



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 07:02 AM JST

PDB ID : 5YLZ
EMDB ID : EMD-6839
Title : Cryo-EM Structure of the Post-catalytic Spliceosome from *Saccharomyces cerevisiae* at 3.6 angstrom
Authors : Wan, R.; Yan, C.; Bai, R.; Lei, J.; Shi, Y.
Deposited on : 2017-10-20
Resolution : 3.60 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

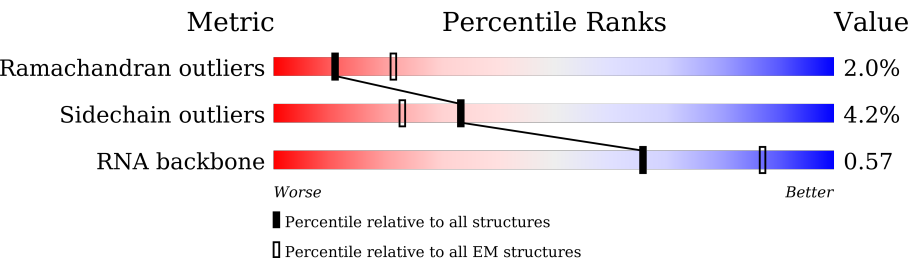
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2413	<div><div>11%</div><div>76%</div><div>20%</div></div>
2	B	214	<div><div>13%</div><div>41%</div><div>14%</div><div>45%</div></div>
3	C	1008	<div><div>9%</div><div>84%</div><div>13%</div></div>
4	D	112	<div><div>14%</div><div>61%</div><div>30%</div><div>8%</div></div>
5	E	369	<div><div>7%</div><div>7%</div><div>9%</div><div>83%</div></div>
6	F	1175	<div><div>6%</div><div>92%</div></div>
7	G	175	<div><div>89%</div><div>82%</div><div>6%</div><div>11%</div></div>
8	H	859	<div><div>65%</div><div>61%</div><div>35%</div></div>

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Mol	Chain	Length	Quality of chain
9	I	687	
10	J	590	
11	K	215	
12	L	157	
13	T	455	
14	M	364	
15	N	339	
16	O	451	
17	P	175	
18	Q	379	
19	R	135	
20	S	577	
21	U	251	
22	V	382	
23	W	1145	
24	a	196	
24	h	196	
25	b	94	
25	i	94	
26	c	86	
26	j	86	
27	d	77	
27	k	77	
28	e	101	
28	l	101	

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Mol	Chain	Length	Quality of chain
29	f	146	
29	m	146	
30	g	110	
30	n	110	
31	o	238	
32	p	111	
33	q	503	
33	r	503	
33	s	503	
33	t	503	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 76247 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1931	Total	C	N	O	S	0	0
			15931	10239	2737	2897	58		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	117	Total	C	N	O	P	0	0
			2465	1104	414	830	117		

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	878	Total	C	N	O	S	0	0
			7019	4529	1166	1295	29		

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 5 is a RNA chain called mRNA/intron lariat.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	62	Total	C	N	O	P	0	0
			1310	590	224	434	62		

- Molecule 6 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	91	Total	C	N	O	P	0	0
			1909	854	309	655	91		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	156	Total	C	N	O	S	0	0
			926	585	160	180	1		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	562	Total	C	N	O	S	0	0
			3012	1844	572	595	1		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	517	Total	C	N	O	S	0	0
			3424	2130	643	643	8		

- Molecule 10 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	432	Total	C	N	O	S	0	0
			2949	1827	545	569	8		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			777	476	143	157	1		

- Molecule 12 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 13 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	344	Total	C	N	O	S	0	0
			2357	1504	414	432	7		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	185	Total	C	N	O	S	0	0
			1472	930	256	271	15		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 16 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	337	Total	C	N	O	S	0	0
			2646	1669	466	501	10		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	69	Total	C	N	O	S	0	0
			560	351	112	96	1		

- Molecule 18 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	201	Total	C	N	O	S	0	0
			1583	988	290	298	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	207	Total	C	N	O	S	0	0
			1701	1096	275	323	7		

- Molecule 21 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	148	Total	C	N	O	S	0	0
			1202	780	204	214	4		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	88	Total	C	N	O		0	0
			554	350	100	104			

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	703	Total	C	N	O	S	0	0
			5553	3521	941	1060	31		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
24	h	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
25	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	70	Total	C	N	O	S	0	0
			554	355	98	100	1		
26	j	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	k	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
28	l	81	Total	C	N	O	S	0	0
			616	393	107	114	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
29	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	n	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	o	135	Total	C	N	O	0	0
			841	538	142	161		

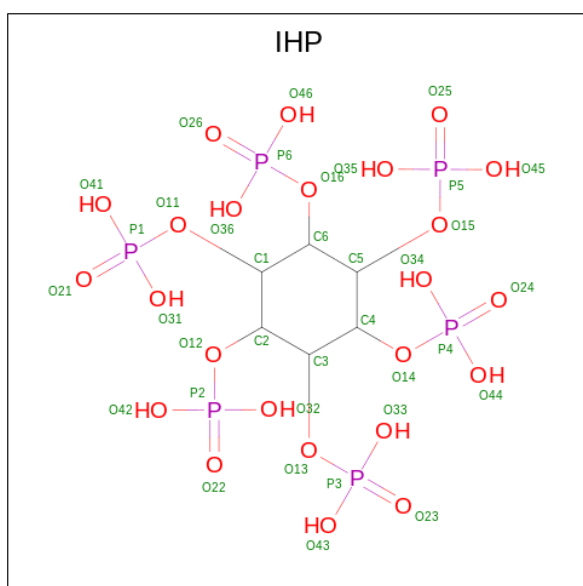
- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	p	81	Total	C	N	O	0	0
			513	332	89	92		

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

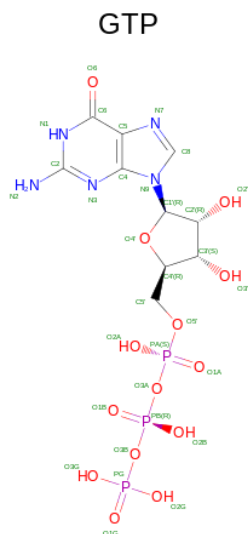
Mol	Chain	Residues	Atoms					AltConf	Trace
33	q	129	Total	C	N	O	S	0	0
			850	537	137	174	2		
33	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		
33	s	126	Total	C	N	O	S	0	0
			830	525	134	169	2		
33	t	128	Total	C	N	O	S	0	0
			843	532	136	173	2		

- Molecule 34 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 35 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



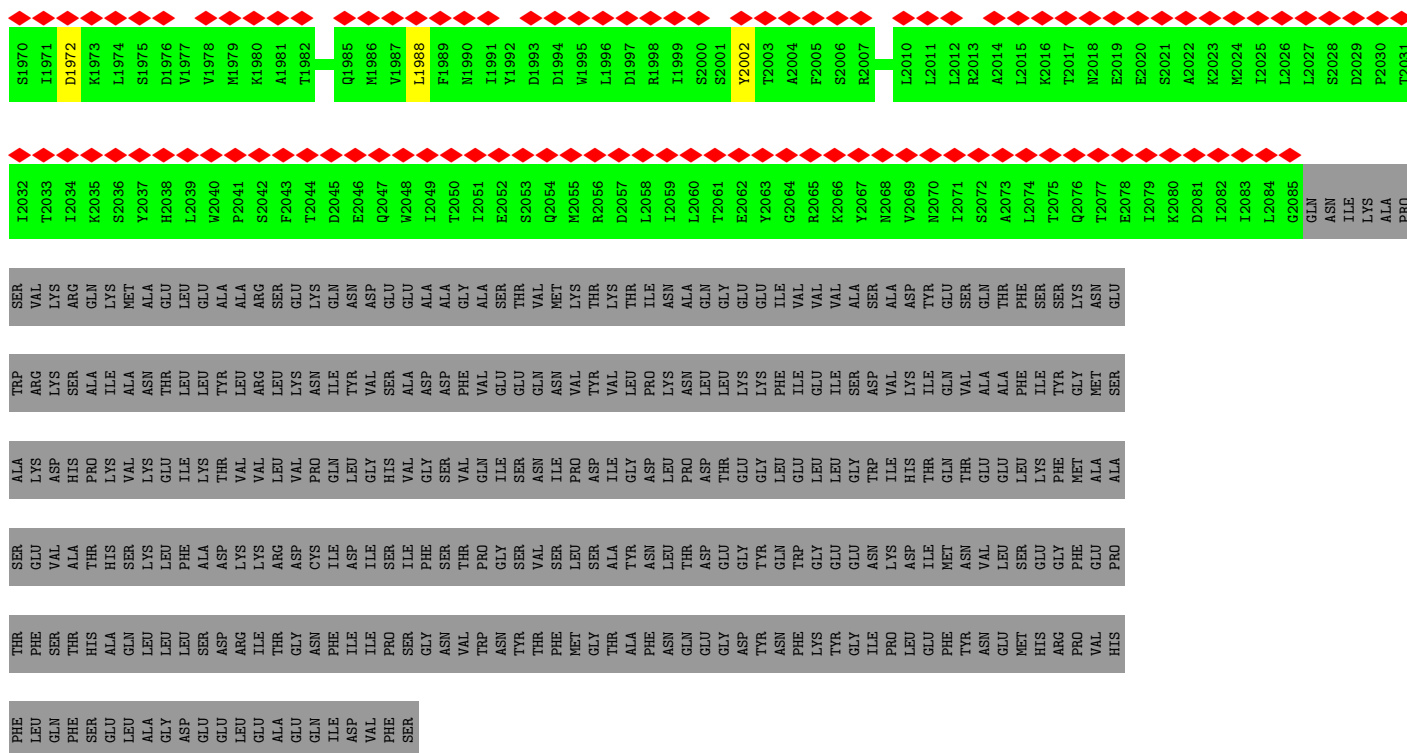
Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

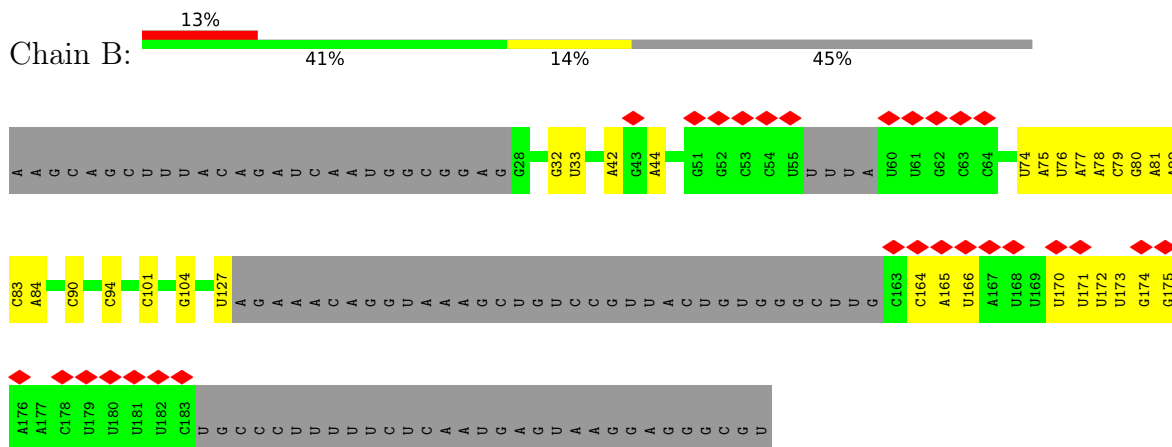
Mol	Chain	Residues	Atoms	AltConf
36	C	1	Total Mg 1 1	0
36	D	5	Total Mg 5 5	0

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

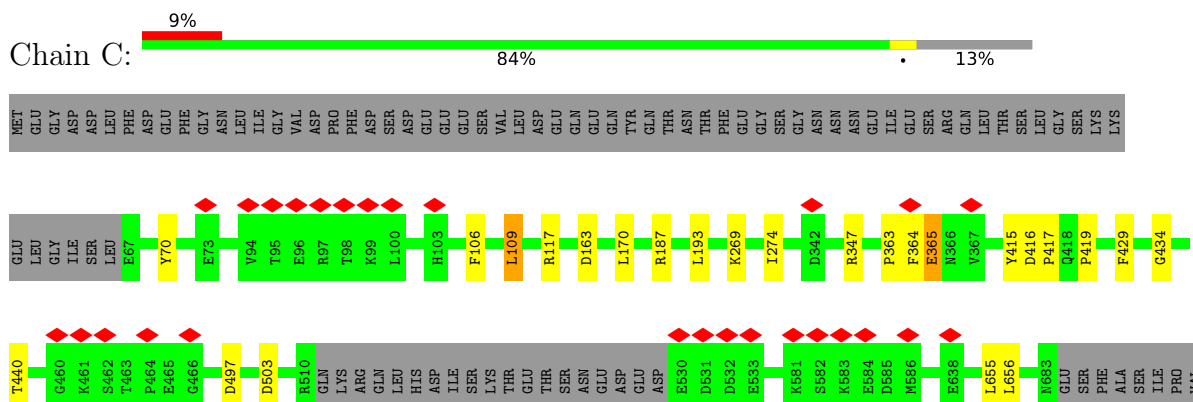
Mol	Chain	Residues	Atoms		AltConf
37	L	3	Total 3	Zn 3	0
37	M	2	Total 2	Zn 2	0
37	N	1	Total 1	Zn 1	0

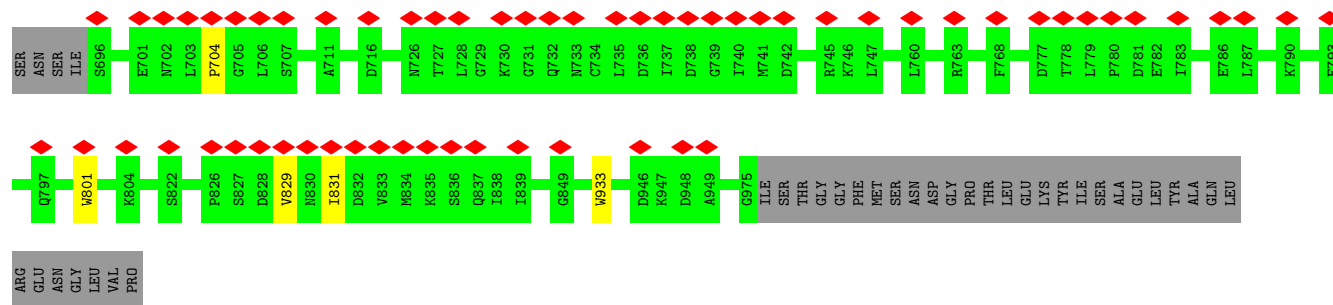


- Molecule 2: U5 snRNA

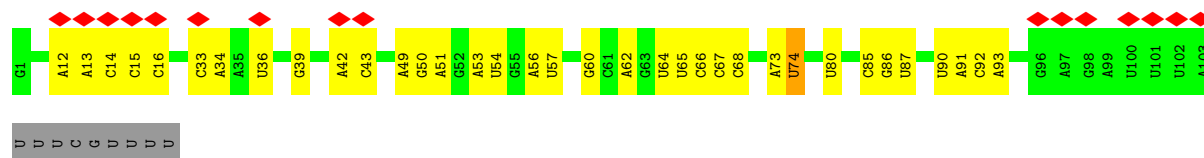


- Molecule 3: Pre-mRNA-splicing factor SNU114

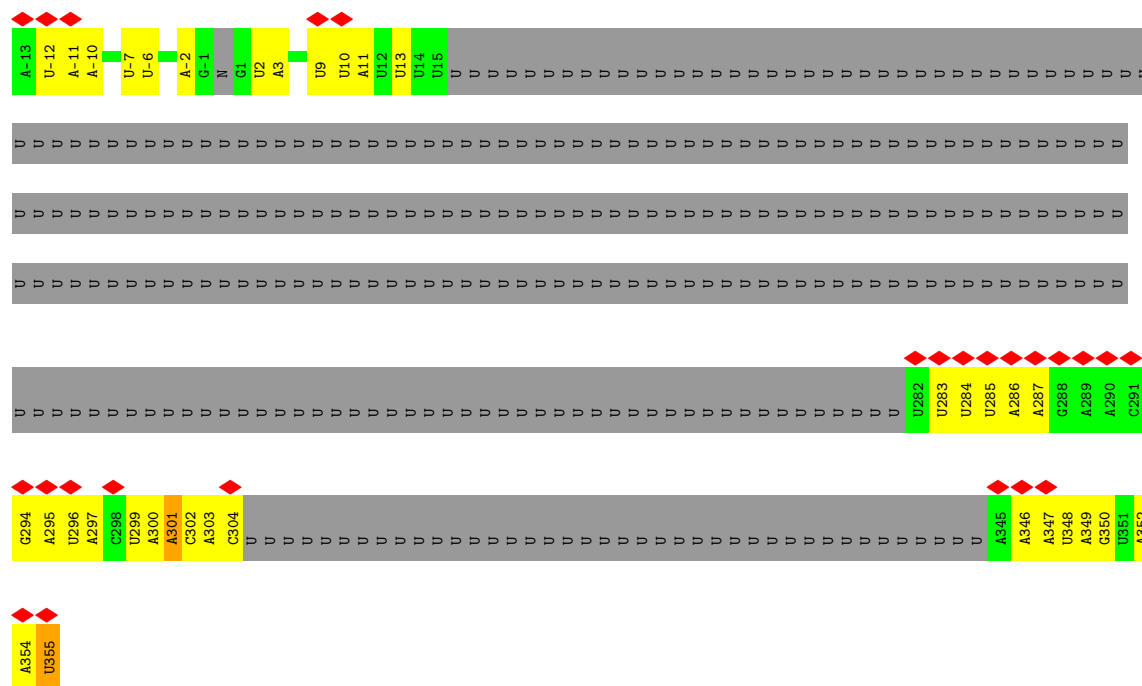




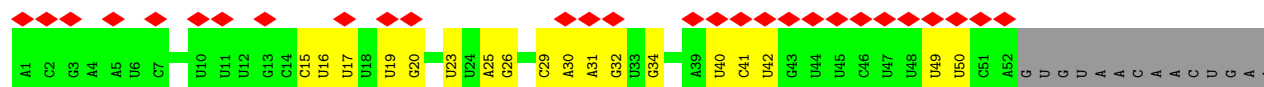
• Molecule 4: U6 snRNA

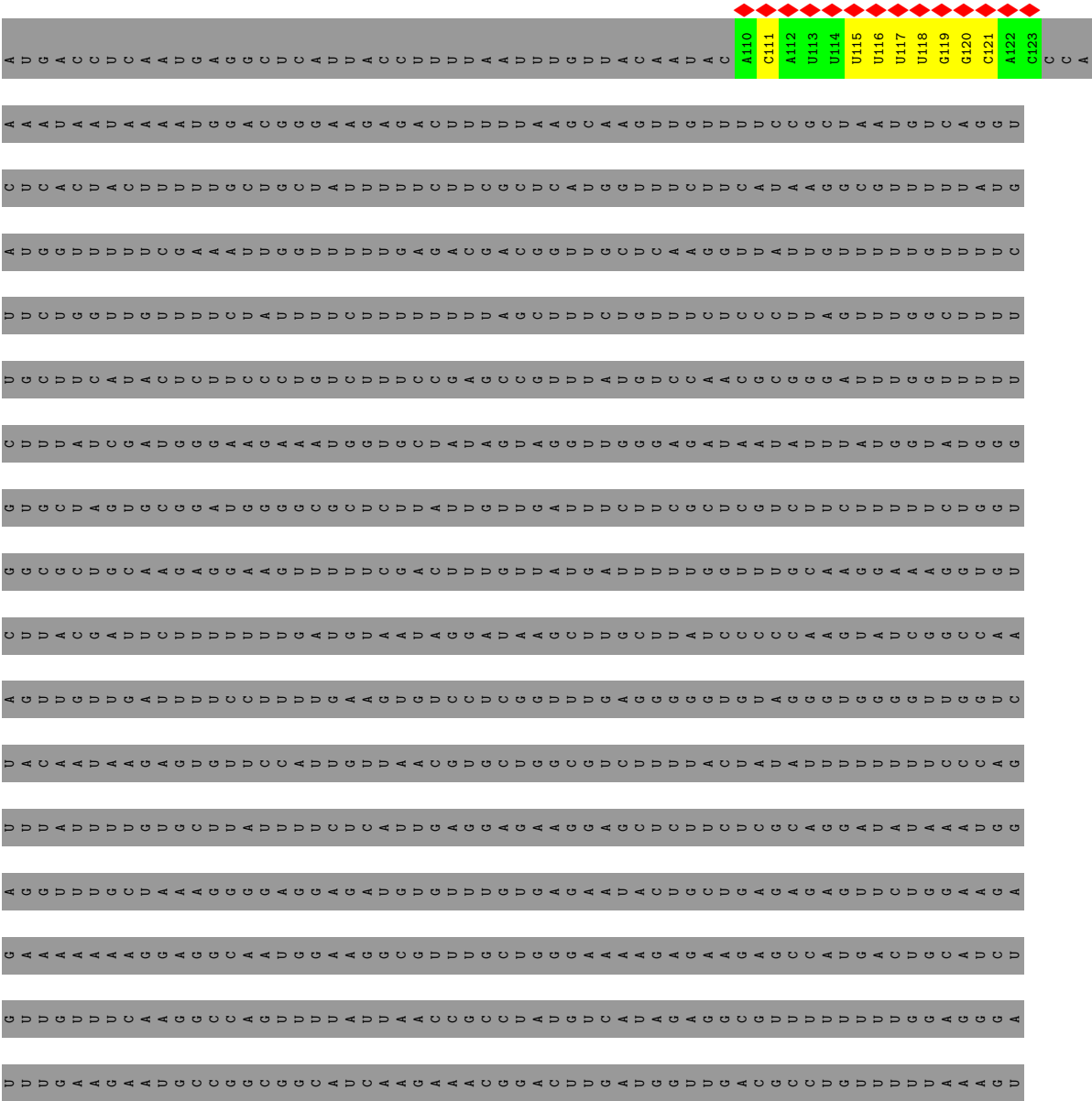


• Molecule 5: mRNA/intron lariat

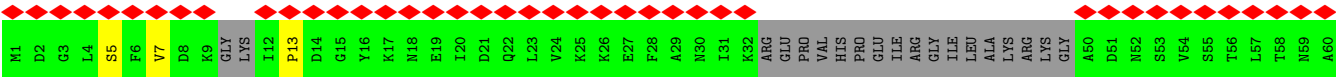
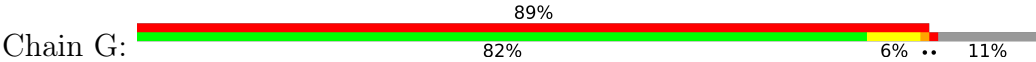


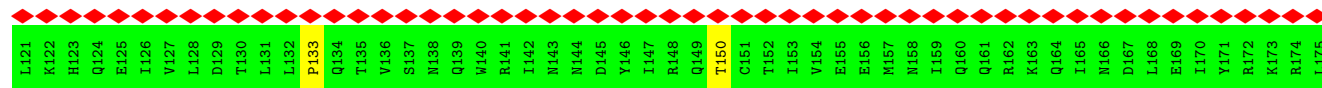
• Molecule 6: U2 snRNA



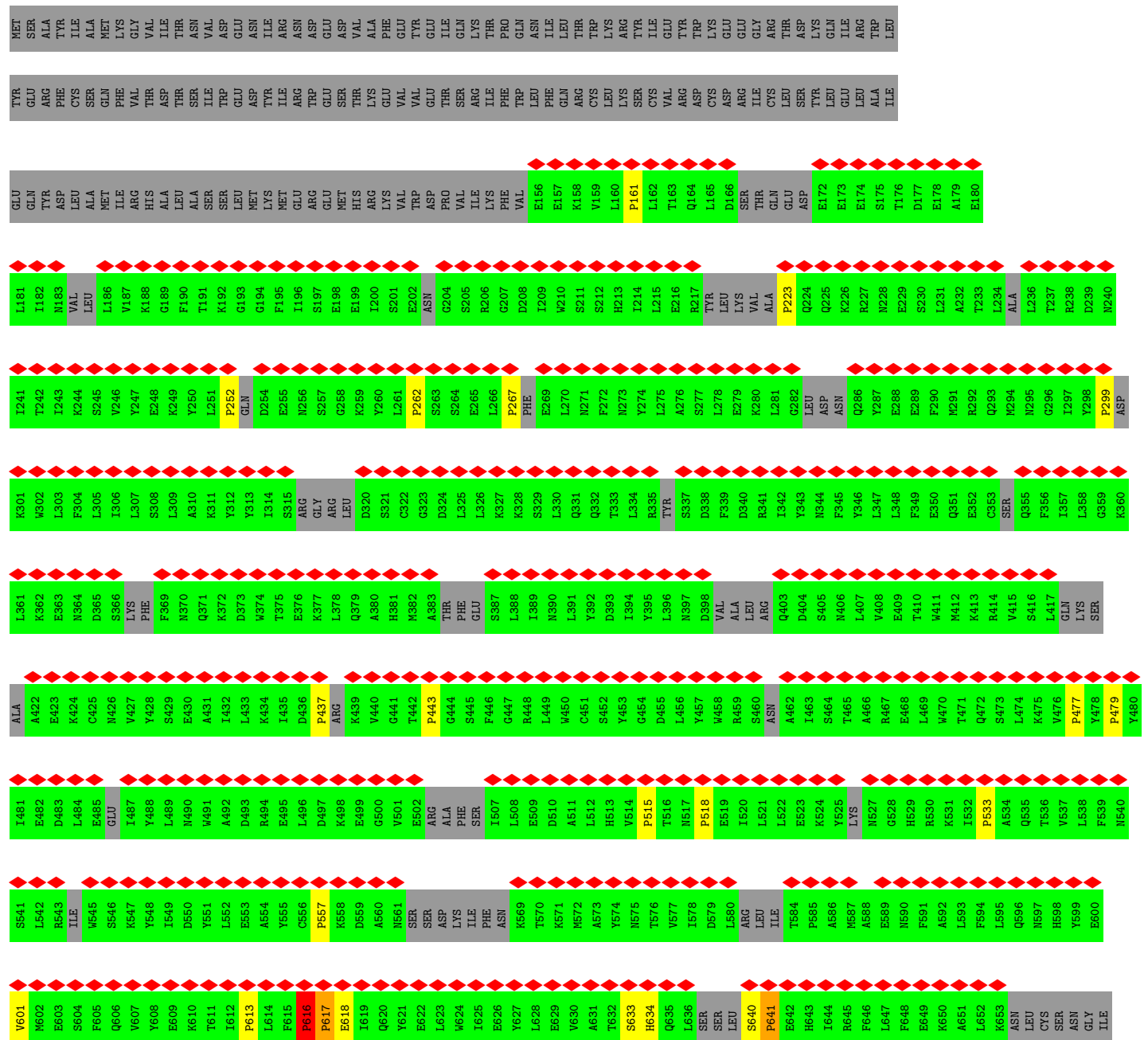


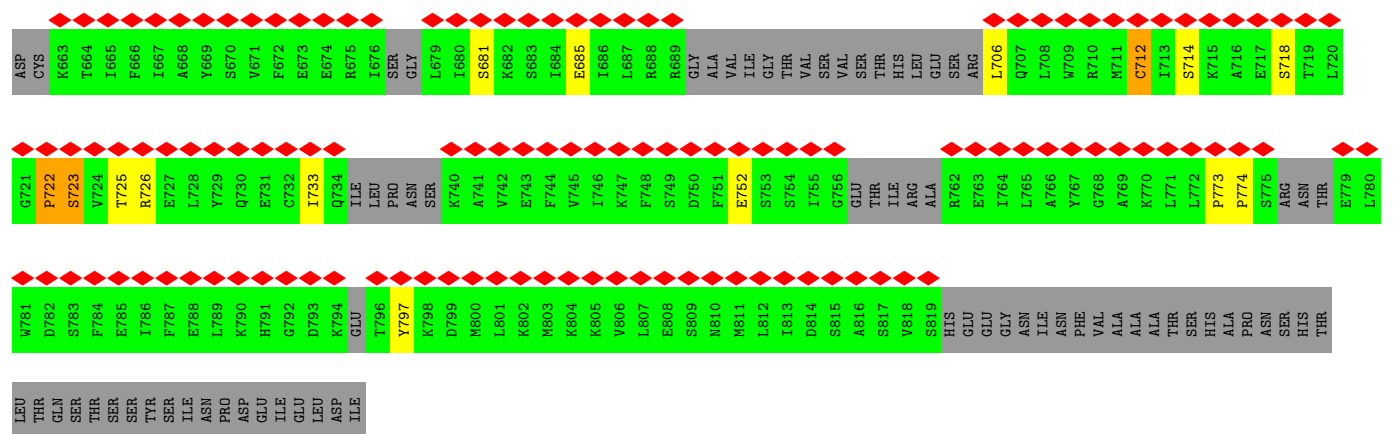
● Molecule 7: Pre-mRNA-splicing factor SNT309



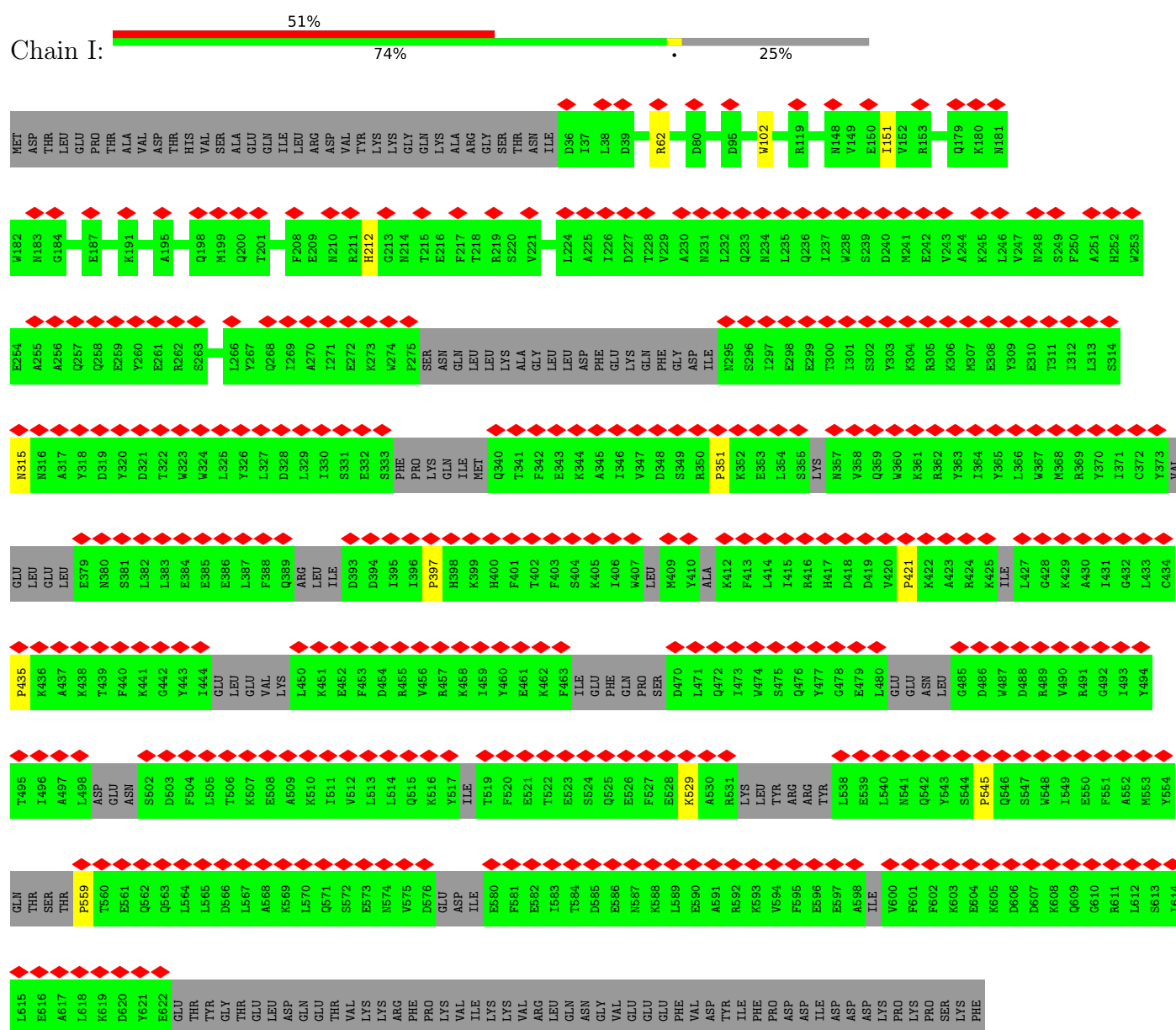


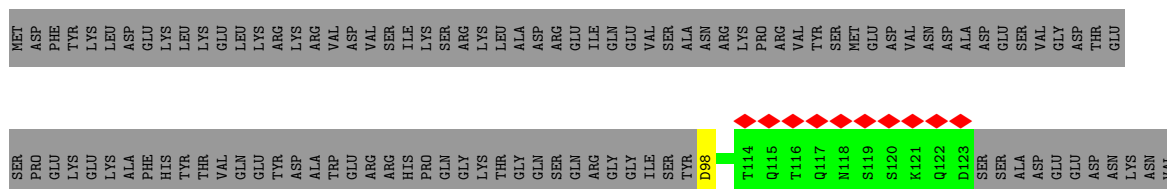
Chain H: 65% 61% 35%



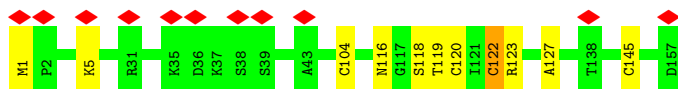


• Molecule 9: Pre-mRNA-splicing factor CLF1

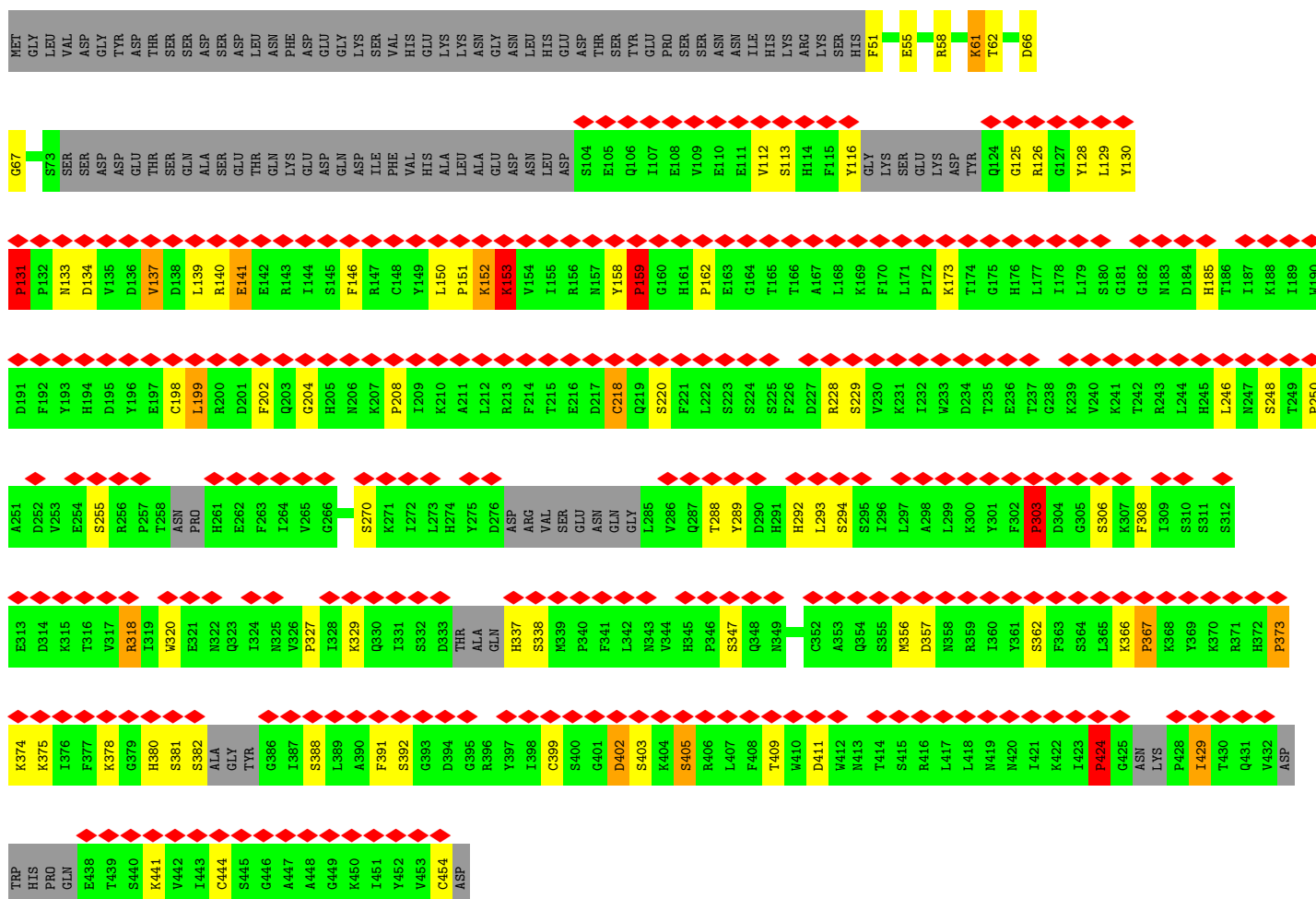




- Molecule 12: Pre-mRNA-splicing factor BUD31



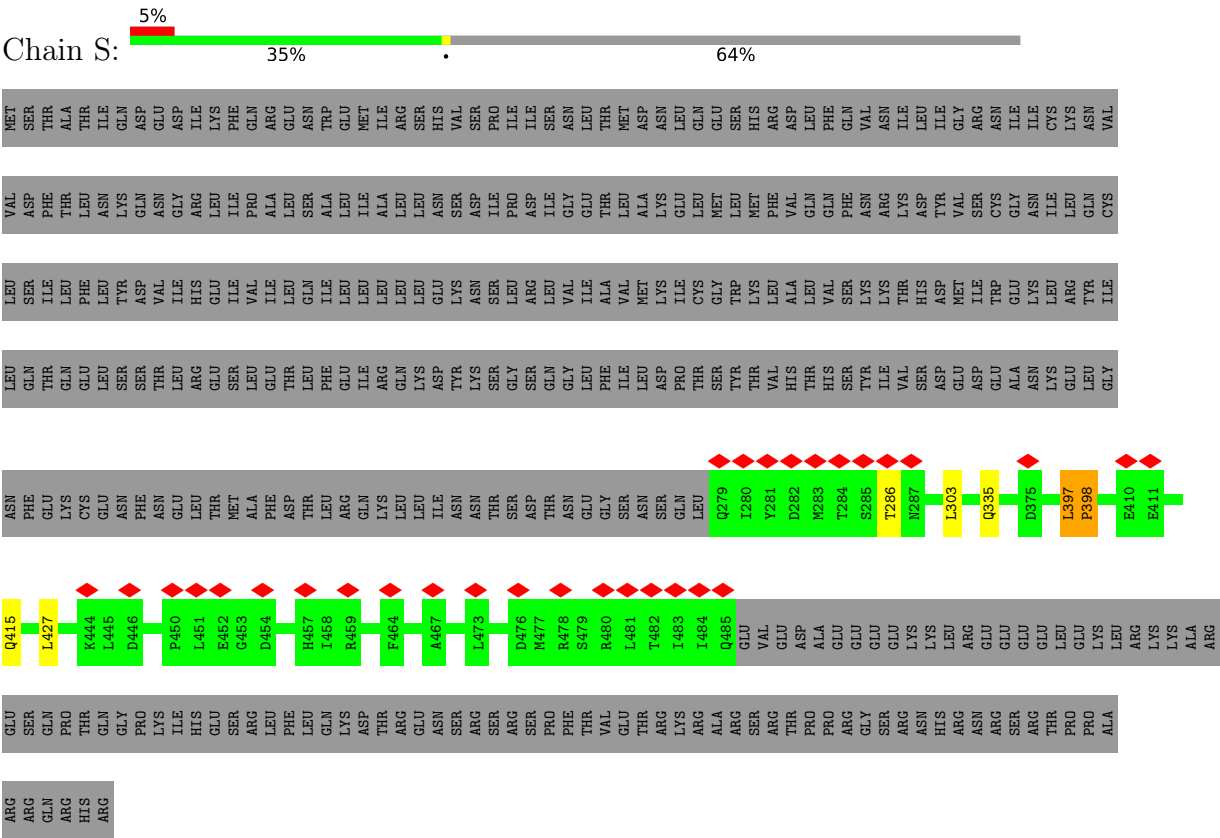
- Molecule 13: Pre-mRNA-processing factor 17



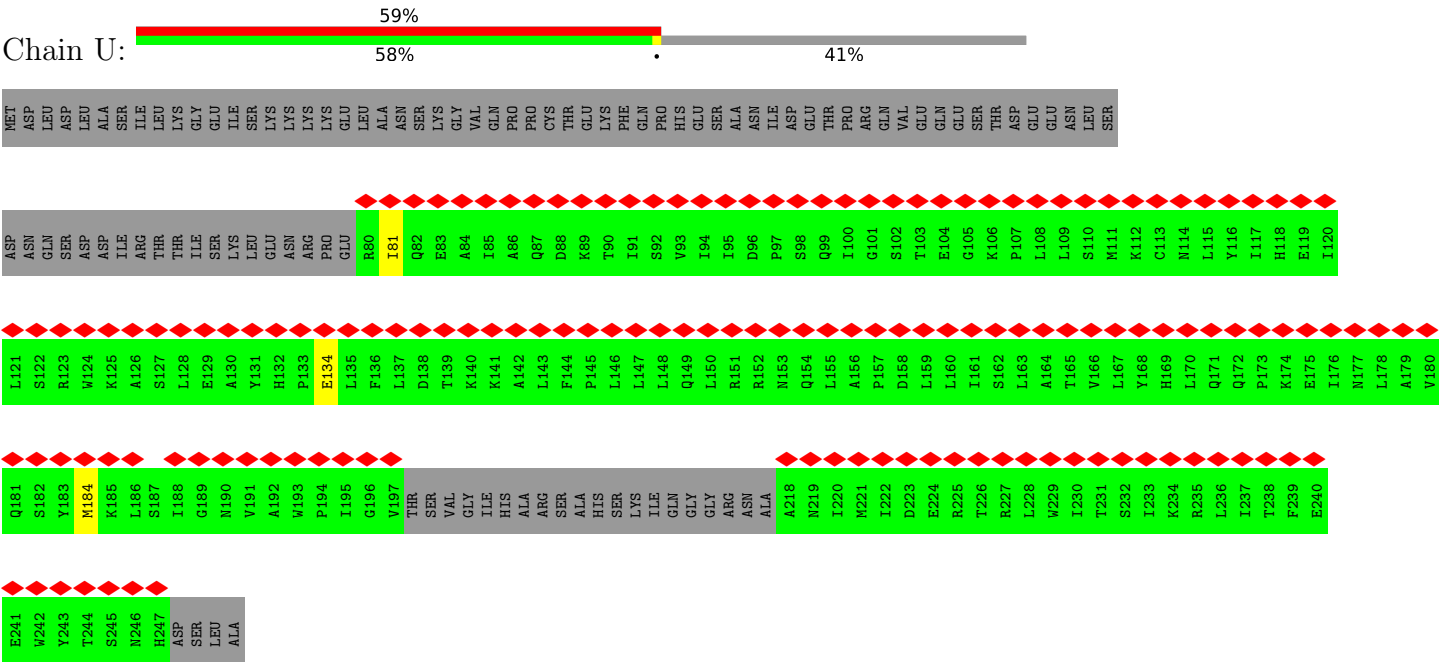
- Molecule 14: Pre-mRNA-splicing factor SLT11



• Molecule 20: Pre-mRNA-splicing factor CWC22



• Molecule 21: Pre-mRNA-splicing factor 18



• Molecule 22: Pre-mRNA-splicing factor SLU7

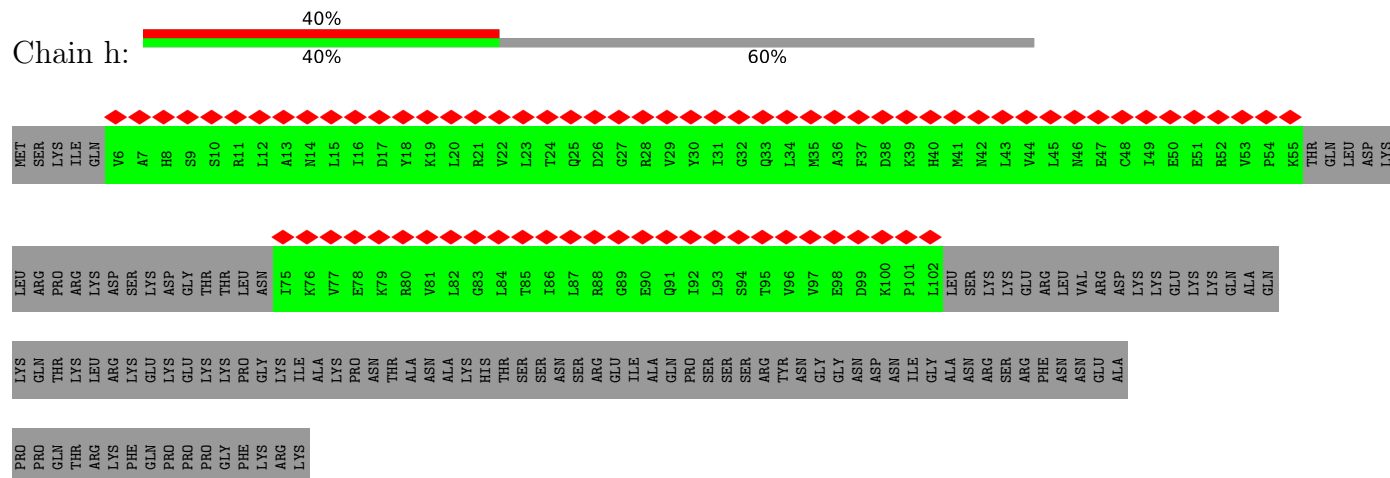


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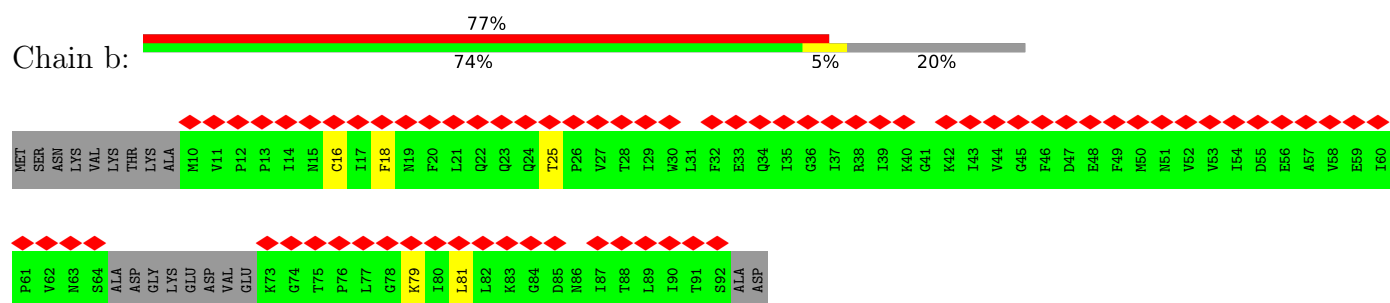
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PRO
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GLY
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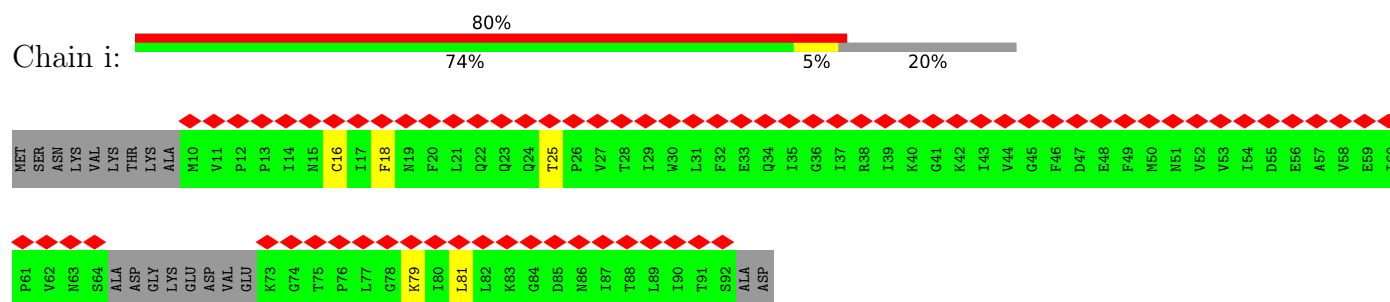
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B



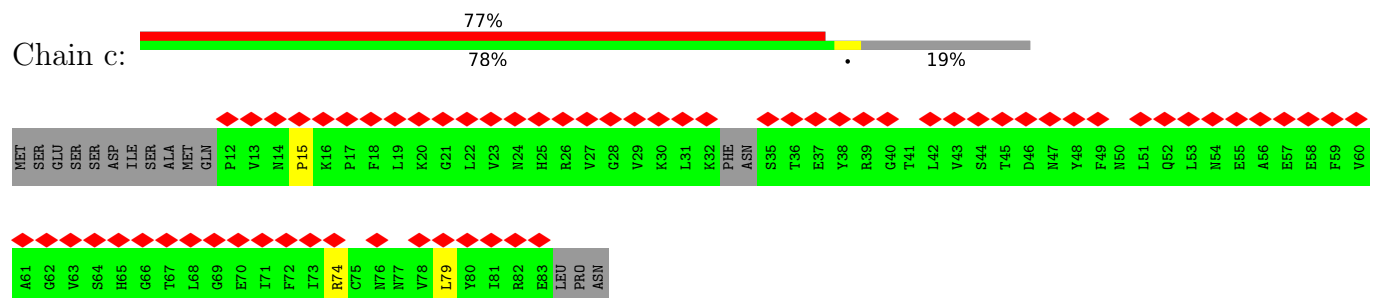
• Molecule 25: Small nuclear ribonucleoprotein E



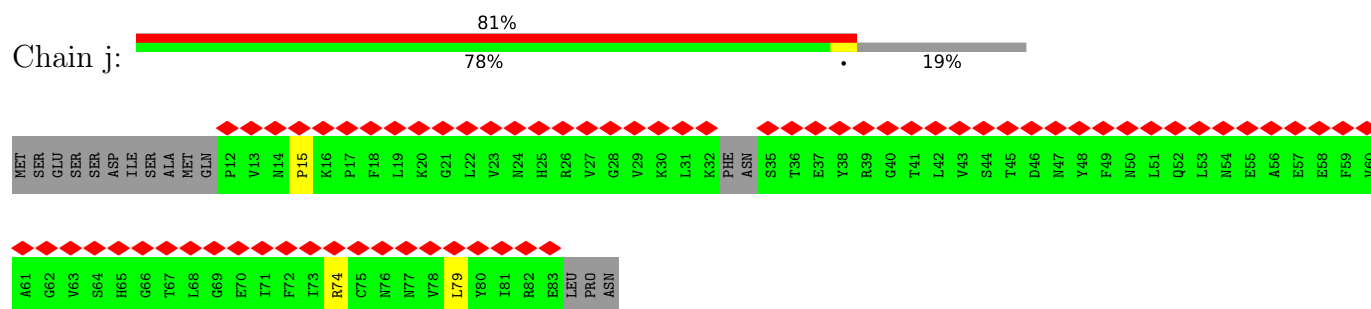
• Molecule 25: Small nuclear ribonucleoprotein E



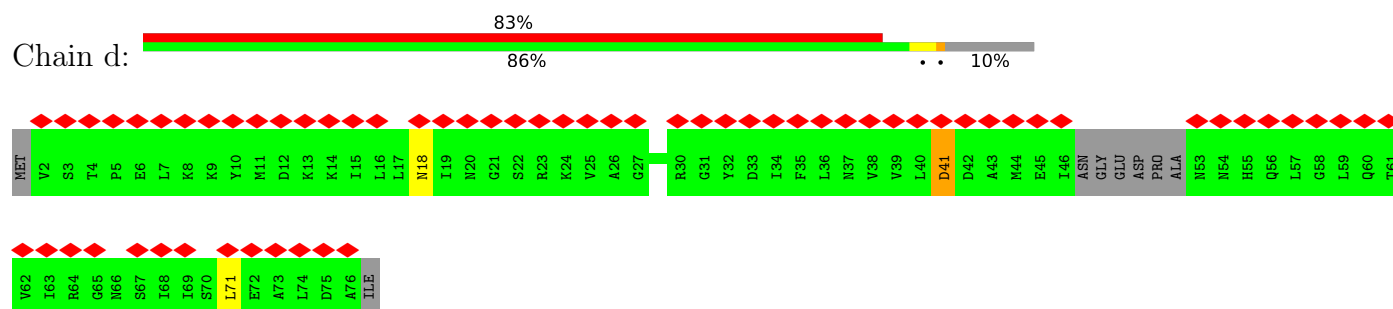
• Molecule 26: Small nuclear ribonucleoprotein F



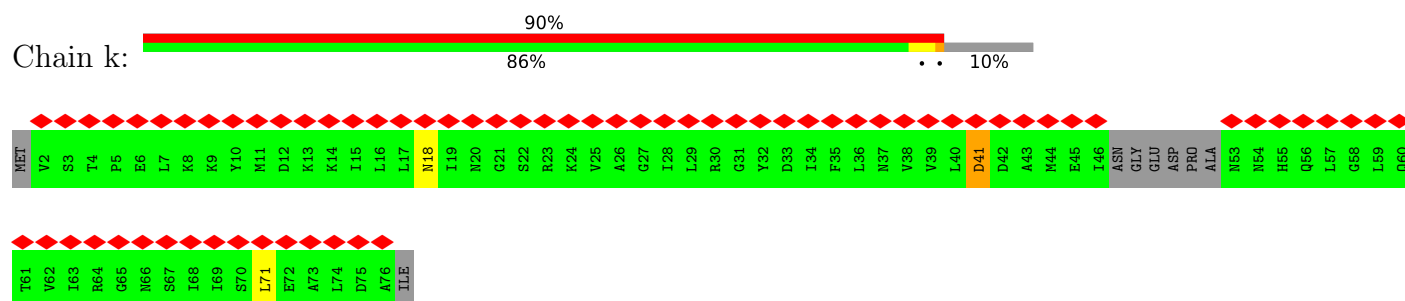
- Molecule 26: Small nuclear ribonucleoprotein F



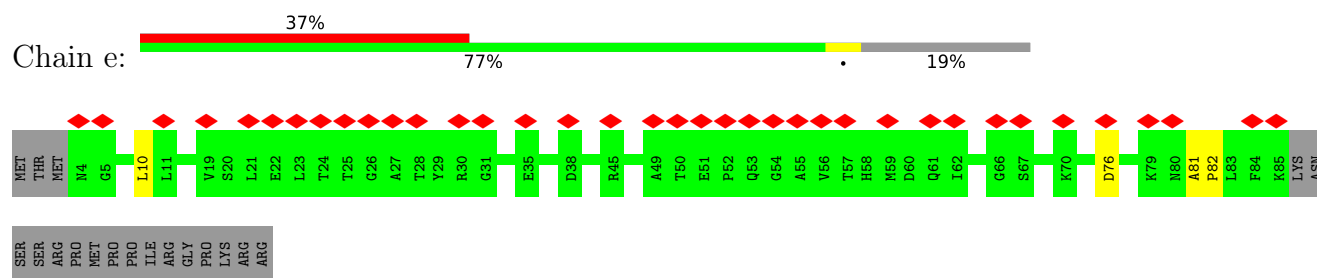
- Molecule 27: Small nuclear ribonucleoprotein G



- Molecule 27: Small nuclear ribonucleoprotein G

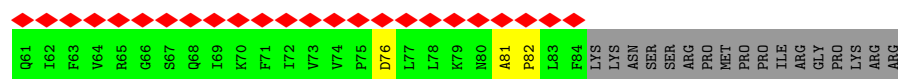


- Molecule 28: Small nuclear ribonucleoprotein Sm D3

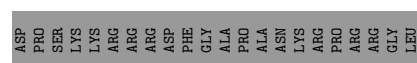
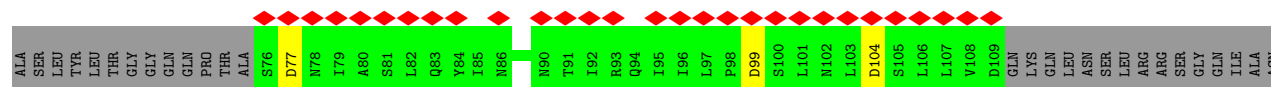
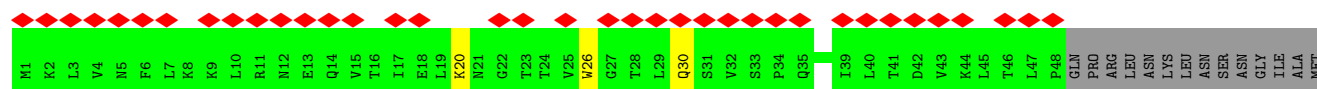
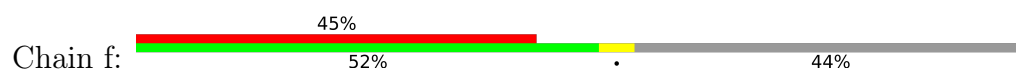


- Molecule 28: Small nuclear ribonucleoprotein Sm D3

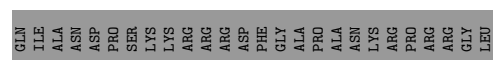
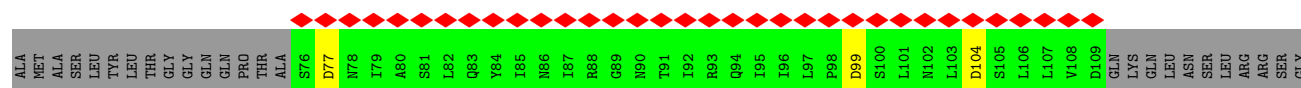




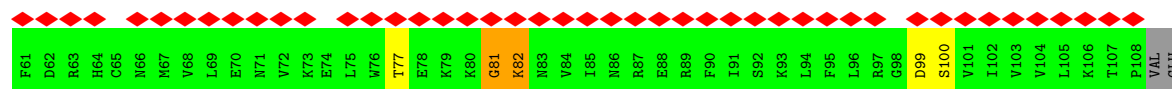
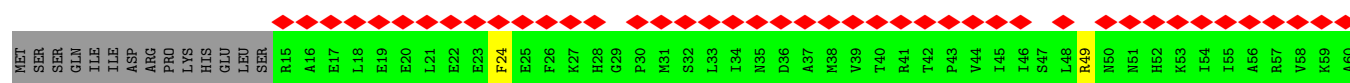
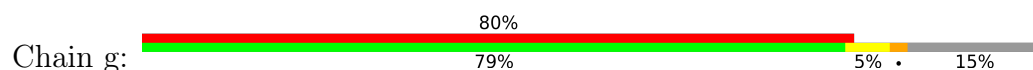
• Molecule 29: Small nuclear ribonucleoprotein Sm D1



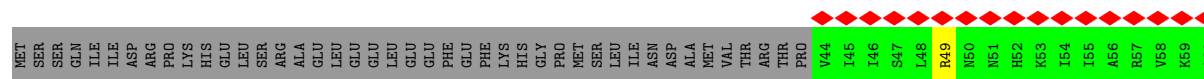
• Molecule 29: Small nuclear ribonucleoprotein Sm D1

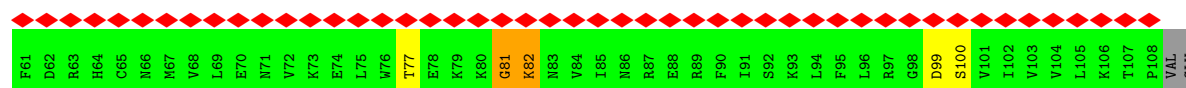


• Molecule 30: Small nuclear ribonucleoprotein Sm D2

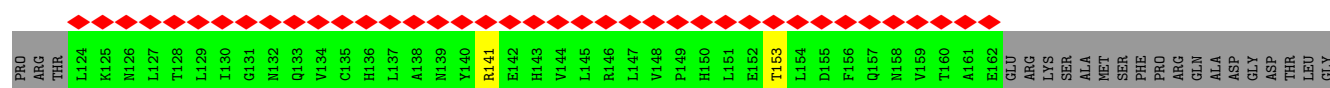
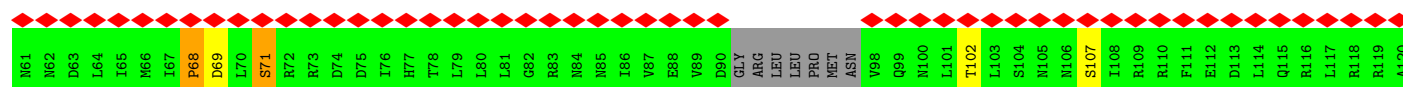
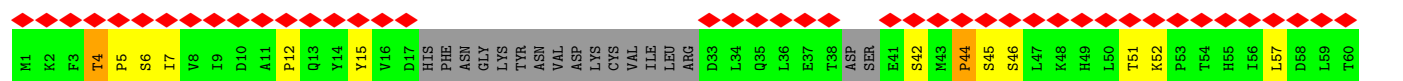


• Molecule 30: Small nuclear ribonucleoprotein Sm D2

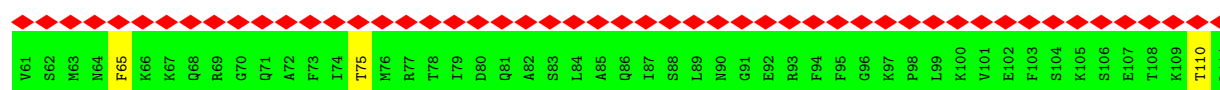
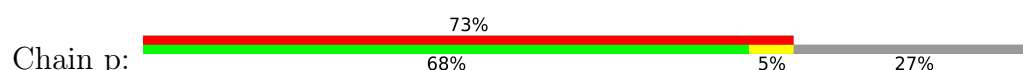




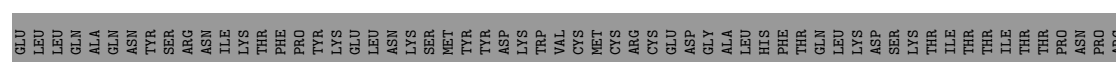
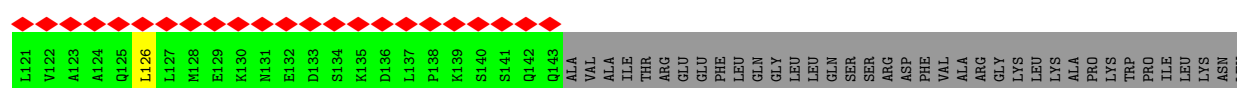
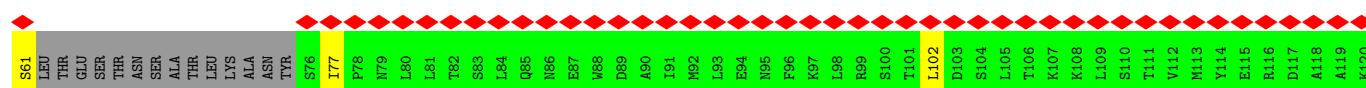
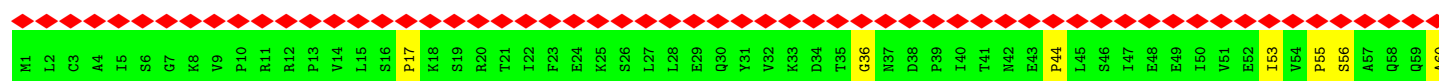
• Molecule 31: U2 small nuclear ribonucleoprotein A'

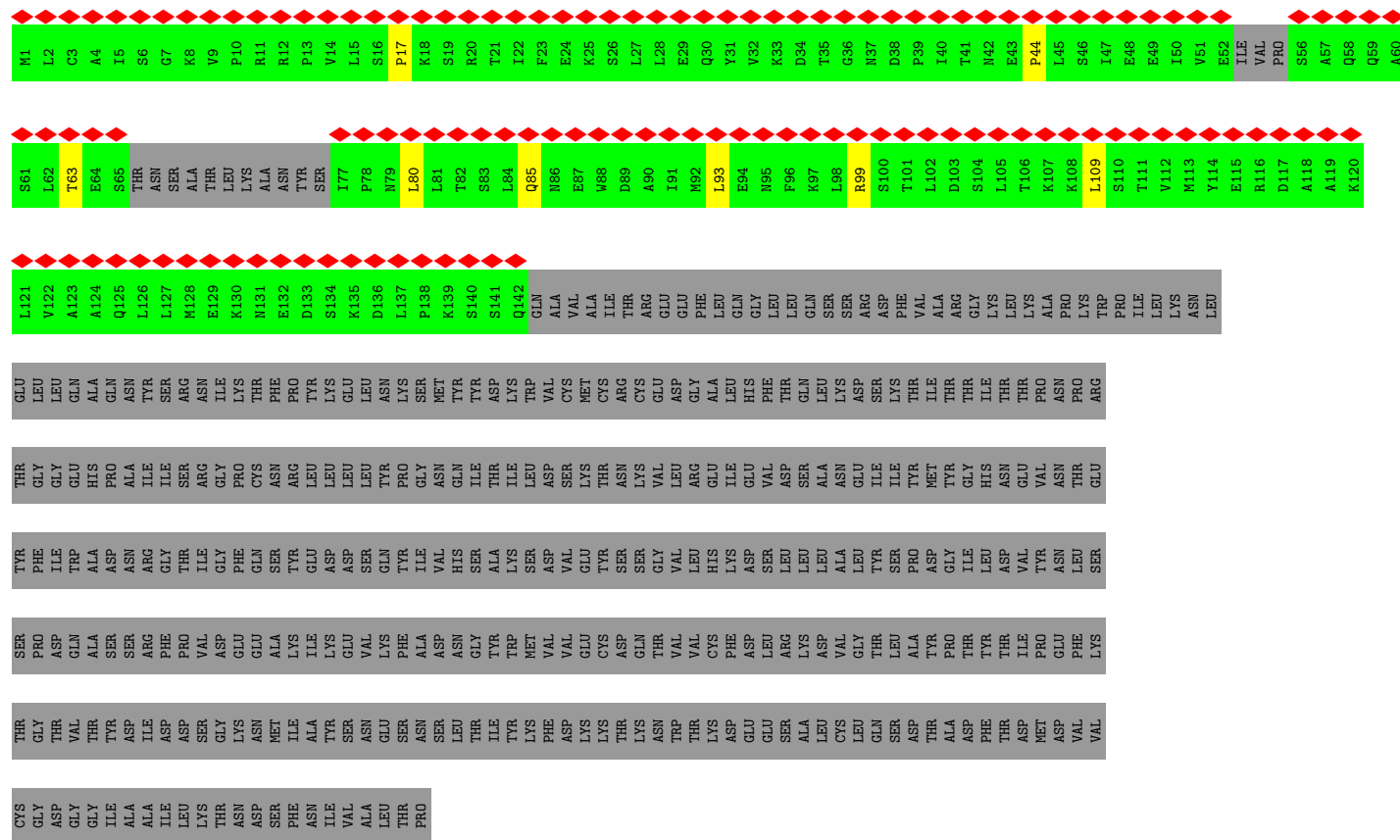


• Molecule 32: U2 small nuclear ribonucleoprotein B''



• Molecule 33: Pre-mRNA-processing factor 19





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.230	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.034	Depositor
Map size (\AA)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, IHP, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	7/16338 (0.0%)	0.94	27/22145 (0.1%)
2	B	0.37	0/2747	0.70	0/4267
3	C	0.67	1/7168 (0.0%)	0.85	3/9707 (0.0%)
4	D	0.46	3/2452 (0.1%)	0.69	0/3817
5	E	0.41	2/1461 (0.1%)	0.68	0/2260
6	F	0.73	11/2123 (0.5%)	1.09	19/3295 (0.6%)
7	G	0.42	0/924	0.56	2/1244 (0.2%)
8	H	0.66	8/2991 (0.3%)	0.63	22/4072 (0.5%)
9	I	0.48	1/3459 (0.0%)	0.61	6/4708 (0.1%)
10	J	0.49	1/2967 (0.0%)	0.68	9/3994 (0.2%)
11	K	0.42	0/780	0.63	0/1036
12	L	0.72	0/1315	0.89	2/1759 (0.1%)
13	T	1.25	24/2390 (1.0%)	1.10	20/3200 (0.6%)
14	M	0.57	0/1496	0.85	0/2014
15	N	0.57	0/2135	0.83	3/2871 (0.1%)
16	O	1.13	5/2704 (0.2%)	1.18	12/3676 (0.3%)
17	P	0.85	0/574	0.98	2/766 (0.3%)
18	Q	0.66	0/1604	0.87	1/2160 (0.0%)
19	R	0.41	0/191	0.73	0/254
20	S	0.60	0/1732	0.84	2/2330 (0.1%)
21	U	0.29	0/1227	0.50	0/1665
22	V	0.98	1/555 (0.2%)	0.90	2/742 (0.3%)
23	W	0.72	1/5660 (0.0%)	1.24	44/7653 (0.6%)
24	a	0.38	0/636	0.61	0/856
24	h	0.37	0/615	0.61	0/829
25	b	0.43	0/585	0.62	0/795
25	i	0.43	0/585	0.62	0/795
26	c	0.44	0/564	0.65	1/761 (0.1%)
26	j	0.44	0/564	0.66	1/761 (0.1%)
27	d	0.37	0/532	0.60	0/715
27	k	0.37	0/532	0.60	0/715
28	e	0.40	0/634	0.71	0/859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	l	0.40	0/625	0.70	0/848
29	f	0.41	0/649	0.61	0/880
29	m	0.42	0/649	0.61	0/880
30	g	0.45	0/753	0.69	2/1013 (0.2%)
30	n	0.43	0/535	0.66	2/717 (0.3%)
31	o	1.03	9/839 (1.1%)	1.65	11/1127 (1.0%)
32	p	0.83	4/514 (0.8%)	1.32	2/686 (0.3%)
33	q	0.41	0/856	0.54	0/1155
33	r	0.39	0/828	0.54	1/1117 (0.1%)
33	s	0.40	0/835	0.53	0/1126
33	t	0.40	0/848	0.56	0/1143
All	All	0.69	78/78171 (0.1%)	0.88	196/107413 (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
1	A	0	8
3	C	0	3
9	I	0	1
10	J	0	3
12	L	0	5
13	T	0	2
14	M	0	5
15	N	0	1
16	O	0	11
18	Q	0	3
20	S	0	3
23	W	0	35
27	d	0	1
27	k	0	1
28	e	0	2
28	l	0	2
30	g	0	2
30	n	0	2
All	All	0	90

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	444	CYS	CB-SG	-22.89	1.43	1.82
13	T	454	CYS	CB-SG	-18.67	1.50	1.82
13	T	185	HIS	CB-CG	18.43	1.83	1.50
13	T	399	CYS	CB-SG	-17.51	1.52	1.82
8	H	712	CYS	CB-SG	-17.09	1.53	1.82
22	V	302	LEU	CA-CB	-10.62	1.29	1.53
6	F	1096	C	O3'-P	-10.04	1.49	1.61
10	J	145	GLU	CD-OE2	9.54	1.36	1.25
13	T	362	SER	CB-OG	9.30	1.54	1.42
13	T	306	SER	CB-OG	9.03	1.53	1.42
8	H	723	SER	CB-OG	8.62	1.53	1.42
8	H	718	SER	CB-OG	8.52	1.53	1.42
1	A	716	ARG	CD-NE	-8.41	1.32	1.46
1	A	708	TRP	CB-CG	-8.19	1.35	1.50
13	T	388	SER	CB-OG	8.09	1.52	1.42
8	H	714	SER	CB-OG	7.92	1.52	1.42
13	T	113	SER	CB-OG	7.89	1.52	1.42
8	H	681	SER	CB-OG	7.74	1.52	1.42
4	D	74	U	C2-N3	7.64	1.43	1.37
13	T	381	SER	CB-OG	7.63	1.52	1.42
5	E	301	A	C3'-O3'	7.58	1.52	1.42
13	T	382	SER	CB-OG	7.52	1.52	1.42
31	o	46	SER	CB-OG	7.51	1.52	1.42
6	F	1096	C	C1'-N1	7.48	1.59	1.48
6	F	1120	G	C1'-N9	-7.35	1.36	1.46
13	T	270	SER	CB-OG	7.35	1.51	1.42
6	F	1118	U	C1'-N1	7.32	1.59	1.48
31	o	45	SER	CB-OG	7.26	1.51	1.42
13	T	248	SER	CB-OG	7.17	1.51	1.42
32	p	33	SER	CB-OG	7.09	1.51	1.42
13	T	220	SER	CB-OG	7.07	1.51	1.42
13	T	218	CYS	CA-CB	-7.06	1.38	1.53
31	o	69	ASP	CA-CB	-6.98	1.38	1.53
31	o	6	SER	CB-OG	6.97	1.51	1.42
6	F	1101	C	C1'-N1	6.86	1.59	1.48
6	F	1111	U	C1'-N1	6.77	1.58	1.48
8	H	633	SER	CB-OG	6.77	1.51	1.42
16	O	251	TRP	CE3-CZ3	-6.76	1.26	1.38
6	F	1119	C	C1'-N1	6.71	1.58	1.48
6	F	1115	G	C1'-N9	-6.63	1.37	1.46
4	D	74	U	C4-O4	6.33	1.28	1.23
6	F	1109	C	C1'-N1	6.11	1.57	1.48
13	T	405	SER	CA-CB	-6.08	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	229	SER	CB-OG	6.07	1.50	1.42
9	I	102	TRP	CB-CG	-5.98	1.39	1.50
13	T	403	SER	CA-CB	-5.97	1.44	1.52
31	o	42	SER	CB-OG	5.92	1.50	1.42
4	D	74	U	C5-C6	5.90	1.39	1.34
16	O	251	TRP	CE2-CZ2	-5.85	1.29	1.39
13	T	255	SER	CB-OG	5.82	1.49	1.42
31	o	102	THR	CB-OG1	5.78	1.54	1.43
8	H	640	SER	CB-OG	5.75	1.49	1.42
6	F	121	C	C1'-N1	5.72	1.57	1.48
13	T	347	SER	CB-OG	5.71	1.49	1.42
1	A	298	TYR	CG-CD2	-5.64	1.31	1.39
16	O	198	PHE	CB-CG	-5.61	1.41	1.51
31	o	15	TYR	CB-CG	-5.60	1.43	1.51
6	F	1112	G	C1'-N9	-5.59	1.39	1.46
13	T	288	THR	CB-OG1	5.55	1.54	1.43
31	o	51	THR	CB-OG1	5.50	1.54	1.43
13	T	409	THR	CB-OG1	5.48	1.54	1.43
13	T	318	ARG	CZ-NH1	5.38	1.40	1.33
16	O	251	TRP	CB-CG	-5.28	1.40	1.50
8	H	685	GLU	CB-CG	-5.26	1.42	1.52
32	p	75	THR	CB-OG1	5.23	1.53	1.43
32	p	110	THR	CB-OG1	5.20	1.53	1.43
13	T	141	GLU	CB-CG	-5.18	1.42	1.52
5	E	355	U	C1'-N1	5.15	1.56	1.48
1	A	1602	PRO	N-CD	5.12	1.55	1.47
31	o	153	THR	CB-OG1	5.10	1.53	1.43
32	p	65	PHE	CB-CG	-5.10	1.42	1.51
16	O	202	GLU	CA-C	-5.08	1.39	1.52
13	T	151	PRO	N-CD	5.04	1.54	1.47
23	W	294	PRO	N-CD	5.03	1.54	1.47
1	A	753	TYR	N-CA	-5.02	1.36	1.46
1	A	667	TYR	CB-CG	-5.02	1.44	1.51
1	A	823	TRP	CE3-CZ3	-5.02	1.29	1.38
3	C	933	TRP	CB-CG	-5.01	1.41	1.50

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	130	TYR	N-CA-C	16.80	156.37	111.00
13	T	152	LYS	CB-CA-C	-16.28	77.83	110.40
13	T	153	LYS	N-CA-CB	12.84	133.71	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1110	U	C5-C4-O4	11.77	132.96	125.90
1	A	284	ARG	NE-CZ-NH2	11.66	126.13	120.30
23	W	1077	ARG	NE-CZ-NH2	11.64	126.12	120.30
13	T	130	TYR	CB-CA-C	-11.43	87.55	110.40
1	A	284	ARG	NE-CZ-NH1	-11.31	114.64	120.30
23	W	538	ARG	NE-CZ-NH2	10.85	125.72	120.30
13	T	424	PRO	N-CA-CB	10.62	116.05	103.30
6	F	1107	C	N1-C2-O2	-10.09	112.84	118.90
23	W	471	ARG	NE-CZ-NH2	10.07	125.33	120.30
23	W	497	ARG	NE-CZ-NH2	9.28	124.94	120.30
23	W	957	TYR	CB-CG-CD2	-9.04	115.58	121.00
23	W	442	ARG	NE-CZ-NH2	9.03	124.81	120.30
6	F	1109	C	O4'-C1'-N1	8.81	115.25	108.20
31	o	44	PRO	N-CA-CB	8.80	113.86	103.30
1	A	1739	ARG	NE-CZ-NH2	-8.65	115.97	120.30
13	T	125	GLY	N-CA-C	-8.51	91.84	113.10
6	F	1112	G	P-O3'-C3'	8.46	129.85	119.70
13	T	131	PRO	N-CA-CB	-8.42	93.20	103.30
13	T	153	LYS	N-CA-C	-8.30	88.60	111.00
6	F	1107	C	C5'-C4'-O4'	-8.27	99.18	109.10
6	F	1110	U	N3-C4-O4	-7.91	113.86	119.40
18	Q	77	LEU	CA-CB-CG	-7.87	97.20	115.30
23	W	992	ARG	NE-CZ-NH2	7.74	124.17	120.30
23	W	461	ARG	NE-CZ-NH2	7.69	124.15	120.30
23	W	1036	ARG	NE-CZ-NH2	7.67	124.14	120.30
23	W	522	GLU	CB-CA-C	7.65	125.71	110.40
6	F	1107	C	P-O3'-C3'	7.55	128.76	119.70
6	F	1107	C	N3-C2-O2	7.54	127.18	121.90
23	W	714	ARG	NE-CZ-NH2	7.54	124.07	120.30
23	W	805	ARG	NE-CZ-NH2	7.54	124.07	120.30
20	S	397	LEU	C-N-CD	-7.53	104.04	120.60
6	F	1110	U	N1-C2-O2	7.51	128.05	122.80
23	W	811	ARG	NE-CZ-NH2	7.41	124.00	120.30
23	W	909	ARG	NE-CZ-NH2	7.29	123.95	120.30
31	o	5	PRO	N-CA-CB	7.27	112.02	103.30
31	o	42	SER	N-CA-CB	-7.24	99.64	110.50
23	W	519	TYR	CB-CG-CD2	-7.14	116.72	121.00
6	F	1111	U	P-O5'-C5'	-7.13	109.49	120.90
16	O	211	LEU	CA-CB-CG	-7.12	98.92	115.30
1	A	1370	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	854	ARG	NE-CZ-NH1	-7.07	116.77	120.30
23	W	751	ARG	NE-CZ-NH2	6.99	123.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1110	U	N3-C2-O2	-6.98	117.32	122.20
13	T	318	ARG	NE-CZ-NH2	-6.88	116.86	120.30
6	F	1108	A	O4'-C1'-N9	-6.87	102.70	108.20
1	A	461	LEU	CB-CG-CD2	-6.87	99.33	111.00
23	W	969	ARG	NE-CZ-NH2	6.87	123.73	120.30
31	o	12	PRO	N-CA-CB	6.77	111.43	103.30
16	O	197	LEU	CB-CG-CD2	6.77	122.51	111.00
1	A	622	MET	CG-SD-CE	-6.69	89.50	100.20
16	O	193	ARG	NE-CZ-NH2	-6.67	116.96	120.30
22	V	275	THR	C-N-CA	-6.66	105.04	121.70
8	H	617	PRO	CA-CB-CG	6.58	117.31	104.80
8	H	613	PRO	N-CA-CB	6.54	111.15	103.30
23	W	1030	PHE	CB-CG-CD2	-6.53	116.23	120.80
20	S	427	LEU	CB-CG-CD2	-6.48	99.98	111.00
8	H	722	PRO	N-CA-CB	6.42	111.00	103.30
10	J	334	PRO	N-CA-CB	6.35	110.92	103.30
13	T	303	PRO	N-CA-CB	6.35	110.92	103.30
16	O	193	ARG	NE-CZ-NH1	6.35	123.47	120.30
13	T	402	ASP	CB-CG-OD2	-6.35	112.59	118.30
16	O	238	LEU	CB-CA-C	-6.34	98.15	110.20
23	W	1105	GLU	CB-CA-C	6.34	123.08	110.40
31	o	4	THR	N-CA-CB	-6.33	98.28	110.30
31	o	57	LEU	N-CA-CB	6.32	123.03	110.40
23	W	626	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	A	224	MET	CA-CB-CG	6.25	123.92	113.30
13	T	162	PRO	N-CA-CB	6.24	110.79	103.30
23	W	537	ARG	NE-CZ-NH2	6.18	123.39	120.30
23	W	805	ARG	NE-CZ-NH1	-6.15	117.22	120.30
8	H	479	PRO	N-CA-CB	6.12	110.65	103.30
16	O	197	LEU	CB-CG-CD1	-6.09	100.64	111.00
8	H	223	PRO	N-CA-CB	6.07	110.58	103.30
23	W	1067	VAL	CA-CB-CG2	6.07	120.00	110.90
17	P	30	LEU	CA-CB-CG	-6.06	101.37	115.30
23	W	562	TYR	C-N-CA	6.05	136.82	121.70
8	H	443	PRO	N-CA-CB	6.05	110.56	103.30
8	H	515	PRO	N-CA-CB	6.03	110.54	103.30
3	C	656	LEU	CA-CB-CG	-6.02	101.45	115.30
8	H	299	PRO	N-CA-CB	6.01	110.51	103.30
13	T	208	PRO	N-CA-CB	6.00	110.49	103.30
8	H	641	PRO	CA-CB-CG	5.99	116.19	104.80
23	W	489	ARG	NE-CZ-NH1	5.99	123.30	120.30
31	o	141	ARG	CD-NE-CZ	5.99	131.99	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	774	PRO	N-CA-CB	5.98	110.47	103.30
10	J	418	PRO	N-CA-CB	5.97	110.47	103.30
8	H	616	PRO	N-CA-CB	5.96	110.45	103.30
8	H	267	PRO	N-CA-CB	5.96	110.45	103.30
8	H	477	PRO	N-CA-CB	5.95	110.44	103.30
9	I	435	PRO	N-CA-CB	5.95	110.43	103.30
1	A	716	ARG	NE-CZ-NH2	-5.94	117.33	120.30
8	H	161	PRO	N-CA-CB	5.94	110.43	103.30
8	H	557	PRO	N-CA-CB	5.94	110.42	103.30
31	o	7	ILE	CA-CB-CG1	5.92	122.25	111.00
1	A	1145	MET	CG-SD-CE	-5.90	90.76	100.20
23	W	559	ASP	CB-CG-OD1	5.88	123.59	118.30
9	I	397	PRO	N-CA-CB	5.88	110.35	103.30
8	H	533	PRO	N-CA-CB	5.87	110.34	103.30
6	F	1107	C	C5-C4-N4	-5.87	116.09	120.20
1	A	674	MET	CG-SD-CE	-5.85	90.83	100.20
8	H	262	PRO	N-CA-CB	5.85	110.32	103.30
8	H	252	PRO	N-CA-CB	5.85	110.31	103.30
9	I	559	PRO	N-CA-CB	5.84	110.30	103.30
13	T	402	ASP	CB-CG-OD1	5.83	123.55	118.30
8	H	437	PRO	N-CA-CB	5.83	110.29	103.30
6	F	1111	U	C5'-C4'-C3'	-5.82	106.68	116.00
23	W	547	ARG	NE-CZ-NH2	5.82	123.21	120.30
9	I	545	PRO	N-CA-CB	5.82	110.29	103.30
1	A	551	LEU	CB-CG-CD2	-5.82	101.11	111.00
17	P	12	ARG	NE-CZ-NH1	5.82	123.21	120.30
8	H	773	PRO	N-CA-CB	5.81	110.27	103.30
9	I	351	PRO	N-CA-CB	5.81	110.27	103.30
15	N	114	ARG	NE-CZ-NH2	-5.80	117.40	120.30
7	G	105	PRO	CA-CB-CG	5.80	115.82	104.80
13	T	131	PRO	C-N-CD	5.80	140.58	128.40
10	J	376	PRO	N-CA-CB	5.78	110.23	103.30
1	A	893	ARG	NE-CZ-NH2	-5.78	117.41	120.30
6	F	1110	U	O3'-P-O5'	-5.77	93.04	104.00
1	A	526	LEU	CA-CB-CG	-5.75	102.08	115.30
23	W	293	SER	C-N-CD	5.74	140.46	128.40
13	T	373	PRO	N-CA-CB	5.74	110.19	103.30
1	A	831	ARG	NE-CZ-NH1	5.73	123.17	120.30
31	o	68	PRO	N-CA-CB	5.71	110.16	103.30
9	I	421	PRO	N-CA-CB	5.70	110.14	103.30
13	T	159	PRO	N-CA-CB	5.70	110.14	103.30
8	H	518	PRO	N-CA-CB	5.69	110.13	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1601	ILE	C-N-CD	5.68	140.33	128.40
16	O	292	LEU	CA-CB-CG	-5.67	102.27	115.30
12	L	145	CYS	CA-CB-SG	5.65	124.16	114.00
3	C	347	ARG	NE-CZ-NH1	5.59	123.09	120.30
23	W	547	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	1339	LEU	CB-CG-CD2	-5.57	101.53	111.00
30	g	81	GLY	CA-C-N	-5.55	104.98	117.20
13	T	367	PRO	N-CA-CB	5.55	109.96	103.30
23	W	1067	VAL	CG1-CB-CG2	-5.55	102.03	110.90
30	n	81	GLY	CA-C-N	-5.55	105.00	117.20
1	A	712	LEU	CB-CG-CD2	-5.54	101.59	111.00
16	O	316	LEU	CA-CB-CG	-5.53	102.57	115.30
15	N	104	LEU	CB-CG-CD2	5.53	120.40	111.00
13	T	424	PRO	CA-CB-CG	5.48	115.20	104.80
16	O	217	ILE	CG1-CB-CG2	-5.47	99.37	111.40
1	A	531	LEU	CA-CB-CG	-5.46	102.73	115.30
26	j	74	ARG	NE-CZ-NH1	5.43	123.01	120.30
10	J	339	PRO	N-CA-CB	5.42	109.80	103.30
10	J	467	PRO	N-CA-CB	5.39	109.77	103.30
12	L	123	ARG	NE-CZ-NH2	-5.36	117.62	120.30
13	T	289	TYR	CB-CG-CD2	-5.36	117.78	121.00
10	J	432	PRO	N-CA-CB	5.33	109.70	103.30
10	J	447	PRO	N-CA-CB	5.33	109.69	103.30
1	A	1320	LEU	CA-CB-CG	-5.32	103.06	115.30
10	J	424	PRO	N-CA-CB	5.32	109.69	103.30
1	A	831	ARG	NE-CZ-NH2	-5.32	117.64	120.30
7	G	77	PRO	CA-CB-CG	5.32	114.90	104.80
23	W	480	ARG	NE-CZ-NH2	5.32	122.96	120.30
23	W	751	ARG	NE-CZ-NH1	-5.29	117.65	120.30
33	r	62	LEU	CA-CB-CG	-5.25	103.22	115.30
1	A	262	ASP	N-CA-C	5.24	125.16	111.00
31	o	71	SER	N-CA-CB	-5.24	102.64	110.50
6	F	1113	U	O4'-C1'-C2'	-5.23	100.57	105.80
1	A	742	VAL	CB-CA-C	-5.21	101.50	111.40
23	W	565	ARG	NE-CZ-NH2	5.20	122.90	120.30
15	N	231	ASP	CB-CG-OD1	5.20	122.98	118.30
23	W	538	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
6	F	1119	C	OP1-P-OP2	-5.20	111.81	119.60
23	W	575	ARG	NE-CZ-NH2	5.20	122.90	120.30
23	W	558	HIS	CB-CA-C	5.18	120.76	110.40
10	J	374	PRO	N-CA-CB	5.17	109.50	103.30
1	A	1339	LEU	CB-CG-CD1	5.17	119.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	506	GLY	N-CA-C	5.15	125.97	113.10
23	W	640	SER	N-CA-C	5.14	124.89	111.00
23	W	591	ASP	CB-CG-OD1	5.14	122.92	118.30
6	F	20	G	P-O3'-C3'	5.11	125.84	119.70
1	A	1499	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	A	237	MET	CG-SD-CE	-5.11	92.03	100.20
30	n	82	LYS	N-CA-C	5.11	124.78	111.00
16	O	133	ARG	NE-CZ-NH2	-5.10	117.75	120.30
23	W	650	CYS	CA-CB-SG	-5.10	104.82	114.00
26	c	74	ARG	NE-CZ-NH1	5.10	122.85	120.30
23	W	497	ARG	CD-NE-CZ	5.09	130.73	123.60
30	g	82	LYS	N-CA-C	5.08	124.72	111.00
23	W	957	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	1302	LEU	CB-CG-CD1	-5.07	102.39	111.00
31	o	107	SER	N-CA-CB	-5.07	102.90	110.50
8	H	617	PRO	N-CA-CB	5.06	109.38	103.30
22	V	246	THR	CA-CB-OG1	5.06	119.63	109.00
23	W	786	ARG	NE-CZ-NH2	5.05	122.83	120.30
32	p	33	SER	N-CA-CB	5.05	118.08	110.50
3	C	187	ARG	NE-CZ-NH2	-5.03	117.78	120.30
32	p	46	VAL	CA-CB-CG2	5.03	118.45	110.90
16	O	264	GLY	N-CA-C	5.03	125.66	113.10
6	F	1096	C	OP2-P-O3'	5.02	116.25	105.20
16	O	205	THR	CB-CA-C	-5.02	98.04	111.60
23	W	912	LEU	O-C-N	-5.01	114.68	122.70

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1375	LEU	Peptide
1	A	1432	GLU	Peptide
1	A	1809	ASN	Peptide
1	A	239	PHE	Peptide
1	A	288	GLU	Peptide
1	A	539	PRO	Peptide
1	A	907	ASN	Peptide
3	C	170	LEU	Peptide
3	C	365	GLU	Peptide
3	C	70	TYR	Peptide
9	I	212	HIS	Peptide

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Mol	Chain	Res	Type	Group
10	J	224	MET	Peptide
10	J	65	PHE	Peptide
10	J	81	PRO	Peptide
12	L	1	MET	Peptide
12	L	104	CYS	Peptide
12	L	116	ASN	Peptide
12	L	118	SER	Peptide
12	L	5	LYS	Peptide
14	M	103	GLU	Peptide
14	M	291	ILE	Peptide
14	M	45	HIS	Peptide
14	M	94	VAL	Peptide
14	M	98	ASN	Peptide
15	N	203	THR	Peptide
16	O	123	PRO	Peptide
16	O	155	PHE	Peptide
16	O	278	ASP	Peptide
16	O	284	SER	Peptide
16	O	336	LEU	Peptide
16	O	351	GLY	Peptide
16	O	431	THR	Peptide
16	O	434	LYS	Peptide
16	O	435	GLU	Peptide
16	O	437	GLU	Peptide
16	O	441	ALA	Peptide
18	Q	103	ASN	Peptide
18	Q	84	ASN	Peptide
18	Q	85	SER	Peptide
20	S	335	GLN	Peptide
20	S	397	LEU	Mainchain,Peptide
13	T	366	LYS	Peptide
13	T	67	GLY	Peptide
23	W	1037	ASP	Peptide
23	W	1042	TYR	Sidechain
23	W	1064	TYR	Sidechain
23	W	1067	VAL	Peptide
23	W	1076	SER	Peptide
23	W	1077	ARG	Sidechain
23	W	1081	SER	Peptide
23	W	1103	ASP	Peptide
23	W	439	LYS	Peptide
23	W	440	ASP	Sidechain

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Mol	Chain	Res	Type	Group
23	W	446	GLN	Peptide
23	W	468	TYR	Peptide
23	W	474	LEU	Peptide
23	W	480	ARG	Sidechain
23	W	486	TYR	Sidechain
23	W	489	ARG	Sidechain
23	W	505	VAL	Peptide
23	W	512	LYS	Peptide
23	W	522	GLU	Peptide
23	W	537	ARG	Sidechain
23	W	562	TYR	Peptide
23	W	566	PHE	Peptide
23	W	575	ARG	Sidechain
23	W	646	TYR	Sidechain
23	W	666	TYR	Sidechain
23	W	729	PRO	Peptide
23	W	786	ARG	Peptide
23	W	808	ARG	Sidechain
23	W	811	ARG	Sidechain
23	W	840	ARG	Sidechain
23	W	911	LEU	Peptide
23	W	916	ASP	Peptide
23	W	940	LYS	Peptide
23	W	957	TYR	Sidechain
23	W	967	TYR	Sidechain
27	d	41	ASP	Peptide
28	e	81	ALA	Mainchain,Peptide
30	g	81	GLY	Mainchain,Peptide
27	k	41	ASP	Peptide
28	l	81	ALA	Mainchain,Peptide
30	n	81	GLY	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1925/2413 (80%)	1558 (81%)	328 (17%)	39 (2%)	7	41
3	C	872/1008 (86%)	735 (84%)	121 (14%)	16 (2%)	8	43
7	G	150/175 (86%)	134 (89%)	13 (9%)	3 (2%)	7	41
8	H	496/859 (58%)	474 (96%)	16 (3%)	6 (1%)	13	51
9	I	481/687 (70%)	433 (90%)	45 (9%)	3 (1%)	25	64
10	J	414/590 (70%)	368 (89%)	35 (8%)	11 (3%)	5	35
11	K	92/215 (43%)	84 (91%)	7 (8%)	1 (1%)	14	53
12	L	155/157 (99%)	118 (76%)	34 (22%)	3 (2%)	8	42
13	T	326/455 (72%)	283 (87%)	21 (6%)	22 (7%)	1	15
14	M	177/364 (49%)	137 (77%)	36 (20%)	4 (2%)	6	38
15	N	259/339 (76%)	219 (85%)	35 (14%)	5 (2%)	8	42
16	O	335/451 (74%)	268 (80%)	58 (17%)	9 (3%)	5	35
17	P	63/175 (36%)	50 (79%)	10 (16%)	3 (5%)	2	22
18	Q	193/379 (51%)	156 (81%)	29 (15%)	8 (4%)	3	26
19	R	25/135 (18%)	20 (80%)	5 (20%)	0	100	100
20	S	205/577 (36%)	166 (81%)	36 (18%)	3 (2%)	10	47
21	U	144/251 (57%)	140 (97%)	4 (3%)	0	100	100
22	V	82/382 (22%)	71 (87%)	9 (11%)	2 (2%)	6	37
23	W	697/1145 (61%)	600 (86%)	72 (10%)	25 (4%)	3	29
24	a	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
24	h	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
25	b	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
25	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
26	c	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	47
26	j	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	47
27	d	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
28	e	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	50
28	l	79/101 (78%)	69 (87%)	9 (11%)	1 (1%)	12	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	f	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
29	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
30	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	14	53
30	n	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	9	46
31	o	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	9	46
32	p	77/111 (69%)	75 (97%)	2 (3%)	0	100	100
33	q	125/503 (25%)	115 (92%)	6 (5%)	4 (3%)	4	31
33	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	5	36
33	s	120/503 (24%)	115 (96%)	4 (3%)	1 (1%)	19	59
33	t	122/503 (24%)	116 (95%)	6 (5%)	0	100	100
All	All	8803/14738 (60%)	7603 (86%)	1021 (12%)	179 (2%)	11	41

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	ASN
1	A	645	ASP
1	A	1404	HIS
1	A	1405	ILE
1	A	1540	ASN
3	C	364	PHE
7	G	77	PRO
8	H	616	PRO
8	H	797	TYR
9	I	315	ASN
10	J	417	PRO
10	J	418	PRO
13	T	112	VAL
13	T	131	PRO
13	T	133	ASN
13	T	137	VAL
13	T	141	GLU
13	T	153	LYS
13	T	158	TYR
13	T	159	PRO
13	T	173	LYS
13	T	218	CYS
13	T	246	LEU

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Mol	Chain	Res	Type
13	T	303	PRO
13	T	424	PRO
14	M	99	VAL
16	O	279	PRO
18	Q	36	LYS
18	Q	112	ILE
23	W	475	PRO
23	W	507	GLU
23	W	526	SER
23	W	640	SER
23	W	773	VAL
23	W	774	ASP
23	W	912	LEU
23	W	1082	GLN
31	o	68	PRO
33	q	53	ILE
33	q	77	ILE
33	r	64	GLU
1	A	410	ILE
1	A	480	TYR
1	A	741	ILE
1	A	1033	ASN
1	A	1419	ASP
1	A	1964	PRO
3	C	363	PRO
7	G	110	GLU
8	H	601	VAL
8	H	618	GLU
10	J	82	ASN
10	J	230	THR
10	J	415	ILE
12	L	119	THR
13	T	61	LYS
13	T	199	LEU
13	T	357	ASP
15	N	151	LEU
16	O	435	GLU
17	P	8	GLN
18	Q	49	SER
20	S	398	PRO
23	W	448	LEU
23	W	566	PHE

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Mol	Chain	Res	Type
23	W	605	ALA
23	W	724	GLU
23	W	729	PRO
23	W	788	GLY
23	W	913	SER
23	W	975	TYR
23	W	1061	GLY
23	W	1076	SER
1	A	240	PRO
1	A	543	ASN
1	A	618	SER
1	A	1347	ARG
1	A	1628	ASP
1	A	2002	TYR
3	C	106	PHE
3	C	109	LEU
3	C	655	LEU
3	C	704	PRO
7	G	80	ASN
8	H	634	HIS
8	H	752	GLU
13	T	294	SER
14	M	61	CYS
15	N	92	HIS
16	O	124	GLU
16	O	244	ARG
17	P	159	ASP
18	Q	102	ALA
18	Q	109	SER
20	S	286	THR
23	W	292	THR
23	W	435	THR
23	W	1040	VAL
33	r	20	ARG
33	s	17	PRO
1	A	128	TYR
1	A	230	ASP
1	A	259	GLU
1	A	701	CYS
1	A	1077	ASN
1	A	1866	PHE
3	C	117	ARG

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Mol	Chain	Res	Type
3	C	829	VAL
9	I	529	LYS
10	J	231	SER
12	L	127	ALA
13	T	405	SER
13	T	429	ILE
14	M	17	LEU
16	O	278	ASP
16	O	340	SER
17	P	9	LEU
18	Q	86	ASN
18	Q	166	PRO
22	V	263	GLU
28	e	82	PRO
30	g	82	LYS
28	l	82	PRO
30	n	82	LYS
1	A	779	ALA
1	A	1233	ARG
1	A	1411	ASP
1	A	1491	ILE
1	A	1941	LEU
1	A	1972	ASP
3	C	274	ILE
3	C	365	GLU
3	C	801	TRP
10	J	16	VAL
10	J	203	PRO
10	J	218	VAL
11	K	210	GLU
12	L	122	CYS
13	T	204	GLY
15	N	110	ASP
15	N	205	LEU
16	O	265	HIS
22	V	333	PRO
23	W	641	ALA
23	W	941	ASP
23	W	1062	LYS
33	q	60	ALA
1	A	377	VAL
1	A	1015	PRO

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Mol	Chain	Res	Type
1	A	1165	LEU
1	A	1377	SER
3	C	416	ASP
3	C	440	THR
10	J	419	SER
13	T	146	PHE
13	T	250	PRO
14	M	93	LEU
16	O	393	VAL
20	S	415	GLN
1	A	407	VAL
1	A	644	VAL
3	C	417	PRO
3	C	434	GLY
9	I	151	ILE
26	c	15	PRO
26	j	15	PRO
31	o	52	LYS
33	q	36	GLY
1	A	379	ILE
3	C	831	ILE
23	W	723	GLY
10	J	225	PRO
18	Q	219	ILE
1	A	266	LEU
1	A	696	GLY
1	A	1199	ILE
16	O	277	VAL
15	N	163	VAL
33	r	36	GLY

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	A	1751/2182 (80%)	1715 (98%)	36 (2%)	53 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	794/910 (87%)	785 (99%)	9 (1%)	73	88
7	G	36/165 (22%)	26 (72%)	10 (28%)	0	3
8	H	57/786 (7%)	47 (82%)	10 (18%)	2	12
9	I	219/633 (35%)	218 (100%)	1 (0%)	88	95
10	J	212/525 (40%)	206 (97%)	6 (3%)	43	72
11	K	88/193 (46%)	86 (98%)	2 (2%)	50	76
12	L	141/141 (100%)	139 (99%)	2 (1%)	67	85
13	T	177/413 (43%)	130 (73%)	47 (27%)	0	3
14	M	171/332 (52%)	167 (98%)	4 (2%)	50	76
15	N	224/296 (76%)	220 (98%)	4 (2%)	59	81
16	O	295/397 (74%)	290 (98%)	5 (2%)	60	82
17	P	56/151 (37%)	54 (96%)	2 (4%)	35	67
18	Q	173/328 (53%)	171 (99%)	2 (1%)	71	87
19	R	21/121 (17%)	20 (95%)	1 (5%)	25	60
20	S	192/538 (36%)	190 (99%)	2 (1%)	76	88
21	U	134/225 (60%)	131 (98%)	3 (2%)	52	77
22	V	24/346 (7%)	22 (92%)	2 (8%)	11	42
23	W	613/1029 (60%)	559 (91%)	54 (9%)	10	40
24	a	70/176 (40%)	70 (100%)	0	100	100
24	h	67/176 (38%)	67 (100%)	0	100	100
25	b	65/83 (78%)	60 (92%)	5 (8%)	13	45
25	i	65/83 (78%)	60 (92%)	5 (8%)	13	45
26	c	61/77 (79%)	60 (98%)	1 (2%)	62	83
26	j	61/77 (79%)	60 (98%)	1 (2%)	62	83
27	d	58/66 (88%)	55 (95%)	3 (5%)	23	58
27	k	58/66 (88%)	55 (95%)	3 (5%)	23	58
28	e	69/89 (78%)	67 (97%)	2 (3%)	42	72
28	l	68/89 (76%)	66 (97%)	2 (3%)	42	72
29	f	77/129 (60%)	71 (92%)	6 (8%)	12	44
29	m	77/129 (60%)	71 (92%)	6 (8%)	12	44
30	g	79/103 (77%)	74 (94%)	5 (6%)	18	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	n	59/103 (57%)	55 (93%)	4 (7%)	16	50
31	o	45/219 (20%)	42 (93%)	3 (7%)	16	50
32	p	26/100 (26%)	25 (96%)	1 (4%)	33	66
33	q	63/451 (14%)	56 (89%)	7 (11%)	6	31
33	r	60/451 (13%)	55 (92%)	5 (8%)	11	42
33	s	59/451 (13%)	52 (88%)	7 (12%)	5	27
33	t	62/451 (14%)	54 (87%)	8 (13%)	4	24
All	All	6627/13280 (50%)	6351 (96%)	276 (4%)	33	63

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LEU
1	A	231	ARG
1	A	285	PRO
1	A	419	THR
1	A	514	TYR
1	A	518	VAL
1	A	549	LYS
1	A	622	MET
1	A	643	ASN
1	A	653	ILE
1	A	660	ILE
1	A	716	ARG
1	A	740	GLU
1	A	757	GLU
1	A	842	LYS
1	A	929	LEU
1	A	1094	ASP
1	A	1113	ILE
1	A	1315	ARG
1	A	1326	THR
1	A	1339	LEU
1	A	1342	LEU
1	A	1367	ILE
1	A	1576	GLU
1	A	1579	SER
1	A	1584	SER
1	A	1588	LYS
1	A	1589	LYS

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Mol	Chain	Res	Type
1	A	1591	THR
1	A	1592	HIS
1	A	1595	ARG
1	A	1598	LEU
1	A	1604	ARG
1	A	1629	LEU
1	A	1866	PHE
1	A	1988	LEU
3	C	109	LEU
3	C	163	ASP
3	C	193	LEU
3	C	269	LYS
3	C	415	TYR
3	C	419	PRO
3	C	429	PHE
3	C	497	ASP
3	C	503	ASP
7	G	5	SER
7	G	7	VAL
7	G	13	PRO
7	G	77	PRO
7	G	96	PRO
7	G	100	THR
7	G	105	PRO
7	G	108	SER
7	G	133	PRO
7	G	150	THR
8	H	616	PRO
8	H	617	PRO
8	H	641	PRO
8	H	706	LEU
8	H	712	CYS
8	H	722	PRO
8	H	723	SER
8	H	725	THR
8	H	726	ARG
8	H	733	ILE
9	I	62	ARG
10	J	504	PRO
10	J	505	PRO
10	J	517	VAL
10	J	523	LEU

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Mol	Chain	Res	Type
10	J	532	PRO
10	J	550	PRO
11	K	98	ASP
11	K	145	LYS
12	L	120	CYS
12	L	122	CYS
13	T	51	PHE
13	T	55	GLU
13	T	58	ARG
13	T	61	LYS
13	T	62	THR
13	T	66	ASP
13	T	116	TYR
13	T	126	ARG
13	T	128	TYR
13	T	129	LEU
13	T	131	PRO
13	T	134	ASP
13	T	137	VAL
13	T	139	LEU
13	T	140	ARG
13	T	150	LEU
13	T	152	LYS
13	T	153	LYS
13	T	159	PRO
13	T	198	CYS
13	T	199	LEU
13	T	202	PHE
13	T	228	ARG
13	T	292	HIS
13	T	293	LEU
13	T	303	PRO
13	T	308	PHE
13	T	318	ARG
13	T	320	TRP
13	T	327	PRO
13	T	329	LYS
13	T	337	HIS
13	T	338	SER
13	T	356	MET
13	T	367	PRO
13	T	373	PRO

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Mol	Chain	Res	Type
13	T	374	LYS
13	T	375	LYS
13	T	378	LYS
13	T	380	HIS
13	T	391	PHE
13	T	392	SER
13	T	402	ASP
13	T	411	ASP
13	T	424	PRO
13	T	429	ILE
13	T	441	LYS
14	M	34	CYS
14	M	55	ILE
14	M	73	CYS
14	M	99	VAL
15	N	104	LEU
15	N	146	LEU
15	N	169	ASP
15	N	231	ASP
16	O	182	VAL
16	O	261	THR
16	O	308	LYS
16	O	343	THR
16	O	447	SER
17	P	35	THR
17	P	36	THR
18	Q	43	PHE
18	Q	81	LYS
19	R	24	LEU
20	S	303	LEU
20	S	398	PRO
21	U	81	ILE
21	U	134	GLU
21	U	184	MET
22	V	261	SER
22	V	277	THR
23	W	292	THR
23	W	293	SER
23	W	295	GLU
23	W	301	GLN
23	W	429	GLN
23	W	448	LEU

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Mol	Chain	Res	Type
23	W	475	PRO
23	W	480	ARG
23	W	482	THR
23	W	489	ARG
23	W	502	LEU
23	W	507	GLU
23	W	513	THR
23	W	517	THR
23	W	521	ASP
23	W	555	LYS
23	W	556	VAL
23	W	559	ASP
23	W	587	GLU
23	W	596	LYS
23	W	598	SER
23	W	613	ASP
23	W	649	ASN
23	W	699	THR
23	W	716	LYS
23	W	740	SER
23	W	742	ILE
23	W	758	ASN
23	W	765	THR
23	W	767	ASP
23	W	811	ARG
23	W	812	THR
23	W	821	TYR
23	W	826	PHE
23	W	835	VAL
23	W	845	HIS
23	W	864	MET
23	W	870	ASN
23	W	883	GLN
23	W	894	LEU
23	W	913	SER
23	W	980	CYS
23	W	1006	LYS
23	W	1010	LYS
23	W	1040	VAL
23	W	1062	LYS
23	W	1065	GLU
23	W	1077	ARG

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Mol	Chain	Res	Type
23	W	1081	SER
23	W	1082	GLN
23	W	1085	SER
23	W	1087	GLU
23	W	1099	TYR
23	W	1100	LYS
25	b	16	CYS
25	b	18	PHE
25	b	25	THR
25	b	79	LYS
25	b	81	LEU
26	c	79	LEU
27	d	18	ASN
27	d	41	ASP
27	d	71	LEU
28	e	10	LEU
28	e	76	ASP
29	f	20	LYS
29	f	26	TRP
29	f	30	GLN
29	f	77	ASP
29	f	99	ASP
29	f	104	ASP
30	g	24	PHE
30	g	49	ARG
30	g	77	THR
30	g	99	ASP
30	g	100	SER
25	i	16	CYS
25	i	18	PHE
25	i	25	THR
25	i	79	LYS
25	i	81	LEU
26	j	79	LEU
27	k	18	ASN
27	k	41	ASP
27	k	71	LEU
28	l	10	LEU
28	l	76	ASP
29	m	20	LYS
29	m	26	TRP
29	m	30	GLN

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Mol	Chain	Res	Type
29	m	77	ASP
29	m	99	ASP
29	m	104	ASP
30	n	49	ARG
30	n	77	THR
30	n	99	ASP
30	n	100	SER
31	o	4	THR
31	o	44	PRO
31	o	71	SER
32	p	38	LYS
33	q	17	PRO
33	q	44	PRO
33	q	55	PRO
33	q	56	SER
33	q	61	SER
33	q	102	LEU
33	q	126	LEU
33	r	17	PRO
33	r	44	PRO
33	r	63	THR
33	r	93	LEU
33	r	99	ARG
33	s	17	PRO
33	s	26	SER
33	s	44	PRO
33	s	63	THR
33	s	96	PHE
33	s	109	LEU
33	s	134	SER
33	t	17	PRO
33	t	44	PRO
33	t	63	THR
33	t	80	LEU
33	t	85	GLN
33	t	93	LEU
33	t	99	ARG
33	t	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	265	ASN
1	A	405	ASN
1	A	429	ASN
1	A	541	ASN
1	A	558	GLN
1	A	658	ASN
1	A	659	HIS
1	A	685	HIS
1	A	705	GLN
1	A	784	GLN
1	A	785	HIS
1	A	796	ASN
1	A	861	GLN
1	A	864	GLN
1	A	976	GLN
1	A	1005	GLN
1	A	1011	ASN
1	A	1097	HIS
1	A	1156	HIS
1	A	1202	ASN
1	A	1281	ASN
1	A	1376	ASN
1	A	1500	HIS
1	A	1529	ASN
1	A	1532	HIS
1	A	1592	HIS
1	A	1594	GLN
1	A	1603	ASN
1	A	1626	GLN
1	A	1782	ASN
1	A	1827	GLN
1	A	1856	ASN
1	A	1888	HIS
1	A	1985	GLN
1	A	2018	ASN
3	C	82	ASN
3	C	84	GLN
3	C	101	GLN
3	C	143	HIS
3	C	158	HIS
3	C	183	GLN
3	C	251	GLN

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Mol	Chain	Res	Type
3	C	289	ASN
3	C	310	ASN
3	C	764	ASN
3	C	776	ASN
3	C	794	GLN
3	C	830	ASN
3	C	869	HIS
9	I	67	GLN
9	I	79	HIS
10	J	31	HIS
10	J	72	GLN
10	J	214	ASN
11	K	202	GLN
13	T	161	HIS
13	T	292	HIS
13	T	337	HIS
13	T	358	ASN
13	T	380	HIS
14	M	72	GLN
14	M	209	ASN
15	N	91	HIS
15	N	202	GLN
15	N	227	ASN
15	N	252	HIS
16	O	181	HIS
16	O	223	HIS
16	O	265	HIS
16	O	382	HIS
16	O	428	GLN
16	O	445	ASN
17	P	5	HIS
17	P	173	HIS
18	Q	37	ASN
18	Q	87	ASN
18	Q	171	ASN
19	R	4	ASN
20	S	354	HIS
20	S	457	HIS
21	U	87	GLN
21	U	169	HIS
21	U	171	GLN
23	W	606	HIS

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Mol	Chain	Res	Type
23	W	701	GLN
23	W	989	HIS
25	b	34	GLN
25	b	86	ASN
27	d	66	ASN
28	e	41	ASN
29	f	30	GLN
25	i	34	GLN
25	i	86	ASN
26	j	52	GLN
27	k	66	ASN
28	l	41	ASN
29	m	30	GLN
30	n	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	114/214 (53%)	27 (23%)	3 (2%)
4	D	102/112 (91%)	31 (30%)	5 (4%)
5	E	57/369 (15%)	34 (59%)	6 (10%)
6	F	88/1175 (7%)	30 (34%)	8 (9%)
All	All	361/1870 (19%)	122 (33%)	22 (6%)

All (122) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	32	G
2	B	33	U
2	B	42	A
2	B	44	A
2	B	74	U
2	B	75	A
2	B	76	U
2	B	77	A
2	B	79	C
2	B	80	G
2	B	81	A
2	B	82	A
2	B	84	A
2	B	90	C

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Mol	Chain	Res	Type
2	B	94	C
2	B	101	C
2	B	104	G
2	B	127	U
2	B	164	C
2	B	165	A
2	B	166	U
2	B	170	U
2	B	171	U
2	B	172	U
2	B	173	U
2	B	174	G
2	B	175	G
4	D	12	A
4	D	13	A
4	D	14	C
4	D	15	C
4	D	16	C
4	D	33	C
4	D	34	A
4	D	36	U
4	D	39	G
4	D	43	C
4	D	49	A
4	D	50	G
4	D	51	A
4	D	54	U
4	D	57	U
4	D	60	G
4	D	62	A
4	D	65	U
4	D	66	C
4	D	67	C
4	D	68	C
4	D	73	A
4	D	74	U
4	D	80	U
4	D	85	C
4	D	86	G
4	D	87	U
4	D	90	U
4	D	91	A

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Mol	Chain	Res	Type
4	D	92	C
4	D	93	A
5	E	-12	U
5	E	-11	A
5	E	-10	A
5	E	-7	U
5	E	-6	U
5	E	-2	A
5	E	2	U
5	E	3	A
5	E	9	U
5	E	10	U
5	E	11	A
5	E	13	U
5	E	284	U
5	E	285	U
5	E	286	A
5	E	287	A
5	E	292	U
5	E	294	G
5	E	295	A
5	E	296	U
5	E	297	A
5	E	300	A
5	E	301	A
5	E	302	C
5	E	303	A
5	E	304	C
5	E	346	A
5	E	347	A
5	E	348	U
5	E	349	A
5	E	350	G
5	E	353	A
5	E	354	A
5	E	355	U
6	F	15	C
6	F	16	U
6	F	17	U
6	F	19	U
6	F	23	U
6	F	25	A

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Mol	Chain	Res	Type
6	F	26	G
6	F	30	A
6	F	31	A
6	F	32	G
6	F	34	G
6	F	40	U
6	F	41	C
6	F	42	U
6	F	49	U
6	F	50	U
6	F	111	C
6	F	115	U
6	F	116	U
6	F	117	U
6	F	118	U
6	F	119	G
6	F	120	G
6	F	1099	G
6	F	1107	C
6	F	1108	A
6	F	1111	U
6	F	1112	G
6	F	1114	G
6	F	1120	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	78	A
2	B	83	C
2	B	172	U
4	D	14	C
4	D	42	A
4	D	53	A
4	D	56	A
4	D	64	U
5	E	9	U
5	E	283	U
5	E	294	G
5	E	299	U
5	E	301	A
5	E	352	A

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Mol	Chain	Res	Type
6	F	29	C
6	F	30	A
6	F	31	A
6	F	40	U
6	F	41	C
6	F	117	U
6	F	1107	C
6	F	1111	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](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	IHP	A	3000	-	36,36,36	0.70	0	54,60,60	0.96	0
35	GTP	C	1500	36	26,34,34	1.35	3 (11%)	32,54,54	2.46	12 (37%)

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	IHP	A	3000	-	-	15/30/54/54	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	GTP	C	1500	36	-	5/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	1500	GTP	C6-N1	-3.52	1.32	1.37
35	C	1500	GTP	PB-O1B	-2.77	1.41	1.50
35	C	1500	GTP	C4-N3	-2.35	1.31	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	1500	GTP	PB-O3B-PG	-6.13	111.78	132.83
35	C	1500	GTP	PA-O3A-PB	-5.30	114.65	132.83
35	C	1500	GTP	O6-C6-N1	4.93	126.47	120.65
35	C	1500	GTP	O6-C6-C5	-4.54	115.51	124.37
35	C	1500	GTP	O4'-C1'-C2'	3.61	112.19	106.93
35	C	1500	GTP	O4'-C4'-C3'	3.42	111.88	105.11
35	C	1500	GTP	C2-N1-C6	-2.57	120.36	125.10
35	C	1500	GTP	O2A-PA-O1A	2.48	124.48	112.24
35	C	1500	GTP	O3B-PG-O1G	-2.41	97.84	111.19
35	C	1500	GTP	C5-C6-N1	2.30	118.02	113.95
35	C	1500	GTP	C8-N7-C5	2.21	107.20	102.99
35	C	1500	GTP	PA-O5'-C5'	-2.01	109.89	121.68

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	3000	IHP	C1-C6-O16-P6
34	A	3000	IHP	C5-C6-O16-P6
34	A	3000	IHP	C2-O12-P2-O22
34	A	3000	IHP	C3-O13-P3-O43
35	C	1500	GTP	C5'-O5'-PA-O3A
35	C	1500	GTP	C5'-O5'-PA-O1A
35	C	1500	GTP	O4'-C4'-C5'-O5'
35	C	1500	GTP	C3'-C4'-C5'-O5'
34	A	3000	IHP	C4-O14-P4-O24
34	A	3000	IHP	C4-C5-O15-P5
34	A	3000	IHP	C6-C5-O15-P5
35	C	1500	GTP	C5'-O5'-PA-O2A

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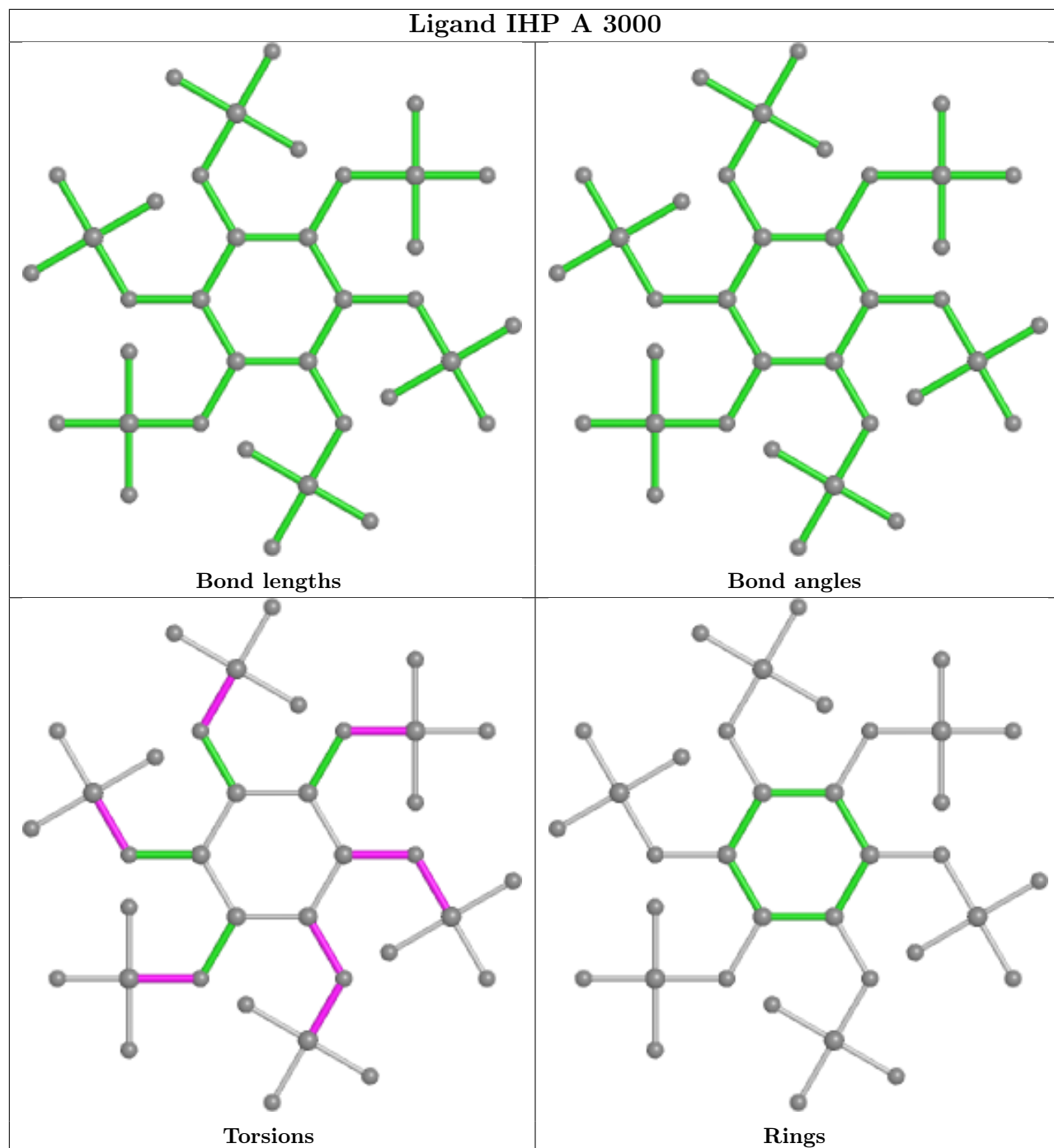
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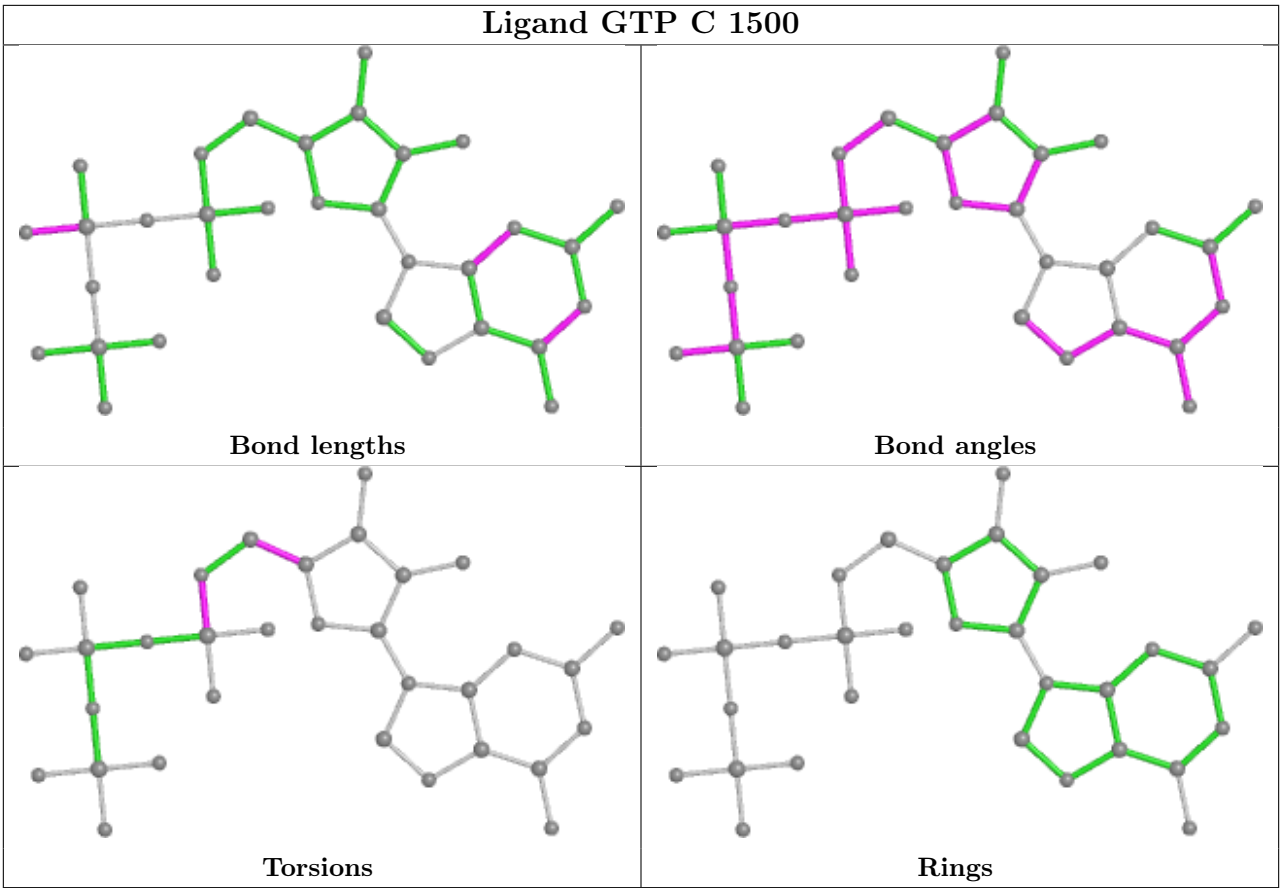
Mol	Chain	Res	Type	Atoms
34	A	3000	IHP	C1-O11-P1-O21
34	A	3000	IHP	C5-O15-P5-O25
34	A	3000	IHP	C6-O16-P6-O26
34	A	3000	IHP	C1-O11-P1-O31
34	A	3000	IHP	C3-O13-P3-O33
34	A	3000	IHP	C4-O14-P4-O44
34	A	3000	IHP	C6-O16-P6-O36
34	A	3000	IHP	C6-O16-P6-O46

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	350:G	O3'	351:U	P	3.39

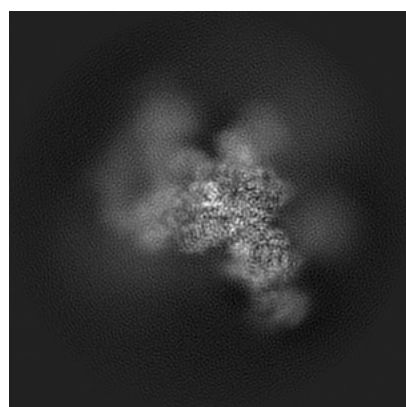
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6839. These allow visual inspection of the internal detail of the map and identification of artifacts.

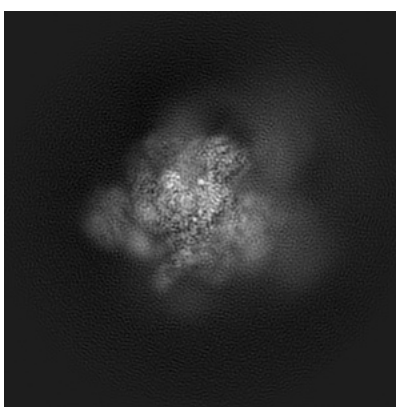
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

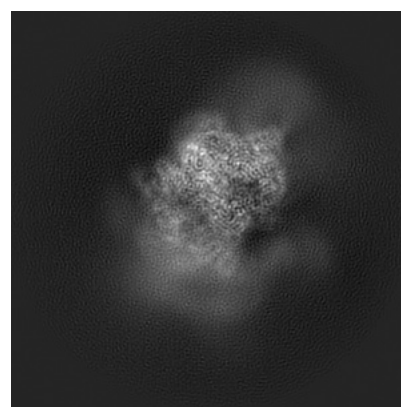
6.1.1 Primary map



X



Y

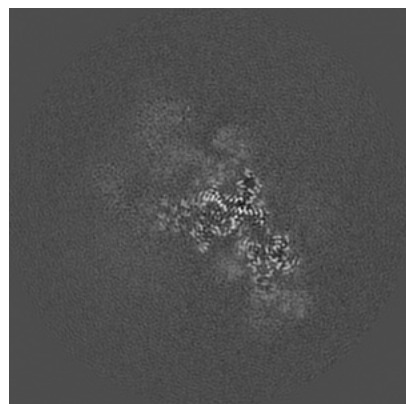


Z

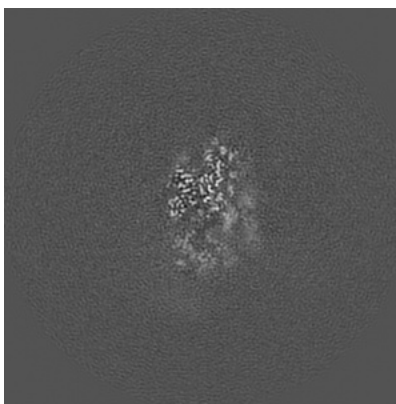
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

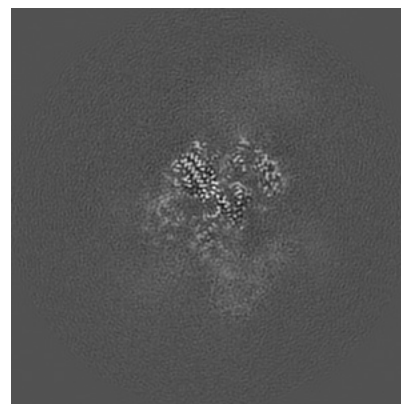
6.2.1 Primary map



X Index: 200



Y Index: 200

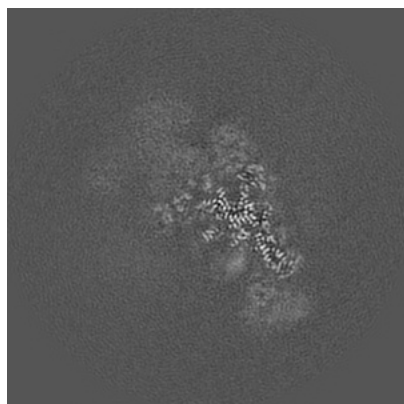


Z Index: 200

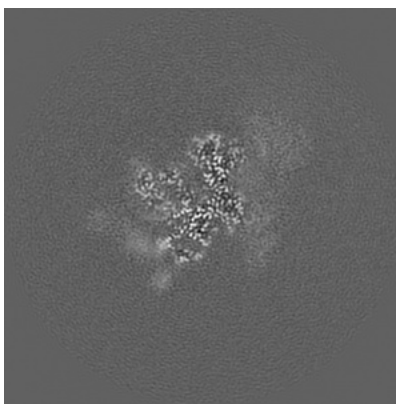
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

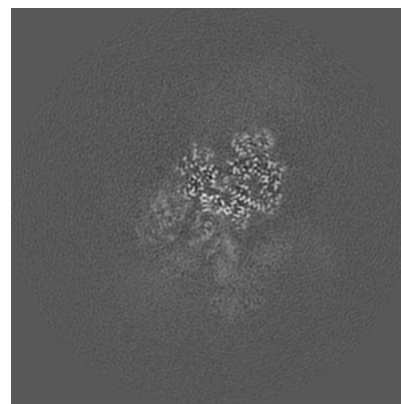
6.3.1 Primary map



X Index: 192



Y Index: 238



Z Index: 206

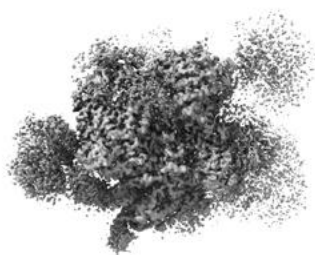
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

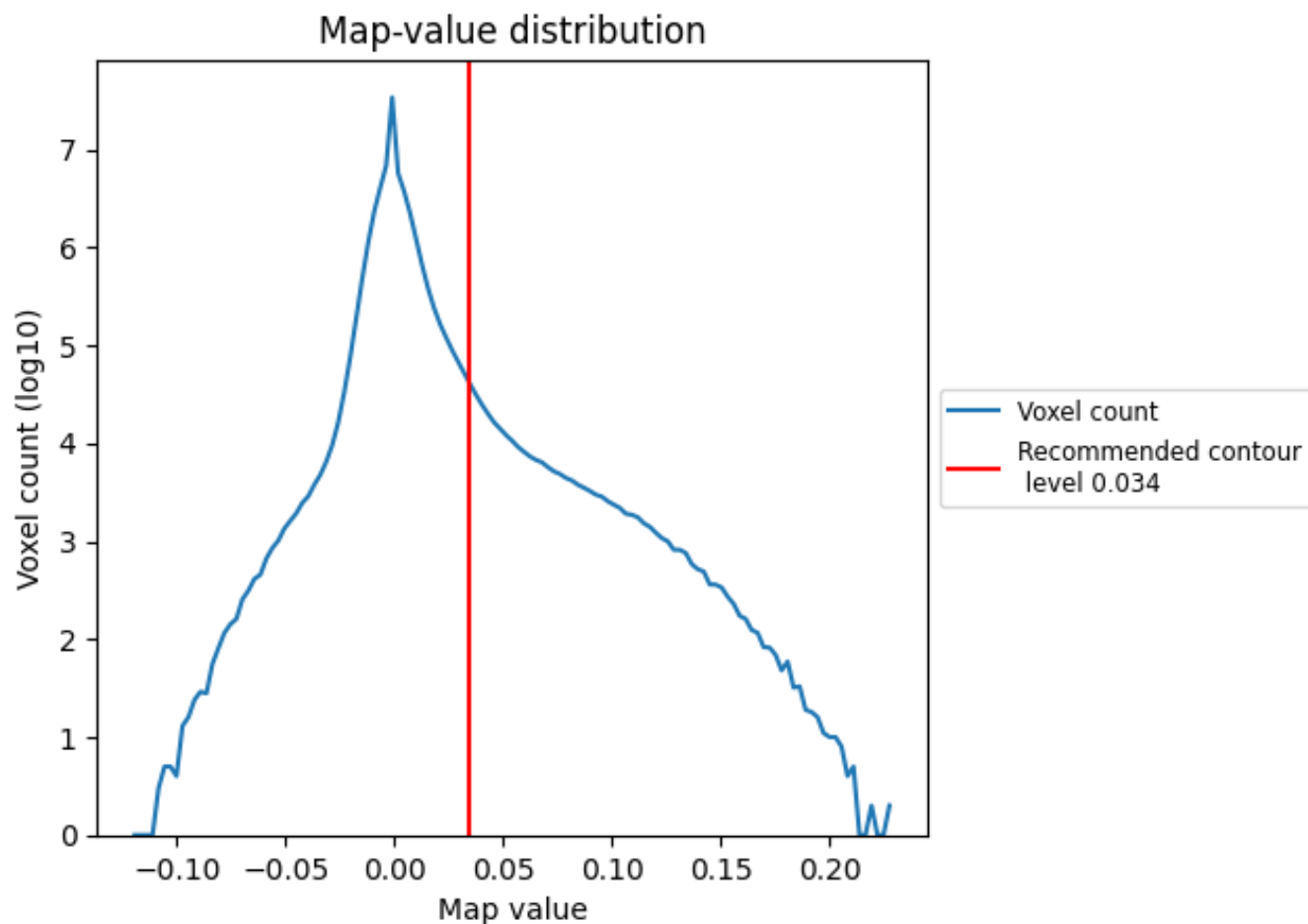
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

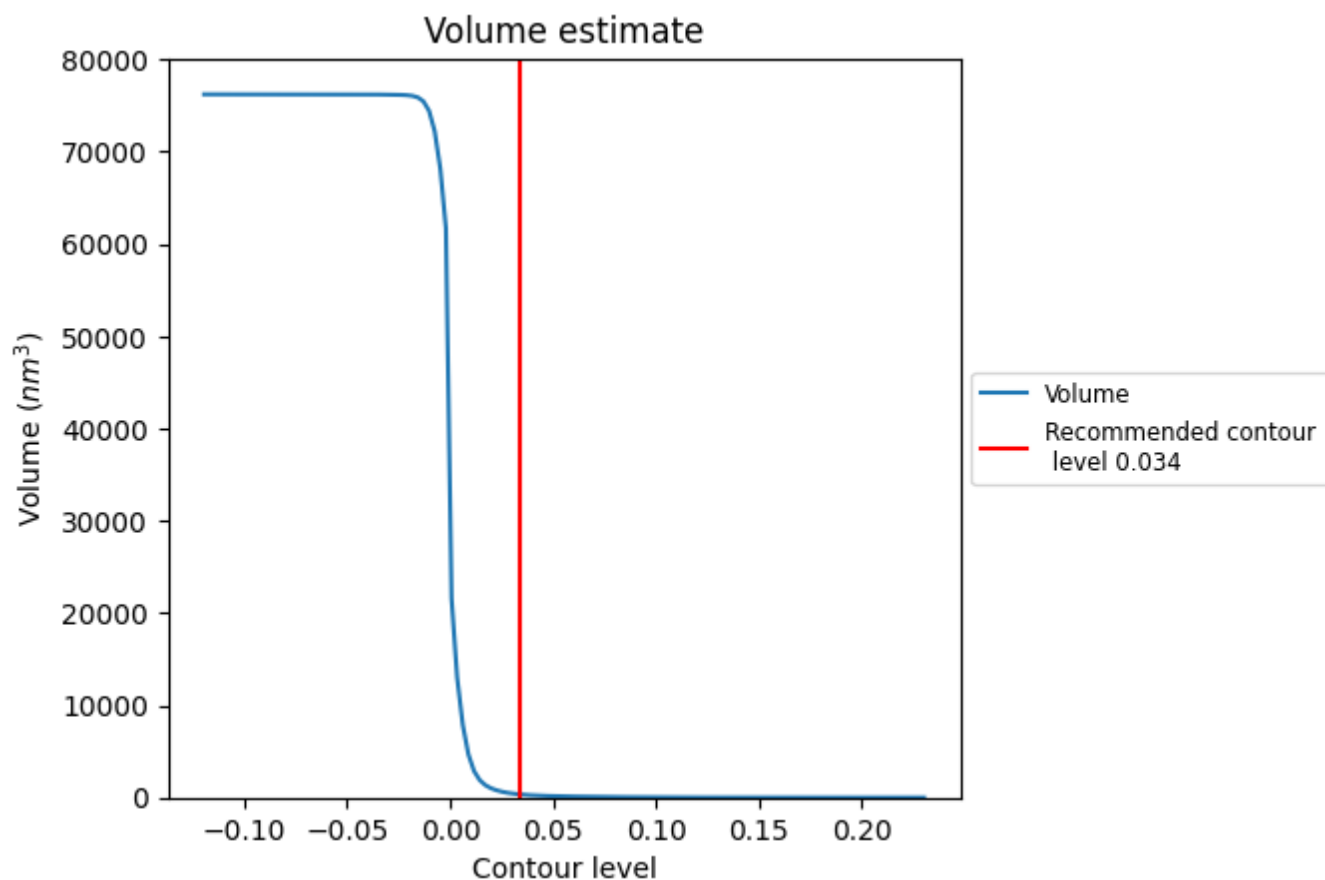
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

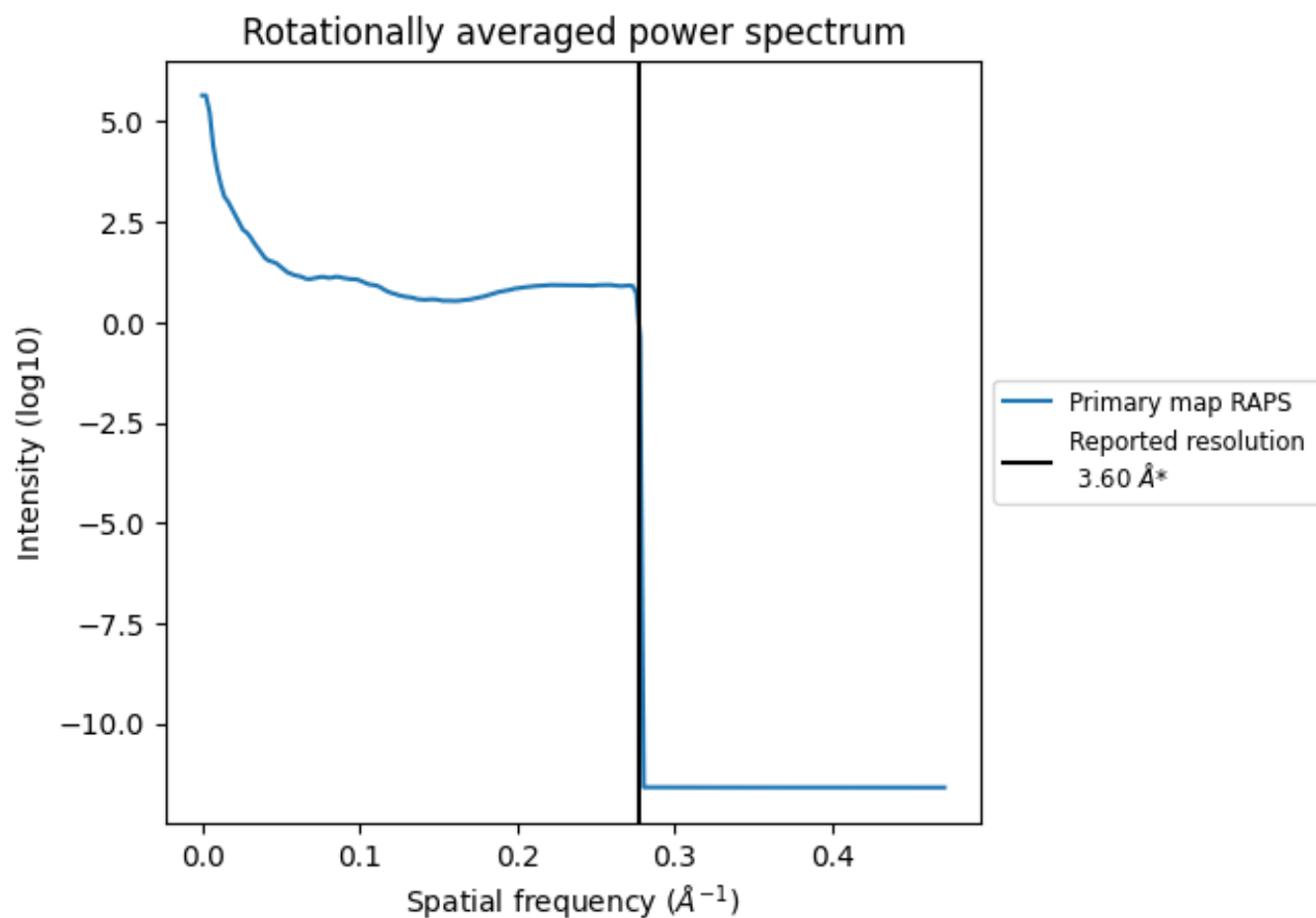
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 343 nm³; this corresponds to an approximate mass of 309 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

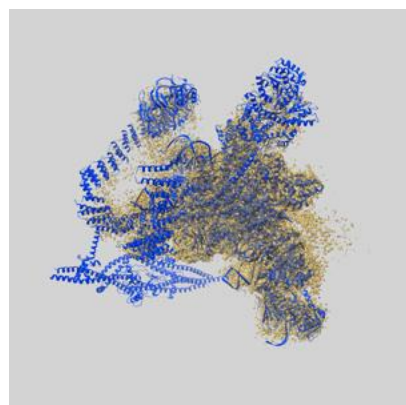
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

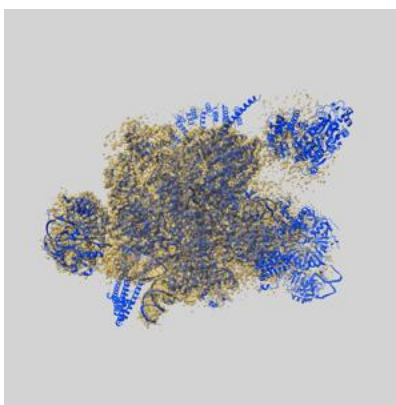
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6839 and PDB model 5YLZ. Per-residue inclusion information can be found in section 3 on page 12.

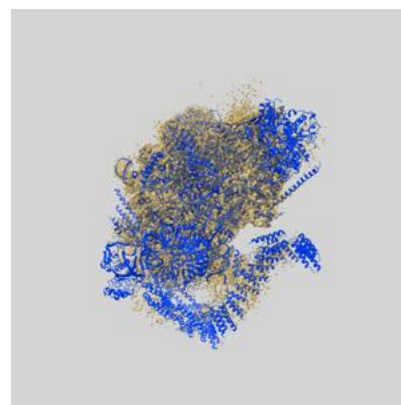
9.1 Map-model overlay [i](#)



X



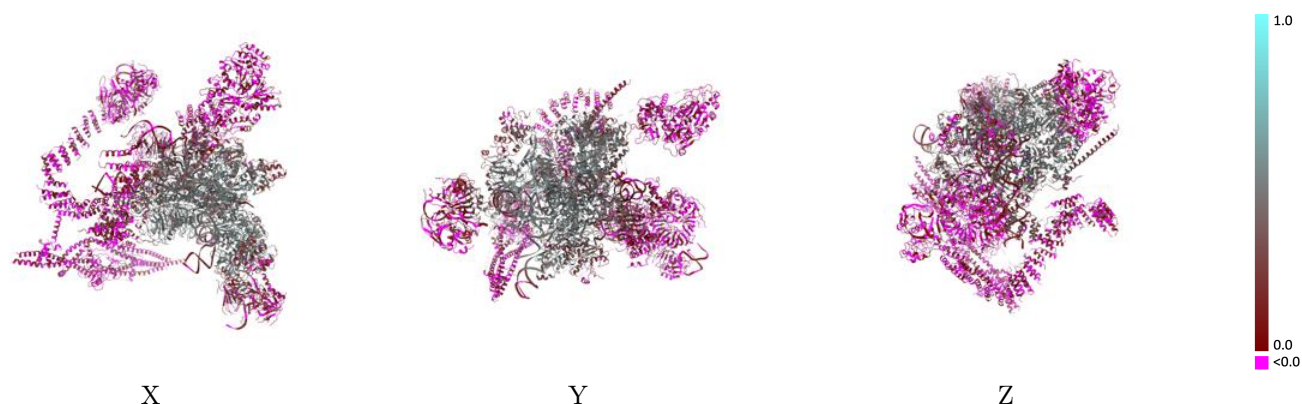
Y



Z

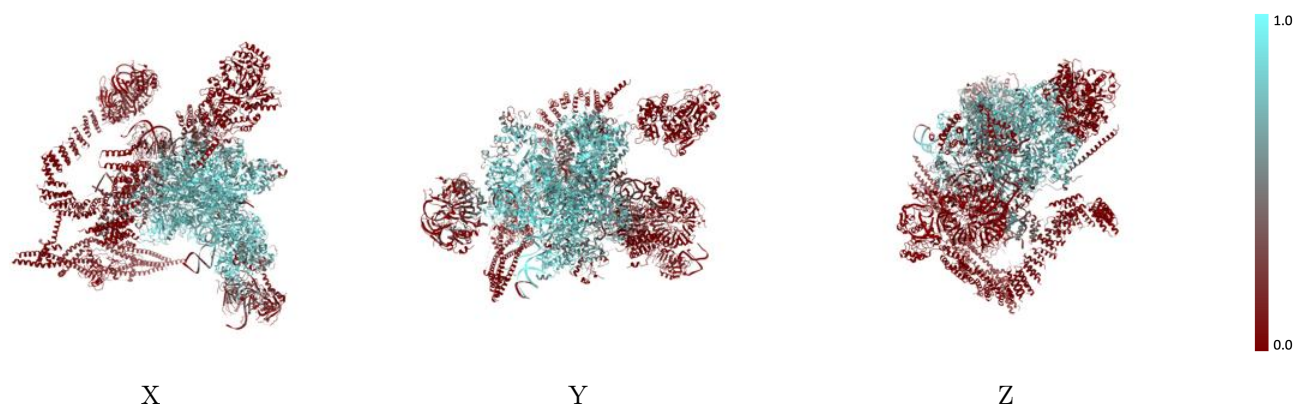
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



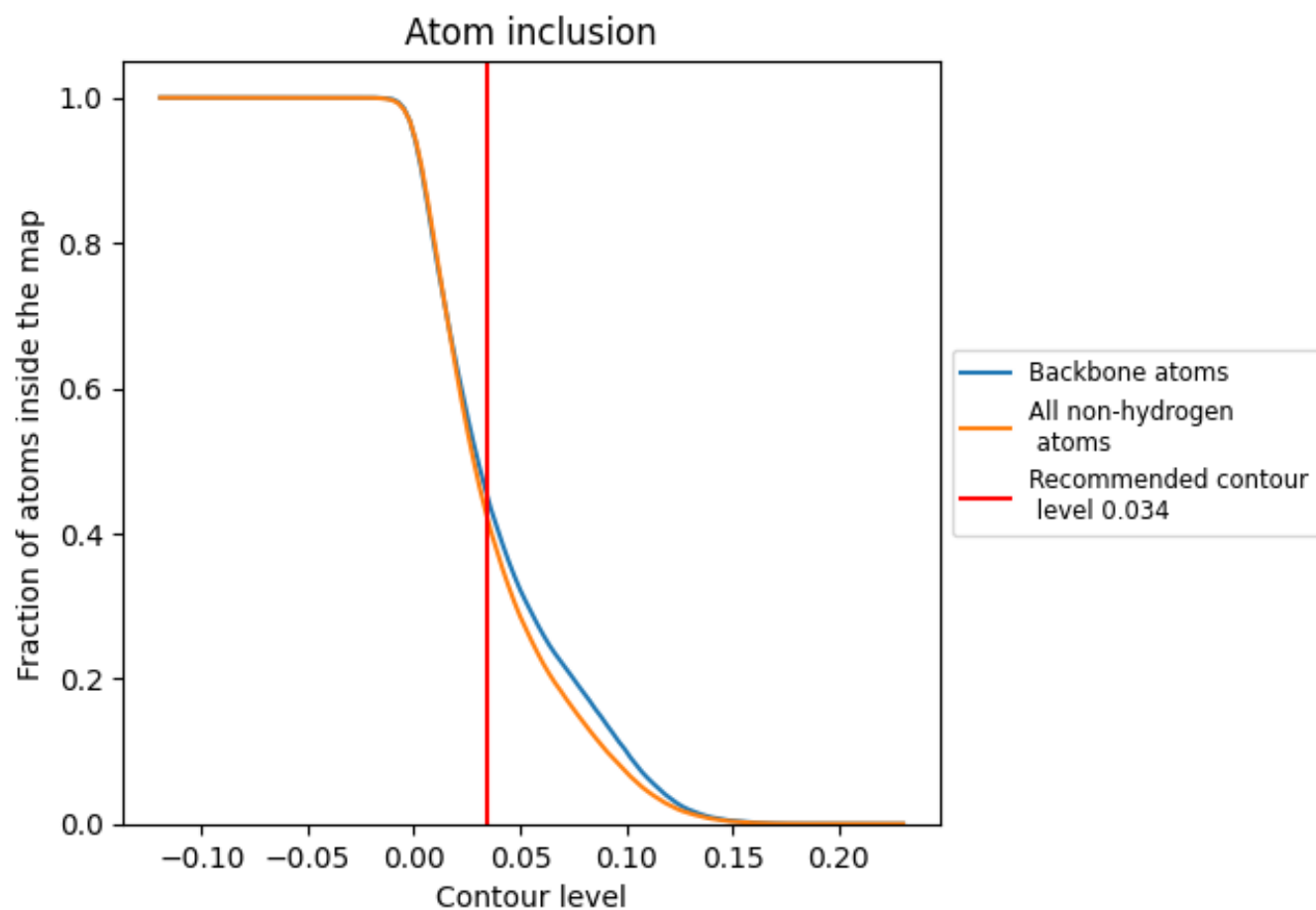
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



















The table lists the average atom inclusion at the recommended contour level (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4272	 0.2510
A	 0.7290	 0.4270
B	 0.7079	 0.3360
C	 0.7331	 0.4230
D	 0.7560	 0.3550
E	 0.4947	 0.2470
F	 0.2525	 0.1240
G	 0.0000	 0.0080
H	 0.0190	 0.0080
I	 0.3308	 0.2120
J	 0.3032	 0.1980
K	 0.3325	 0.2530
L	 0.7893	 0.4380
M	 0.4135	 0.3100
N	 0.5739	 0.3440
O	 0.8106	 0.4820
P	 0.6784	 0.4730
Q	 0.4653	 0.3650
R	 0.5401	 0.4360
S	 0.6812	 0.3860
T	 0.1841	 0.1280
U	 0.0204	 0.0470
V	 0.0238	 0.0620
W	 0.0314	 0.0290
a	 0.2707	 0.1470
b	 0.1136	 0.0690
c	 0.1160	 0.0480
d	 0.1862	 0.1130
e	 0.4256	 0.2570
f	 0.2311	 0.0990
g	 0.1257	 0.0380
h	 0.0067	 0.0070
i	 0.0052	 -0.0350
j	 0.0129	 -0.0110
k	 0.0038	 -0.0070



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Chain	Atom inclusion	Q-score
l	 0.0049	 0.0330
m	 0.0267	 -0.0240
n	 0.0194	 0.0030
o	 0.0024	 0.0180
p	 0.0000	 0.0110
q	 0.0000	 -0.0150
r	 0.0000	 0.0230
s	 0.0000	 -0.0180
t	 0.0000	 0.0140