



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 10:44 AM JST

PDB ID : 5GMK
EMDB ID : EMD-9525
Title : Cryo-EM structure of the Catalytic Step I spliceosome (C complex) at 3.4 angstrom resolution
Authors : Wan, R.; Yan, C.; Bai, R.; Huang, G.; Shi, Y.
Deposited on : 2016-07-14
Resolution : 3.40 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:

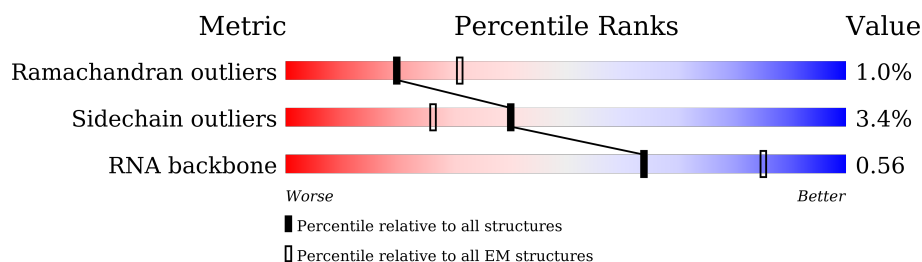
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	
2	C	1008	
3	D	214	
4	E	112	
5	L	1175	
6	M	29	
7	B	13	
8	N	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	135	
10	O	451	
11	P	379	
12	Q	364	
13	R	339	
14	S	175	
15	T	157	
16	Z	577	
17	c	587	
18	d	687	
19	F	278	
20	G	179	
21	H	235	
22	I	215	
23	v	859	
24	n	455	
25	o	503	
25	p	503	
25	q	503	
25	r	503	
26	t	175	
27	k	196	
27	s	196	
28	i	94	
28	u	94	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	h	86	<div>81%</div> <div>78% 19%</div>
29	w	86	<div>81%</div> <div>78% 19%</div>
30	j	77	<div>88%</div> <div>86% 10%</div>
30	x	77	<div>90%</div> <div>86% 10%</div>
31	l	101	<div>60%</div> <div>77% 19%</div>
31	y	101	<div>81%</div> <div>77% 19%</div>
32	m	146	<div>56%</div> <div>52% 44%</div>
32	z	146	<div>56%</div> <div>52% 44%</div>
33	e	110	<div>59%</div> <div>54% 41%</div>
33	g	110	<div>85%</div> <div>79% 5% 15%</div>
34	a	111	<div>73%</div> <div>68% 5% 27%</div>
35	b	238	<div>57%</div> <div>48% 7% 43%</div>

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 75273 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	1910	Total	C	N	O	S	0	0
			15775	10142	2709	2867	57		

- Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

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

- Molecule 3 is a RNA chain called U5 snRNA.

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

- Molecule 4 is a RNA chain called U6 snRNA.

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

- Molecule 5 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	127	Total	C	N	O	P	0	0
			2673	1197	445	904	127		

- Molecule 6 is a RNA chain called Intron_BPS.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	29	Total	C	N	O	P	0	0
			608	274	101	204	29		

- Molecule 7 is a RNA chain called 5'-Exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	13	Total	C	N	O	P	0	0
			275	124	47	91	13		

- Molecule 8 is a RNA chain called 5'-Splicing Site.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	15	Total	C	N	O	P	0	0
			312	140	45	112	15		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC21.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor PRP46.

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

- Molecule 11 is a protein called Pre-mRNA-processing protein 45.

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

- Molecule 12 is a protein called Pre-mRNA-splicing factor SLT11.

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

- Molecule 13 is a protein called Pre-mRNA-splicing factor CWC2.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC15.

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

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

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	447	Total	C	N	O	S	0	0
			3651	2343	602	688	18		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	436	Total	C	N	O	S	0	0
			2971	1841	549	573	8		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	549	Total	C	N	O	S	0	0
			3590	2232	675	675	8		

- Molecule 19 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	115	Total	C	N	O	S	0	0
			937	592	167	169	9		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	41	Total	C	N	O	S	0	0
			342	215	63	63	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	95	Total	C	N	O	S	0	0
			810	506	152	151	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	673	Total	C	N	O	S	0	0
			3580	2190	683	706	1		

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	n	299	Total	C	N	O	S	0	0
			1890	1175	340	369	6		

- Molecule 25 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	o	126	Total	C	N	O	S	0	0
			830	525	134	169	2		
25	p	128	Total	C	N	O	S	0	0
			843	532	136	173	2		
25	q	387	Total	C	N	O	S	0	0
			2345	1471	402	464	8		
25	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SNT309.

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

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
27	s	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein E.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	70	Total	C	N	O	S	0	0
			554	355	98	100	1		
29	w	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
30	x	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	l	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	y	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

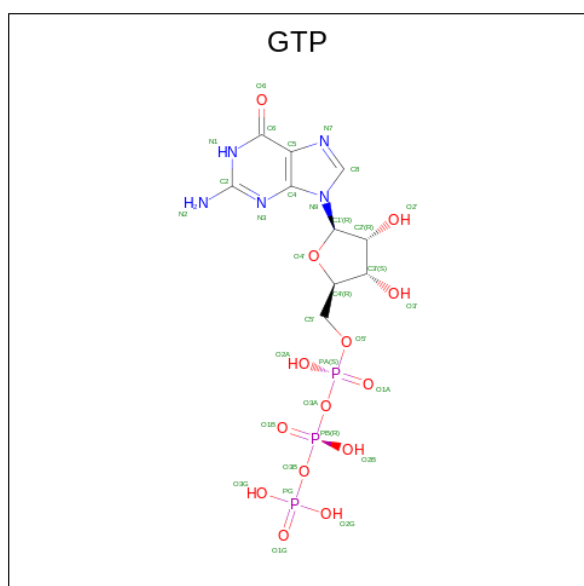
- Molecule 34 is a protein called U2 small nuclear ribonucleoprotein B''.

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

- Molecule 35 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	
37	E	5	Total	Mg	0
			5	5	

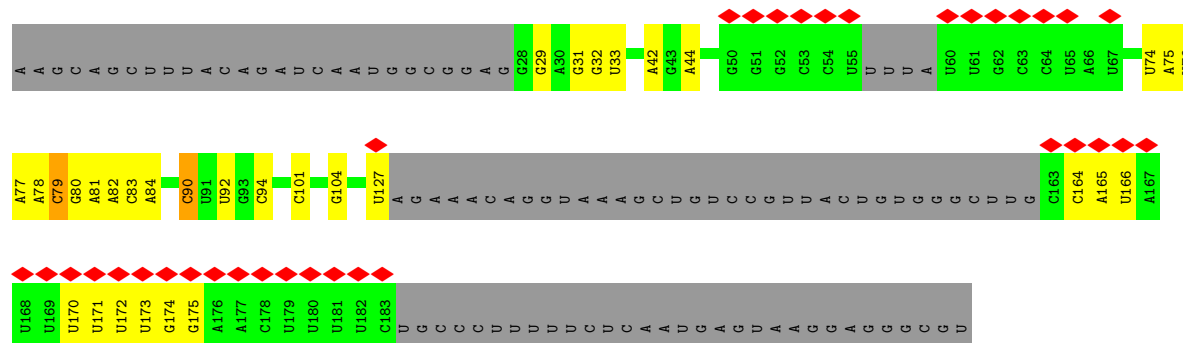
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	Q	2	Total	Zn	0
			2	2	
38	R	1	Total	Zn	0
			1	1	
38	T	3	Total	Zn	0
			3	3	
38	F	1	Total	Zn	0
			1	1	

GLU
LYS
TYR
ILE
SER
ALA
GLU
LEU
TYR
GLN
ALA
LEU
ARG
GLU
ASN
GLY
LEU
VAL
PRO

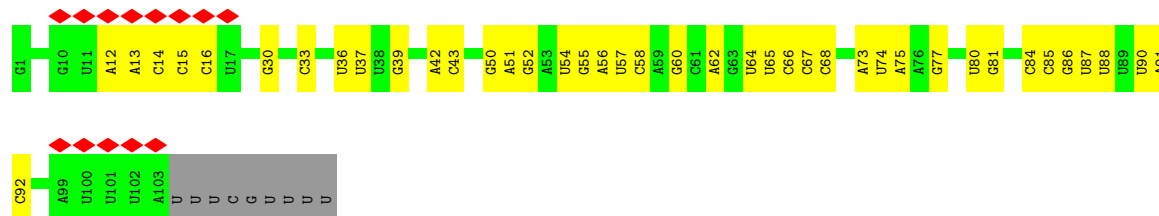
• Molecule 3: U5 snRNA

Chain D: 16% 40% 14% 45%



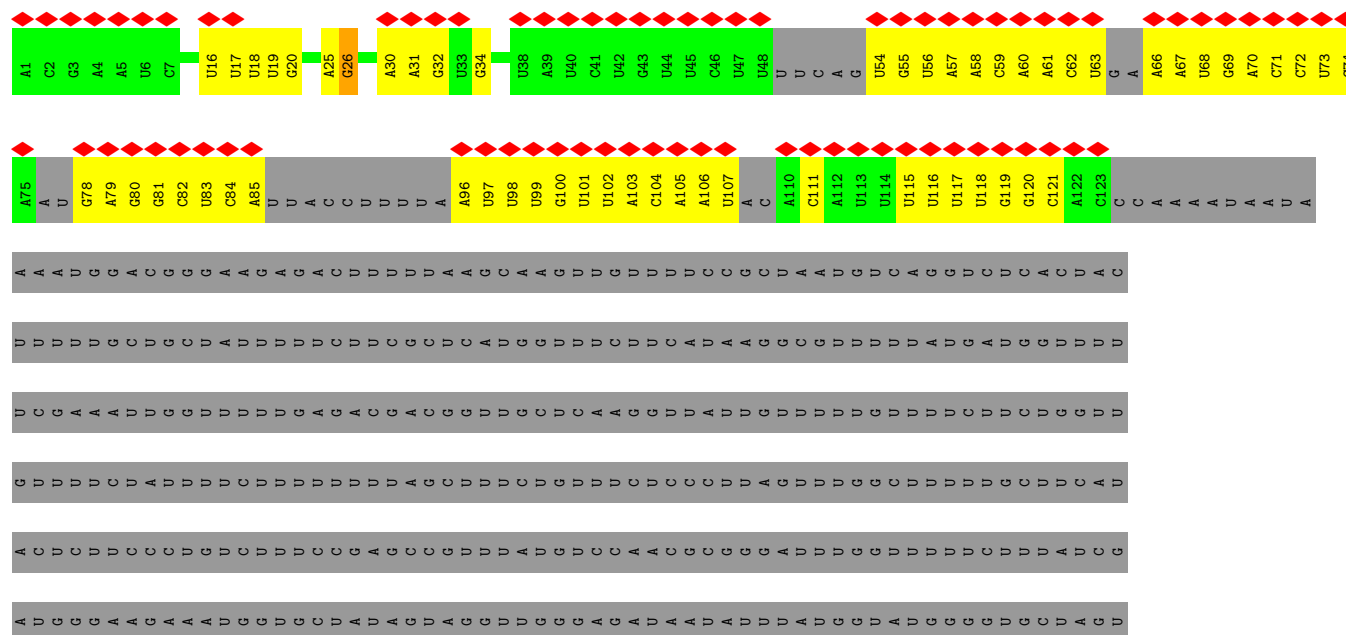
• Molecule 4: U6 snRNA

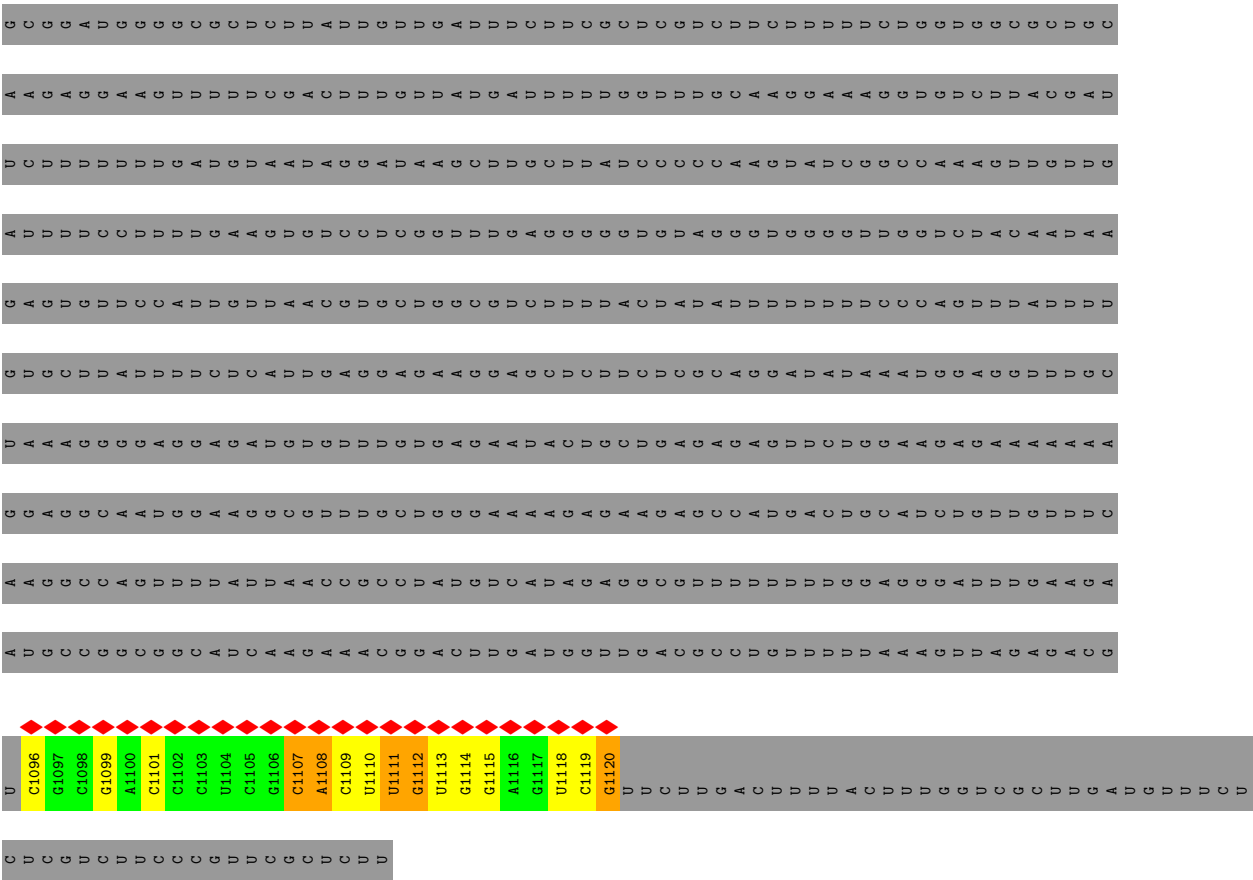
Chain E: 12% 55% 37% 8%



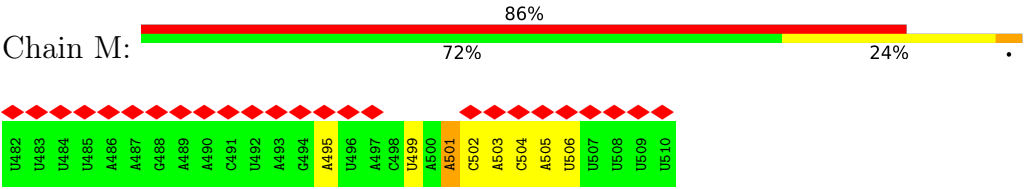
• Molecule 5: U2 snRNA

Chain L: 9% 5% 6% 89%





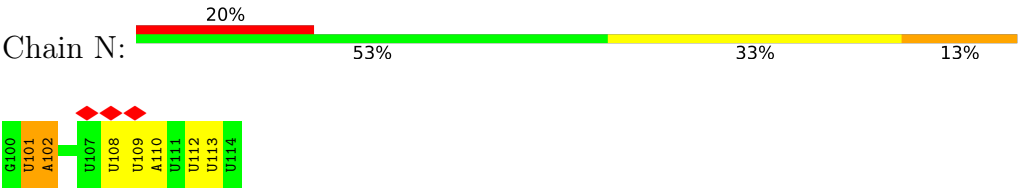
• Molecule 6: Intron_BPS



• Molecule 7: 5'-Exon

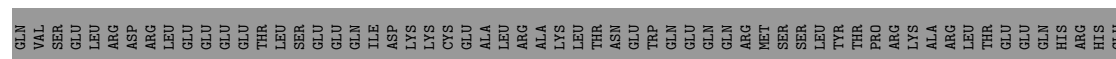


• Molecule 8: 5'-Splicing Site

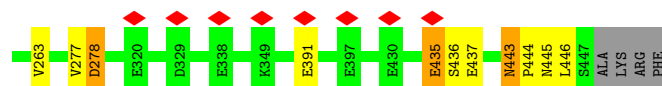
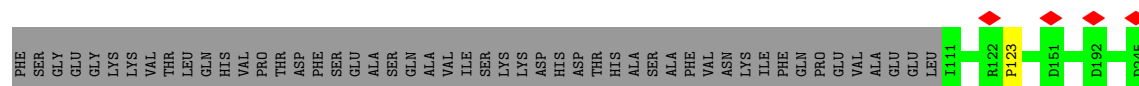
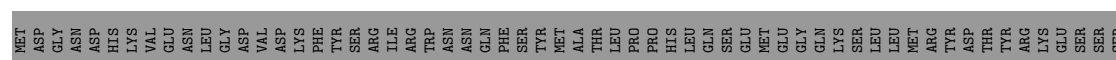


• Molecule 9: Pre-mRNA-splicing factor CWC21

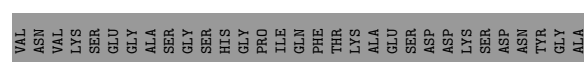
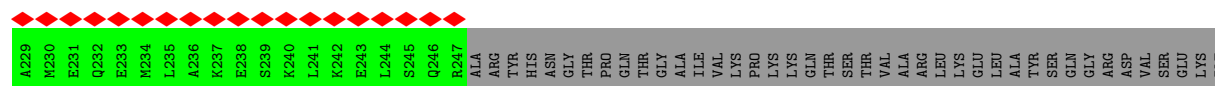
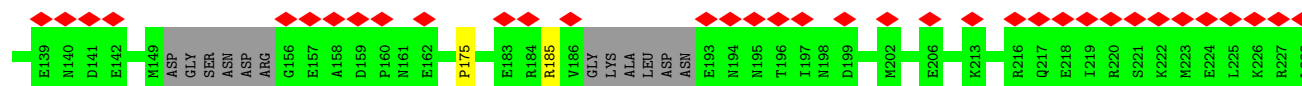
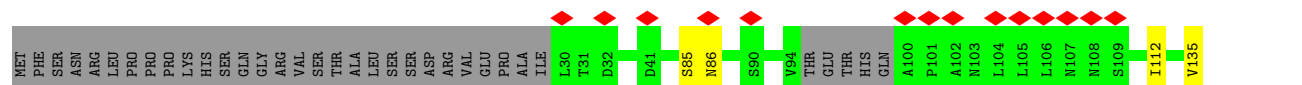
Chain J:



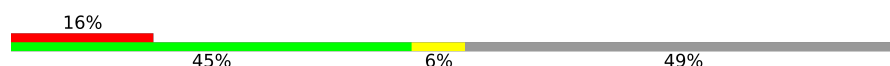
Chain O:



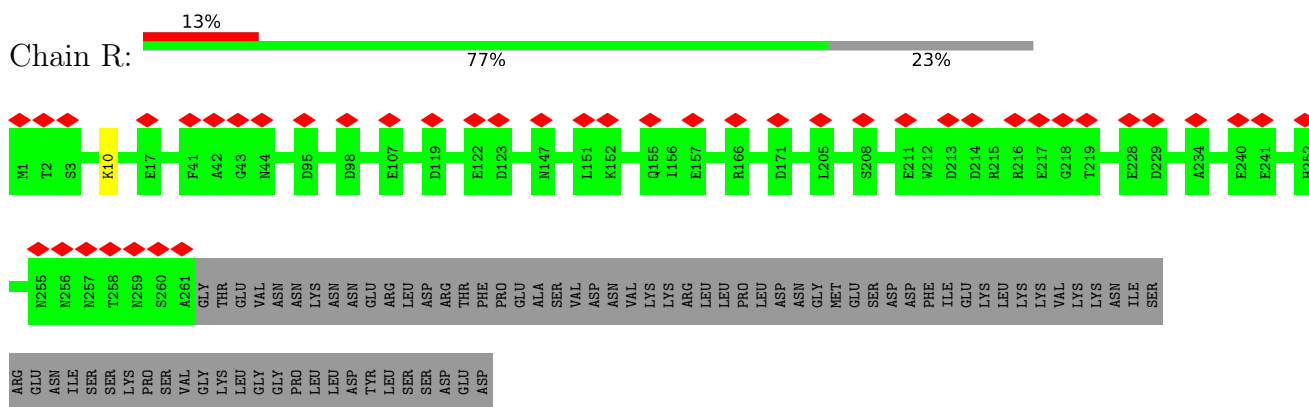
Chain P:



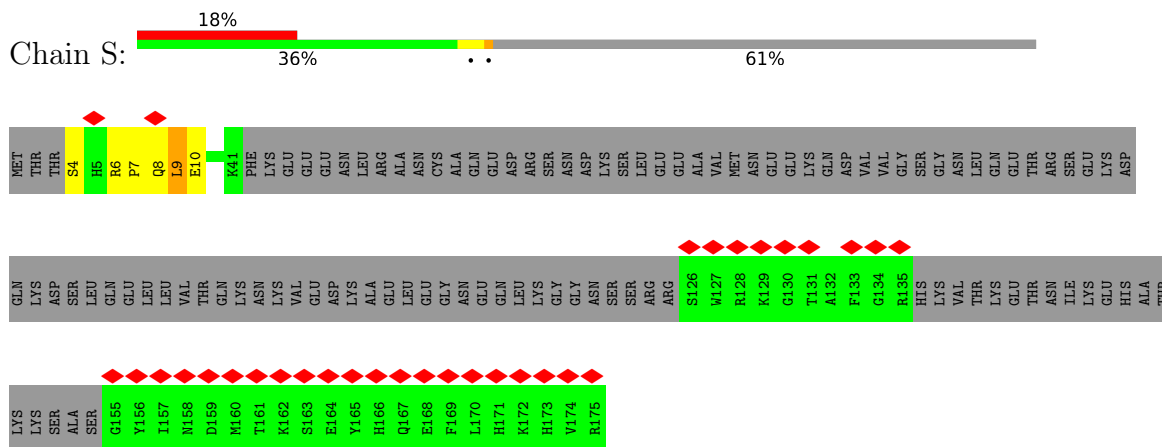
Chain Q:



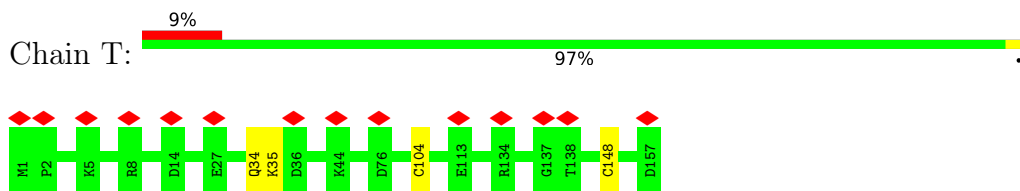
- Molecule 13: Pre-mRNA-splicing factor CWC2



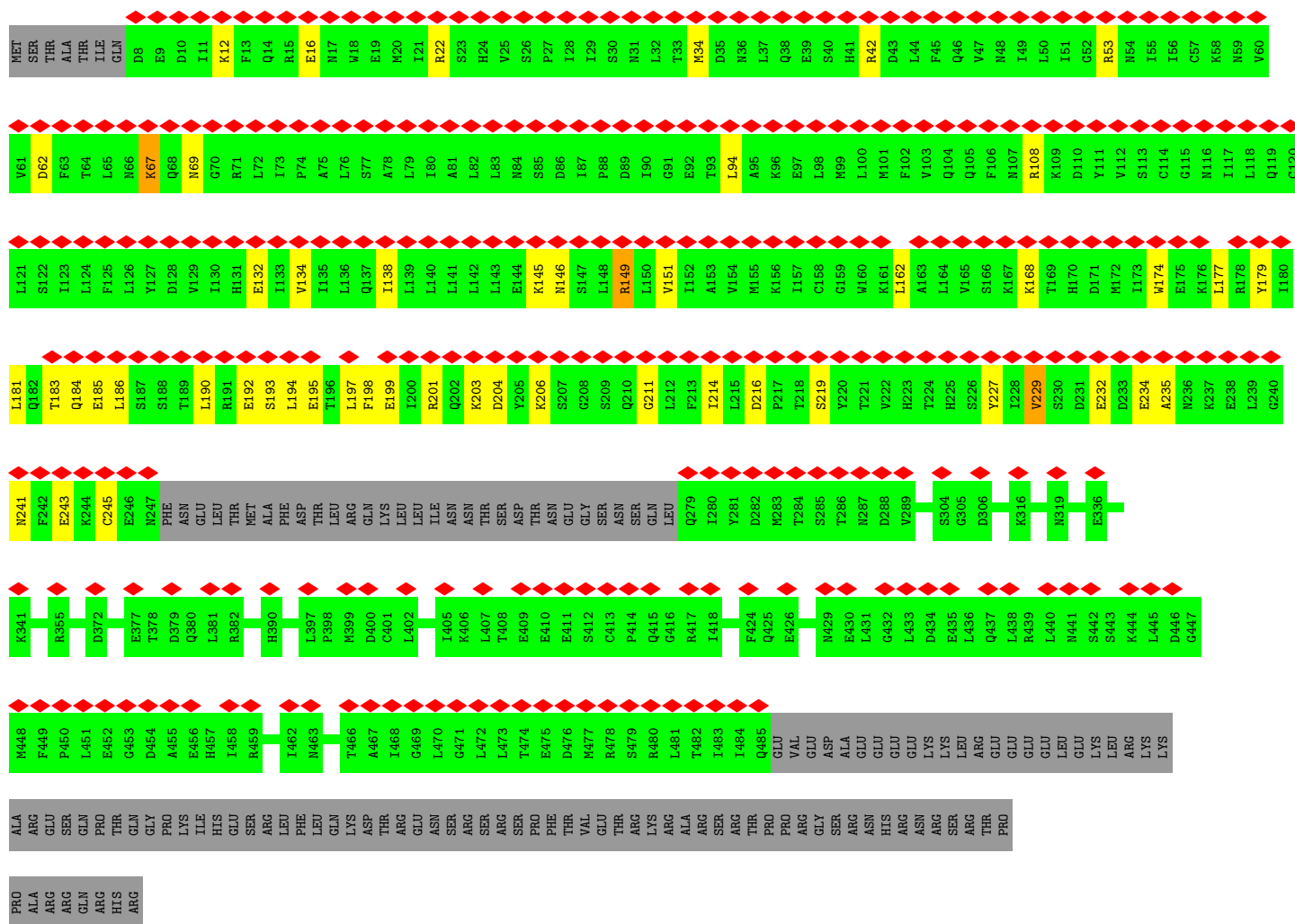
- Molecule 14: Pre-mRNA-splicing factor CWC15



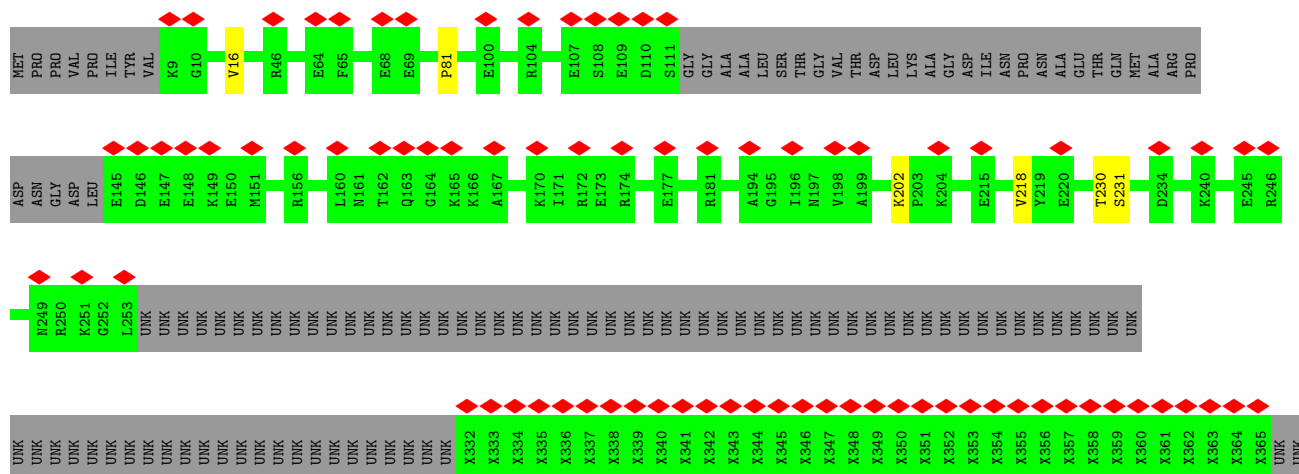
- Molecule 15: Pre-mRNA-splicing factor BUD31



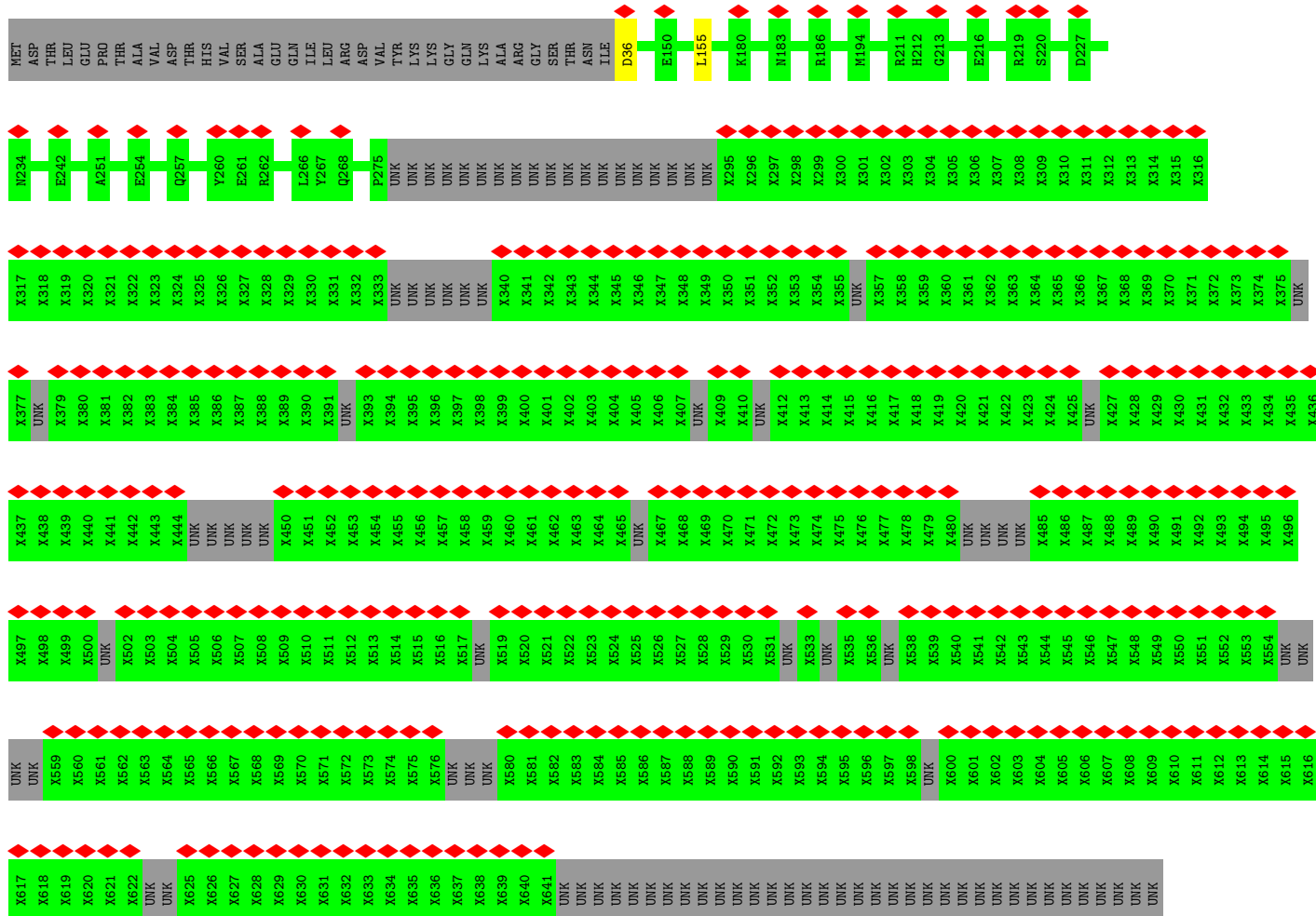
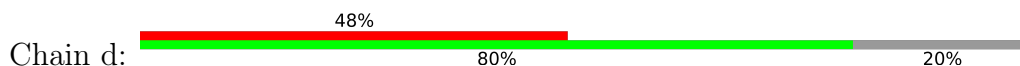
- Molecule 16: Pre-mRNA-splicing factor CWC22



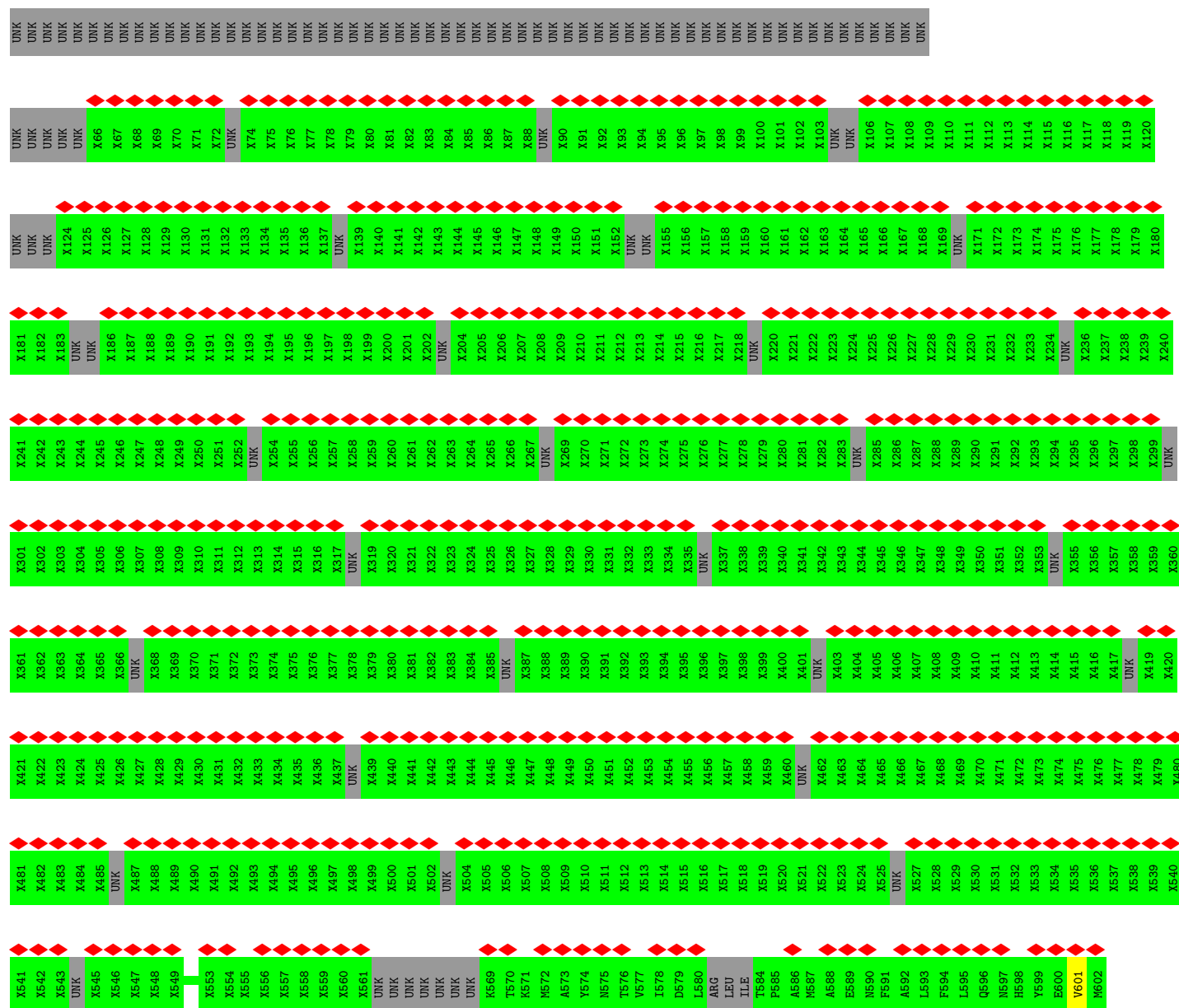
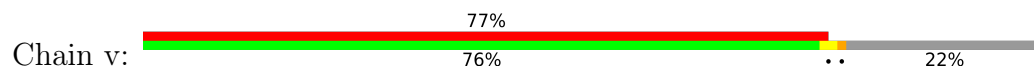
• Molecule 17: Pre-mRNA-splicing factor CEF1

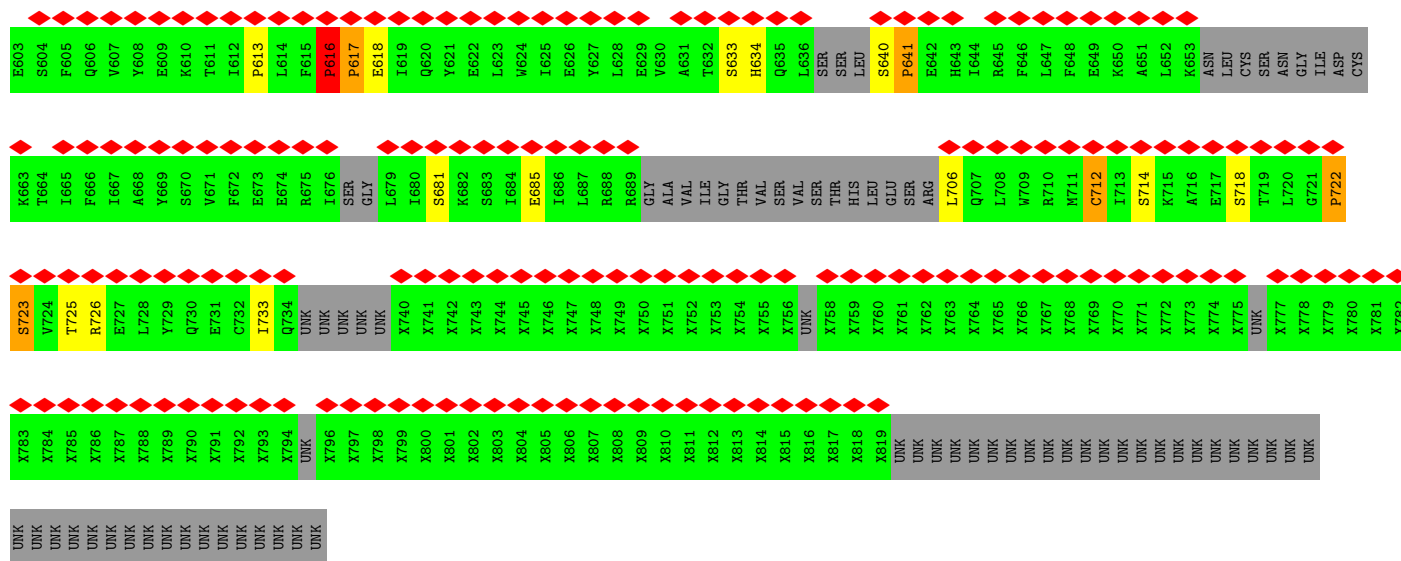


- Molecule 18: Pre-mRNA-splicing factor CLF1

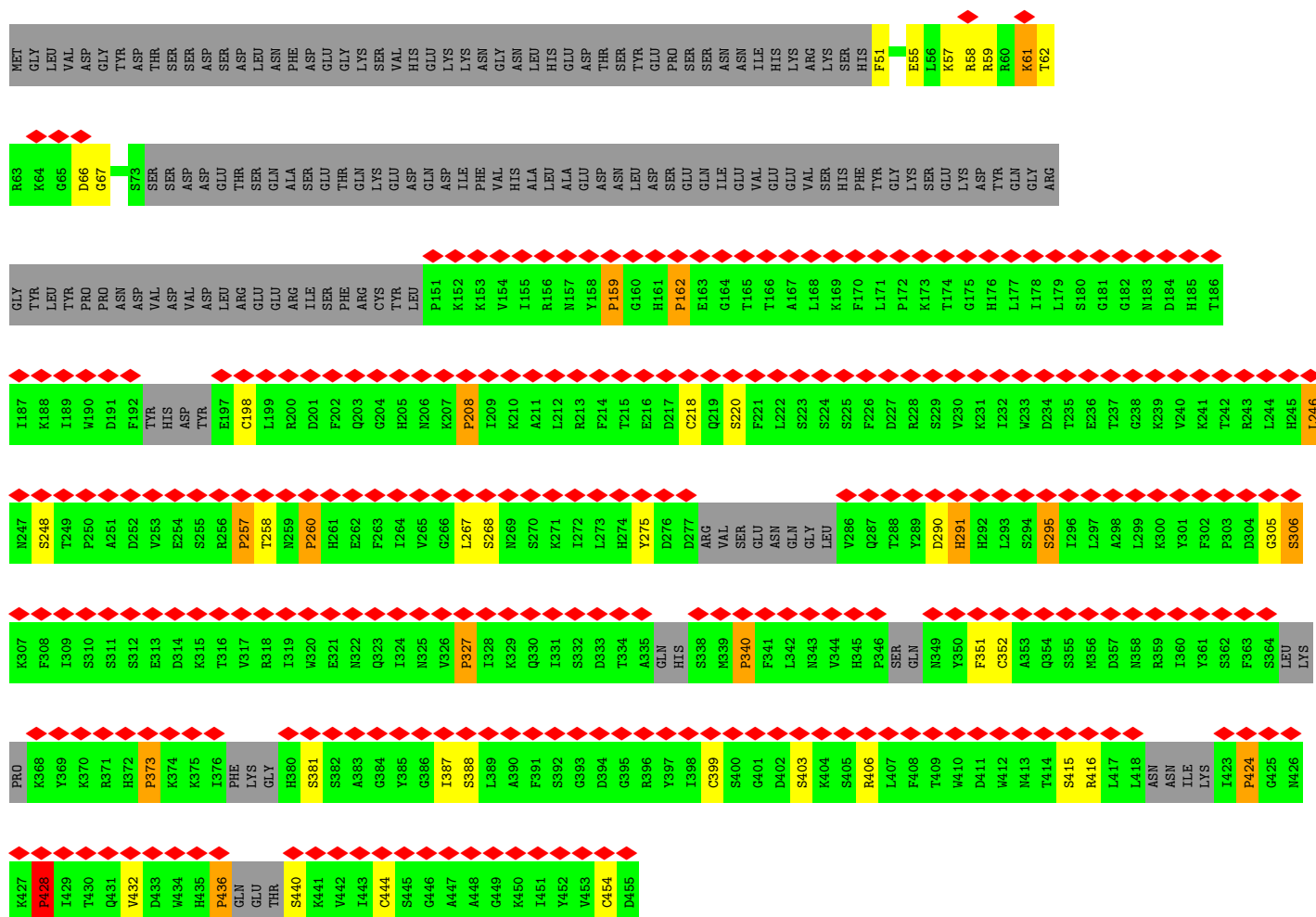


- Molecule 23: Pre-mRNA-splicing factor SYF1

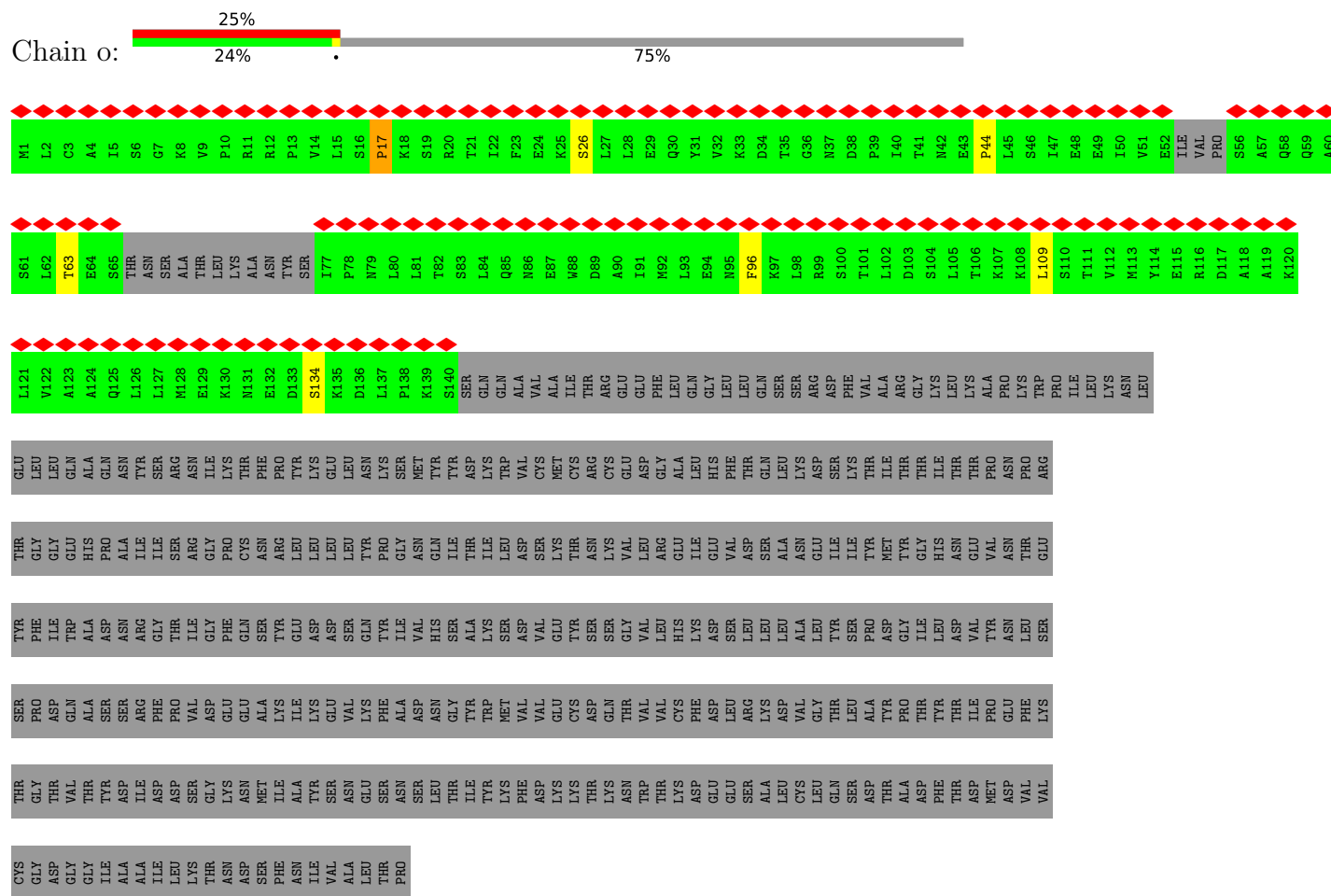




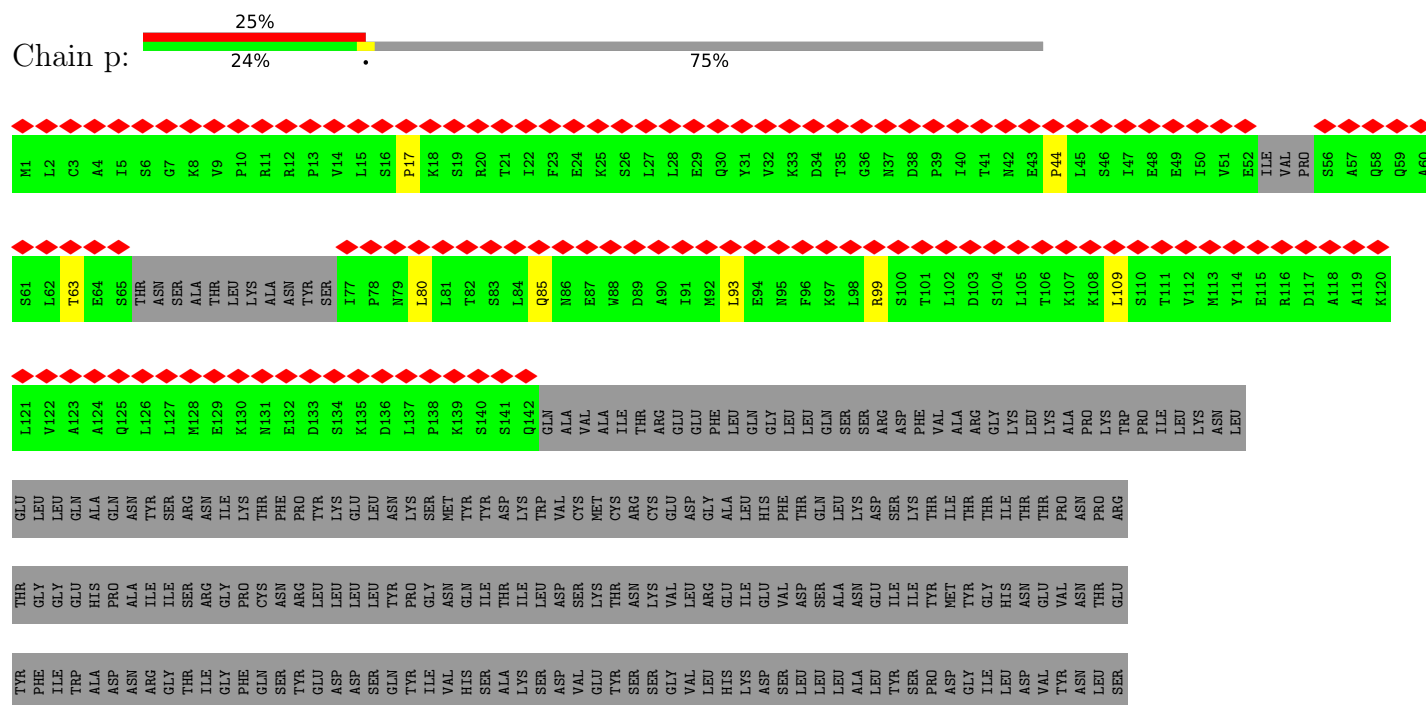
• Molecule 24: Pre-mRNA-processing factor 17



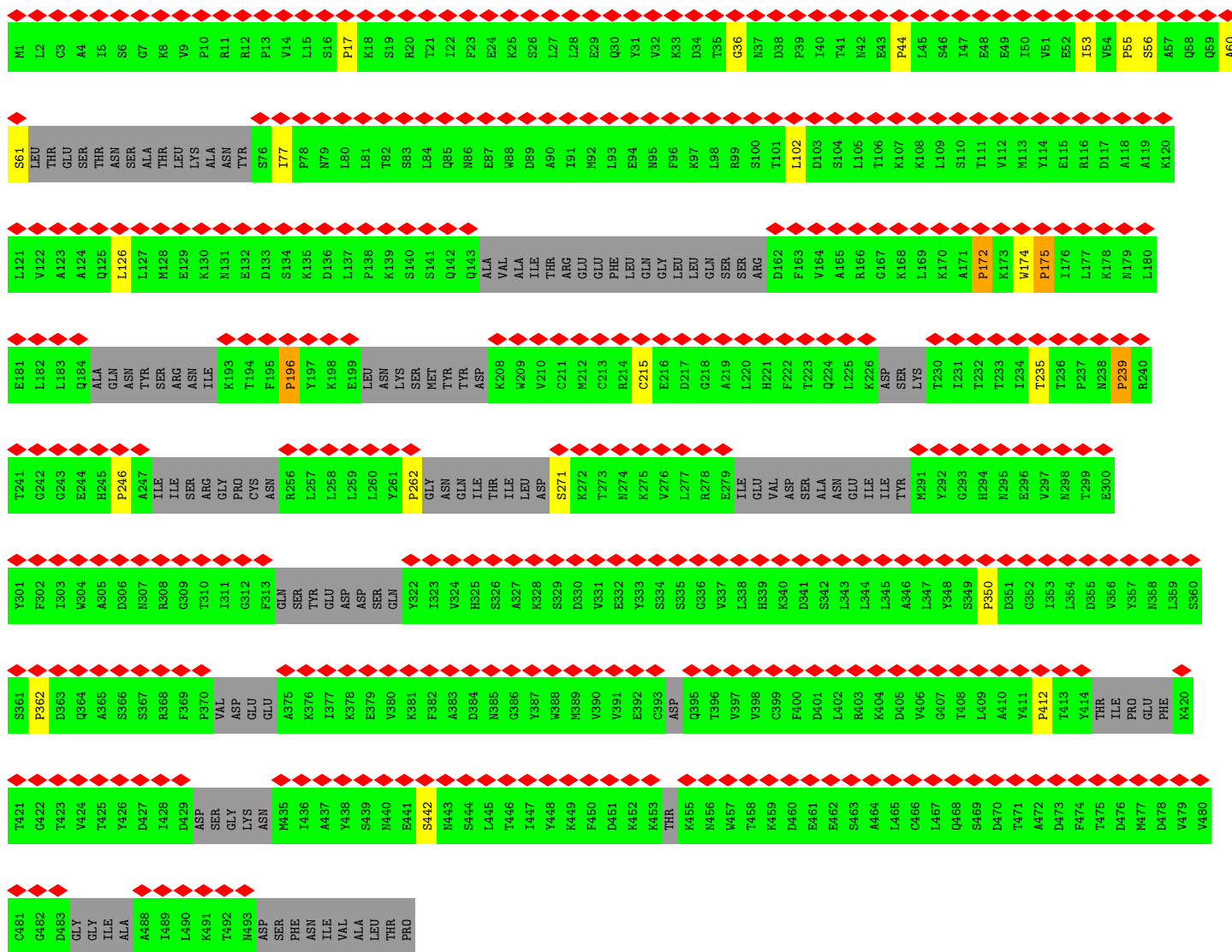
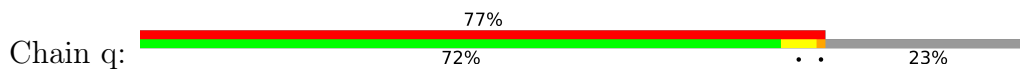
- Molecule 25: Pre-mRNA-processing factor 19



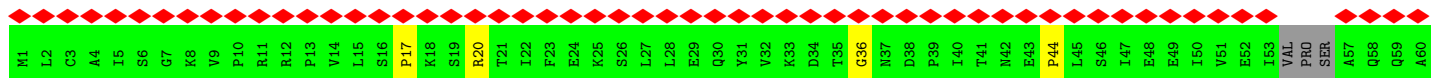
- Molecule 25: Pre-mRNA-processing factor 19

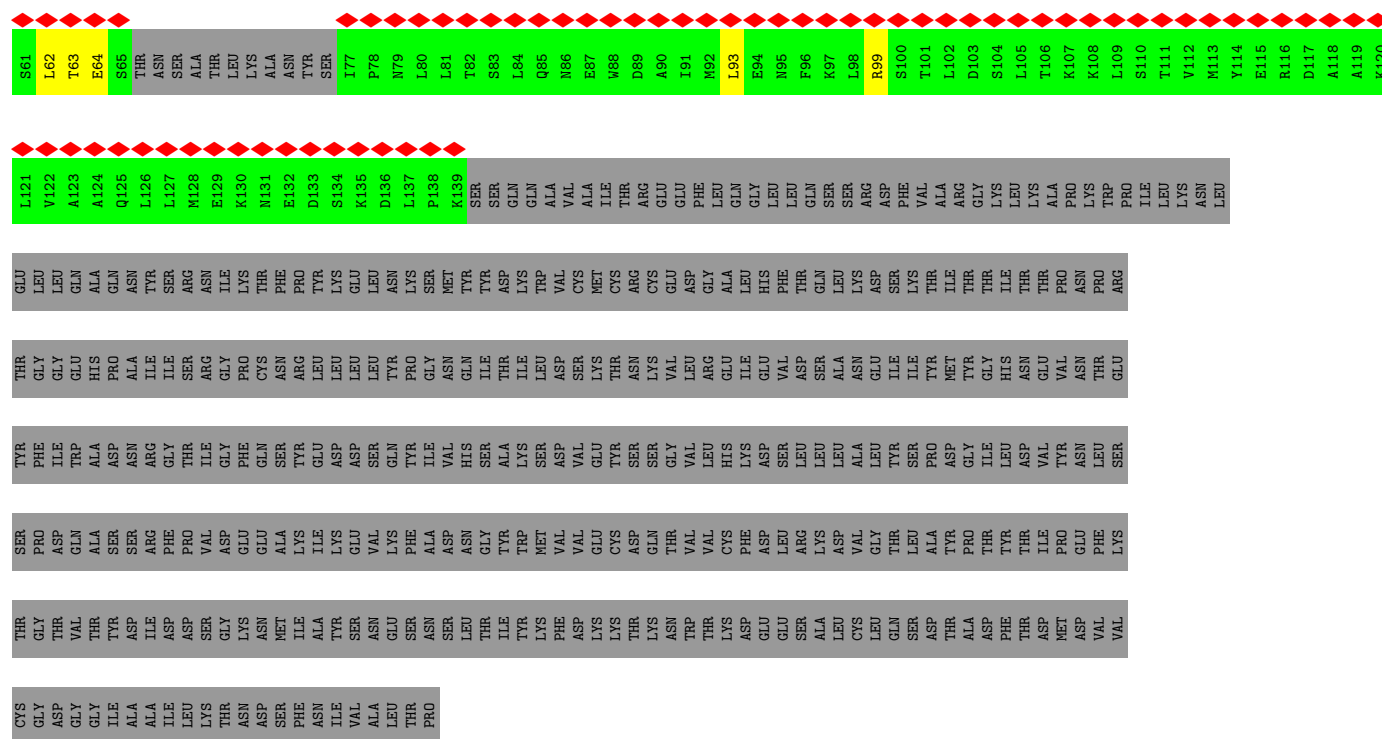


- Molecule 25: Pre-mRNA-processing factor 19

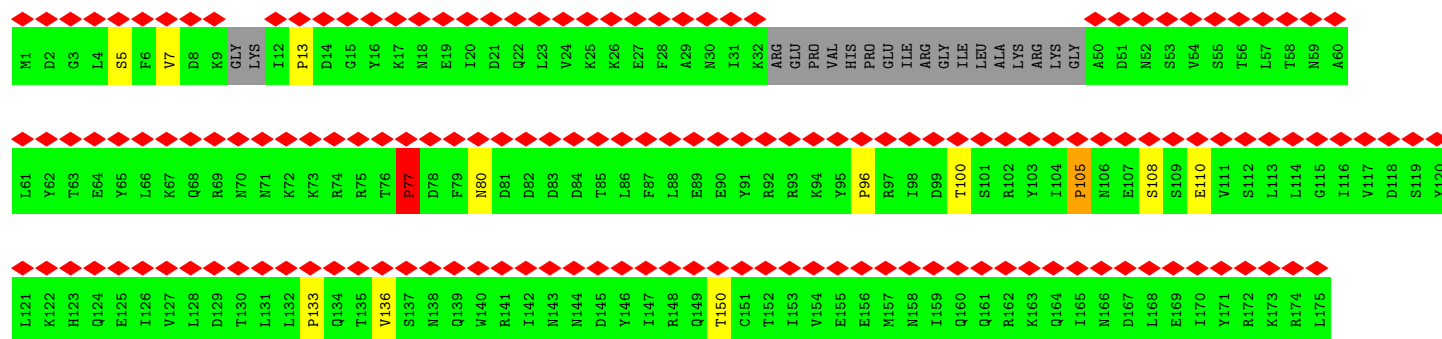
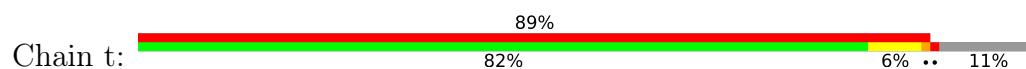


- Molecule 25: Pre-mRNA-processing factor 19

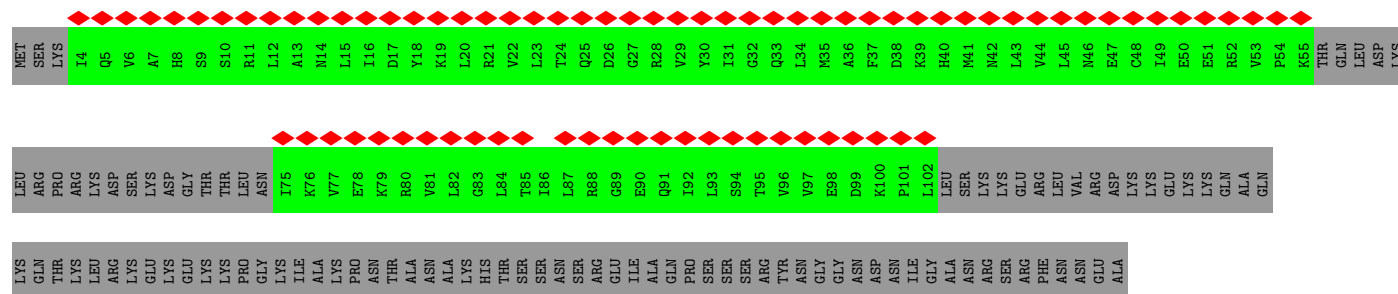
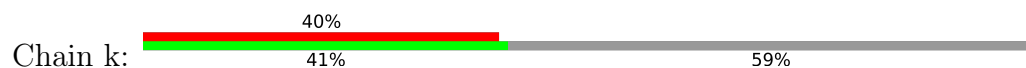




• Molecule 26: Pre-mRNA-splicing factor SNT309



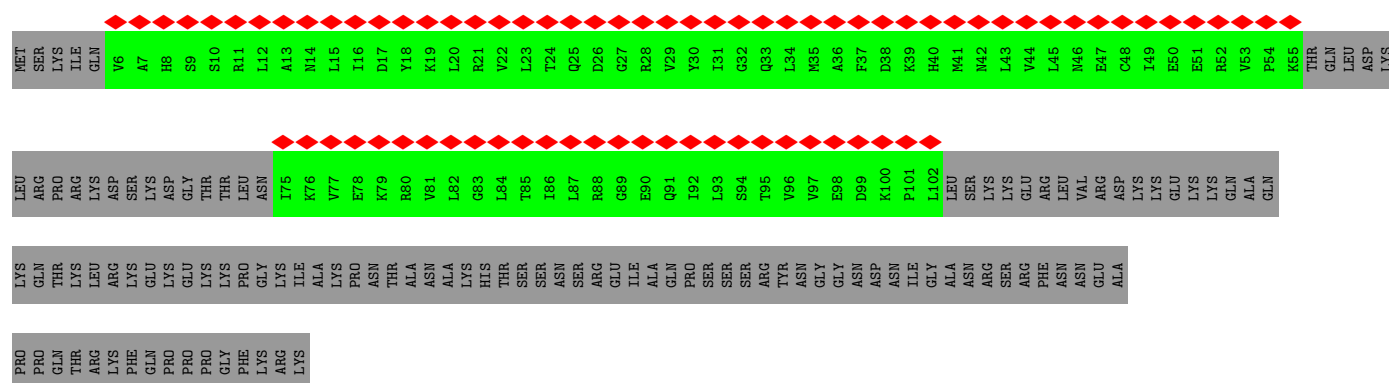
• Molecule 27: Small nuclear ribonucleoprotein-associated protein B



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

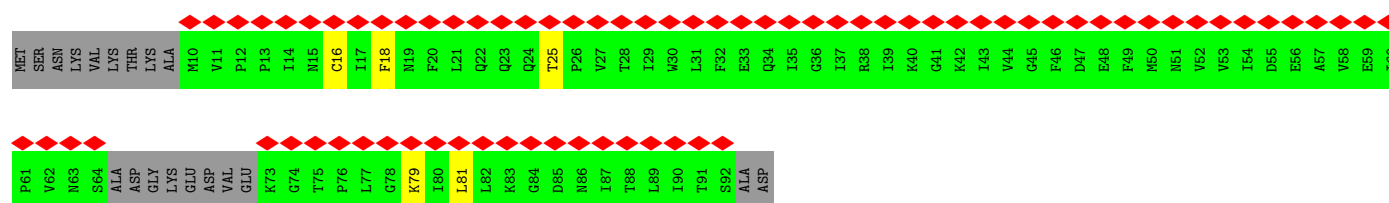
• Molecule 27: Small nuclear ribonucleoprotein-associated protein B

Chain s: 




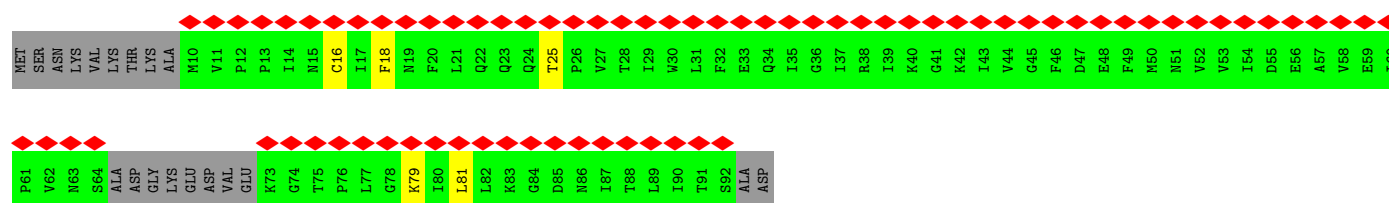
• Molecule 28: Small nuclear ribonucleoprotein E

Chain i: 




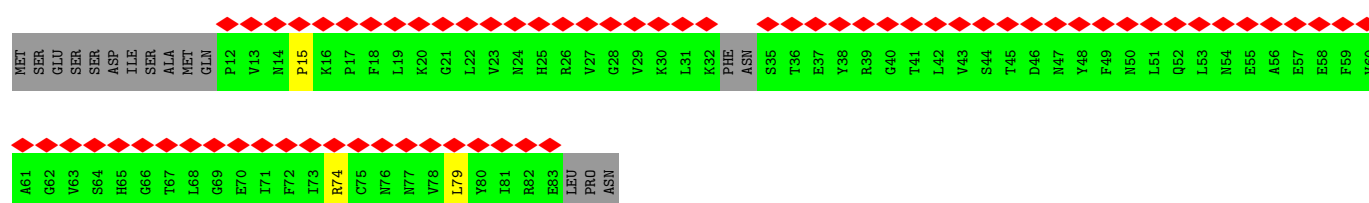
• Molecule 28: Small nuclear ribonucleoprotein E

Chain u: 

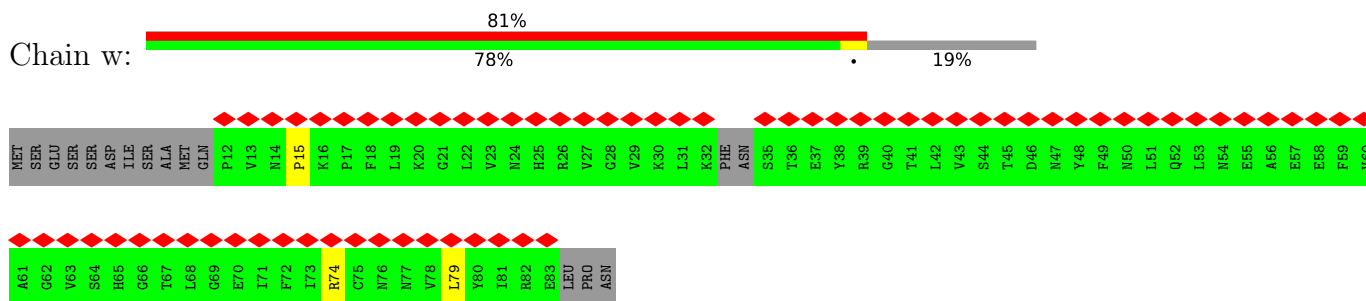


• Molecule 29: Small nuclear ribonucleoprotein F

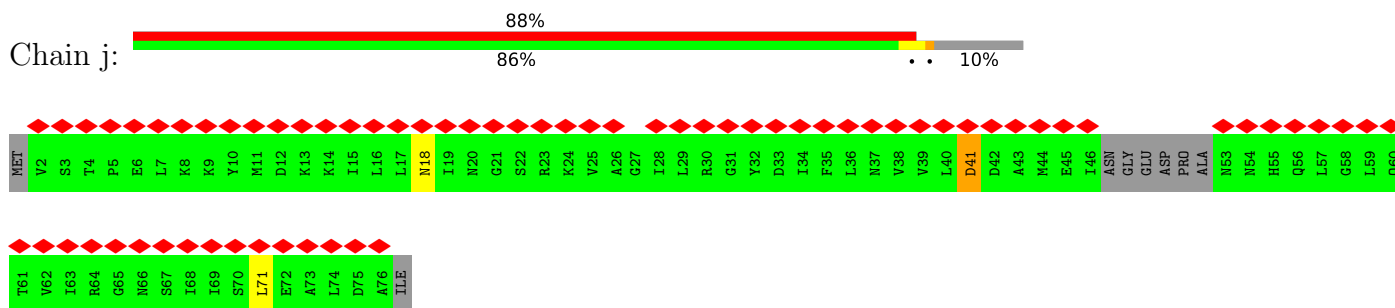
Chain h: 



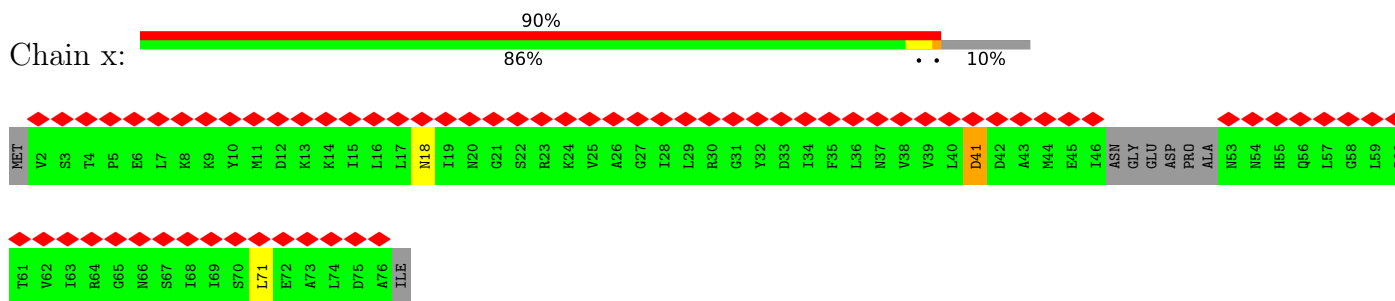
• Molecule 29: Small nuclear ribonucleoprotein F



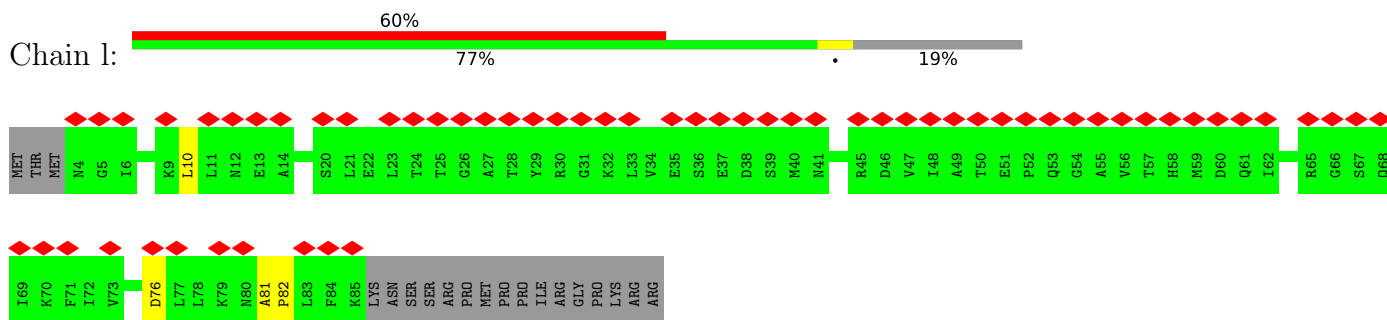
• Molecule 30: Small nuclear ribonucleoprotein G



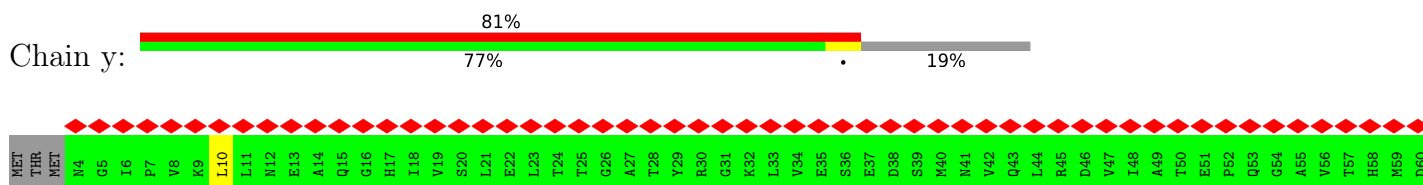
• Molecule 30: Small nuclear ribonucleoprotein G

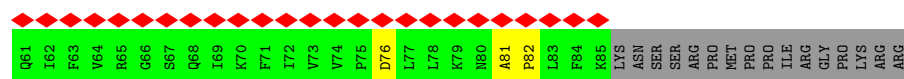


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

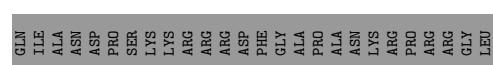
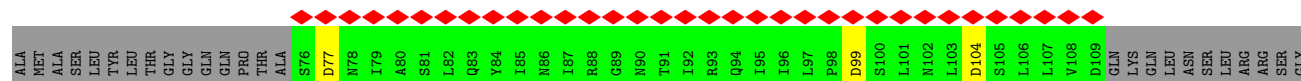
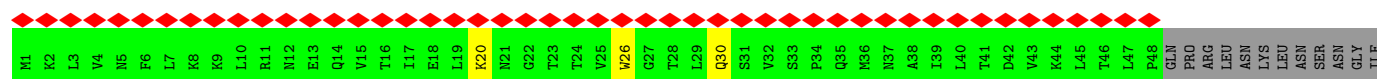


• Molecule 31: Small nuclear ribonucleoprotein Sm D3

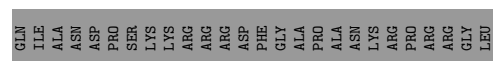
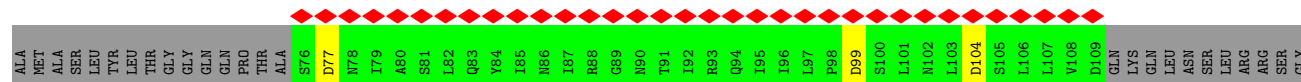




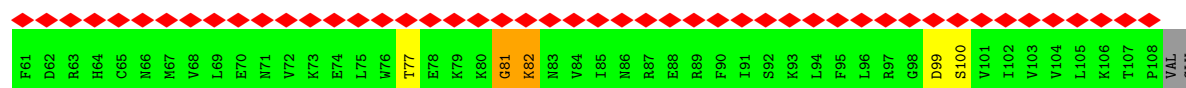
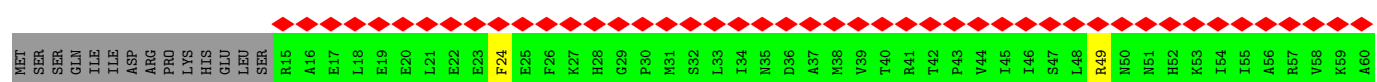
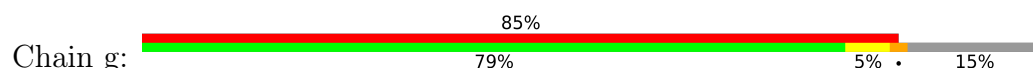
• Molecule 32: Small nuclear ribonucleoprotein Sm D1



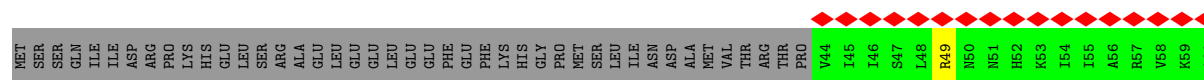
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

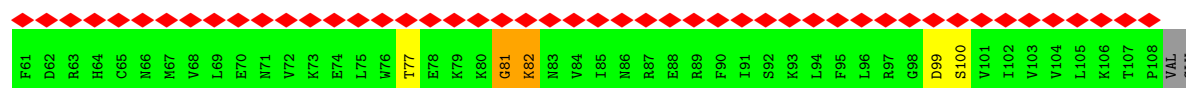


• Molecule 33: Small nuclear ribonucleoprotein Sm D2

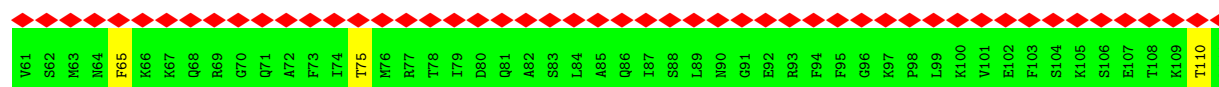
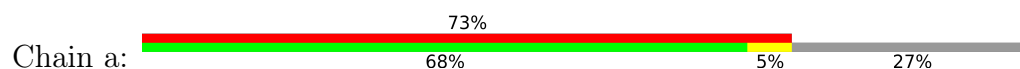


• Molecule 33: Small nuclear ribonucleoprotein Sm D2

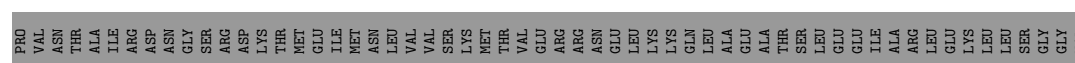
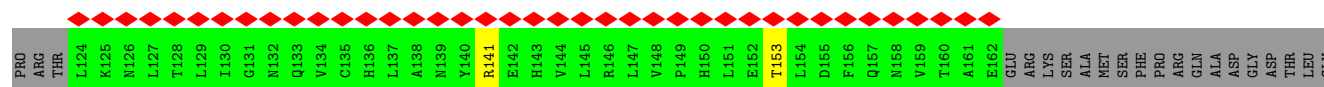
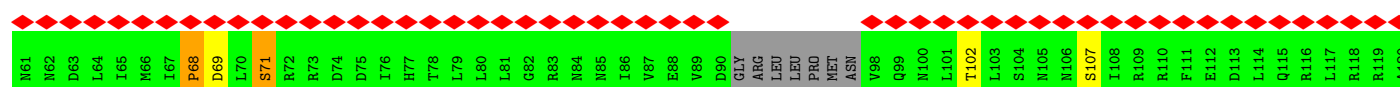
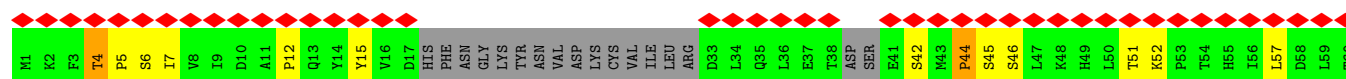




• Molecule 34: U2 small nuclear ribonucleoprotein B''



• Molecule 35: U2 small nuclear ribonucleoprotein A'



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.7	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	0.240	Depositor
Minimum map value	-0.120	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0413	Depositor
Map size (Å)	522.4, 522.4, 522.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3060001, 1.3060001, 1.3060001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GTP

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	0.48	3/16178 (0.0%)	0.60	6/21929 (0.0%)
2	C	0.47	1/7168 (0.0%)	0.57	3/9707 (0.0%)
3	D	0.73	0/2747	0.93	2/4267 (0.0%)
4	E	0.76	1/2452 (0.0%)	0.96	3/3817 (0.1%)
5	L	0.94	33/2974 (1.1%)	1.51	88/4610 (1.9%)
6	M	0.73	2/678 (0.3%)	1.01	3/1051 (0.3%)
7	B	1.01	1/307 (0.3%)	0.95	0/475
8	N	1.27	5/346 (1.4%)	1.29	10/535 (1.9%)
9	J	0.41	0/191	0.57	0/254
10	O	0.57	0/2704	0.63	1/3676 (0.0%)
11	P	0.42	2/1604 (0.1%)	0.52	0/2160
12	Q	0.47	1/1496 (0.1%)	0.62	0/2014
13	R	0.44	0/2135	0.56	0/2871
14	S	0.46	1/574 (0.2%)	0.56	0/766
15	T	0.51	1/1315 (0.1%)	0.61	0/1759
16	Z	0.50	0/3712	0.85	7/5004 (0.1%)
17	c	0.41	1/2405 (0.0%)	0.50	0/3218
18	d	0.49	0/2107	0.54	1/2852 (0.0%)
19	F	0.37	0/955	0.55	0/1277
20	G	0.27	0/346	0.51	0/462
21	H	0.33	0/826	0.54	0/1108
22	I	0.34	0/826	0.47	0/1097
23	v	1.04	8/905 (0.9%)	0.76	6/1214 (0.5%)
24	n	1.48	19/1900 (1.0%)	0.89	15/2537 (0.6%)
25	o	0.40	0/835	0.53	0/1126
25	p	0.40	0/848	0.55	0/1143
25	q	0.44	0/2342	0.65	0/3139
25	r	0.39	0/828	0.54	1/1117 (0.1%)
26	t	0.42	0/924	0.56	2/1244 (0.2%)
27	k	0.37	0/636	0.61	0/856
27	s	0.37	0/615	0.61	0/829
28	i	0.42	0/585	0.62	0/795

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	u	0.42	0/585	0.62	0/795
29	h	0.44	0/564	0.65	1/761 (0.1%)
29	w	0.44	0/564	0.65	1/761 (0.1%)
30	j	0.37	0/532	0.60	0/715
30	x	0.37	0/532	0.60	0/715
31	l	0.40	0/634	0.70	0/859
31	y	0.40	0/634	0.70	0/859
32	m	0.41	0/649	0.61	0/880
32	z	0.41	0/649	0.61	0/880
33	e	0.43	0/535	0.67	2/717 (0.3%)
33	g	0.45	0/753	0.69	2/1013 (0.2%)
34	a	0.82	4/514 (0.8%)	1.32	2/686 (0.3%)
35	b	1.03	9/839 (1.1%)	1.65	11/1127 (1.0%)
All	All	0.59	92/72448 (0.1%)	0.75	167/99677 (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
2	C	0	2
10	O	0	6
11	P	0	1
12	Q	0	3
16	Z	0	5
17	c	0	1
20	G	0	1
24	n	0	4
30	j	0	1
30	x	0	1
31	l	0	2
31	y	0	2
33	e	0	2
33	g	0	2
All	All	0	41

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	399	CYS	CB-SG	-24.10	1.41	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	444	CYS	CB-SG	-22.82	1.43	1.82
24	n	454	CYS	CB-SG	-19.98	1.48	1.82
24	n	218	CYS	CB-SG	-19.56	1.49	1.82
24	n	352	CYS	CB-SG	-18.84	1.50	1.82
24	n	198	CYS	CB-SG	-17.69	1.52	1.82
23	v	712	CYS	CB-SG	-17.09	1.53	1.82
7	B	98	A	O3'-P	-11.86	1.47	1.61
5	L	1096	C	O3'-P	-9.98	1.49	1.61
8	N	102	A	O3'-P	-9.15	1.50	1.61
23	v	718	SER	CB-OG	8.60	1.53	1.42
23	v	723	SER	CB-OG	8.51	1.53	1.42
4	E	84	C	O3'-P	-8.03	1.51	1.61
23	v	714	SER	CB-OG	7.93	1.52	1.42
24	n	440	SER	CB-OG	7.88	1.52	1.42
23	v	681	SER	CB-OG	7.79	1.52	1.42
24	n	248	SER	CB-OG	7.58	1.52	1.42
5	L	59	C	C1'-N1	7.51	1.60	1.48
5	L	1096	C	C1'-N1	7.50	1.59	1.48
5	L	71	C	C1'-N1	7.47	1.59	1.48
35	b	46	SER	CB-OG	7.43	1.51	1.42
5	L	82	C	C1'-N1	7.43	1.59	1.48
5	L	84	C	C1'-N1	7.38	1.59	1.48
24	n	381	SER	CB-OG	7.37	1.51	1.42
5	L	1118	U	C1'-N1	7.36	1.59	1.48
5	L	1120	G	C1'-N9	-7.30	1.36	1.46
35	b	45	SER	CB-OG	7.29	1.51	1.42
8	N	101	U	C2-N3	-7.20	1.32	1.37
24	n	246	LEU	CA-CB	-7.09	1.37	1.53
34	a	33	SER	CB-OG	7.03	1.51	1.42
35	b	6	SER	CB-OG	7.00	1.51	1.42
35	b	69	ASP	CA-CB	-6.97	1.38	1.53
5	L	63	U	C1'-N1	6.95	1.59	1.48
5	L	97	U	C1'-N1	6.92	1.59	1.48
5	L	99	U	C1'-N1	6.91	1.59	1.48
23	v	633	SER	CB-OG	6.89	1.51	1.42
5	L	98	U	C1'-N1	6.88	1.59	1.48
5	L	107	U	C1'-N1	6.87	1.59	1.48
5	L	101	U	C1'-N1	6.86	1.59	1.48
5	L	54	U	C1'-N1	6.85	1.59	1.48
5	L	56	U	C1'-N1	6.85	1.59	1.48
5	L	26	G	O3'-P	-6.84	1.52	1.61
5	L	102	U	C1'-N1	6.80	1.58	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	68	U	C1'-N1	6.80	1.58	1.48
5	L	73	U	C1'-N1	6.79	1.58	1.48
5	L	1111	U	C1'-N1	6.79	1.58	1.48
5	L	1119	C	C1'-N1	6.78	1.58	1.48
5	L	83	U	C1'-N1	6.77	1.58	1.48
5	L	1101	C	C1'-N1	6.77	1.58	1.48
24	n	415	SER	CB-OG	6.66	1.50	1.42
17	c	202	LYS	C-N	-6.63	1.21	1.34
24	n	268	SER	CB-OG	6.58	1.50	1.42
5	L	1115	G	C1'-N9	-6.54	1.37	1.46
6	M	501	A	C6-N1	-6.41	1.31	1.35
6	M	502	C	O3'-P	6.34	1.68	1.61
5	L	62	C	C1'-N1	6.33	1.58	1.48
5	L	104	C	C1'-N1	6.29	1.58	1.48
5	L	72	C	C1'-N1	6.25	1.58	1.48
5	L	74	C	C1'-N1	6.24	1.58	1.48
8	N	102	A	N3-C4	-6.16	1.31	1.34
15	T	148	CYS	CB-SG	-6.15	1.71	1.82
5	L	1109	C	C1'-N1	6.05	1.57	1.48
24	n	220	SER	CB-OG	5.98	1.50	1.42
35	b	42	SER	CB-OG	5.94	1.50	1.42
24	n	388	SER	CB-OG	5.88	1.49	1.42
24	n	403	SER	CB-OG	5.85	1.49	1.42
35	b	102	THR	CB-OG1	5.78	1.54	1.43
23	v	640	SER	CB-OG	5.73	1.49	1.42
24	n	351	PHE	CB-CG	-5.70	1.41	1.51
5	L	121	C	C1'-N1	5.67	1.57	1.48
35	b	15	TYR	CB-CG	-5.64	1.43	1.51
5	L	1112	G	C1'-N9	-5.58	1.39	1.46
35	b	51	THR	CB-OG1	5.57	1.54	1.43
8	N	102	A	C6-N1	-5.57	1.31	1.35
5	L	34	G	O3'-P	-5.50	1.54	1.61
24	n	275	TYR	CB-CG	-5.47	1.43	1.51
1	A	1206	CYS	C-N	-5.45	1.21	1.34
24	n	432	VAL	CB-CG1	-5.41	1.41	1.52
1	A	902	PRO	N-CD	5.36	1.55	1.47
12	Q	215	PRO	N-CD	5.35	1.55	1.47
1	A	899	PRO	N-CD	5.33	1.55	1.47
8	N	102	A	C5-C4	-5.32	1.35	1.38
23	v	685	GLU	CB-CG	-5.32	1.42	1.52
34	a	75	THR	CB-OG1	5.21	1.53	1.43
34	a	110	THR	CB-OG1	5.17	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	175	PRO	N-CD	5.17	1.55	1.47
11	P	135	VAL	C-N	-5.16	1.22	1.34
14	S	7	PRO	N-CD	5.11	1.55	1.47
24	n	291	HIS	CA-CB	-5.07	1.42	1.53
34	a	65	PHE	CB-CG	-5.07	1.42	1.51
2	C	464	PRO	N-CD	5.06	1.54	1.47
35	b	153	THR	CB-OG1	5.05	1.53	1.43

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	PRO	O-C-N	-28.27	77.47	122.70
6	M	502	C	O3'-P-O5'	-12.66	79.95	104.00
5	L	1110	U	C5-C4-O4	12.01	133.11	125.90
6	M	502	C	P-O3'-C3'	11.50	133.50	119.70
5	L	1107	C	N1-C2-O2	-10.12	112.83	118.90
16	Z	42	ARG	NE-CZ-NH2	9.67	125.14	120.30
6	M	502	C	OP1-P-O3'	9.22	125.49	105.20
1	A	483	PRO	CA-C-N	8.96	136.92	117.20
16	Z	22	ARG	NE-CZ-NH2	8.95	124.77	120.30
5	L	1109	C	O4'-C1'-N1	8.86	115.29	108.20
35	b	44	PRO	N-CA-CB	8.83	113.89	103.30
8	N	101	U	C5-C6-N1	-8.48	118.46	122.70
5	L	1112	G	P-O3'-C3'	8.30	129.66	119.70
5	L	1107	C	C5'-C4'-O4'	-8.27	99.18	109.10
8	N	101	U	N1-C2-N3	8.16	119.80	114.90
5	L	1110	U	N3-C4-O4	-8.13	113.71	119.40
5	L	1107	C	N3-C2-O2	7.56	127.19	121.90
5	L	1107	C	P-O3'-C3'	7.54	128.75	119.70
5	L	1110	U	N1-C2-O2	7.44	128.01	122.80
24	n	428	PRO	N-CA-CB	7.35	112.12	103.30
35	b	5	PRO	N-CA-CB	7.27	112.03	103.30
35	b	42	SER	N-CA-CB	-7.24	99.64	110.50
5	L	68	U	OP2-P-O3'	7.23	121.10	105.20
5	L	99	U	OP2-P-O3'	7.23	121.10	105.20
5	L	59	C	OP2-P-O3'	7.22	121.09	105.20
5	L	97	U	OP2-P-O3'	7.22	121.09	105.20
5	L	102	U	OP2-P-O3'	7.22	121.09	105.20
5	L	74	C	OP2-P-O3'	7.22	121.09	105.20
5	L	56	U	OP2-P-O3'	7.22	121.08	105.20
5	L	69	G	OP2-P-O3'	7.22	121.08	105.20
5	L	70	A	OP2-P-O3'	7.22	121.08	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	55	G	OP2-P-O3'	7.22	121.08	105.20
5	L	54	U	OP2-P-O3'	7.22	121.08	105.20
5	L	78	G	OP2-P-O3'	7.22	121.08	105.20
5	L	81	G	OP2-P-O3'	7.22	121.08	105.20
5	L	103	A	OP2-P-O3'	7.22	121.08	105.20
5	L	104	C	OP2-P-O3'	7.22	121.08	105.20
5	L	67	A	OP2-P-O3'	7.21	121.07	105.20
5	L	100	G	OP2-P-O3'	7.21	121.07	105.20
5	L	82	C	OP2-P-O3'	7.21	121.07	105.20
5	L	101	U	OP2-P-O3'	7.21	121.06	105.20
5	L	105	A	OP2-P-O3'	7.21	121.07	105.20
5	L	66	A	OP2-P-O3'	7.21	121.06	105.20
5	L	71	C	OP2-P-O3'	7.21	121.06	105.20
5	L	57	A	OP2-P-O3'	7.21	121.06	105.20
5	L	83	U	OP2-P-O3'	7.21	121.06	105.20
5	L	96	A	OP2-P-O3'	7.21	121.06	105.20
5	L	62	C	OP2-P-O3'	7.21	121.05	105.20
5	L	73	U	OP2-P-O3'	7.21	121.05	105.20
5	L	80	G	OP2-P-O3'	7.21	121.06	105.20
5	L	98	U	OP2-P-O3'	7.21	121.05	105.20
5	L	79	A	OP2-P-O3'	7.20	121.05	105.20
5	L	61	A	OP2-P-O3'	7.20	121.05	105.20
5	L	106	A	OP2-P-O3'	7.20	121.04	105.20
5	L	58	A	OP2-P-O3'	7.20	121.04	105.20
5	L	60	A	OP2-P-O3'	7.19	121.01	105.20
5	L	72	C	OP2-P-O3'	7.19	121.01	105.20
8	N	101	U	C2-N1-C1'	-7.12	109.16	117.70
5	L	1111	U	P-O5'-C5'	-7.11	109.53	120.90
8	N	101	U	C2-N3-C4	-7.08	122.75	127.00
16	Z	108	ARG	NE-CZ-NH2	7.03	123.81	120.30
5	L	1110	U	N3-C2-O2	-6.95	117.33	122.20
5	L	1108	A	O4'-C1'-N9	-6.94	102.65	108.20
5	L	71	C	O3'-P-O5'	-6.80	91.08	104.00
5	L	104	C	O3'-P-O5'	-6.80	91.08	104.00
5	L	70	A	O3'-P-O5'	-6.80	91.08	104.00
5	L	54	U	O3'-P-O5'	-6.79	91.10	104.00
5	L	73	U	O3'-P-O5'	-6.79	91.10	104.00
5	L	78	G	O3'-P-O5'	-6.79	91.10	104.00
5	L	80	G	O3'-P-O5'	-6.79	91.10	104.00
5	L	106	A	O3'-P-O5'	-6.79	91.10	104.00
5	L	79	A	O3'-P-O5'	-6.79	91.10	104.00
5	L	81	G	O3'-P-O5'	-6.79	91.10	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	U	N3-C2-O2	-6.79	117.45	122.20
5	L	82	C	O3'-P-O5'	-6.78	91.11	104.00
5	L	83	U	O3'-P-O5'	-6.78	91.11	104.00
5	L	57	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	102	U	O3'-P-O5'	-6.78	91.12	104.00
5	L	58	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	67	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	74	C	O3'-P-O5'	-6.78	91.12	104.00
5	L	56	U	O3'-P-O5'	-6.78	91.12	104.00
5	L	66	A	O3'-P-O5'	-6.78	91.12	104.00
5	L	99	U	O3'-P-O5'	-6.78	91.13	104.00
5	L	103	A	O3'-P-O5'	-6.78	91.13	104.00
5	L	105	A	O3'-P-O5'	-6.78	91.13	104.00
5	L	72	C	O3'-P-O5'	-6.77	91.13	104.00
5	L	59	C	O3'-P-O5'	-6.77	91.13	104.00
5	L	96	A	O3'-P-O5'	-6.77	91.13	104.00
5	L	98	U	O3'-P-O5'	-6.77	91.13	104.00
5	L	68	U	O3'-P-O5'	-6.77	91.14	104.00
5	L	101	U	O3'-P-O5'	-6.77	91.14	104.00
5	L	55	G	O3'-P-O5'	-6.77	91.14	104.00
5	L	97	U	O3'-P-O5'	-6.77	91.14	104.00
5	L	100	G	O3'-P-O5'	-6.77	91.14	104.00
5	L	61	A	O3'-P-O5'	-6.76	91.15	104.00
5	L	62	C	O3'-P-O5'	-6.76	91.15	104.00
5	L	69	G	O3'-P-O5'	-6.76	91.15	104.00
5	L	60	A	O3'-P-O5'	-6.76	91.16	104.00
35	b	12	PRO	N-CA-CB	6.67	111.31	103.30
23	v	617	PRO	CA-CB-CG	6.62	117.37	104.80
23	v	613	PRO	N-CA-CB	6.53	111.13	103.30
23	v	722	PRO	N-CA-CB	6.49	111.09	103.30
35	b	4	THR	N-CA-CB	-6.31	98.31	110.30
35	b	57	LEU	N-CA-CB	6.31	123.01	110.40
10	O	443	ASN	C-N-CD	6.29	141.62	128.40
16	Z	149	ARG	NE-CZ-NH2	6.19	123.40	120.30
24	n	257	PRO	N-CA-CB	6.18	110.72	103.30
24	n	159	PRO	N-CA-CB	6.16	110.70	103.30
24	n	373	PRO	N-CA-CB	6.14	110.67	103.30
1	A	1882	LEU	C-N-CA	-6.13	106.38	121.70
24	n	208	PRO	N-CA-CB	6.12	110.64	103.30
3	D	79	C	C2-N1-C1'	6.02	125.42	118.80
24	n	424	PRO	N-CA-CB	6.02	110.52	103.30
23	v	641	PRO	CA-CB-CG	5.98	116.16	104.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	458	ILE	C-N-CD	5.97	140.95	128.40
23	v	616	PRO	N-CA-CB	5.96	110.45	103.30
35	b	7	ILE	CA-CB-CG1	5.95	122.31	111.00
35	b	141	ARG	CD-NE-CZ	5.93	131.90	123.60
8	N	101	U	N3-C4-O4	-5.91	115.26	119.40
5	L	1107	C	C5-C4-N4	-5.88	116.08	120.20
1	A	1419	ASP	CB-CG-OD1	5.84	123.55	118.30
5	L	1111	U	C5'-C4'-C3'	-5.83	106.67	116.00
5	L	1110	U	O3'-P-O5'	-5.80	92.99	104.00
24	n	162	PRO	N-CA-CB	5.79	110.25	103.30
24	n	373	PRO	CA-CB-CG	5.78	115.79	104.80
2	C	656	LEU	CA-CB-CG	-5.77	102.03	115.30
26	t	105	PRO	CA-CB-CG	5.77	115.76	104.80
2	C	463	THR	C-N-CD	5.75	140.48	128.40
16	Z	53	ARG	NE-CZ-NH2	5.75	123.18	120.30
24	n	327	PRO	N-CA-CB	5.70	110.14	103.30
24	n	436	PRO	N-CA-CB	5.69	110.13	103.30
24	n	436	PRO	CA-CB-CG	5.64	115.51	104.80
35	b	68	PRO	N-CA-CB	5.63	110.06	103.30
8	N	101	U	C6-N1-C1'	5.61	129.05	121.20
1	A	901	PRO	C-N-CD	5.60	140.16	128.40
8	N	101	U	C5-C4-O4	5.58	129.25	125.90
24	n	260	PRO	N-CA-CB	5.57	109.98	103.30
33	e	81	GLY	CA-C-N	-5.57	104.96	117.20
1	A	898	ILE	C-N-CD	5.55	140.05	128.40
24	n	306	SER	N-CA-CB	-5.54	102.19	110.50
33	g	81	GLY	CA-C-N	-5.53	105.03	117.20
4	E	77	G	C6-C5-N7	-5.49	127.11	130.40
26	t	77	PRO	CA-CB-CG	5.31	114.89	104.80
4	E	58	C	C2-N1-C1'	5.28	124.61	118.80
24	n	340	PRO	N-CA-CB	5.28	109.63	103.30
5	L	1113	U	O4'-C1'-C2'	-5.27	100.53	105.80
8	N	102	A	OP2-P-O3'	5.25	116.76	105.20
25	r	62	LEU	CA-CB-CG	-5.22	103.28	115.30
35	b	71	SER	N-CA-CB	-5.22	102.67	110.50
8	N	102	A	P-O3'-C3'	-5.21	113.45	119.70
18	d	36	ASP	CB-CG-OD2	5.19	122.97	118.30
29	h	74	ARG	NE-CZ-NH1	5.18	122.89	120.30
4	E	55	G	N3-C4-N9	5.17	129.10	126.00
16	Z	42	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
5	L	1119	C	OP1-P-OP2	-5.16	111.86	119.60
16	Z	62	ASP	CB-CG-OD1	5.16	122.94	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	295	SER	N-CA-CB	-5.14	102.79	110.50
23	v	617	PRO	N-CA-CB	5.11	109.44	103.30
33	e	82	LYS	N-CA-C	5.09	124.75	111.00
34	a	33	SER	N-CA-CB	5.08	118.12	110.50
33	g	82	LYS	N-CA-C	5.07	124.70	111.00
29	w	74	ARG	NE-CZ-NH1	5.07	122.84	120.30
34	a	46	VAL	CA-CB-CG2	5.07	118.51	110.90
35	b	107	SER	N-CA-CB	-5.04	102.93	110.50
3	D	90	C	C5-C6-N1	5.01	123.50	121.00
5	L	1096	C	OP2-P-O3'	5.01	116.22	105.20

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1346	PHE	Peptide
1	A	1375	LEU	Peptide
1	A	1377	SER	Peptide
1	A	257	ASN	Peptide
1	A	483	PRO	Mainchain
1	A	539	PRO	Peptide
1	A	773	SER	Peptide
2	C	170	LEU	Peptide
2	C	534	THR	Peptide
20	G	16	LEU	Peptide
10	O	123	PRO	Peptide
10	O	263	VAL	Peptide
10	O	278	ASP	Peptide
10	O	435	GLU	Peptide
10	O	436	SER	Peptide
10	O	437	GLU	Peptide
11	P	85	SER	Peptide
12	Q	103	GLU	Peptide
12	Q	291	ILE	Peptide
12	Q	45	HIS	Peptide
16	Z	211	GLY	Peptide
16	Z	219	SER	Peptide
16	Z	227	TYR	Sidechain
16	Z	232	GLU	Peptide
16	Z	241	ASN	Peptide
17	c	81	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
33	e	81	GLY	Peptide,Mainchain
33	g	81	GLY	Peptide,Mainchain
30	j	41	ASP	Peptide
31	l	81	ALA	Peptide,Mainchain
24	n	290	ASP	Peptide
24	n	305	GLY	Peptide
24	n	67	GLY	Peptide,Mainchain
30	x	41	ASP	Peptide
31	y	81	ALA	Peptide,Mainchain

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	A	1902/2413 (79%)	1744 (92%)	149 (8%)	9 (0%)	29	61
2	C	872/1008 (86%)	796 (91%)	72 (8%)	4 (0%)	29	61
9	J	25/135 (18%)	20 (80%)	5 (20%)	0	100	100
10	O	335/451 (74%)	299 (89%)	31 (9%)	5 (2%)	10	36
11	P	193/379 (51%)	174 (90%)	17 (9%)	2 (1%)	15	46
12	Q	177/364 (49%)	154 (87%)	21 (12%)	2 (1%)	14	44
13	R	259/339 (76%)	241 (93%)	18 (7%)	0	100	100
14	S	63/175 (36%)	55 (87%)	5 (8%)	3 (5%)	2	15
15	T	155/157 (99%)	137 (88%)	16 (10%)	2 (1%)	12	39
16	Z	443/577 (77%)	390 (88%)	44 (10%)	9 (2%)	7	30
17	c	312/587 (53%)	291 (93%)	17 (5%)	4 (1%)	12	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	d	238/687 (35%)	221 (93%)	17 (7%)	0	100	100
19	F	113/278 (41%)	104 (92%)	8 (7%)	1 (1%)	17	49
20	G	39/179 (22%)	37 (95%)	1 (3%)	1 (3%)	5	26
21	H	93/235 (40%)	78 (84%)	14 (15%)	1 (1%)	14	44
22	I	98/215 (46%)	95 (97%)	3 (3%)	0	100	100
23	v	121/859 (14%)	110 (91%)	7 (6%)	4 (3%)	4	22
24	n	279/455 (61%)	242 (87%)	29 (10%)	8 (3%)	4	24
25	o	120/503 (24%)	115 (96%)	4 (3%)	1 (1%)	19	51
25	p	122/503 (24%)	116 (95%)	6 (5%)	0	100	100
25	q	355/503 (71%)	327 (92%)	16 (4%)	12 (3%)	3	21
25	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	5	26
26	t	150/175 (86%)	134 (89%)	13 (9%)	3 (2%)	7	30
27	k	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
27	s	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
28	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
28	u	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
29	h	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	36
29	w	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	36
30	j	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
30	x	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
31	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	39
31	y	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	39
32	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
32	z	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
33	e	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	9	34
33	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	14	44
34	a	77/111 (69%)	75 (97%)	2 (3%)	0	100	100
35	b	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	9	34
All	All	7810/13649 (57%)	7124 (91%)	604 (8%)	82 (1%)	20	46

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	PRO
2	C	364	PHE
2	C	463	THR
16	Z	206	LYS
20	G	17	MET
23	v	616	PRO
24	n	246	LEU
24	n	428	PRO
25	q	53	ILE
25	q	77	ILE
25	q	172	PRO
25	q	174	TRP
25	q	239	PRO
25	q	246	PRO
25	q	362	PRO
25	q	442	SER
25	r	64	GLU
26	t	77	PRO
35	b	68	PRO
1	A	1405	ILE
12	Q	99	VAL
12	Q	255	SER
14	S	8	GLN
14	S	9	LEU
16	Z	67	LYS
16	Z	69	ASN
16	Z	234	GLU
16	Z	235	ALA
17	c	230	THR
21	H	27	LYS
23	v	601	VAL
23	v	618	GLU
24	n	61	LYS
24	n	291	HIS
24	n	406	ARG
25	q	196	PRO
26	t	110	GLU
1	A	484	PHE
2	C	829	VAL
16	Z	204	ASP
23	v	634	HIS
25	o	17	PRO
25	r	20	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	t	80	ASN
1	A	1628	ASP
10	O	444	PRO
11	P	86	ASN
11	P	112	ILE
14	S	10	GLU
17	c	231	SER
24	n	267	LEU
31	l	82	PRO
33	g	82	LYS
31	y	82	PRO
33	e	82	LYS
10	O	278	ASP
10	O	391	GLU
10	O	435	GLU
15	T	35	LYS
15	T	104	CYS
16	Z	146	ASN
16	Z	229	VAL
24	n	416	ARG
25	q	60	ALA
17	c	218	VAL
19	F	110	VAL
16	Z	214	ILE
25	q	36	GLY
29	h	15	PRO
29	w	15	PRO
35	b	52	LYS
1	A	407	VAL
1	A	562	ILE
10	O	277	VAL
25	q	175	PRO
1	A	264	ILE
1	A	377	VAL
1	A	741	ILE
17	c	16	VAL
24	n	387	ILE
2	C	363	PRO
25	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	1736/2182 (80%)	1721 (99%)	15 (1%)	78	90
2	C	794/910 (87%)	789 (99%)	5 (1%)	86	94
9	J	21/121 (17%)	21 (100%)	0	100	100
10	O	295/397 (74%)	292 (99%)	3 (1%)	76	88
11	P	173/328 (53%)	172 (99%)	1 (1%)	86	94
12	Q	171/332 (52%)	154 (90%)	17 (10%)	8	27
13	R	224/296 (76%)	223 (100%)	1 (0%)	91	95
14	S	56/151 (37%)	53 (95%)	3 (5%)	22	52
15	T	141/141 (100%)	140 (99%)	1 (1%)	84	92
16	Z	417/538 (78%)	382 (92%)	35 (8%)	11	36
17	c	212/316 (67%)	206 (97%)	6 (3%)	43	70
18	d	219/249 (88%)	218 (100%)	1 (0%)	88	94
19	F	105/256 (41%)	103 (98%)	2 (2%)	57	78
20	G	39/163 (24%)	39 (100%)	0	100	100
21	H	88/216 (41%)	87 (99%)	1 (1%)	73	86
22	I	92/193 (48%)	92 (100%)	0	100	100
23	v	58/152 (38%)	48 (83%)	10 (17%)	2	8
24	n	124/413 (30%)	102 (82%)	22 (18%)	2	6
25	o	60/451 (13%)	53 (88%)	7 (12%)	5	20
25	p	62/451 (14%)	54 (87%)	8 (13%)	4	16
25	q	124/451 (28%)	107 (86%)	17 (14%)	3	14
25	r	60/451 (13%)	55 (92%)	5 (8%)	11	36
26	t	40/165 (24%)	29 (72%)	11 (28%)	0	1
27	k	70/176 (40%)	70 (100%)	0	100	100
27	s	67/176 (38%)	67 (100%)	0	100	100
28	i	65/83 (78%)	60 (92%)	5 (8%)	13	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	u	65/83 (78%)	60 (92%)	5 (8%)	13	40
29	h	61/77 (79%)	60 (98%)	1 (2%)	62	81
29	w	61/77 (79%)	60 (98%)	1 (2%)	62	81
30	j	58/66 (88%)	55 (95%)	3 (5%)	23	53
30	x	58/66 (88%)	55 (95%)	3 (5%)	23	53
31	l	69/89 (78%)	67 (97%)	2 (3%)	42	69
31	y	69/89 (78%)	67 (97%)	2 (3%)	42	69
32	m	77/129 (60%)	71 (92%)	6 (8%)	12	39
32	z	77/129 (60%)	71 (92%)	6 (8%)	12	39
33	e	59/103 (57%)	55 (93%)	4 (7%)	16	45
33	g	79/103 (77%)	74 (94%)	5 (6%)	18	47
34	a	26/100 (26%)	25 (96%)	1 (4%)	33	61
35	b	47/219 (22%)	44 (94%)	3 (6%)	17	47
All	All	6319/11088 (57%)	6101 (97%)	218 (3%)	40	65

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	144	ASN
1	A	234	PHE
1	A	376	ARG
1	A	488	ARG
1	A	489	THR
1	A	495	ARG
1	A	588	LEU
1	A	612	LYS
1	A	640	ARG
1	A	737	ARG
1	A	900	PHE
1	A	903	LEU
1	A	908	ASP
1	A	928	ARG
2	C	176	ARG
2	C	177	TYR
2	C	458	ILE
2	C	461	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	465	GLU
10	O	443	ASN
10	O	445	ASN
10	O	446	LEU
11	P	185	ARG
12	Q	50	LYS
12	Q	51	ARG
12	Q	53	ASN
12	Q	55	ILE
12	Q	119	LYS
12	Q	120	LEU
12	Q	126	THR
12	Q	209	ASN
12	Q	213	SER
12	Q	217	TRP
12	Q	220	THR
12	Q	222	THR
12	Q	226	LEU
12	Q	227	LEU
12	Q	245	LYS
12	Q	248	CYS
12	Q	252	ARG
13	R	10	LYS
14	S	4	SER
14	S	6	ARG
14	S	9	LEU
15	T	34	GLN
16	Z	12	LYS
16	Z	16	GLU
16	Z	34	MET
16	Z	67	LYS
16	Z	94	LEU
16	Z	132	GLU
16	Z	134	VAL
16	Z	138	ILE
16	Z	145	LYS
16	Z	149	ARG
16	Z	151	VAL
16	Z	162	LEU
16	Z	168	LYS
16	Z	174	TRP
16	Z	177	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Z	179	TYR
16	Z	181	LEU
16	Z	183	THR
16	Z	184	GLN
16	Z	185	GLU
16	Z	186	LEU
16	Z	190	LEU
16	Z	192	GLU
16	Z	193	SER
16	Z	194	LEU
16	Z	195	GLU
16	Z	197	LEU
16	Z	198	PHE
16	Z	199	GLU
16	Z	201	ARG
16	Z	203	LYS
16	Z	216	ASP
16	Z	229	VAL
16	Z	243	GLU
16	Z	245	CYS
17	c	504	PRO
17	c	505	PRO
17	c	517	VAL
17	c	523	LEU
17	c	532	PRO
17	c	550	PRO
18	d	155	LEU
19	F	42	ARG
19	F	62	ARG
21	H	3	ARG
23	v	616	PRO
23	v	617	PRO
23	v	641	PRO
23	v	706	LEU
23	v	712	CYS
23	v	722	PRO
23	v	723	SER
23	v	725	THR
23	v	726	ARG
23	v	733	ILE
24	n	51	PHE
24	n	55	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	n	57	LYS
24	n	58	ARG
24	n	59	ARG
24	n	61	LYS
24	n	62	THR
24	n	66	ASP
24	n	159	PRO
24	n	162	PRO
24	n	208	PRO
24	n	257	PRO
24	n	258	THR
24	n	260	PRO
24	n	295	SER
24	n	306	SER
24	n	327	PRO
24	n	340	PRO
24	n	373	PRO
24	n	424	PRO
24	n	428	PRO
24	n	436	PRO
25	o	17	PRO
25	o	26	SER
25	o	44	PRO
25	o	63	THR
25	o	96	PHE
25	o	109	LEU
25	o	134	SER
25	p	17	PRO
25	p	44	PRO
25	p	63	THR
25	p	80	LEU
25	p	85	GLN
25	p	93	LEU
25	p	99	ARG
25	p	109	LEU
25	q	17	PRO
25	q	44	PRO
25	q	55	PRO
25	q	56	SER
25	q	61	SER
25	q	102	LEU
25	q	126	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	q	172	PRO
25	q	175	PRO
25	q	196	PRO
25	q	215	CYS
25	q	235	THR
25	q	239	PRO
25	q	262	PRO
25	q	271	SER
25	q	350	PRO
25	q	412	PRO
25	r	17	PRO
25	r	44	PRO
25	r	63	THR
25	r	93	LEU
25	r	99	ARG
26	t	5	SER
26	t	7	VAL
26	t	13	PRO
26	t	77	PRO
26	t	96	PRO
26	t	100	THR
26	t	105	PRO
26	t	108	SER
26	t	133	PRO
26	t	136	VAL
26	t	150	THR
28	i	16	CYS
28	i	18	PHE
28	i	25	THR
28	i	79	LYS
28	i	81	LEU
29	h	79	LEU
30	j	18	ASN
30	j	41	ASP
30	j	71	LEU
31	l	10	LEU
31	l	76	ASP
32	m	20	LYS
32	m	26	TRP
32	m	30	GLN
32	m	77	ASP
32	m	99	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	m	104	ASP
33	g	24	PHE
33	g	49	ARG
33	g	77	THR
33	g	99	ASP
33	g	100	SER
28	u	16	CYS
28	u	18	PHE
28	u	25	THR
28	u	79	LYS
28	u	81	LEU
29	w	79	LEU
30	x	18	ASN
30	x	41	ASP
30	x	71	LEU
31	y	10	LEU
31	y	76	ASP
32	z	20	LYS
32	z	26	TRP
32	z	30	GLN
32	z	77	ASP
32	z	99	ASP
32	z	104	ASP
33	e	49	ARG
33	e	77	THR
33	e	99	ASP
33	e	100	SER
34	a	38	LYS
35	b	4	THR
35	b	44	PRO
35	b	71	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	265	ASN
1	A	405	ASN
1	A	429	ASN
1	A	658	ASN
1	A	659	HIS
1	A	705	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	848	ASN
1	A	868	GLN
1	A	1011	ASN
1	A	1156	HIS
1	A	1368	GLN
1	A	1376	ASN
1	A	1449	ASN
1	A	1529	ASN
1	A	1532	HIS
1	A	1652	HIS
1	A	1667	GLN
1	A	1737	GLN
1	A	1863	HIS
1	A	1947	HIS
1	A	2018	ASN
2	C	82	ASN
2	C	101	GLN
2	C	158	HIS
2	C	183	GLN
2	C	251	GLN
2	C	289	ASN
2	C	683	ASN
2	C	764	ASN
2	C	817	GLN
2	C	830	ASN
2	C	869	HIS
10	O	126	HIS
10	O	215	GLN
10	O	344	ASN
10	O	382	HIS
10	O	428	GLN
11	P	37	ASN
11	P	174	ASN
12	Q	53	ASN
12	Q	209	ASN
12	Q	225	GLN
13	R	58	HIS
13	R	91	HIS
13	R	92	HIS
13	R	150	HIS
13	R	155	GLN
13	R	191	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	R	201	ASN
13	R	227	ASN
13	R	248	ASN
14	S	5	HIS
14	S	8	GLN
14	S	34	HIS
14	S	173	HIS
15	T	34	GLN
15	T	57	HIS
15	T	112	ASN
15	T	116	ASN
15	T	143	HIS
16	Z	170	HIS
16	Z	184	GLN
16	Z	310	HIS
16	Z	354	HIS
16	Z	457	HIS
17	c	82	ASN
17	c	83	GLN
18	d	79	HIS
19	F	35	ASN
19	F	65	ASN
21	H	18	GLN
21	H	53	GLN
21	H	93	GLN
22	I	200	ASN
28	i	34	GLN
28	i	86	ASN
30	j	66	ASN
31	l	41	ASN
32	m	30	GLN
28	u	34	GLN
28	u	86	ASN
29	w	52	GLN
30	x	66	ASN
31	y	41	ASN
32	z	30	GLN
33	e	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	114/214 (53%)	30 (26%)	3 (2%)
4	E	102/112 (91%)	34 (33%)	7 (6%)
5	L	120/1175 (10%)	25 (20%)	5 (4%)
6	M	28/29 (96%)	7 (25%)	0
7	B	12/13 (92%)	5 (41%)	0
8	N	14/15 (93%)	7 (50%)	1 (7%)
All	All	390/1558 (25%)	108 (27%)	16 (4%)

All (108) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	29	G
3	D	31	G
3	D	32	G
3	D	33	U
3	D	42	A
3	D	44	A
3	D	74	U
3	D	75	A
3	D	76	U
3	D	77	A
3	D	79	C
3	D	80	G
3	D	81	A
3	D	82	A
3	D	84	A
3	D	90	C
3	D	92	U
3	D	94	C
3	D	101	C
3	D	104	G
3	D	127	U
3	D	164	C
3	D	165	A
3	D	166	U
3	D	170	U
3	D	171	U
3	D	172	U
3	D	173	U
3	D	174	G
3	D	175	G
4	E	12	A
4	E	13	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	14	C
4	E	15	C
4	E	16	C
4	E	30	G
4	E	33	C
4	E	36	U
4	E	37	U
4	E	39	G
4	E	43	C
4	E	50	G
4	E	51	A
4	E	52	G
4	E	54	U
4	E	57	U
4	E	60	G
4	E	62	A
4	E	65	U
4	E	66	C
4	E	67	C
4	E	68	C
4	E	73	A
4	E	74	U
4	E	75	A
4	E	80	U
4	E	81	G
4	E	85	C
4	E	86	G
4	E	87	U
4	E	88	U
4	E	90	U
4	E	91	A
4	E	92	C
5	L	16	U
5	L	17	U
5	L	18	U
5	L	19	U
5	L	20	G
5	L	25	A
5	L	26	G
5	L	30	A
5	L	31	A
5	L	32	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	85	A
5	L	111	C
5	L	115	U
5	L	116	U
5	L	117	U
5	L	118	U
5	L	119	G
5	L	120	G
5	L	1099	G
5	L	1107	C
5	L	1108	A
5	L	1111	U
5	L	1112	G
5	L	1114	G
5	L	1120	G
6	M	495	A
6	M	499	U
6	M	501	A
6	M	503	A
6	M	504	C
6	M	505	A
6	M	506	U
7	B	88	U
7	B	89	A
7	B	90	A
7	B	93	U
7	B	94	U
8	N	101	U
8	N	102	A
8	N	108	U
8	N	109	U
8	N	110	A
8	N	112	U
8	N	113	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	78	A
3	D	83	C
3	D	172	U
4	E	14	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	42	A
4	E	51	A
4	E	56	A
4	E	64	U
4	E	66	C
4	E	74	U
5	L	17	U
5	L	19	U
5	L	117	U
5	L	1107	C
5	L	1111	U
8	N	108	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, 13 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	GTP	C	1500	37	26,34,34	1.33	2 (7%)	32,54,54	1.97	7 (21%)

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
36	GTP	C	1500	37	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	1500	GTP	C5-C6	-4.66	1.38	1.47
36	C	1500	GTP	C5-C4	-2.07	1.37	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	1500	GTP	PB-O3B-PG	-6.23	111.45	132.83
36	C	1500	GTP	PA-O3A-PB	-4.27	118.18	132.83
36	C	1500	GTP	C5-C6-N1	3.30	119.77	113.95
36	C	1500	GTP	C3'-C2'-C1'	3.17	105.75	100.98
36	C	1500	GTP	C2-N1-C6	-3.07	119.44	125.10
36	C	1500	GTP	C8-N7-C5	2.92	108.56	102.99
36	C	1500	GTP	O6-C6-C5	-2.41	119.66	124.37

There are no chirality outliers.

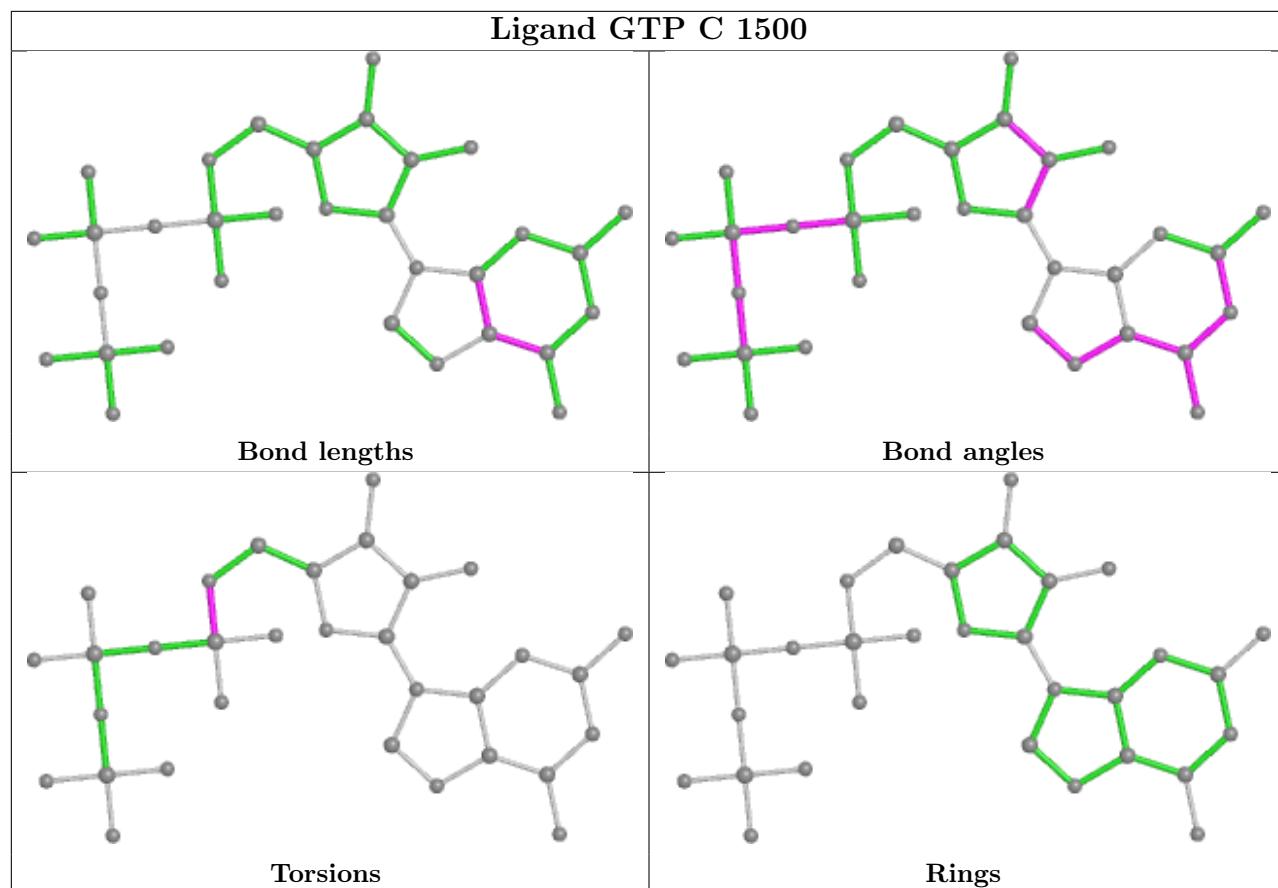
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	C	1500	GTP	C5'-O5'-PA-O3A
36	C	1500	GTP	C5'-O5'-PA-O1A
36	C	1500	GTP	C5'-O5'-PA-O2A

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](#)

There are no chain breaks in this entry.

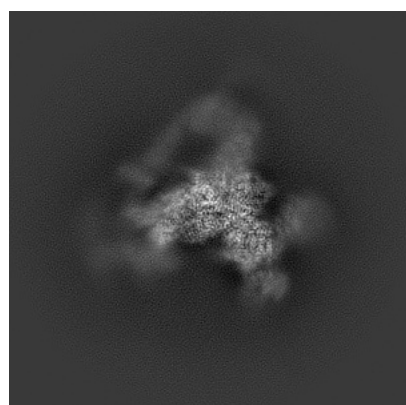
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9525. These allow visual inspection of the internal detail of the map and identification of artifacts.

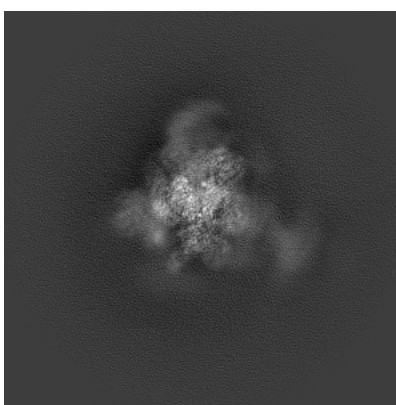
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

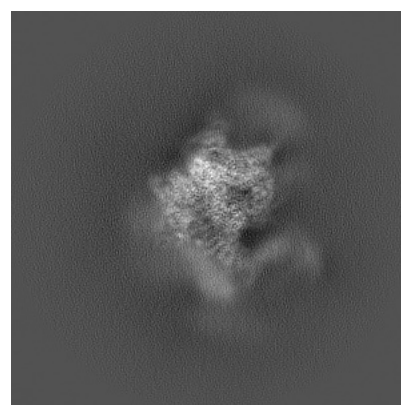
6.1.1 Primary map



X



Y

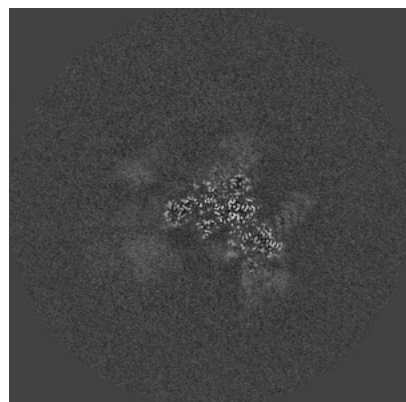


Z

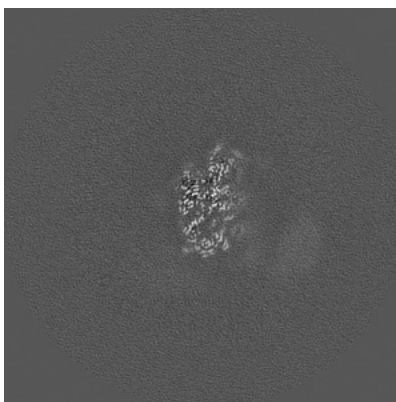
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

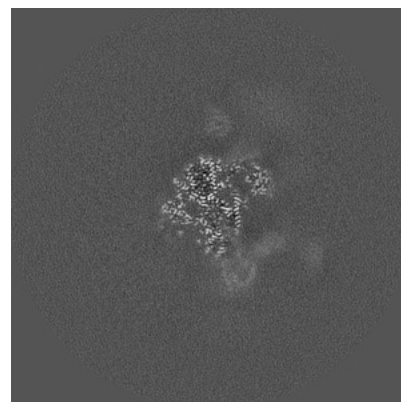
6.2.1 Primary map



X Index: 200



Y Index: 200

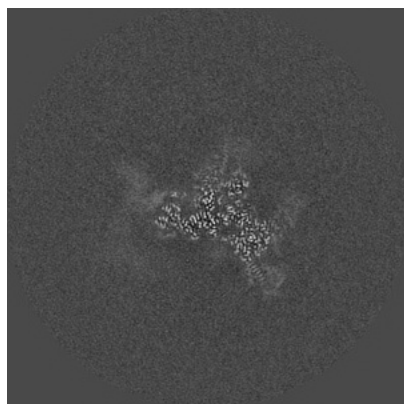


Z Index: 200

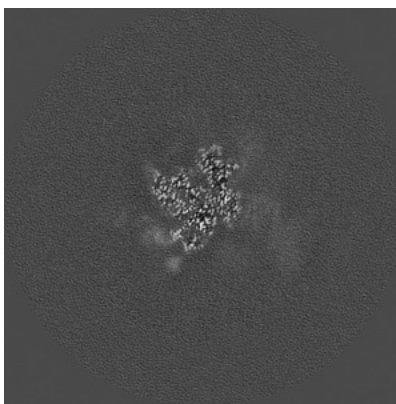
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

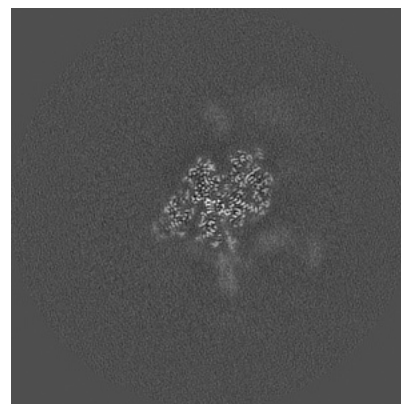
6.3.1 Primary map



X Index: 211



Y Index: 230



Z Index: 207

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 0.0413. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

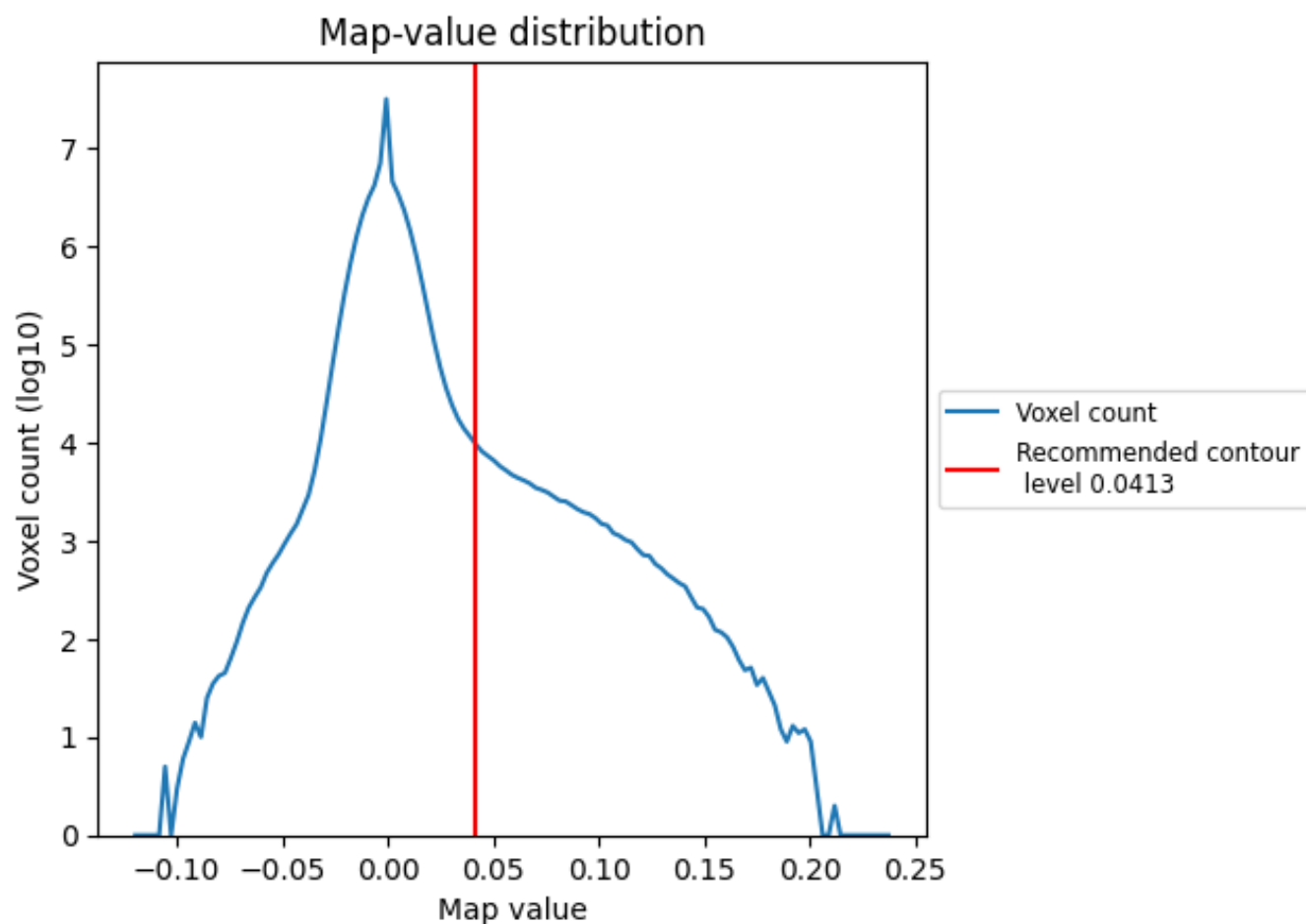
6.5 Mask visualisation

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

7 Map analysis [i](#)

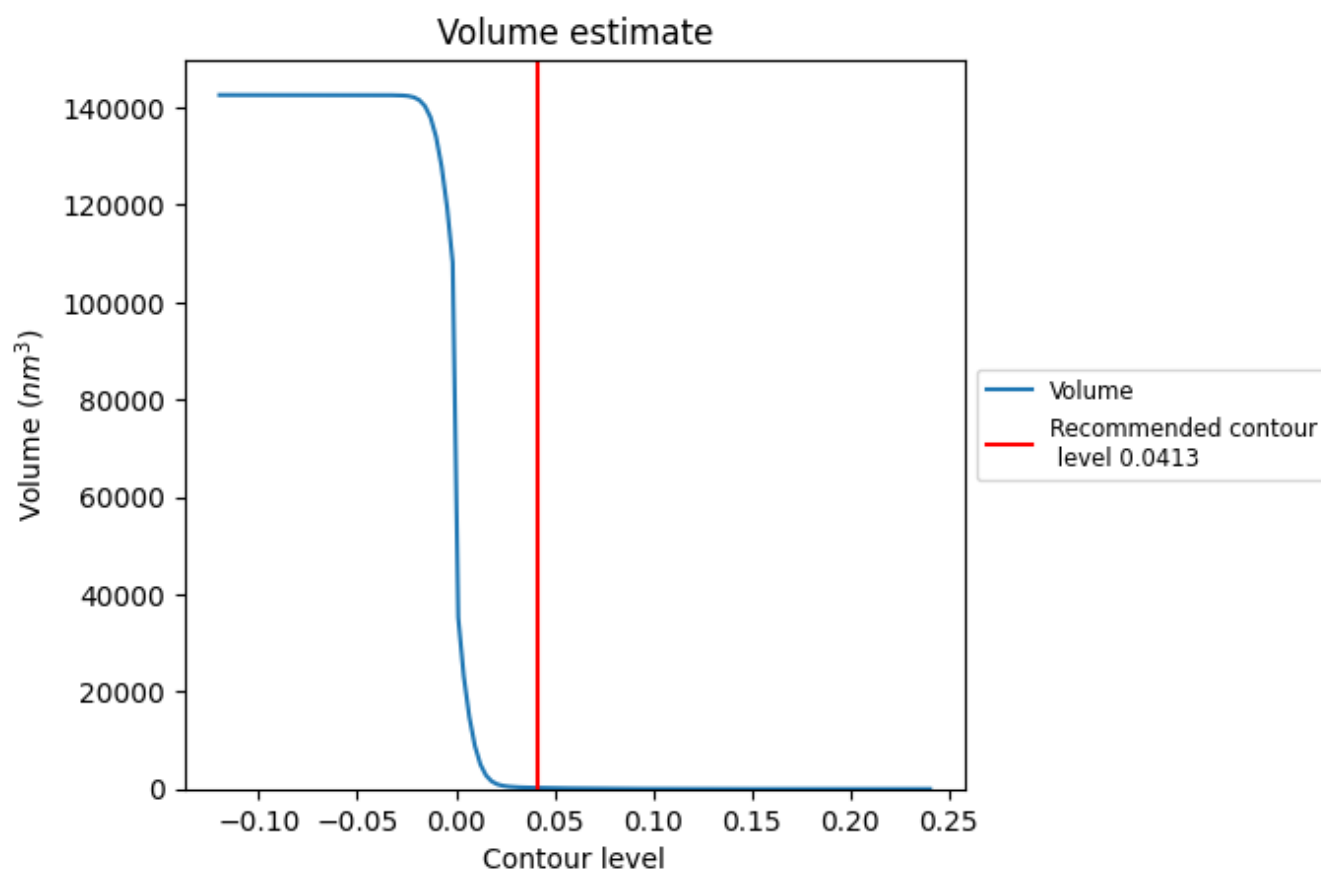
This section contains the results of statistical analysis of the map.

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.

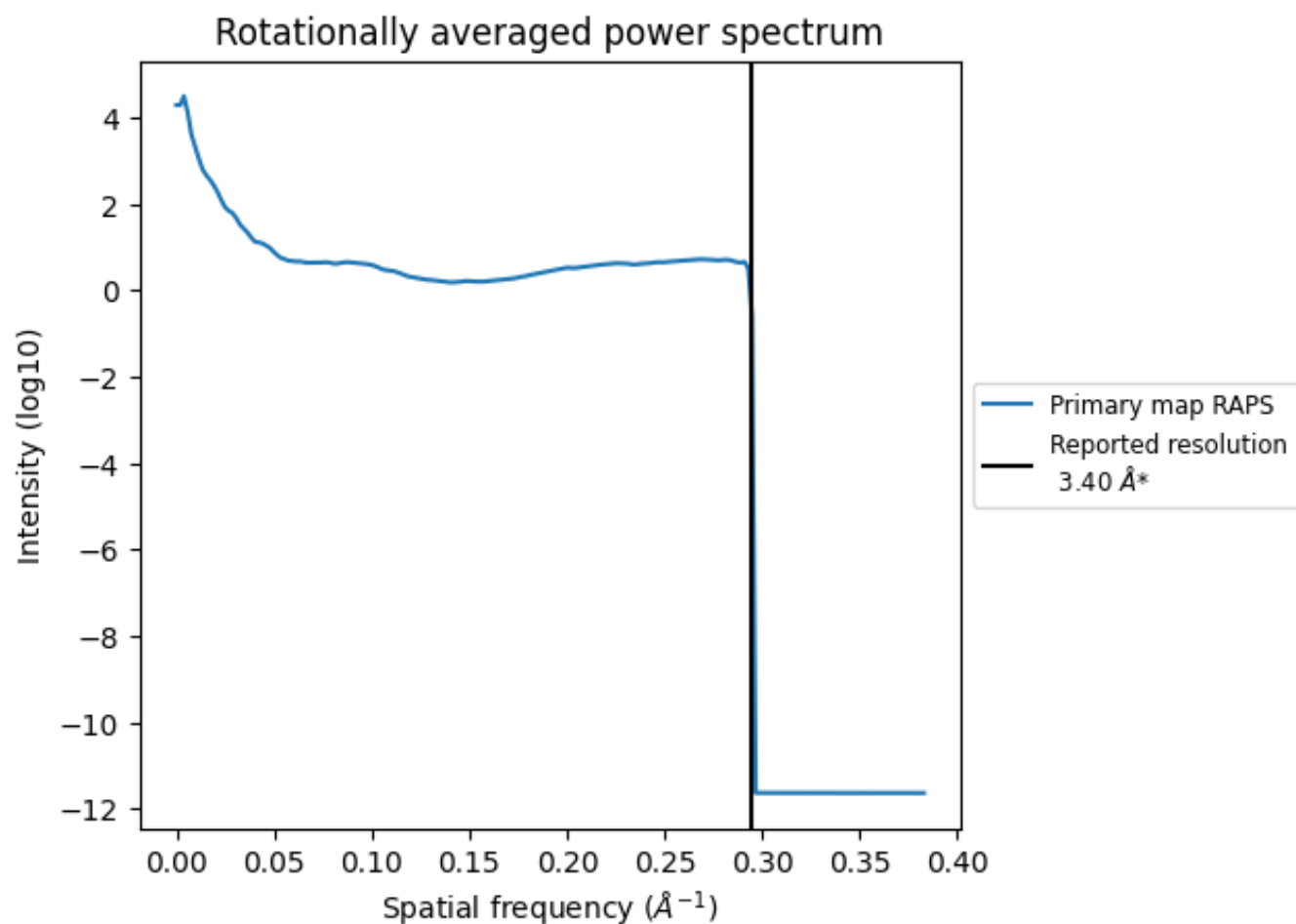
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm^3 ; this corresponds to an approximate mass of 208 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 0.294 Å⁻¹

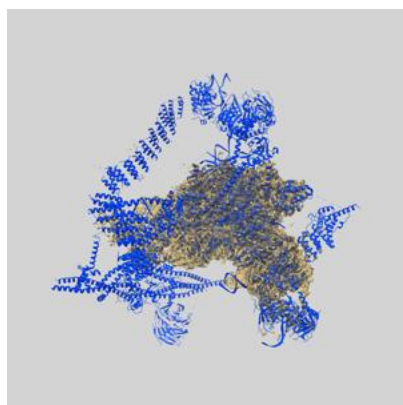
8 Fourier-Shell correlation ⓘ

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

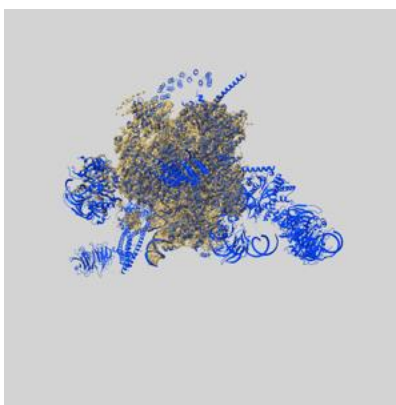
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9525 and PDB model 5GMK. Per-residue inclusion information can be found in section [3](#) on page [12](#).

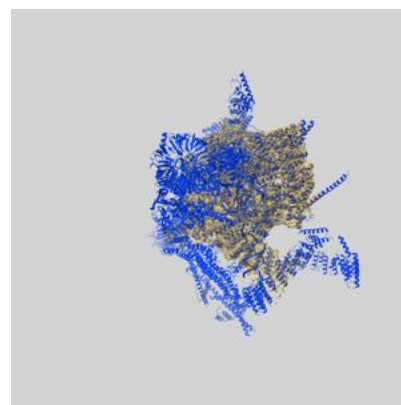
9.1 Map-model overlay [i](#)



X



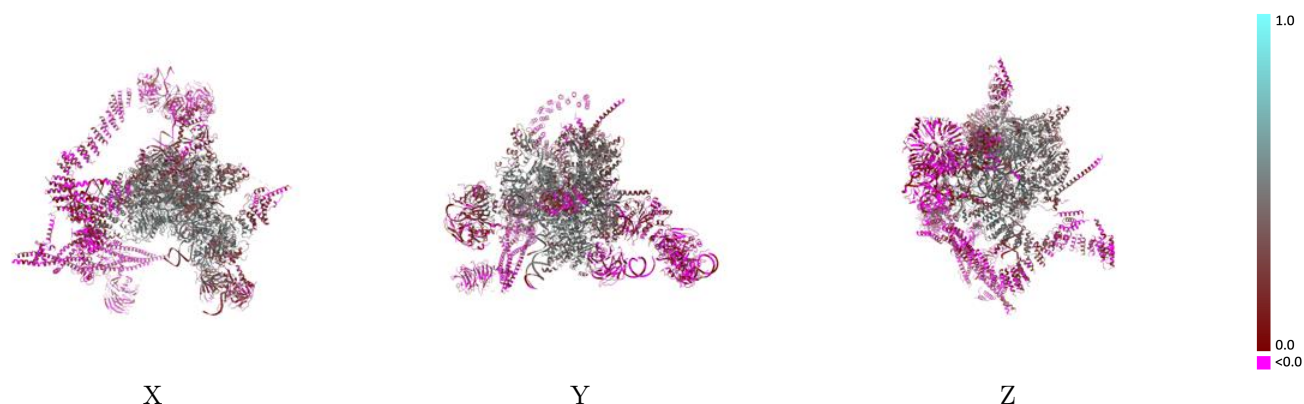
Y



Z

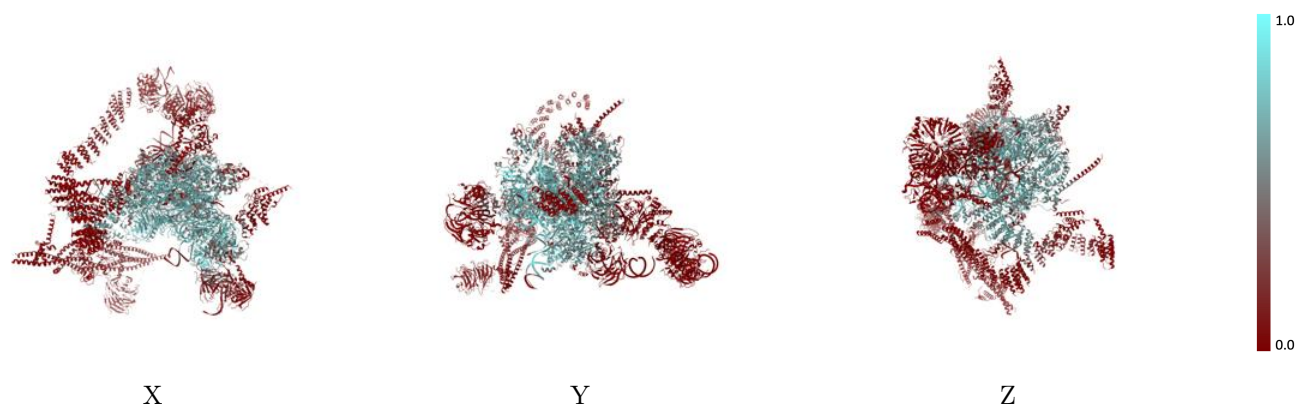
The images above show the 3D surface view of the map at the recommended contour level 0.0413 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



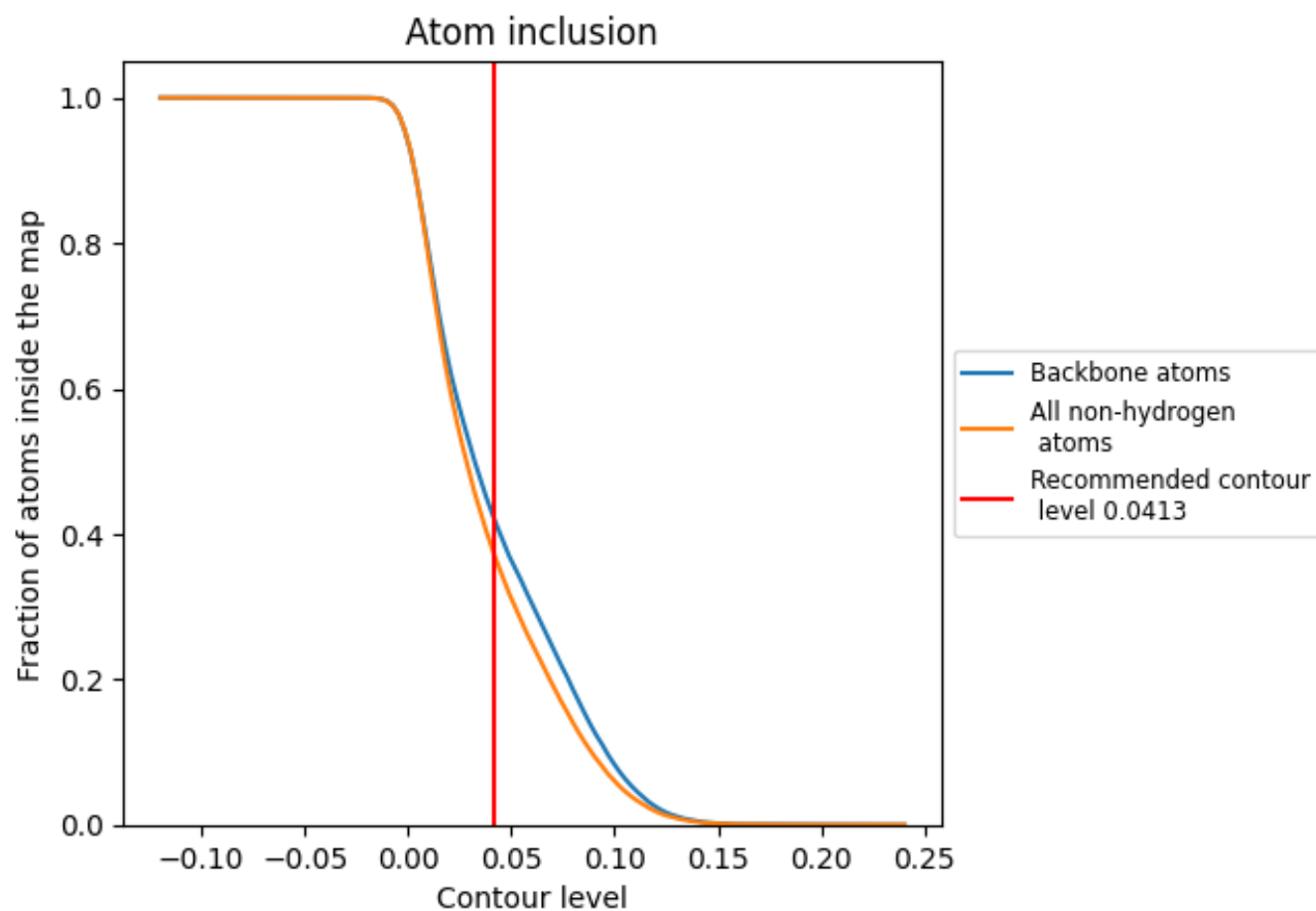
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0413).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 42% of all backbone atoms, 37% 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 (0.0413) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3748	 0.2790
A	 0.5814	 0.4060
B	 0.5600	 0.4420
C	 0.6551	 0.4330
D	 0.6349	 0.3920
E	 0.7214	 0.4230
F	 0.1436	 0.3760
G	 0.1399	 0.3200
H	 0.0992	 0.3320
I	 0.4218	 0.3730
J	 0.5455	 0.4740
L	 0.1586	 0.1240
M	 0.1168	 0.1810
N	 0.6026	 0.4150
O	 0.7512	 0.4890
P	 0.5039	 0.3740
Q	 0.5389	 0.4270
R	 0.6403	 0.4260
S	 0.4455	 0.4390
T	 0.6916	 0.4540
Z	 0.2319	 0.2360
a	 0.0000	 0.0020
b	 0.0000	 0.0090
c	 0.3235	 0.2250
d	 0.3836	 0.2600
e	 0.0000	 -0.0120
g	 0.0110	 0.1290
h	 0.0074	 0.0820
i	 0.0140	 0.1390
j	 0.0691	 0.2270
k	 0.0810	 0.2660
l	 0.2735	 0.3460
m	 0.0252	 0.1360
n	 0.0571	 0.0280
o	 0.0000	 -0.0230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	 0.0000	 0.0070
q	 0.0000	 -0.0060
r	 0.0000	 0.0490
s	 0.0000	 0.0380
t	 0.0000	 -0.0000
u	 0.0000	 -0.0020
v	 0.0403	 0.0590
w	 0.0000	 0.0260
x	 0.0000	 0.0060
y	 0.0000	 0.0170
z	 0.0000	 0.0090