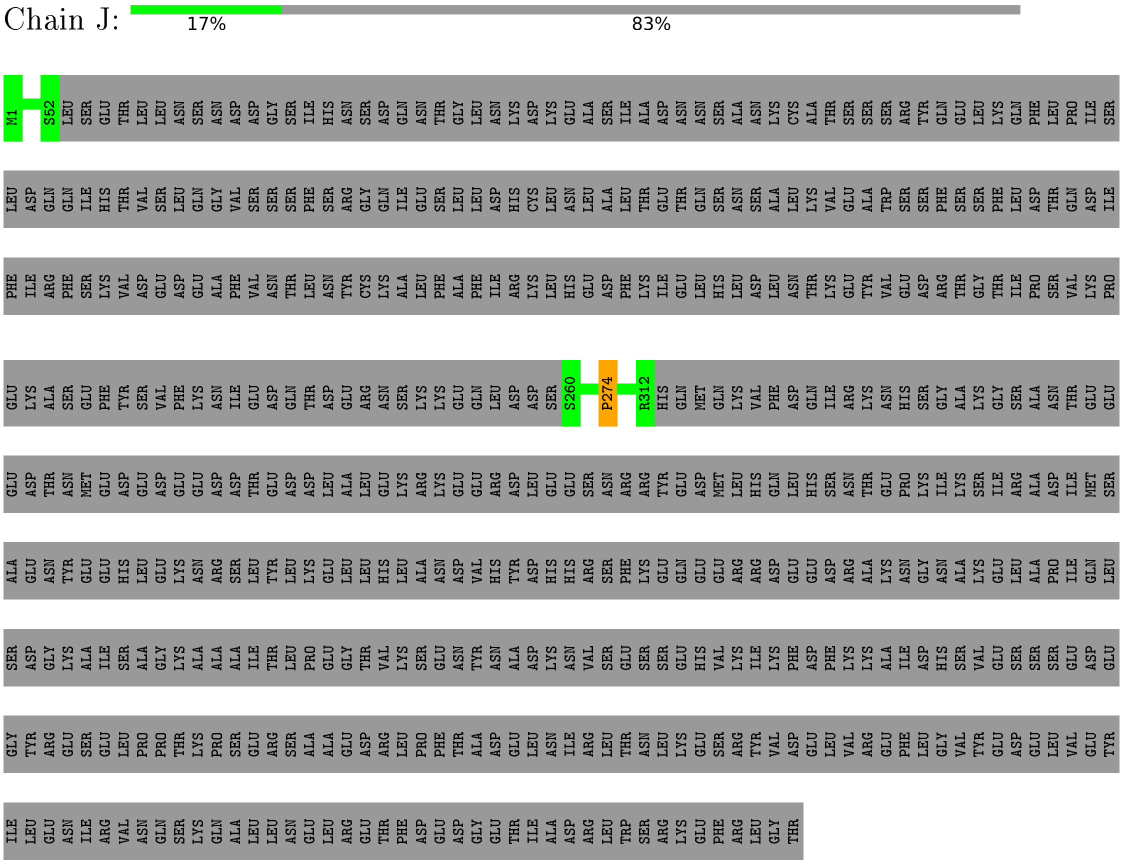
- Molecule 3: U1 small nuclear ribonucleoprotein component PRP42

Chain E:

There are no outlier residues recorded for this chain.

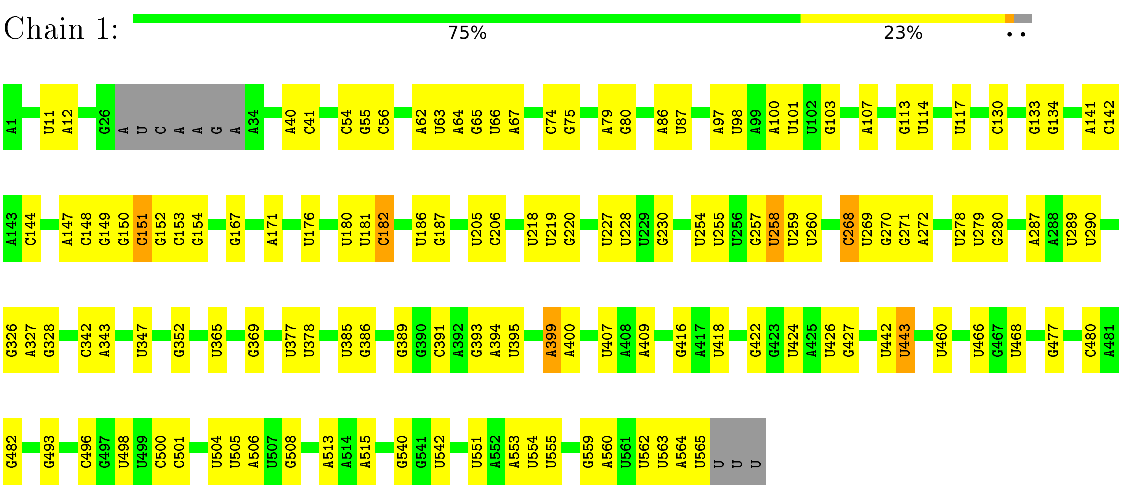
• Molecule 4: U1 small nuclear ribonucleoprotein component SNU71

Chain J:



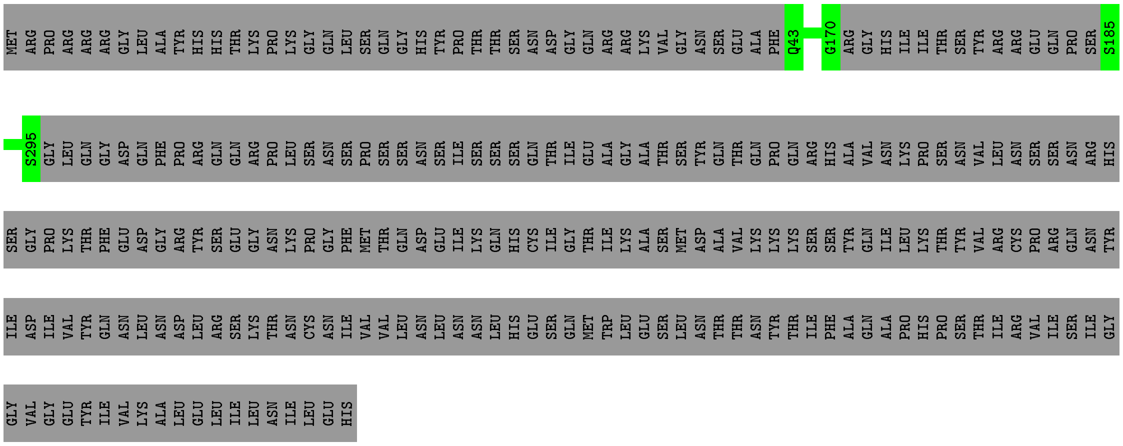
• Molecule 5: U1 snRNA

Chain 1:



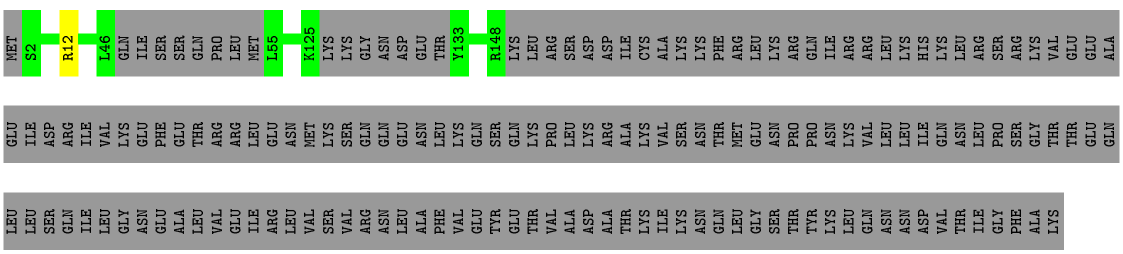
• Molecule 6: 56 kDa U1 small nuclear ribonucleoprotein component

Chain G:



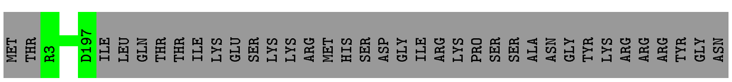
• Molecule 7: U1 small nuclear ribonucleoprotein A

Chain A:



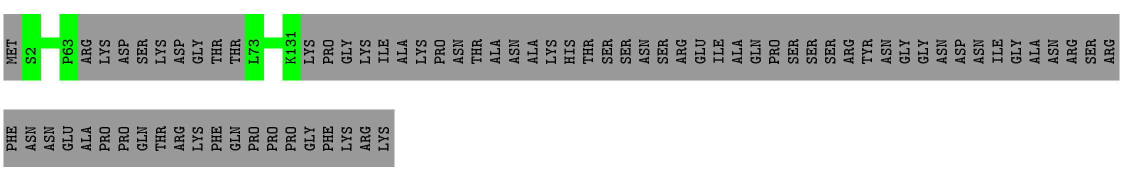
• Molecule 8: U1 small nuclear ribonucleoprotein C

Chain C:



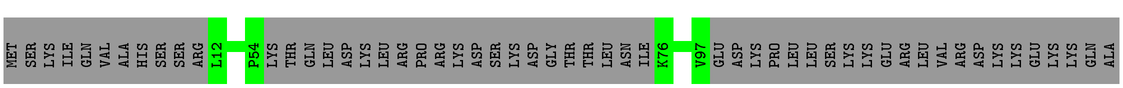
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B

Chain b:



• Molecule 9: Small nuclear ribonucleoprotein-associated protein B

Chain s:



GLN LYS GLN THR LYS LEU ARG LYS GLU LYS GLU LYS LYS PRO GLY LYS ILE ALA LYS PRO ASN THR ALA ASN ALA LYS HIS THR SER SER ASN SER ARG GLU ILE ALA GLN PRO SER SER SER ARG TYR ASN GLY GLY ASN ASP ASN ILE GLY ALA ASN ARG SER ARG PHE ASN ASN GLU

ALA PRO PRO GLN THR ARG LYS PHE GLN PRO PRO GLY PHE LYS ARG LYS

• Molecule 10: Small nuclear ribonucleoprotein Sm D3

Chain d: 92% 8%

MET THR M3 I95 ARG GLY PRO LYS ARG ARG

• Molecule 10: Small nuclear ribonucleoprotein Sm D3

Chain v: 81% 19%

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

• Molecule 11: Small nuclear ribonucleoprotein E

Chain e: 81% • 18%

MET SER ASN LYS VAL LYS THR K8 Q34 N63 SER ALA ASP GLY LYS GLU ASP VAL GLU K73 A93 ASP

• Molecule 11: Small nuclear ribonucleoprotein E

Chain w: 82% 18%

MET SER ASN LYS VAL LYS THR LYS ALA M10 N63 SER ALA ASP GLY LYS GLU ASP V71 A93 ASP

• Molecule 12: Small nuclear ribonucleoprotein F

Chain f: 85% 15%

MET SER GLU SER SER ASP ILE SER ALA MET GLN P12 L84 PRO ASN

• Molecule 12: Small nuclear ribonucleoprotein F

Chain x: 85% 15%

MET SER GLU SER SER ASP ILE SER ALA MET GLN P12 L84 PRO ASN

• Molecule 13: Small nuclear ribonucleoprotein G

Chain g: 91% • 6%

MET V2 N20 G21 G48 GLU ASP PRO ALA N53 I77

• Molecule 13: Small nuclear ribonucleoprotein G

Chain y: 94%

MET V2 R30 D50 Q60 A76 ILE

• Molecule 14: Small nuclear ribonucleoprotein Sm D1

Chain h: 73% 27%

M1 Q49 PRO ARG LEU ASN LYS LEU ASN S58 Q73 PRO THR ALA SER ASP N78 S119 GLY GLN ILE ALA ASN ASP PRO SER LYS LYS ARG ARG ASP PHE GLY ALA PRO ALA ASN LYS ARG PRO ARG GLY LEU

• Molecule 14: Small nuclear ribonucleoprotein Sm D1

Chain t: 49% 51%

M1 P48 GLN PRO ARG LEU ASN LYS LEU ASN SER ASN GLY ILE ALA MET ALA SER LEU TYR LEU THR GLY GLY GLN GLN PRO THR ALA SER ASP N78 L101 ASN LEU ASP SER LEU LEU VAL ASP GLN LYS GLN LEU ASN SER LEU ARG ARG SER GLY GLN ILE ALA ASN ASP PRO

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

• Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain i: 90% 10%

MET SER SER GLN ILE ILE ASP R8 K80 GLY LYS N83 P108 VAL GLU

• Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain u: 84% 16%

MET SER SER GLN ILE ILE ASP ARG PRO LYS HIS GLU LEU SER ARG ALA E17 P108 VAL GLU

• Molecule 16: Protein LUC7

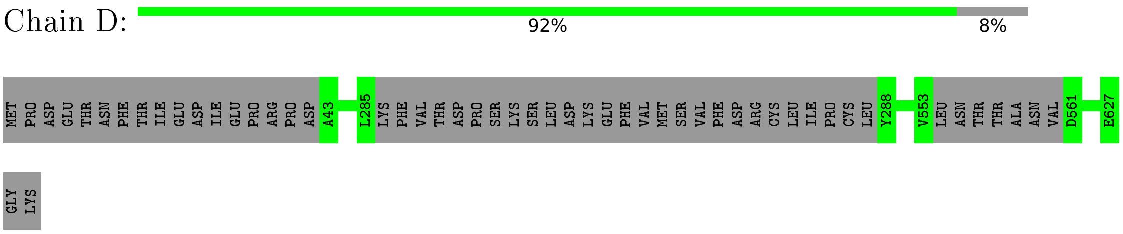
Chain H: 74% 26%

MET SER THR M4 M19 GLY ARG ASP PHE SER PHE ARG HIS ASN ARG TYR SER HIS GLN LYS ARG ASP LEU G38 D140 VAL ARG ILE GLY LEU MET GLY GLN GLU ILE ASP SER LEU ILE ARG ALA ASP GLU VAL SER MET GLY MET LEU GLN SER VAL LYS LEU GLN GLU L172

R244 THR THR ASN ALA SER LYS THR ALA THR THR LEU PRO GLY ARG ARG PHE VAL

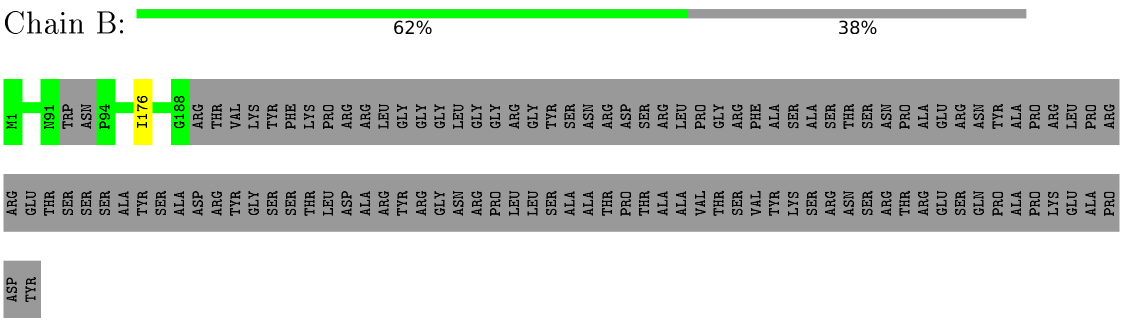
- Molecule 17: Pre-mRNA-processing factor 39

Chain D:



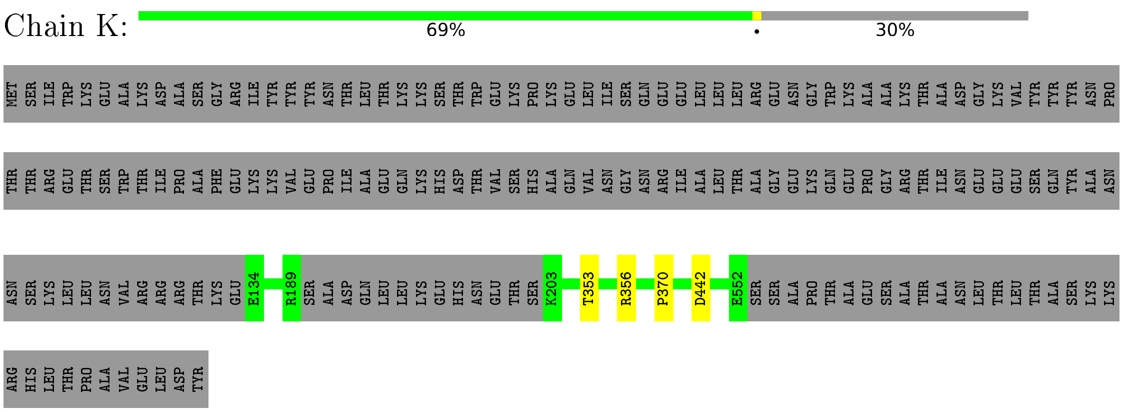
- Molecule 18: U1 small nuclear ribonucleoprotein 70 kDa homolog

Chain B:



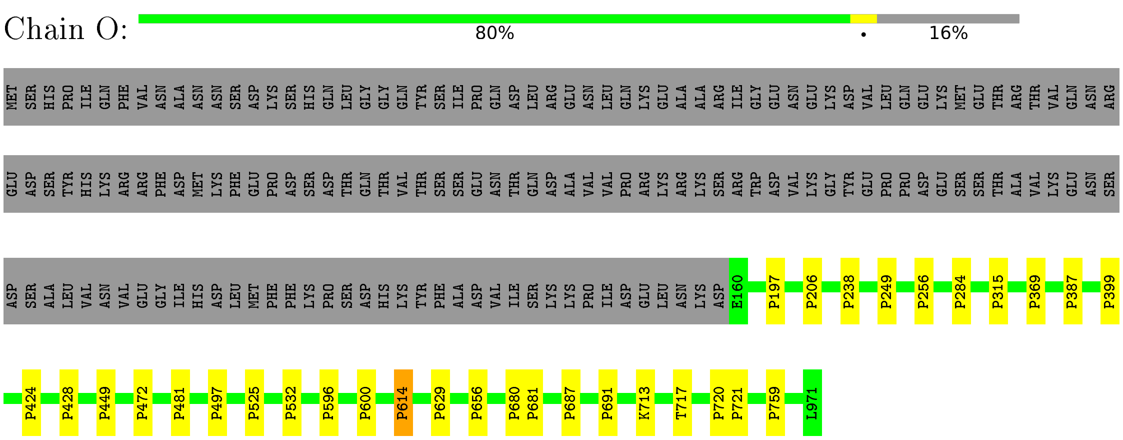
- Molecule 19: Pre-mRNA-processing protein PRP40

Chain K:

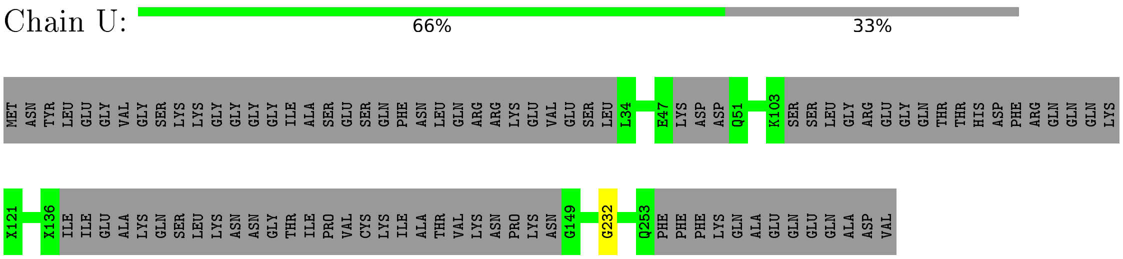


- Molecule 20: U2 snRNP component HSH155

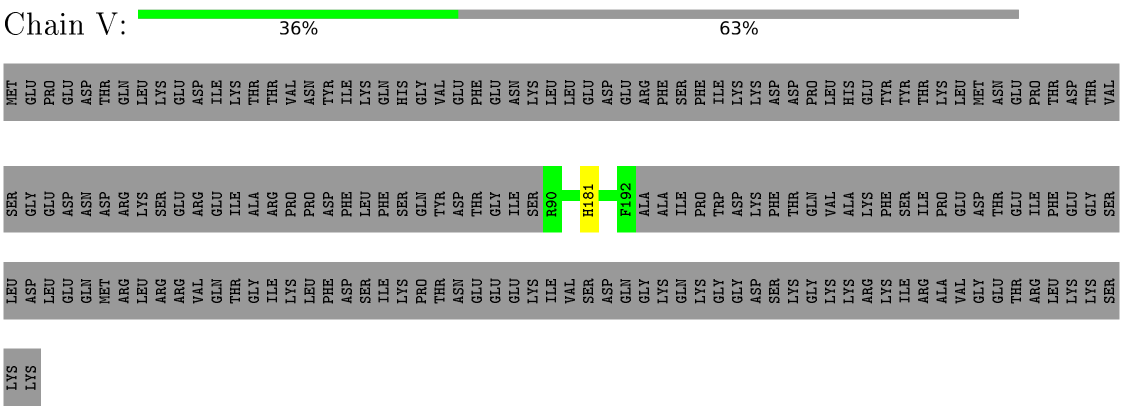
Chain O:



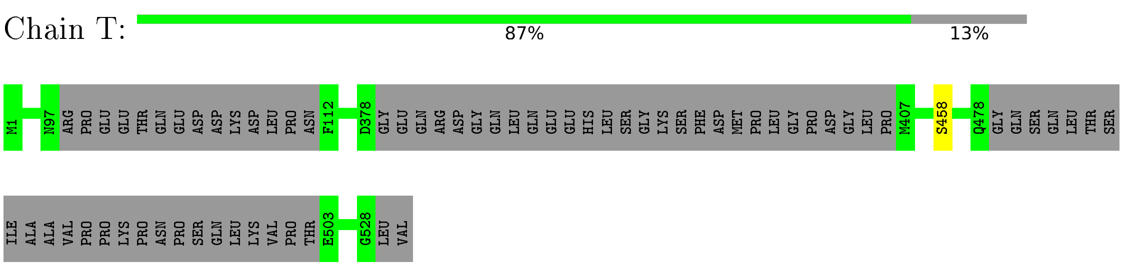
- Molecule 21: Pre-mRNA-splicing factor PRP11



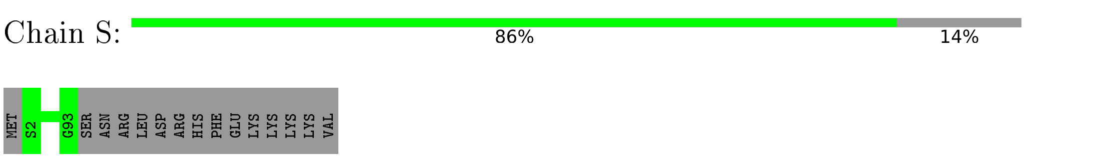
- Molecule 22: Pre-mRNA-splicing factor PRP21



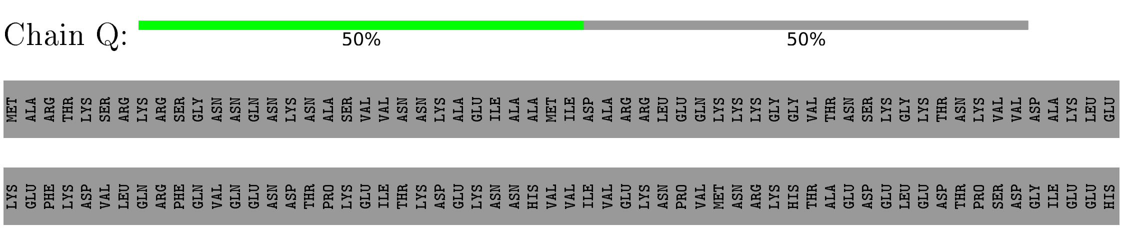
- Molecule 23: Pre-mRNA-splicing factor PRP9



- Molecule 24: Pre-mRNA-splicing factor RDS3



- Molecule 25: Cold sensitive U2 snRNA suppressor 1



LEU SER ALA ARG K125 P213 GLN SER GLY LEU ASP GLY GLN ASP GLU LYS SER LEU LYS GLU ALA SER ARG ALA ARG VAL GLN PRO LYS MET GLY A239 H353 SER ARG SER LYS LYS GLN GLY R361 I368 E376 ASN SER LYS GLU ASP THR GLN ALA ASN ALA GLU ASN GLY

ARG GLN ASP ASP LYS ILE ASP ASP GLU VAL GLU HIS LYS LEU ASP HIS PHE GLN GLU ASP ILE SER GLU VAL THR SER ALA GLU GLU LYS LEU GLU ARG ASN GLU GLU GLU SER GLU LYS GLN LEU TYR THR VAL LEU LYS

- Molecule 26: Pre-mRNA-splicing factor RSE1

Chain P: 86% • 13%

MET TRP GLY GLY GLY LYS MET ALA VAL VAL SER LEU SER PRO HIS THR ALA LYS MET ARG LYS LEU PHE GLY GLN ALA SER THR THR MET ALA TYR ASP GLY LEU LYS ARG GLU ALA GLU ARG ARG THR ARG SER ASP HIS ASN ILE THR MET VAL A53 A107 P133 HIS SER GLY

SER ARG ALA LYS ALA SER ASN W144 S188 N305 ILE THR THR SER LEU SER ASP ASN ASN TYR ASP ALA ASP TYR ASP THR LEU F323 V363 T364 I413 P486 L571 THR PRO ASP GLU ALA THR ARG SER ALA F581 P626 P627 A628 G629 L705 LYS ASP GLN LYS

GLU D711 S784 VAL SER LEU ASN ASN GLU GLU GLU GLU GLU GLU GLU ASP ASP ASP ASP GLU LYS GLU GLU GLU GLU ILE ASN SER SER GLY ALA K814 E890 SER SER VAL ASN LYS GLN GLU GLU ASN GLY GLY GLY ASP GLU SER ASN GLU GLU GLU GLU ASP GLU MET GLU GLU

GLU MET GLU M918 D1013 K1014 I1031 N1265 ASN MET ARG LYS GLU ASP ASP GLU GLU GLU SER GLY SER VAL VAL LEU GLN GLY ARG HIS GLY ILE GLU ASP GLU ILE I1292 I1299 M1361

- Molecule 27: Protein HSH49

Chain R: 81% 19%

MET ASN TYR SER ALA ASP SER GLY N9 A48 V86 THR ASN SER THR GLY THR THR ASN LEU PRO SER ASN ILE SER LYS ASP MET ILE LEU P106 S144 ASN GLY K147 K185 GLU N187 N203 LYS GLU ALA LEU LYS HIS ASN MET LEU LYS

- Molecule 28: RDS3 complex subunit 10

Chain Z: 96% ••

MET A2 I19 E84 ARG

- Molecule 29: U2 small nuclear ribonucleoprotein A'

Chain W: 66% 5% 29%

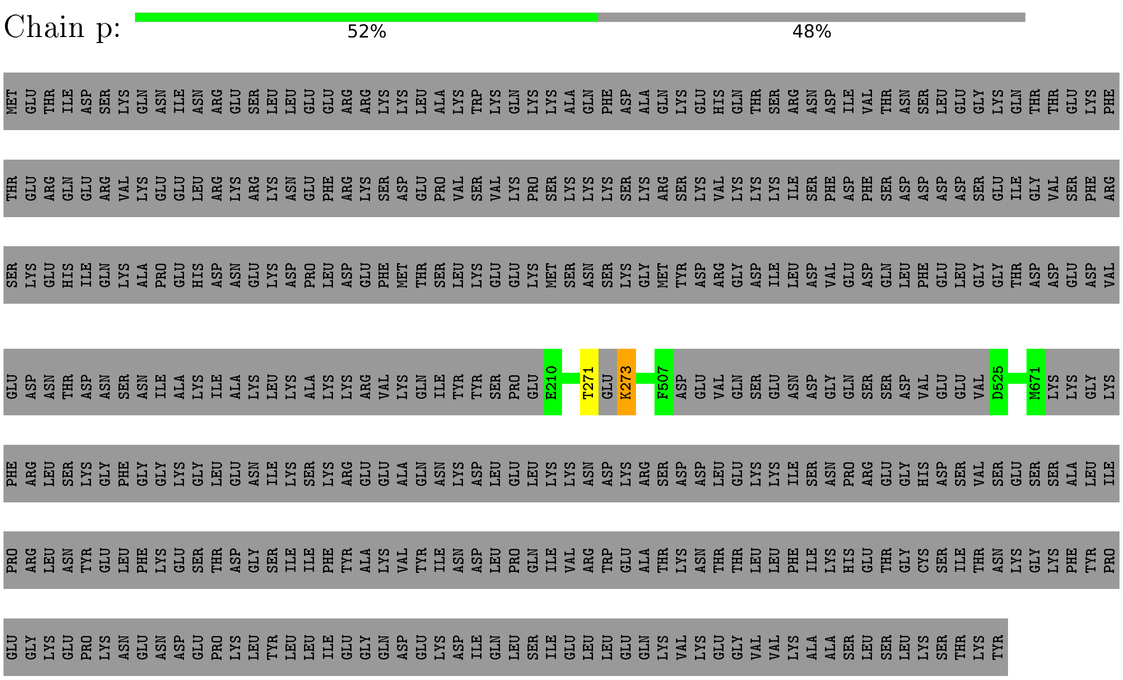
M1 P12 V16 D17 H18 V29 L34 T51 K52 P68 P121 L124 V159 F170 PRO ARG GLN ALA ASP GLY ASP THR LEU GLY PRO VAL ASN THR ALA ILE ARG ASP ASN GLY SER ARG ASP LYS THR MET GLU ILE MET ASN LEU VAL VAL SER LYS MET

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

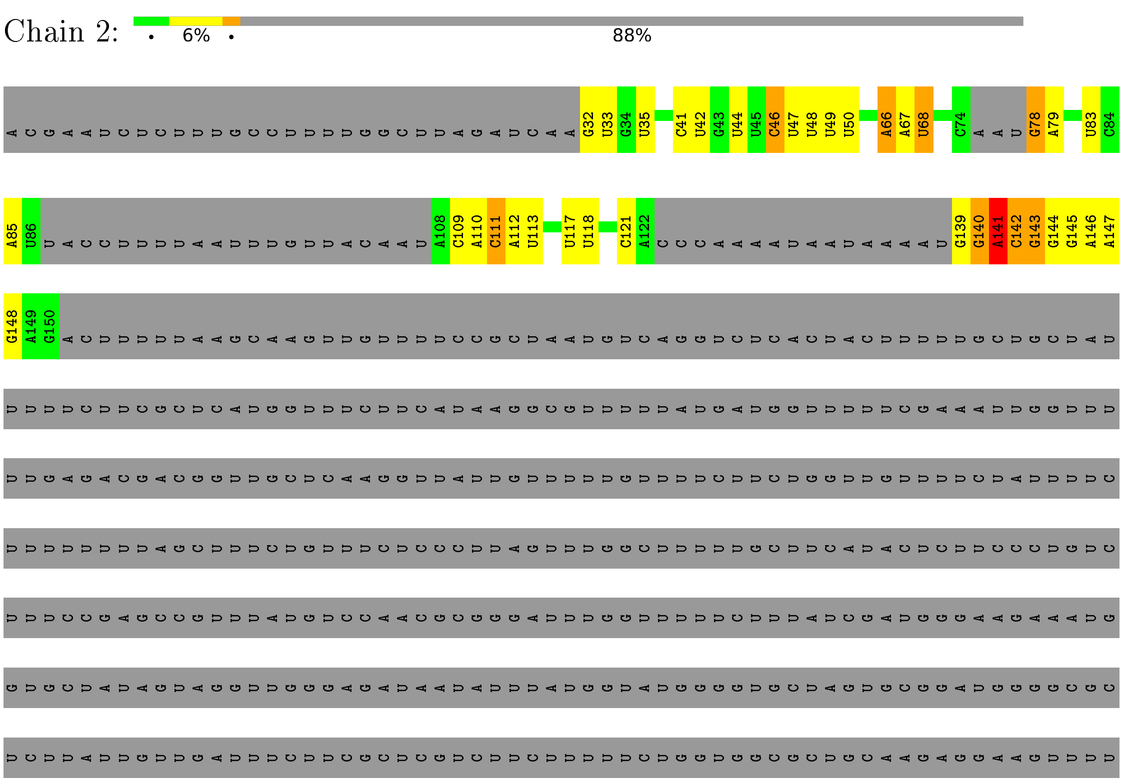
- Molecule 30: U2 small nuclear ribonucleoprotein B"

Chain Y: 75% • 24%

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



• Molecule 32: U2 snRNA



U C G A C U U U G U U A U G A U U U U U G G U U U G C A A G G A A A G G U G U C U U A C G A U U C U U U U U U U G A U G

U A A U A G G A U A A G C U U G C U U A U C C C C C A A G U A U C G G C C A A G U U G U U G A U U U U C C U U U U G A

A G U G U C C U C G G U U U G A G G G G G U G U A G G G U G G G G U U G G U C U A C A A U A A G A G U G U U C C A U U G

U U A A C G U G C U G G C G U C U U U U A C U A U A U U U U U U U U C C C A G U U U A U U U U G U G C U U A U U U U C U

C A U U G A G G A G A A G G A G C U C U U C U C G C A G G A U A U A A A U G G A G G U U U G C U A A A G G G G A G G A G

A U G U G U U U G U G A G A A U A C U G C U G A G A G A G U U C U G G A A G A G A A A A A A G G A G G C A A U G G A A

G G C G U U U G C U G G G A A A A G A G A A G A G C C A U G A C U G C A U C U G U U G U U U C A A G G C C A G U U U U A

U U A A C C G C C U A U G U C A U A G A G G C G U U U U U U U U G G A G G G A U U U G A A G A A U G C C G G C G G C A U

C A A G A A A C G G A C U U G A U G G U U G A C G C C U G U U U U A A A G U U A G1089 A1092 C1093 G1094 U1095 C1096 G1097 C1098 G1099 A1100 C1101 C1102 C1103 U1104 C1105 G1106 C1107 A1108

C U U G U G G1115 A1116 G1117 U1118 C1119 G1120 U1121 U1122 C1123 U1124 U1125 G1126 A1127 C1128 U1129 U1130 U U A C U U U G1138 G1139 U1140 C1141 G1142 C1143 U1144 U1145 G1146 A1147 U1148 G1149 U1150 U1151 U1152 C1153 U1154 C U C G U1159 C1160 U1161 U1162 C1163 C1164 C1165 G1166 U1167 U1168

C1169 G C U C U U

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 $(e^-/\text{Å}^2)$	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 (i)

5.1 Standard geometry (i)

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

All (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
32	2	1092	A	O3'-P	-14.75	1.43	1.61
32	2	1116	A	O3'-P	-11.56	1.47	1.61
32	2	1166	G	O3'-P	10.01	1.73	1.61
32	2	1163	C	O5'-C5'	9.13	1.59	1.44
32	2	1116	A	C3'-O3'	-8.90	1.29	1.42
32	2	1127	A	O3'-P	-8.73	1.50	1.61
32	2	1167	U	O3'-P	8.62	1.71	1.61
32	2	1164	C	O3'-P	-8.20	1.51	1.61
32	2	1162	U	P-O5'	7.59	1.67	1.59
32	2	1163	C	P-O5'	7.44	1.67	1.59
32	2	1117	G	P-O5'	7.25	1.67	1.59
32	2	1096	C	O3'-P	6.97	1.69	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	1154	U	C1'-N1	6.97	1.59	1.48
32	2	1128	C	C5'-C4'	-6.94	1.43	1.51
32	2	1140	U	C1'-N1	6.92	1.59	1.48
32	2	1095	U	O3'-P	6.57	1.69	1.61
32	2	1165	C	O3'-P	6.53	1.69	1.61
2	I	260	G	C1'-N9	-6.51	1.37	1.46
32	2	1169	C	C1'-N1	6.43	1.58	1.48
32	2	145	G	P-O5'	-6.37	1.53	1.59
32	2	1168	U	C5'-C4'	-6.25	1.43	1.51
32	2	1117	G	C5'-C4'	6.19	1.58	1.51
32	2	1162	U	O3'-P	6.18	1.68	1.61
32	2	1162	U	C2-N3	6.09	1.42	1.37
32	2	1165	C	O5'-C5'	6.03	1.54	1.44
32	2	1162	U	O5'-C5'	6.01	1.54	1.44
26	P	188	SER	C-N	-5.99	1.22	1.34
2	I	250	U	C1'-N1	5.98	1.57	1.48
32	2	1151	U	O5'-C5'	-5.95	1.33	1.42
32	2	1163	C	O3'-P	5.88	1.68	1.61
32	2	68	U	C1'-N1	5.72	1.57	1.48
32	2	1161	U	C3'-O3'	-5.71	1.34	1.42
2	I	249	C	C1'-N1	5.70	1.57	1.48
32	2	1162	U	C3'-C2'	-5.64	1.46	1.52
32	2	1097	G	O3'-P	5.63	1.68	1.61
32	2	118	U	C1'-N1	5.62	1.57	1.48
32	2	121	C	C1'-N1	5.50	1.57	1.48
32	2	44	U	C5-C6	5.39	1.39	1.34
32	2	111	C	C1'-N1	5.34	1.56	1.48
32	2	109	C	C1'-N1	5.31	1.56	1.48
32	2	147	A	O3'-P	-5.28	1.54	1.61
2	I	268	U	C1'-N1	5.25	1.56	1.48
32	2	1166	G	C5'-C4'	5.23	1.57	1.51
2	I	246	U	C1'-N1	5.14	1.56	1.48
2	I	247	U	C1'-N1	5.13	1.56	1.48
32	2	85	A	C1'-N9	-5.08	1.39	1.46
32	2	1162	U	C4'-O4'	5.01	1.52	1.45

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
32	2	35	U	O4'-C1'-N1	-20.67	91.67	108.20
31	p	271	THR	O-C-N	-18.58	92.98	122.70
32	2	1162	U	C5'-C4'-O4'	14.83	126.89	109.10
32	2	1093	C	P-O5'-C5'	14.82	144.62	120.90
32	2	1147	A	C5'-C4'-C3'	-14.18	93.31	116.00
32	2	1092	A	C2'-C3'-O3'	14.11	140.54	109.50
32	2	1098	C	N1-C1'-C2'	-13.38	96.61	114.00
32	2	1151	U	C4'-C3'-O3'	-12.56	83.03	109.40
32	2	44	U	C2-N1-C1'	-12.33	102.90	117.70
32	2	1151	U	P-O5'-C5'	11.71	139.64	120.90
32	2	1117	G	C5'-C4'-O4'	11.47	122.86	109.10
32	2	35	U	C2-N1-C1'	-11.45	103.96	117.70
32	2	42	U	C2-N1-C1'	-11.33	104.10	117.70
32	2	145	G	C5'-C4'-C3'	-11.20	98.08	116.00
32	2	1117	G	C5'-C4'-C3'	-10.88	98.59	116.00
32	2	44	U	C2-N3-C4	-10.88	120.47	127.00
32	2	1163	C	C5'-C4'-O4'	10.58	121.79	109.10
5	1	442	U	OP2-P-O3'	-10.46	82.18	105.20
32	2	141	A	N9-C1'-C2'	-10.45	100.41	114.00
5	1	442	U	OP1-P-O3'	-10.44	82.24	105.20
32	2	1126	G	N9-C1'-C2'	-10.07	100.91	114.00
32	2	1163	C	C5'-C4'-C3'	-9.73	100.43	116.00
32	2	1139	G	N9-C1'-C2'	-9.71	101.31	112.00
32	2	1147	A	P-O5'-C5'	9.61	136.27	120.90
20	O	238	PRO	CA-N-CD	-9.29	98.50	111.50
20	O	206	PRO	CA-N-CD	-9.28	98.51	111.50
20	O	424	PRO	CA-N-CD	-9.28	98.50	111.50
20	O	284	PRO	CA-N-CD	-9.28	98.51	111.50
20	O	315	PRO	CA-N-CD	-9.23	98.58	111.50
20	O	249	PRO	CA-N-CD	-9.22	98.59	111.50
20	O	399	PRO	CA-N-CD	-9.20	98.61	111.50
20	O	691	PRO	CA-N-CD	-9.20	98.62	111.50
20	O	596	PRO	CA-N-CD	-9.19	98.63	111.50
32	2	1162	U	C5'-C4'-C3'	-9.17	101.32	116.00
20	O	687	PRO	CA-N-CD	-9.17	98.67	111.50
20	O	449	PRO	CA-N-CD	-9.15	98.69	111.50
20	O	481	PRO	CA-N-CD	-9.14	98.71	111.50
20	O	656	PRO	CA-N-CD	-9.14	98.71	111.50
20	O	759	PRO	CA-N-CD	-9.11	98.75	111.50
32	2	1168	U	C4'-C3'-O3'	-8.99	90.51	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	O	387	PRO	CA-N-CD	-8.98	98.92	111.50
32	2	142	C	N1-C1'-C2'	-8.83	102.29	112.00
20	O	681	PRO	CA-N-CD	-8.80	99.17	111.50
20	O	428	PRO	CA-N-CD	-8.78	99.22	111.50
20	O	197	PRO	CA-N-CD	-8.69	99.33	111.50
32	2	1152	U	P-O5'-C5'	8.68	134.79	120.90
20	O	525	PRO	CA-N-CD	-8.68	99.35	111.50
32	2	1151	U	O4'-C1'-N1	8.67	115.14	108.20
20	O	629	PRO	CA-N-CD	-8.65	99.39	111.50
20	O	472	PRO	CA-N-CD	-8.64	99.40	111.50
20	O	721	PRO	CA-N-CD	-8.64	99.40	111.50
20	O	680	PRO	CA-N-CD	-8.63	99.42	111.50
20	O	614	PRO	CA-N-CD	-8.63	99.42	111.50
20	O	600	PRO	CA-N-CD	-8.60	99.46	111.50
20	O	369	PRO	CA-N-CD	-8.59	99.47	111.50
20	O	256	PRO	CA-N-CD	-8.59	99.47	111.50
20	O	532	PRO	CA-N-CD	-8.57	99.51	111.50
32	2	1148	U	C4'-C3'-O3'	-8.54	91.46	109.40
32	2	1092	A	P-O5'-C5'	8.53	134.55	120.90
4	J	274	PRO	CA-N-CD	-8.53	99.56	111.50
20	O	497	PRO	CA-N-CD	-8.52	99.58	111.50
32	2	44	U	N1-C2-N3	8.46	119.98	114.90
32	2	145	G	P-O5'-C5'	8.32	134.22	120.90
32	2	148	G	C5'-C4'-C3'	-8.30	102.72	116.00
32	2	1165	C	C5'-C4'-C3'	-8.26	102.79	116.00
20	O	720	PRO	CA-N-CD	-8.18	100.05	111.50
32	2	1151	U	C5'-C4'-O4'	8.14	118.86	109.10
32	2	44	U	N3-C4-C5	7.98	119.39	114.60
32	2	1168	U	P-O5'-C5'	-7.91	108.25	120.90
32	2	1167	U	C2'-C3'-O3'	7.88	126.83	109.50
32	2	1092	A	C4'-C3'-O3'	-7.82	92.97	109.40
32	2	1165	C	C5'-C4'-O4'	7.77	118.42	109.10
32	2	1107	C	N1-C1'-C2'	-7.74	103.48	112.00
32	2	1147	A	C4'-C3'-O3'	7.74	128.48	113.00
32	2	1161	U	C5'-C4'-C3'	-7.73	103.62	116.00
32	2	1093	C	C5'-C4'-C3'	-7.71	103.67	116.00
32	2	1169	C	P-O5'-C5'	-7.62	108.70	120.90
32	2	1097	G	C3'-C2'-O2'	7.61	135.38	113.30
32	2	1165	C	C4'-C3'-O3'	7.55	128.11	113.00
32	2	1128	C	C5'-C4'-O4'	7.30	117.86	109.10
32	2	1168	U	C2'-C3'-O3'	7.29	125.55	109.50
32	2	1089	G	C4'-C3'-O3'	7.24	127.47	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1115	G	O5'-P-OP1	-7.23	99.19	105.70
32	2	1159	U	O5'-P-OP1	-7.22	99.20	105.70
32	2	139	G	O5'-P-OP2	-7.21	99.22	105.70
32	2	1089	G	O5'-P-OP2	-7.14	99.28	105.70
5	1	289	U	N3-C2-O2	-7.13	117.21	122.20
32	2	139	G	O5'-P-OP1	-7.12	99.29	105.70
5	1	443	U	OP1-P-OP2	7.11	130.27	119.60
32	2	1089	G	O5'-P-OP1	-7.09	99.32	105.70
32	2	1159	U	O5'-P-OP2	-7.07	99.33	105.70
32	2	1115	G	O5'-P-OP2	-7.04	99.37	105.70
32	2	1115	G	C4'-C3'-O3'	7.03	127.07	113.00
32	2	1096	C	C1'-C2'-O2'	-6.68	90.55	110.60
32	2	148	G	C5'-C4'-O4'	6.61	117.03	109.10
5	1	498	U	N3-C2-O2	-6.61	117.58	122.20
32	2	1129	U	C5'-C4'-O4'	6.60	117.02	109.10
32	2	140	G	N9-C1'-C2'	-6.53	104.82	112.00
32	2	78	G	C2'-C3'-O3'	6.39	123.92	113.70
32	2	1166	G	O5'-C5'-C4'	6.36	123.77	111.70
31	p	271	THR	CA-C-N	6.34	131.14	117.20
32	2	1166	G	C5'-C4'-C3'	6.30	126.09	116.00
32	2	145	G	O4'-C1'-N9	6.29	113.24	108.20
5	1	500	C	C6-N1-C2	-6.29	117.79	120.30
32	2	145	G	O5'-C5'-C4'	-6.23	99.87	111.70
32	2	1092	A	N9-C1'-C2'	6.21	122.08	114.00
32	2	44	U	N1-C1'-C2'	6.17	122.03	114.00
32	2	1152	U	C5'-C4'-C3'	-6.15	106.17	116.00
5	1	289	U	N1-C2-O2	6.13	127.09	122.80
32	2	1096	C	C4'-C3'-O3'	6.12	125.25	113.00
32	2	44	U	C5-C4-O4	-6.08	122.25	125.90
32	2	1151	U	O3'-P-O5'	-6.02	92.57	104.00
32	2	1167	U	P-O3'-C3'	-6.02	112.48	119.70
5	1	148	C	N1-C2-O2	6.00	122.50	118.90
5	1	148	C	C2-N1-C1'	5.98	125.38	118.80
5	1	54	C	C2-N1-C1'	5.96	125.36	118.80
5	1	144	C	C2-N1-C1'	5.96	125.36	118.80
5	1	268	C	P-O3'-C3'	5.90	126.78	119.70
32	2	1162	U	C4'-C3'-O3'	5.87	124.75	113.00
32	2	1167	U	C5'-C4'-O4'	-5.87	102.06	109.10
5	1	144	C	N1-C2-O2	5.84	122.40	118.90
32	2	1108	A	C3'-C2'-C1'	5.81	106.15	101.50
32	2	1115	G	P-O3'-C3'	5.76	126.62	119.70
32	2	1148	U	C5'-C4'-O4'	5.75	116.00	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	151	C	P-O3'-C3'	5.74	126.59	119.70
32	2	1162	U	C2'-C3'-O3'	-5.74	96.88	109.50
5	1	342	C	C6-N1-C2	-5.68	118.03	120.30
32	2	141	A	C4'-C3'-O3'	5.68	124.36	113.00
5	1	258	U	P-O3'-C3'	5.66	126.50	119.70
5	1	399	A	P-O3'-C3'	5.66	126.49	119.70
32	2	1167	U	C5'-C4'-C3'	5.58	124.92	116.00
32	2	1097	G	C2'-C3'-O3'	-5.57	97.25	109.50
32	2	1162	U	P-O3'-C3'	5.51	126.31	119.70
32	2	1151	U	N1-C1'-C2'	5.50	121.15	114.00
32	2	145	G	C3'-C2'-O2'	-5.49	97.38	113.30
32	2	145	G	C5'-C4'-O4'	5.48	115.67	109.10
32	2	1105	C	C4'-C3'-O3'	-5.46	97.94	109.40
31	p	273	LYS	N-CA-C	5.45	125.72	111.00
32	2	1168	U	C4'-C3'-C2'	-5.42	97.18	102.60
32	2	1162	U	C4'-C3'-C2'	5.42	108.02	102.60
5	1	144	C	N3-C2-O2	-5.40	118.12	121.90
5	1	342	C	C5-C6-N1	5.37	123.69	121.00
32	2	1168	U	O3'-P-O5'	-5.32	93.89	104.00
2	I	6	U	N1-C2-O2	5.27	126.49	122.80
5	1	480	C	C6-N1-C2	-5.25	118.20	120.30
5	1	496	C	C6-N1-C2	-5.23	118.21	120.30
32	2	1152	U	O4'-C4'-C3'	5.21	110.27	106.10
5	1	151	C	N1-C2-O2	5.20	122.02	118.90
5	1	182	C	C2-N1-C1'	5.19	124.51	118.80
5	1	347	U	N3-C2-O2	-5.19	118.57	122.20
32	2	46	C	C2'-C3'-O3'	5.16	121.95	113.70
32	2	66	A	C4'-C3'-O3'	5.16	123.31	113.00
32	2	1148	U	P-O5'-C5'	5.14	129.13	120.90
32	2	1163	C	C4'-C3'-O3'	5.13	123.27	113.00
5	1	130	C	N1-C2-O2	5.12	121.97	118.90
5	1	342	C	C2-N1-C1'	5.12	124.43	118.80
5	1	130	C	N3-C2-O2	-5.10	118.33	121.90
32	2	145	G	C4'-C3'-O3'	5.10	123.20	113.00
5	1	144	C	C6-N1-C2	-5.06	118.28	120.30
32	2	1169	C	O5'-C5'-C4'	-5.05	102.10	111.70
32	2	1147	A	O5'-C5'-C4'	5.05	121.29	111.70
5	1	501	C	C5-C6-N1	5.04	123.52	121.00
5	1	391	C	C6-N1-C2	-5.03	118.29	120.30
32	2	66	A	P-O3'-C3'	5.02	125.72	119.70
32	2	146	A	C5'-C4'-C3'	-5.02	107.97	116.00
32	2	145	G	P-O3'-C3'	5.01	125.72	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	1161	U	C5'-C4'-O4'	5.01	115.11	109.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	2	141	A	Sidechain
32	2	143	G	Sidechain
7	A	12	ARG	Peptide
18	B	176	ILE	Peptide
26	P	1013	ASP	Peptide
26	P	1014	LYS	Peptide
23	T	458	SER	Peptide
29	W	16	VAL	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
4	J	274	PRO
19	K	356	ARG
19	K	370	PRO
26	P	363	VAL
26	P	413	ILE
26	P	626	PRO
26	P	629	GLY
29	W	17	ASP
29	W	18	HIS
29	W	51	THR
29	W	68	PRO
29	W	121	PRO
29	W	124	LEU
30	Y	71	GLN
11	e	34	GLN
27	R	48	ALA
29	W	29	VAL
31	p	273	LYS
13	g	21	GLY
19	K	353	THR
19	K	442	ASP
20	O	713	LYS
20	O	717	THR
26	P	107	ALA
26	P	628	ALA
28	Z	19	ILE
29	W	12	PRO
21	U	232	GLY
22	V	181	HIS
13	y	30	ARG
13	y	60	GLN
26	P	364	THR
26	P	486	PRO
29	W	159	VAL
20	O	614	PRO
26	P	1031	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	
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

Continued on next page...

Continued from previous page...

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 (i)

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%)

All (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
2	I	252	A
2	I	253	G
2	I	254	U
2	I	258	A
2	I	265	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	267	A
5	1	11	U
5	1	12	A
5	1	40	A
5	1	41	C
5	1	55	G
5	1	56	C
5	1	62	A
5	1	63	U
5	1	64	A
5	1	65	G
5	1	66	U
5	1	67	A
5	1	74	C
5	1	75	G
5	1	79	A
5	1	80	G
5	1	87	U
5	1	97	A
5	1	98	U
5	1	100	A
5	1	101	U
5	1	103	G
5	1	107	A
5	1	113	G
5	1	114	U
5	1	117	U
5	1	133	G
5	1	134	G
5	1	141	A
5	1	142	C
5	1	147	A
5	1	149	G
5	1	150	G
5	1	151	C
5	1	152	G
5	1	153	C
5	1	154	G
5	1	167	G
5	1	171	A
5	1	176	U
5	1	180	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1	181	U
5	1	182	C
5	1	186	U
5	1	187	G
5	1	205	U
5	1	206	C
5	1	218	U
5	1	219	U
5	1	220	G
5	1	227	U
5	1	228	U
5	1	230	G
5	1	254	U
5	1	255	U
5	1	257	G
5	1	258	U
5	1	259	U
5	1	260	U
5	1	269	U
5	1	270	G
5	1	271	G
5	1	272	A
5	1	278	U
5	1	279	U
5	1	280	G
5	1	287	A
5	1	290	U
5	1	326	G
5	1	327	A
5	1	328	G
5	1	343	A
5	1	352	G
5	1	365	U
5	1	369	G
5	1	377	U
5	1	378	U
5	1	385	U
5	1	386	G
5	1	389	G
5	1	393	G
5	1	394	A
5	1	395	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1	399	A
5	1	400	A
5	1	407	U
5	1	409	A
5	1	416	G
5	1	418	U
5	1	422	G
5	1	424	U
5	1	426	U
5	1	427	G
5	1	443	U
5	1	460	U
5	1	466	U
5	1	468	U
5	1	477	G
5	1	482	G
5	1	493	G
5	1	504	U
5	1	505	U
5	1	506	A
5	1	508	G
5	1	513	A
5	1	515	A
5	1	540	G
5	1	542	U
5	1	551	U
5	1	553	A
5	1	554	U
5	1	555	U
5	1	559	G
5	1	560	A
5	1	562	U
5	1	563	U
5	1	564	A
5	1	565	U
32	2	33	U
32	2	41	C
32	2	46	C
32	2	47	U
32	2	48	U
32	2	49	U
32	2	50	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	66	A
32	2	67	A
32	2	68	U
32	2	79	A
32	2	83	U
32	2	111	C
32	2	112	A
32	2	113	U
32	2	117	U
32	2	140	G
32	2	141	A
32	2	142	C
32	2	143	G
32	2	144	G
32	2	1094	G
32	2	1095	U
32	2	1096	C
32	2	1097	G
32	2	1098	C
32	2	1100	A
32	2	1101	C
32	2	1102	C
32	2	1103	C
32	2	1104	U
32	2	1105	C
32	2	1106	G
32	2	1107	C
32	2	1108	A
32	2	1119	C
32	2	1120	G
32	2	1121	U
32	2	1122	U
32	2	1123	C
32	2	1124	U
32	2	1125	U
32	2	1126	G
32	2	1130	U
32	2	1139	G
32	2	1141	C
32	2	1142	G
32	2	1143	C
32	2	1144	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1145	U
32	2	1146	G
32	2	1150	U
32	2	1151	U

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	1	86	A
5	1	100	A
5	1	113	G
5	1	151	C
5	1	152	G
5	1	258	U
5	1	268	C
5	1	399	A
5	1	505	U
32	2	32	G
32	2	46	C
32	2	66	A
32	2	67	A
32	2	78	G
32	2	110	A
32	2	1095	U
32	2	1096	C
32	2	1097	G
32	2	1100	A
32	2	1101	C
32	2	1102	C
32	2	1105	C
32	2	1107	C
32	2	1119	C
32	2	1120	G
32	2	1121	U
32	2	1122	U
32	2	1123	C
32	2	1124	U
32	2	1125	U
32	2	1138	G
32	2	1141	C
32	2	1142	G
32	2	1144	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1145	U
32	2	1150	U

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.