



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 11:18 pm GMT

PDB ID : 7B9V
EMDB ID : EMD-12106
Title : Yeast C complex spliceosome at 2.8 Angstrom resolution with Prp18/Slu7 bound
Authors : Wilkinson, M.E.; Fica, S.M.; Galej, W.P.; Nagai, K.
Deposited on : 2020-12-14
Resolution : 2.80 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

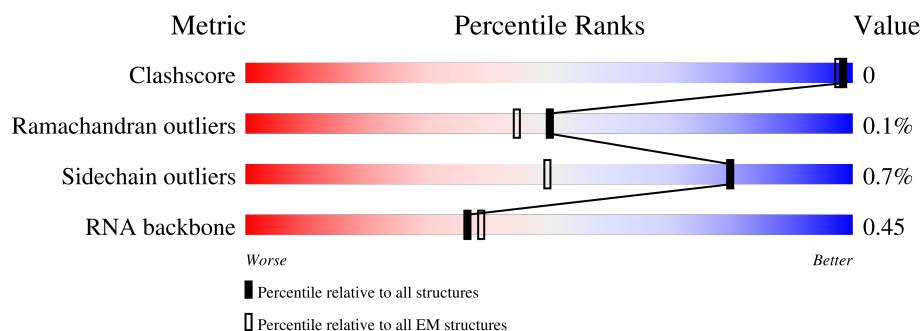
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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







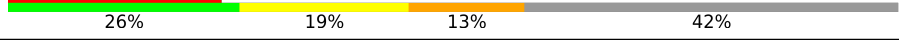


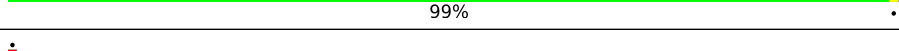
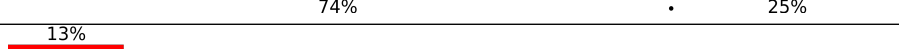
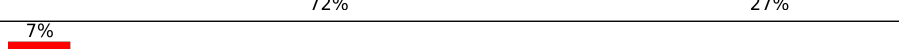


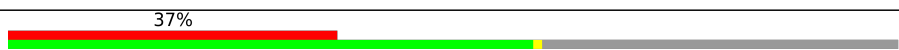

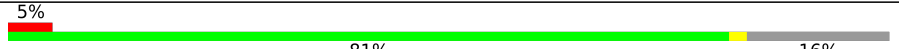










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	1175	<div> <div>6%</div> <div>9% 5% .</div> <div>83%</div> </div>
2	5	214	<div> <div>39%</div> <div>47%</div> <div>30%</div> <div>6%</div> <div>17%</div> </div>
3	6	112	<div> <div>16%</div> <div>67%</div> <div>20%</div> <div>9%</div> </div>
4	A	2413	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>
5	B	2163	<div> <div>25%</div> <div>77%</div> <div>21%</div> </div>
6	C	1008	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
7	D	291	<div> <div>9%</div> <div>66%</div> <div>33%</div> </div>




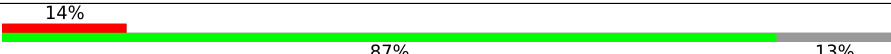
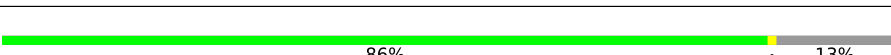
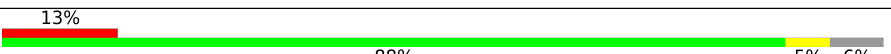
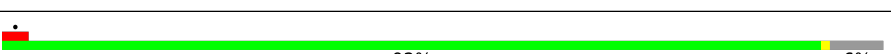
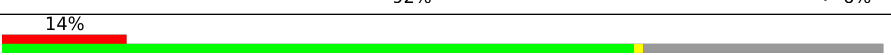

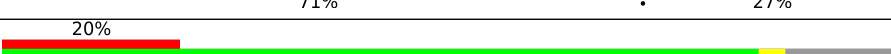
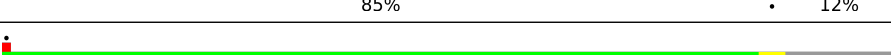

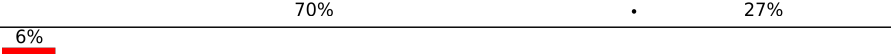





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Mol	Chain	Length	Quality of chain
8	E	47	
9	F	179	
10	G	235	
11	H	577	
12	I	95	
13	J	451	
14	K	379	
15	L	157	
16	M	339	
17	N	364	
18	O	590	
19	P	175	
20	Q	1071	
21	R	135	
22	S	687	
23	T	859	
24	W	238	
25	X	240	
26	Y	111	
27	Z	140	
28	a	251	
29	b	196	
29	k	196	
30	c	382	
31	d	101	

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Mol	Chain	Length	Quality of chain
31	n	101	
32	e	94	
32	p	94	
33	f	86	
33	q	86	
34	g	77	
34	r	77	
35	h	146	
35	l	146	
36	j	110	
36	m	110	
37	o	455	
38	s	175	
39	t	503	
39	u	503	
39	v	503	
39	w	503	
40	y	215	

2 Entry composition [i](#)

There are 45 unique types of molecules in this entry. The entry contains 109105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	196	Total	C	N	O	P	0	0
			4120	1846	681	1399	194		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	178	Total	C	N	O	P	0	0
			3777	1691	660	1249	177		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	102	Total	C	N	O	P	0	0
			2170	972	386	710	102		

- Molecule 4 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2191	Total	C	N	O	S	0	0
			18036	11598	3079	3295	64		

- Molecule 5 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1707	Total	C	N	O	S	0	0
			13675	8758	2279	2583	55		

- Molecule 6 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	898	Total	C	N	O	S	0	0
			7139	4614	1189	1309	27		

- Molecule 7 is a protein called Splicing factor YJU2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	194	Total	C	N	O	S	0	0
			1547	956	280	298	13		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	218	UNK	-	insertion	UNP A0A6L1B9A1
D	219	UNK	-	insertion	UNP A0A6L1B9A1
D	220	UNK	-	insertion	UNP A0A6L1B9A1
D	221	UNK	-	insertion	UNP A0A6L1B9A1
D	222	UNK	-	insertion	UNP A0A6L1B9A1
D	223	UNK	-	insertion	UNP A0A6L1B9A1
D	224	UNK	-	insertion	UNP A0A6L1B9A1
D	225	UNK	-	insertion	UNP A0A6L1B9A1
D	226	UNK	-	insertion	UNP A0A6L1B9A1
D	227	UNK	-	insertion	UNP A0A6L1B9A1
D	228	UNK	-	insertion	UNP A0A6L1B9A1
D	229	UNK	-	insertion	UNP A0A6L1B9A1
D	230	UNK	-	insertion	UNP A0A6L1B9A1
D	231	UNK	-	insertion	UNP A0A6L1B9A1
D	232	UNK	-	insertion	UNP A0A6L1B9A1
D	233	UNK	-	insertion	UNP A0A6L1B9A1
D	234	UNK	-	insertion	UNP A0A6L1B9A1
D	?	-	ASP	deletion	UNP A0A6L1B9A1
D	?	-	ASN	deletion	UNP A0A6L1B9A1
D	?	-	ASN	deletion	UNP A0A6L1B9A1
D	?	-	ASP	deletion	UNP A0A6L1B9A1

- Molecule 8 is a RNA chain called 5' exon of UBC4 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	14	Total	C	N	O	P	0	0
			304	136	59	95	14		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	64	Total	C	N	O	S	0	0
			505	314	92	98	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	72	UNK	LYS	conflict	UNP A0A6A5Q526
F	73	UNK	LYS	conflict	UNP A0A6A5Q526
F	74	UNK	SER	conflict	UNP A0A6A5Q526
F	75	UNK	GLY	conflict	UNP A0A6A5Q526
F	76	UNK	LEU	conflict	UNP A0A6A5Q526
F	77	UNK	GLU	conflict	UNP A0A6A5Q526
F	78	UNK	TRP	conflict	UNP A0A6A5Q526
F	79	UNK	MET	conflict	UNP A0A6A5Q526
F	80	UNK	TYR	conflict	UNP A0A6A5Q526
F	81	UNK	GLN	conflict	UNP A0A6A5Q526

- Molecule 10 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	138	Total	C	N	O	S	0	0
			1090	679	209	199	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	163	UNK	ARG	conflict	UNP A0A6V8S636
G	164	UNK	ASN	conflict	UNP A0A6V8S636
G	165	UNK	ASP	conflict	UNP A0A6V8S636
G	166	UNK	PHE	conflict	UNP A0A6V8S636
G	167	UNK	TYR	conflict	UNP A0A6V8S636
G	168	UNK	TYR	conflict	UNP A0A6V8S636
G	169	UNK	HIS	conflict	UNP A0A6V8S636
G	170	UNK	GLY	conflict	UNP A0A6V8S636
G	171	UNK	LYS	conflict	UNP A0A6V8S636
G	172	UNK	VAL	conflict	UNP A0A6V8S636
G	173	UNK	THR	conflict	UNP A0A6V8S636

- Molecule 11 is a protein called CWC22 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	453	Total	C	N	O	S	0	0
			3705	2383	612	692	18		

- Molecule 12 is a RNA chain called Branched intron and 3' exon of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	55	Total	C	N	O	P	0	0
			1068	476	159	378	55		

- Molecule 13 is a protein called BJ4_G0054360.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	370	Total	C	N	O	S	0	0
			2926	1849	513	553	11		

- Molecule 14 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	182	Total	C	N	O	S	0	0
			1455	911	268	270	6		

- Molecule 15 is a protein called BUD31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	156	Total	C	N	O	S	0	0
			1283	803	239	231	10		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	255	Total	C	N	O	S	0	0
			2048	1297	362	378	11		

- Molecule 17 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	264	Total	C	N	O	S	0	0
			2092	1331	364	382	15		

- Molecule 18 is a protein called Y55_G0042700.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	280	Total	C	N	O	S	0	0
			2143	1347	390	399	7		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	125	ALA	VAL	conflict	UNP A0A6L0ZW46
O	304	UNK	THR	conflict	UNP A0A6L0ZW46
O	305	UNK	LYS	conflict	UNP A0A6L0ZW46
O	306	UNK	GLN	conflict	UNP A0A6L0ZW46

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Chain	Residue	Modelled	Actual	Comment	Reference
O	307	UNK	GLY	conflict	UNP A0A6L0ZW46
O	308	UNK	LYS	conflict	UNP A0A6L0ZW46
O	309	UNK	VAL	conflict	UNP A0A6L0ZW46
O	310	UNK	THR	conflict	UNP A0A6L0ZW46
O	311	UNK	TYR	conflict	UNP A0A6L0ZW46
O	312	UNK	LYS	conflict	UNP A0A6L0ZW46
O	313	UNK	LYS	conflict	UNP A0A6L0ZW46
O	314	UNK	LYS	conflict	UNP A0A6L0ZW46
O	315	UNK	LEU	conflict	UNP A0A6L0ZW46
O	316	UNK	GLU	conflict	UNP A0A6L0ZW46
O	317	UNK	SER	conflict	UNP A0A6L0ZW46
O	318	UNK	LYS	conflict	UNP A0A6L0ZW46
O	319	UNK	ARG	conflict	UNP A0A6L0ZW46
O	320	UNK	GLN	conflict	UNP A0A6L0ZW46
O	321	UNK	LYS	conflict	UNP A0A6L0ZW46
O	322	UNK	LEU	conflict	UNP A0A6L0ZW46
O	323	UNK	ILE	conflict	UNP A0A6L0ZW46
O	324	UNK	GLU	conflict	UNP A0A6L0ZW46
O	325	UNK	ALA	conflict	UNP A0A6L0ZW46
O	326	UNK	GLN	conflict	UNP A0A6L0ZW46
O	327	UNK	ALA	conflict	UNP A0A6L0ZW46

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	74	Total	C	N	O	S	0	0
			607	382	120	104	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	49	ARG	LYS	conflict	UNP A0A6L0Y8G8
P	68	MET	VAL	conflict	UNP A0A6L0Y8G8
P	99	VAL	ILE	conflict	UNP A0A6L0Y8G8

- Molecule 20 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	624	Total	C	N	O	S	0	0
			4959	3184	833	921	21		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	81	Total	C	N	O	S	0	0
			555	336	109	109	1		

- Molecule 22 is a protein called CLF1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	549	Total	C	N	O	S	0	0
			4170	2663	732	762	13		

- Molecule 23 is a protein called SYF1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	720	Total	C	N	O	S	0	0
			5387	3441	914	1015	17		

- Molecule 24 is a protein called HLJ1_G0053790.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	214	Total	C	N	O	S	0	0
			1734	1084	317	324	9		

- Molecule 25 is a protein called Unassigned structure.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 26 is a protein called BJ4_G0027490.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	88	Total	C	N	O	S	0	0
			713	457	124	129	3		

- Molecule 27 is a protein called NTC20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	55	Total	C	N	O	S	0	0
			446	276	85	83	2		

- Molecule 28 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	138	Total	C	N	O	S	0	0
			1132	729	195	205	3		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	93	Total	C	N	O	S	0	0
			752	477	138	134	3		
29	k	102	Total	C	N	O	S	0	0
			830	526	155	146	3		

- Molecule 30 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	37	Total	C	N	O	S	0	0
			293	180	52	56	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	9	GLU	LYS	conflict	UNP A0A6V8RGB0
c	154	ASN	THR	conflict	UNP A0A6V8RGB0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	82	Total	C	N	O	S	0	0
			633	404	109	118	2		
31	n	82	Total	C	N	O	S	0	0
			633	404	109	118	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	77	Total	C	N	O	S	0	0
			606	398	94	111	3		
32	p	77	Total	C	N	O	S	0	0
			606	398	94	111	3		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	75	Total	C	N	O	S	0	0
			601	385	105	110	1		
33	q	75	Total	C	N	O	S	0	0
			601	385	105	110	1		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	72	Total	C	N	O	S	0	0
			557	351	97	107	2		
34	r	72	Total	C	N	O	S	0	0
			557	351	97	107	2		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	106	Total	C	N	O	S	0	0
			819	516	144	156	3		
35	l	106	Total	C	N	O	S	0	0
			819	516	144	156	3		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	97	Total	C	N	O	S	0	0
			795	506	144	141	4		
36	m	97	Total	C	N	O	S	0	0
			795	506	144	141	4		

- Molecule 37 is a protein called CDC40 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	330	Total	C	N	O	P S	0	0
			2673	1696	475	493	1 8		

- Molecule 38 is a protein called SNT309 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	61	Total	C	N	O	S	0	0
			426	277	76	72	1		

- Molecule 39 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	107	Total	C	N	O	S	0	0
			794	511	128	152	3		
39	u	117	Total	C	N	O	S	0	0
			856	551	138	164	3		
39	v	113	Total	C	N	O	S	0	0
			827	532	134	158	3		
39	w	438	Total	C	N	O	S	0	0
			3405	2167	551	670	17		

- Molecule 40 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	134	Total	C	N	O	S	0	0
			1003	618	187	197	1		

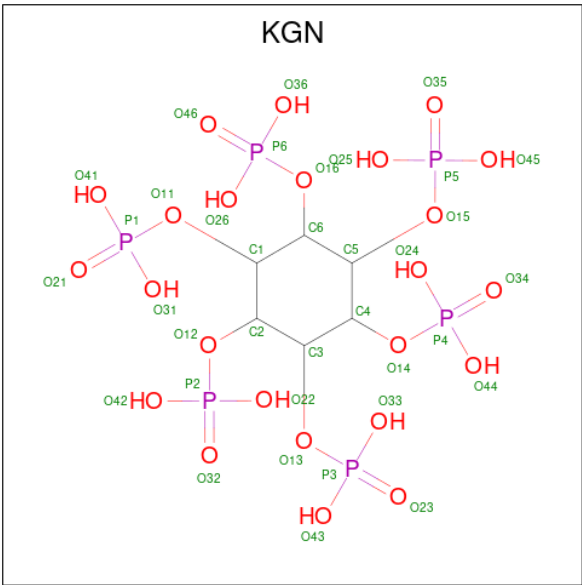
- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	6	5	Total	Mg	0
			5	5	
41	C	1	Total	Mg	0
			1	1	

- Molecule 42 is POTASSIUM ION (three-letter code: K) (formula: K).

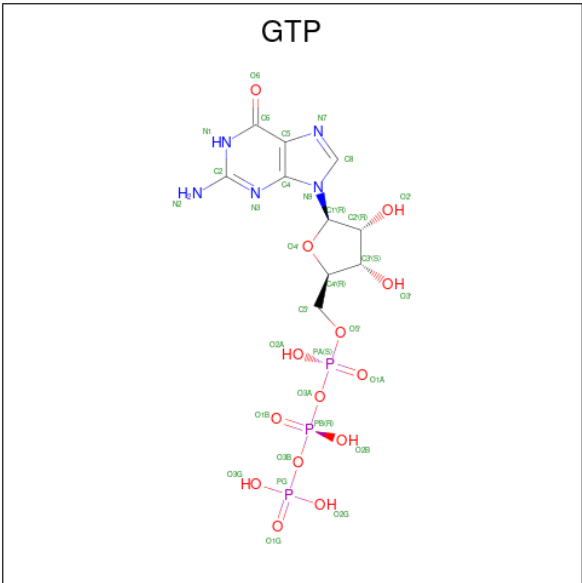
Mol	Chain	Residues	Atoms		AltConf
42	6	1	Total	K	0
			1	1	

- Molecule 43 is D-chiro inositol hexakisphosphate (three-letter code: KGN) (formula: C₆H₁₈O₂₄P₆).



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

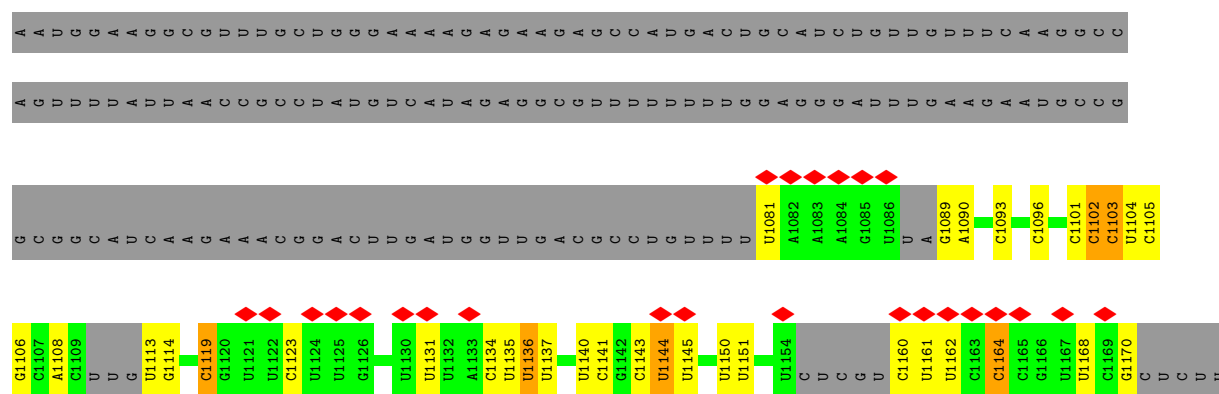
- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



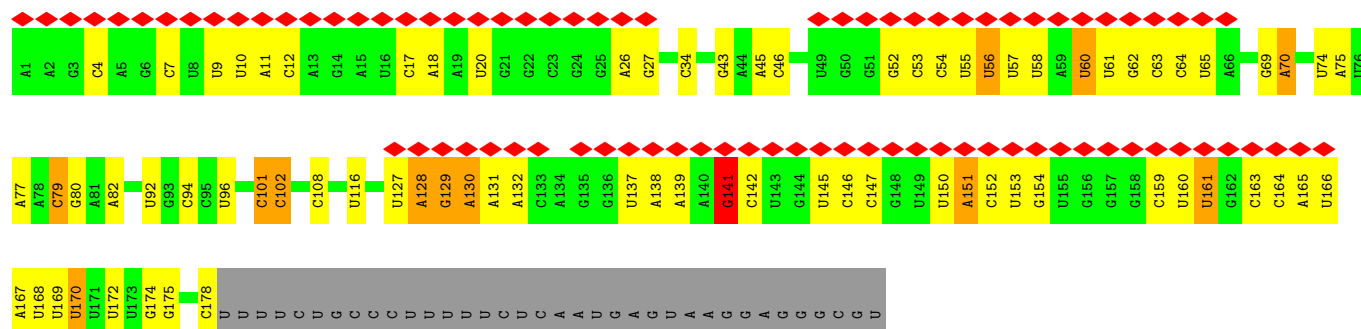
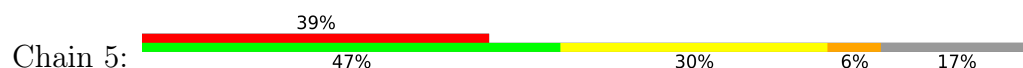
Mol	Chain	Residues	Atoms					AltConf
44	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

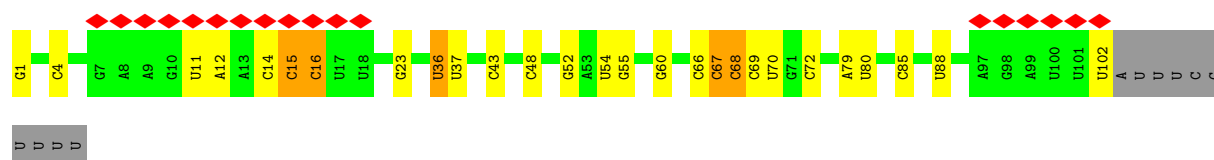
Mol	Chain	Residues	Atoms		AltConf
45	D	1	Total 1	Zn 1	0
45	L	3	Total 3	Zn 3	0
45	M	1	Total 1	Zn 1	0
45	N	2	Total 2	Zn 2	0
45	c	1	Total 1	Zn 1	0



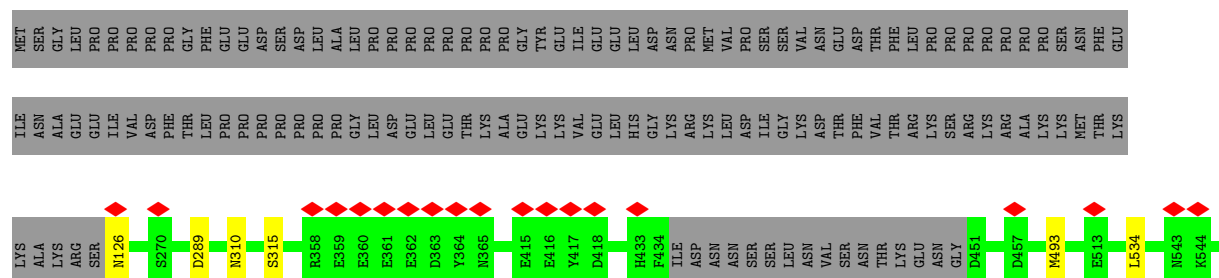
• Molecule 2: U5 snRNA



• Molecule 3: U6 snRNA

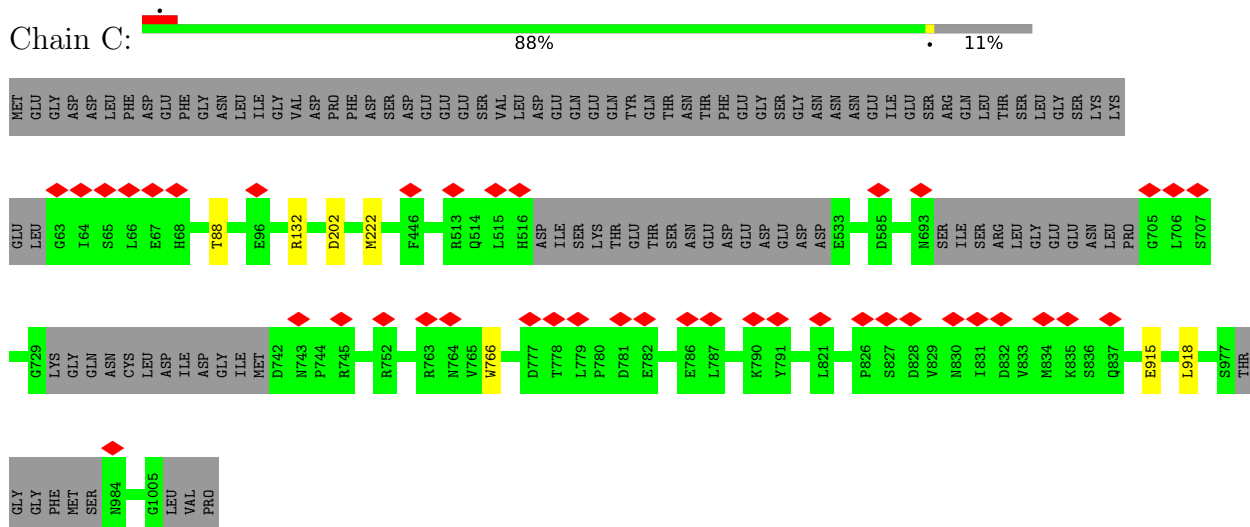


• Molecule 4: Pre-mRNA-splicing factor 8

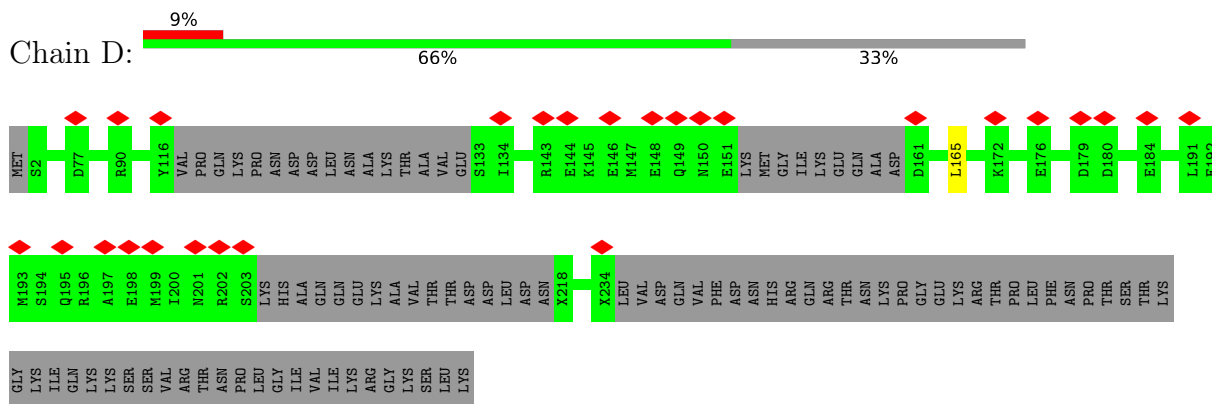


PRO	ALA	ILE	PRO	PRO	VAL	ILE	ASP	LEU	GLU	LYS	LYS	PHE	ASP	GLU	SER	SER	LYS	LEU	MET	T442	V443	T444	K445	E450	G451	S452	F453	K454	R455	V456	K457	P458	Q459	Y460	D461	E462	I463	H464	I465	P466	A467	P468	S469	K470	P471	V472	I473	D474	Y475	K478	E479	P562	I480	T481	S482	L483	P484
E489	A490	F491	P492	S493	S494	E495	T496	L588	T497	S498	L499	N500	P501	F507	E512	M517	L518	T444	I519	C520	A521	P522	T523	G524	S525	G526	K527	T528	N529	I530	A531	L532	L533	T534	V535	L536	K537	A538	L539	S540	H541	L550	N551	L552	S553	A554	I560	A561	P562	L563	K564	A565	L566	R572			
Q575	R576	R577	G582	A586	E587	T588	T589	G590	D591	S592	R593	L594	S595	R596	K597	Q598	I599	D600	L605	V606	P609	D613	T616	R617	N618	S619	G620	N621	L622	V628	R629	L630	I632	I633	D634	E635	I636	D641	D642	E648	R653	A657	S658	K659	Y660	G661											
Q662	E663	I667	I668	G669	L670	S671	A672	V680	G681	R682	L683	R685	K688	E689	G690	L691	S695	S697	F698	P702	L703	T704	Q705	Q706	F707	C708	G709	I710	K711	E712	R713	N714	S715	L716	A725	C726	E736	G737	F743	A754	T755	W756	A762	E763	E764	T767	H768										
K769	L770	T771	K772	N773	D774	A775	G776	N787	V788	L789	D790	L793	R794	K795	L796	I797	E798	S799	G800	I801	G802	T803	G807	L808	T809	R810	S816	E817	A821	D822	G823	L824	L825	Q826	T833	L834	A835	W836	G837	L840	V845	I846	I847	Y853	S854	P855	E856	E861									
L872	E885	G886	I887	I888	I889	S910	Q911	F912	V913	S914	D918	N919	L920	N921	R947	W853	K956	V957	P958	D959	I960	S961	S962	Q965	L966	K967	K968	L973	V974	H975	S976	A977	L978	C979	E983	D990	E997	A998	F1008	R1020	E1021	L1022	D1023	R1033	I1034												
F1035	E1039	E1040	V1044	S1045	V1046	R1047	R1052	Q1056	L1057	L1058	E1059	K1060	A1061	I1065	R1066	E1067	D1068	I1069	D1070	D1071	P1072	Y1083	L1087	K1088	F1089	E1090	G1091	H1102	A1105	G1106	R1107	K1118	K1138	K1150	V1154	R1159	L1160	T1164	D1169	E1174	R1181																
R1184	K1187	Y1188	G1189	M1202	N1207	A1224	D1229	M1230	N1231	V1232	D1245	T1246	D1247	G1248	D1249	S1250	Y1253	D1262	G1265	Q1281	I1293	S1294	E1295	H1299	S1300	E1301	S1307	F1308	N1309	G1310	F1311	K1312	K1316	F1317	P1318	P1319	P1320	L1323	L1324	E1325	N1326	I1327	S1328														
I1329	G1335	M1336	D1337	F1339	S1340	E1341	K1350	Q1354	V1355	F1356	M1361	S1362	N1363	S1370	G1371	K1372	A1380	A1383	R1389	A1395	V1396	Y1397	I1405	D1406	F1407	W1412	L1428	G1429	N1430	D1431	P1432	S1433	L1434	L1455	M1471	I1472	Y1473	D1474	D1475	A1476	Y1488	E1503															
K1504	K1505	I1506	A1518	R1519	T1528	K1529	P1537	S1538	E1539	R1540	I1541	E1542	P1543	L1544	E1545	I1546	K1552	D1553	F1559	N1560	F1561	A1567	A1570	S1571	A1572	A1573	A1574	N1577	R1578	F1584	L1585	P1586	R1587	N1588	M1592	E1593	F1601	A1604	I1605	E1606	V1607	D1608	N1611	Y1612	E1613	E1614											
E1615	K1623	L1624	T1625	D1626	R1630	L1633	I1639	G1643	R1654	Y1658	G1659	A1660	S1667	K1668	D1669	A1672	F1673	D1678	G1684	D1689	G1690	A1691	G1692	H1693	M1701	E1702	L1703	M1706	A1710	S1711	G1712	M1713	D1714	S1715	M1716	A1717	G1718	K1719	M1727	M1728	K1729	K1733															
I1737	E1738	P1739	L1740	Y1745	A1759	M1760	I1763	S1767	Y1768	Y1769	G1790	V1791	D1792	T1794	F1819	D1824	T1825	GLU	ALA	VAL	THR	ALA	GLU	VAL	ASN	GLY	GLY	ASP	ASP	GLU	ALA	T1841	T1846	N1849	A1853	G1857	V1858	F1861	F1866	S1871	S1874	T1875															
L1876	L1883	A1886	V1887	E1888	F1889	E1890	S1891	R1899	R1906	R1912	F1913	P1914	E1915	H1916	T1917	S1918	S1919	G1920	A1932	D1942	F1943	Q1944	D1946	L1947	K1948	D1949	I1950	L1951	E1952	K1953	I1964	L1965	S1966	A1967	N1968	G1969	Y1970	I1984	V1990	H1999	K2009	E2010	I2011	N2012	Y2013												

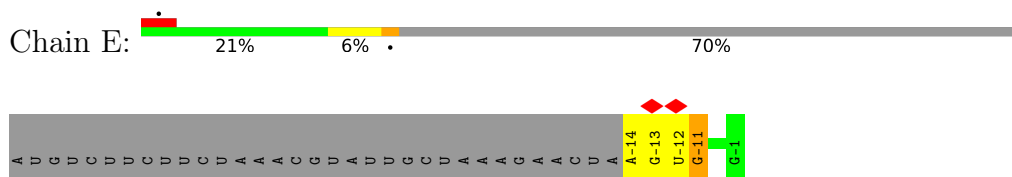
- Molecule 6: Pre-mRNA-splicing factor SNU114



- Molecule 7: Splicing factor YJU2



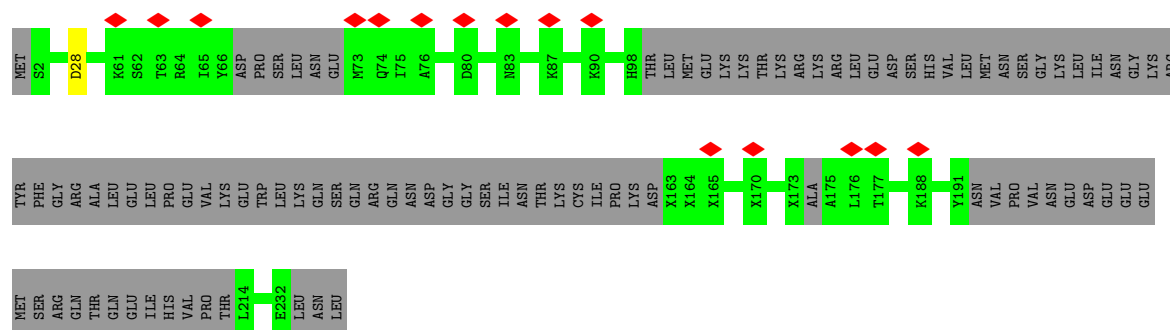
- Molecule 8: 5' exon of UBC4 mRNA



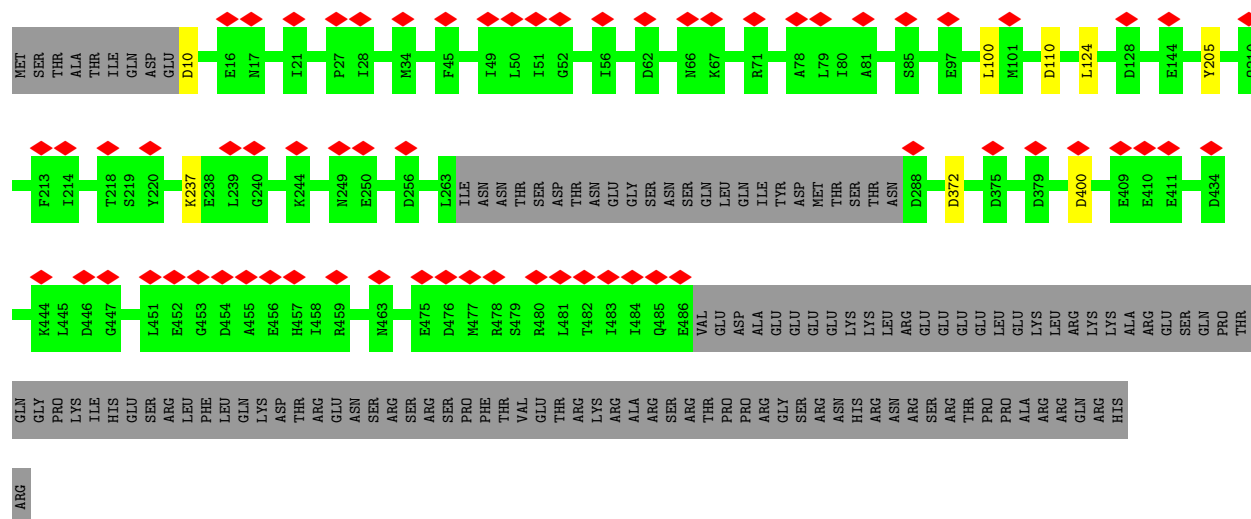
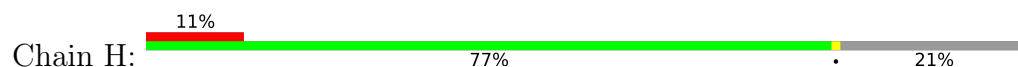
- Molecule 9: Pre-mRNA-splicing factor CWC25



- Molecule 10: Pre-mRNA-splicing factor ISY1



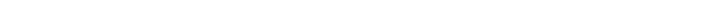
- Molecule 11: CWC22 isoform 1

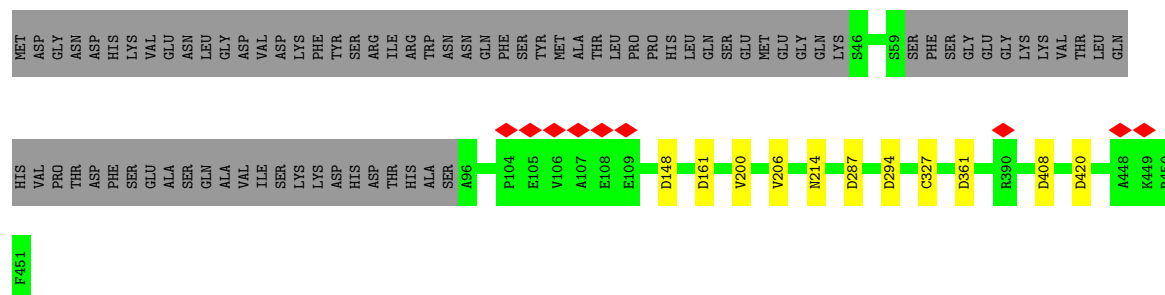


- Molecule 12: Branched intron and 3' exon of UBC4 pre-mRNA



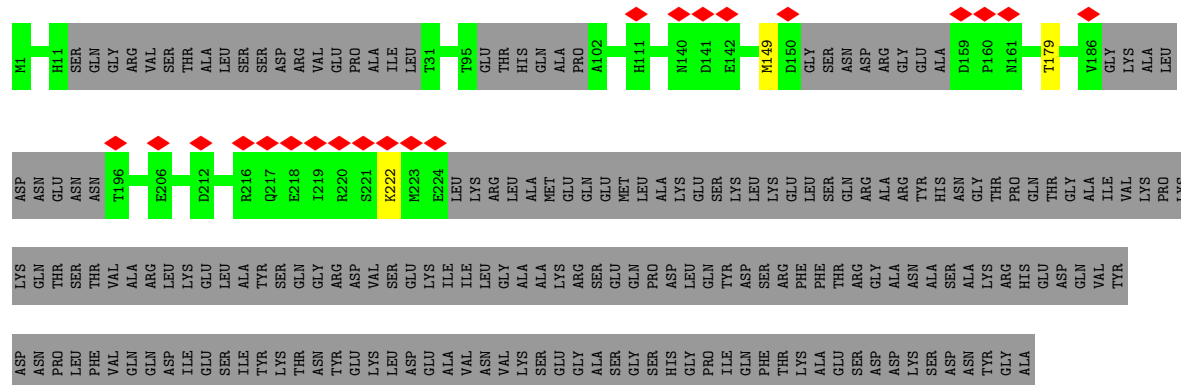
- Molecule 13: BJ4 G0054360.mRNA.1.CDS.1

Chain J:  80% 18%



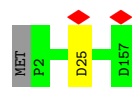
- Molecule 14: Pre-mRNA-processing protein 45

Chain K: 

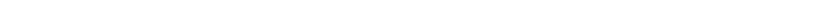


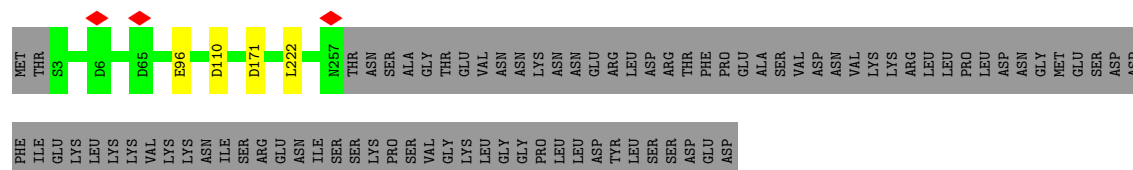
- Molecule 15: BUD31 isoform 1

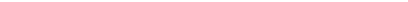
Chain L:  99%



- Molecule 16: Pre-mRNA-splicing factor CWC2

Chain M:  74% 25%



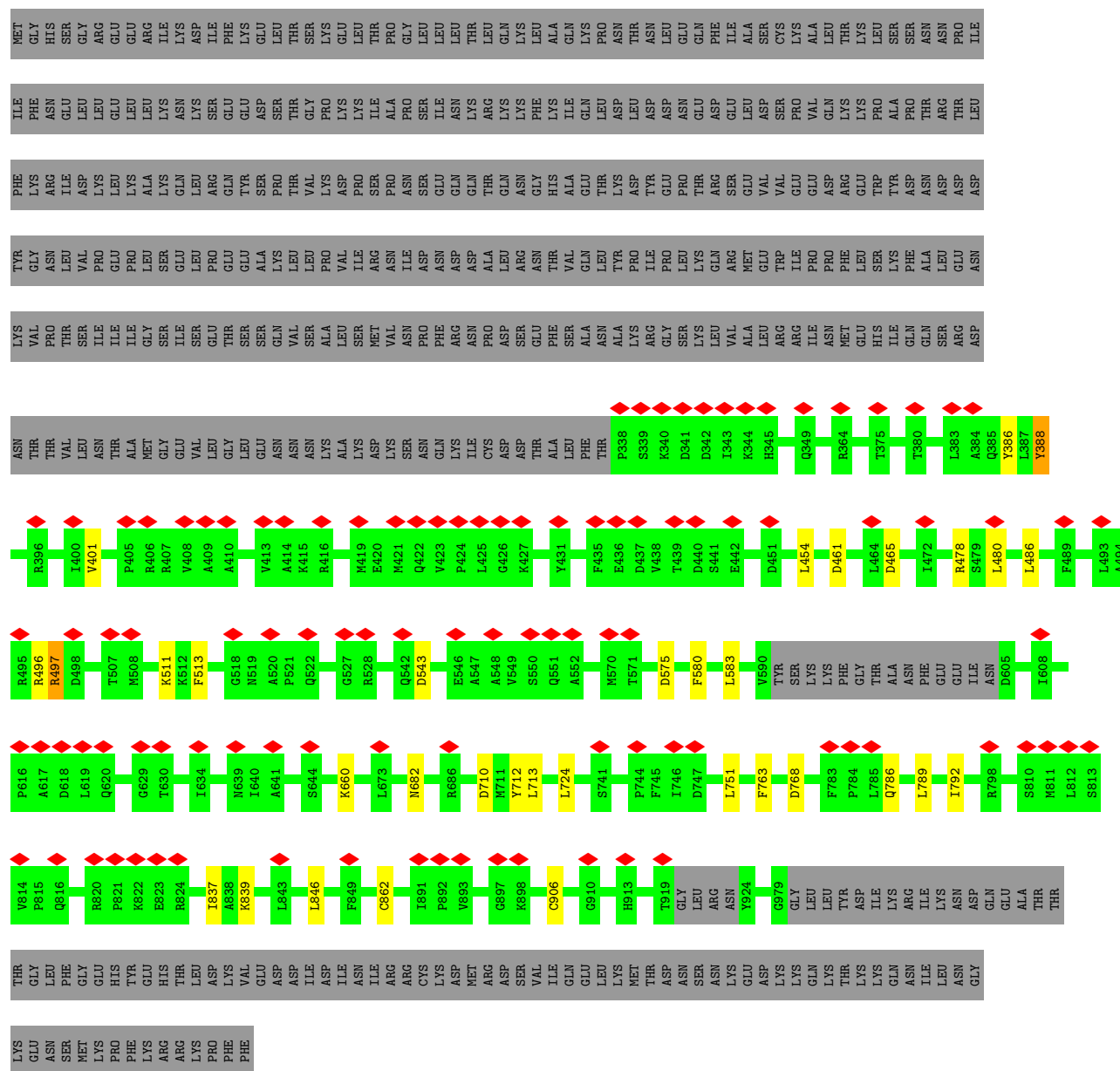
Chain N:  13% 72% 27%

Chain O: 

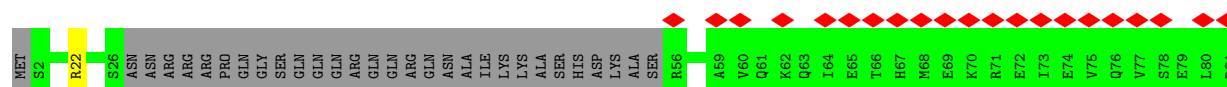
Chain P: 41% 58%

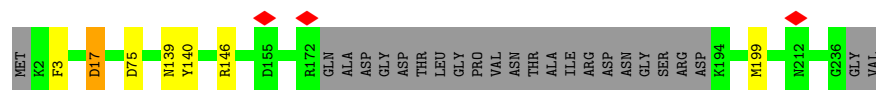


• Molecule 20: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

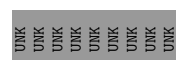


• Molecule 21: Pre-mRNA-splicing factor CWC21

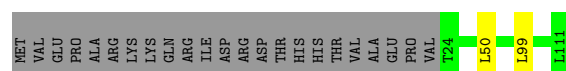
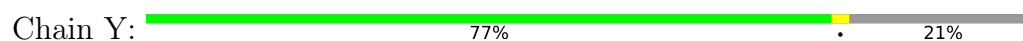




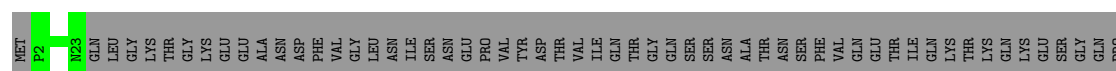
- Molecule 25: Unassigned structure



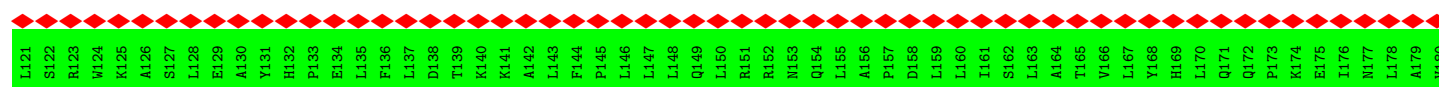
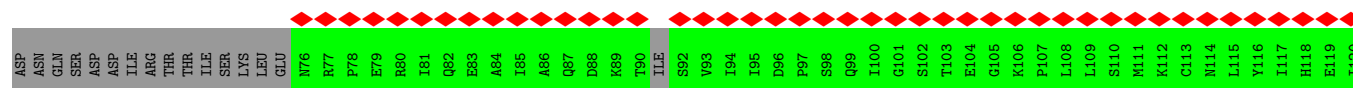
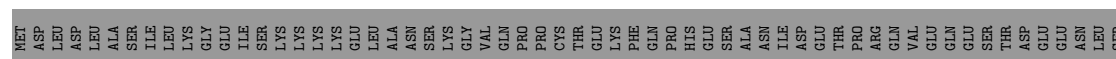
- Molecule 26: BJ4_G0027490.mRNA.1.CDS.1



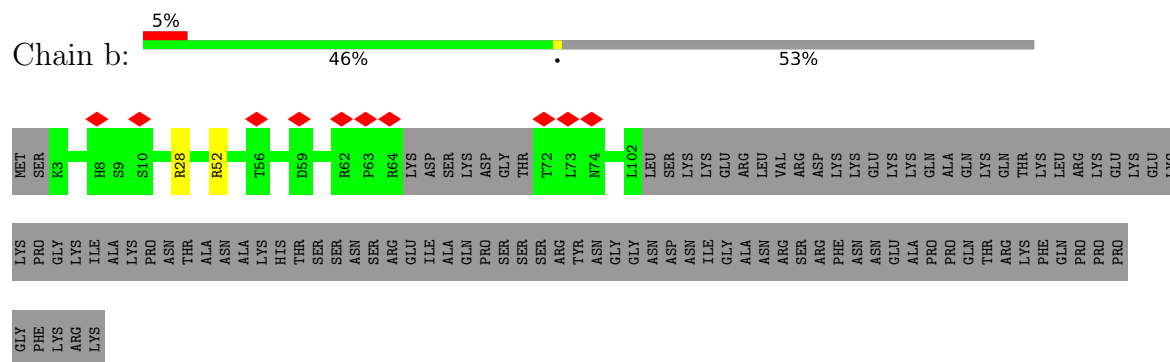
- Molecule 27: NTC20 isoform 1



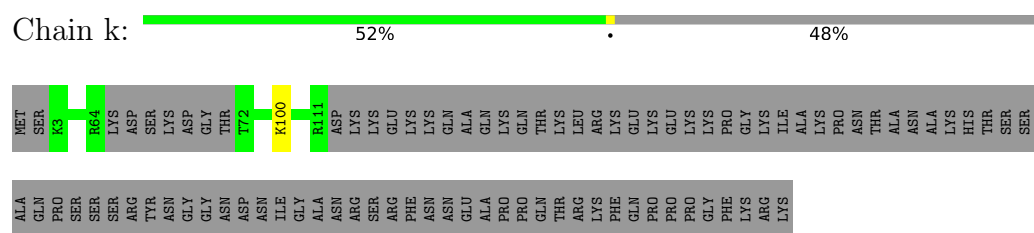
- Molecule 28: Pre-mRNA-splicing factor 18



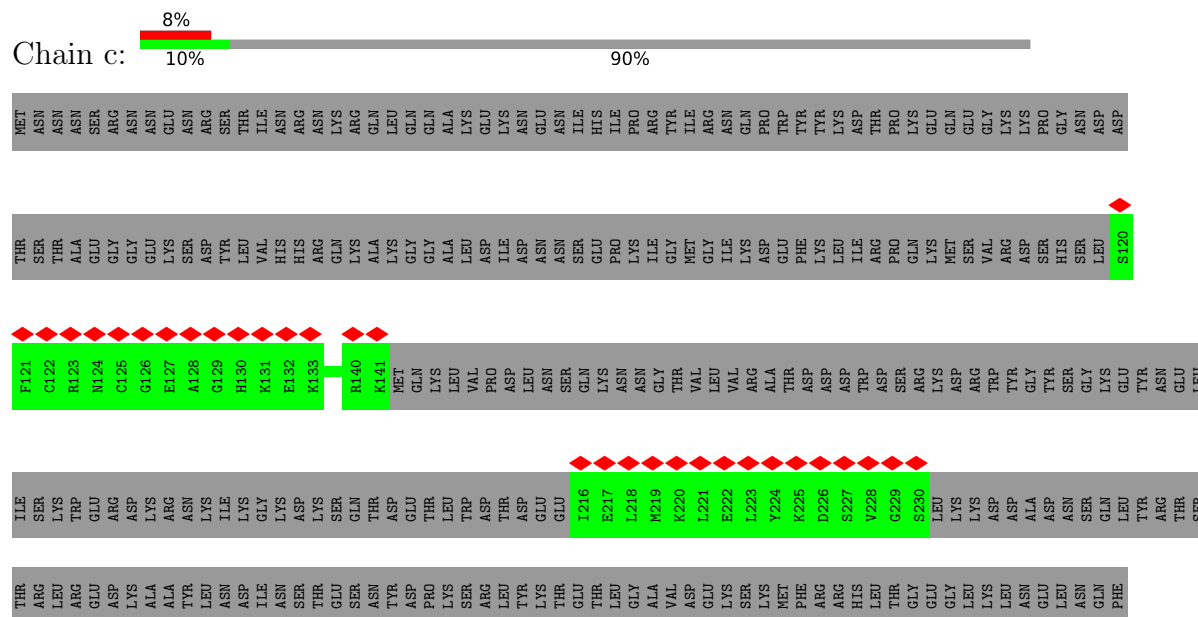
- Molecule 29: Small nuclear ribonucleoprotein-associated protein B

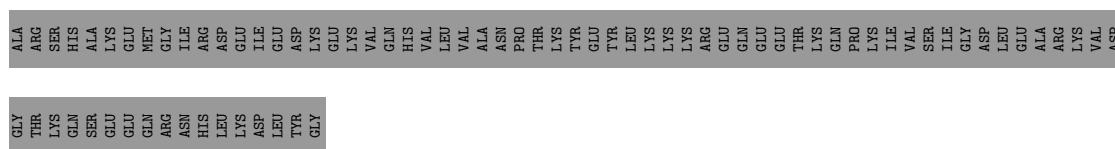


- Molecule 29: Small nuclear ribonucleoprotein-associated protein B

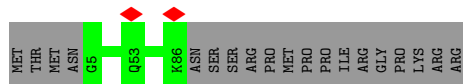
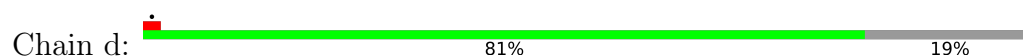


- Molecule 30: Pre-mRNA-splicing factor SLU7

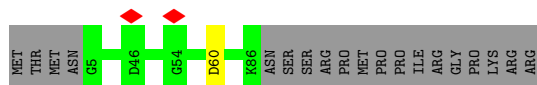
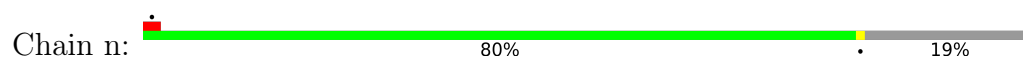




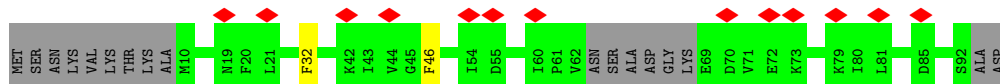
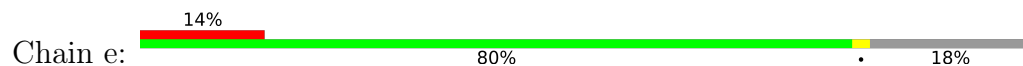
• Molecule 31: Small nuclear ribonucleoprotein Sm D3



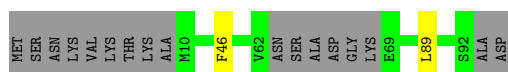
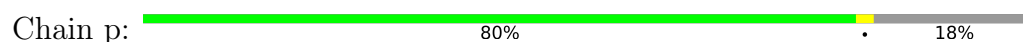
• Molecule 31: Small nuclear ribonucleoprotein Sm D3



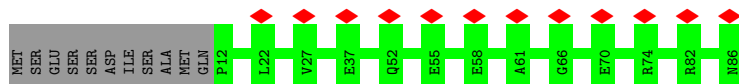
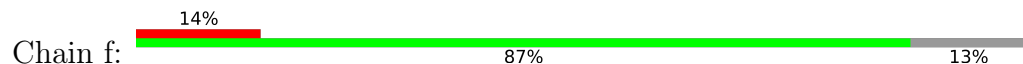
• Molecule 32: Small nuclear ribonucleoprotein E



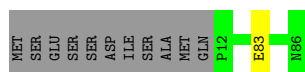
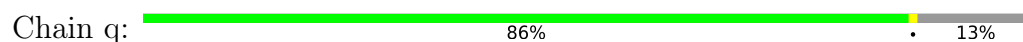
• Molecule 32: Small nuclear ribonucleoprotein E



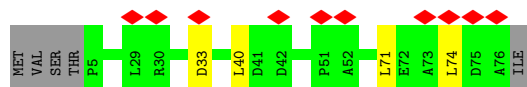
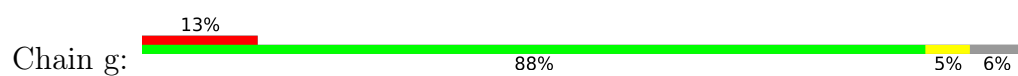
• Molecule 33: Small nuclear ribonucleoprotein F



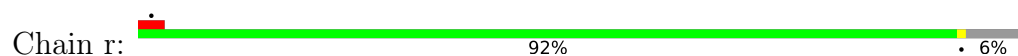
• Molecule 33: Small nuclear ribonucleoprotein F



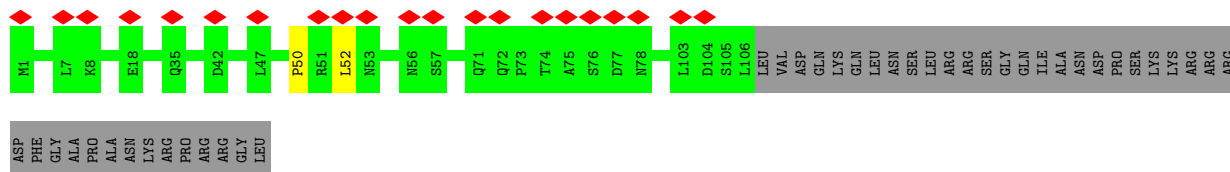
• Molecule 34: Small nuclear ribonucleoprotein G



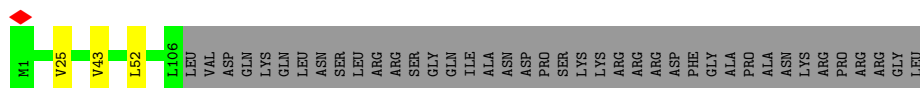
- Molecule 34: Small nuclear ribonucleoprotein G



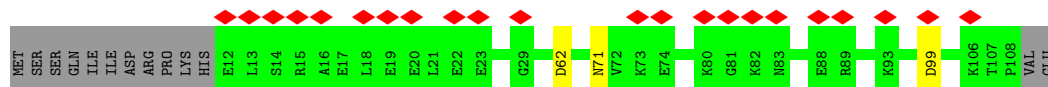
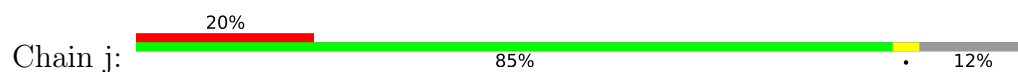
- Molecule 35: Small nuclear ribonucleoprotein Sm D1



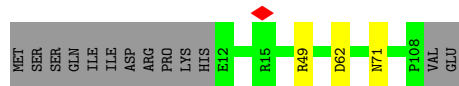
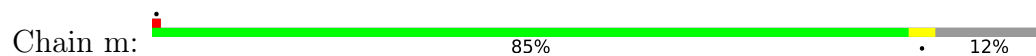
- Molecule 35: Small nuclear ribonucleoprotein Sm D1



- Molecule 36: Small nuclear ribonucleoprotein Sm D2

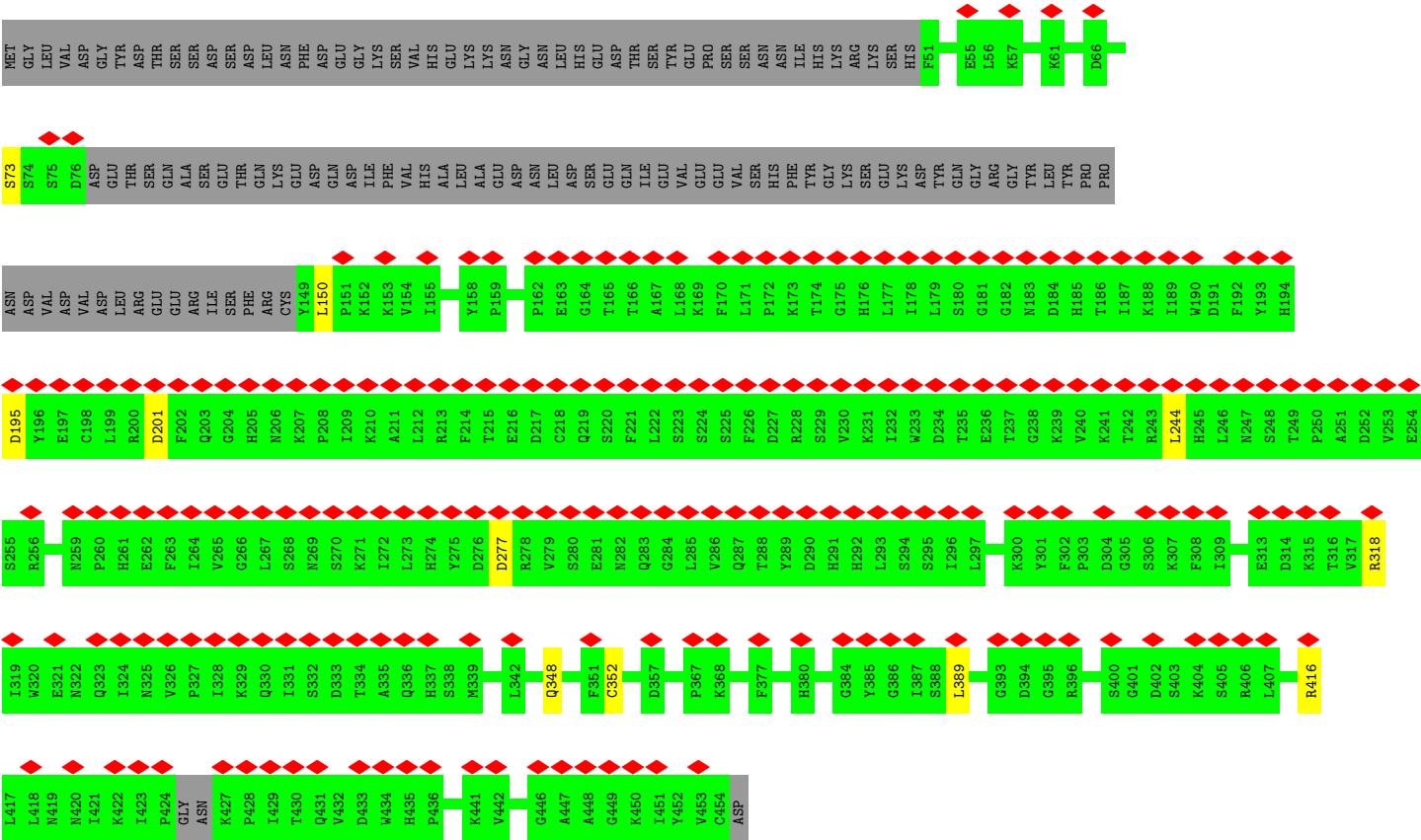


- Molecule 36: Small nuclear ribonucleoprotein Sm D2

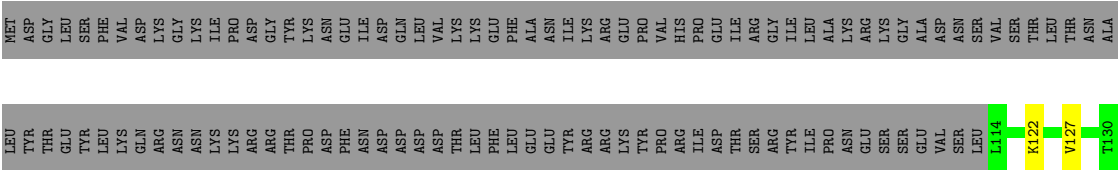


- Molecule 37: CDC40 isoform 1

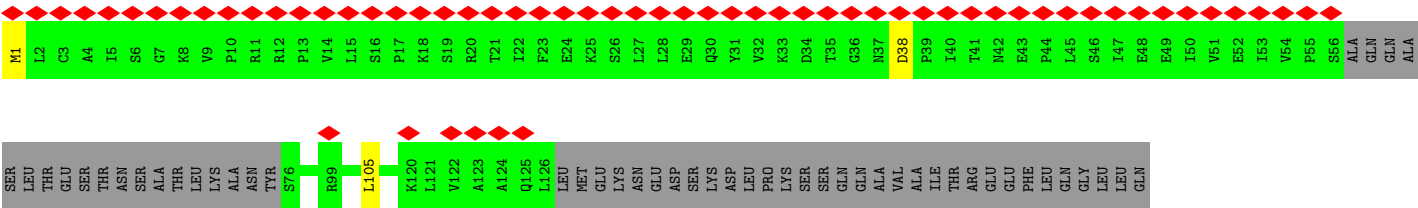




• Molecule 38: SNT309 isoform 1

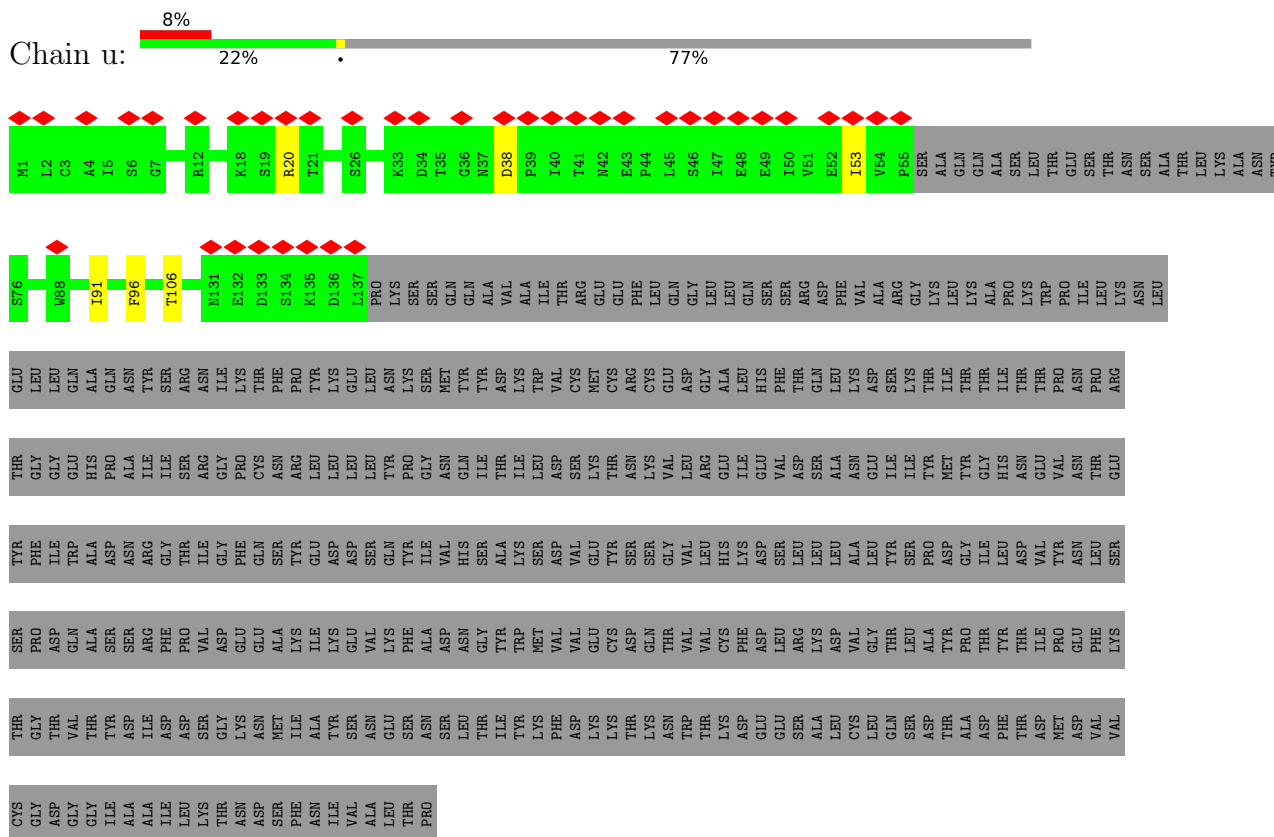


• Molecule 39: Pre-mRNA-processing factor 19

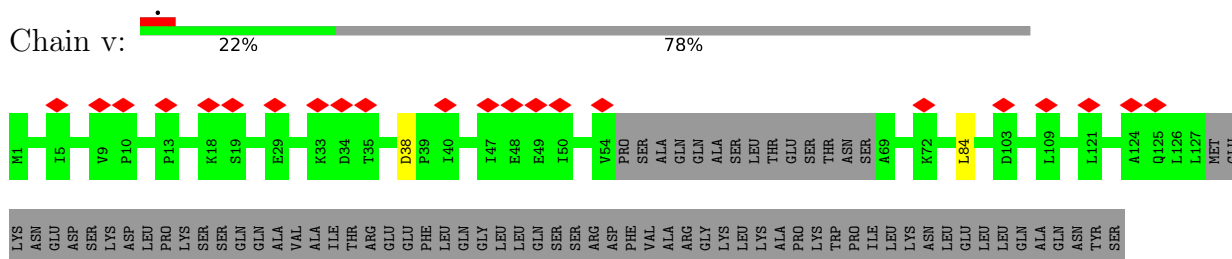


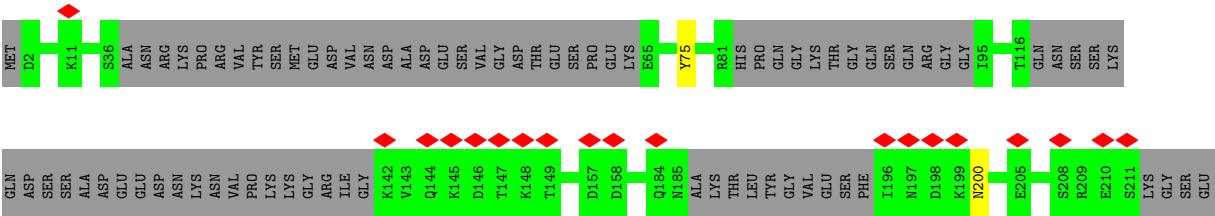
[illegible]

- Molecule 39: Pre-mRNA-processing factor 19



- Molecule 39: Pre-mRNA-processing factor 19





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	403474	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 ($e^-/\text{\AA}^2$)	40	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	140.475	Depositor
Minimum map value	-91.484	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.810	Depositor
Recommended contour level	5	Depositor
Map size (Å)	458.0, 458.0, 458.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.145, 1.145, 1.145	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	0.68	1/4585 (0.0%)	1.65	135/7114 (1.9%)
2	5	0.66	2/4221 (0.0%)	1.60	118/6573 (1.8%)
3	6	0.52	1/2427 (0.0%)	1.35	38/3778 (1.0%)
4	A	0.45	0/18498	0.71	7/25078 (0.0%)
5	B	0.55	2/13971 (0.0%)	0.86	28/18941 (0.1%)
6	C	0.41	0/7291	0.69	1/9875 (0.0%)
7	D	0.44	0/1478	0.73	1/1967 (0.1%)
8	E	0.54	0/341	1.40	8/530 (1.5%)
9	F	0.42	0/459	0.63	0/613
10	G	0.41	0/1051	0.64	1/1406 (0.1%)
11	H	0.44	0/3767	0.73	3/5076 (0.1%)
12	I	0.68	0/1187	1.67	38/1839 (2.1%)
13	J	0.44	1/2989 (0.0%)	0.80	6/4055 (0.1%)
14	K	0.40	0/1479	0.68	0/1995
15	L	0.39	0/1307	0.70	1/1748 (0.1%)
16	M	0.40	0/2094	0.76	4/2815 (0.1%)
17	N	0.43	0/2124	0.73	0/2860
18	O	0.44	0/2049	0.72	0/2748
19	P	0.42	0/623	0.75	1/832 (0.1%)
20	Q	0.61	4/5056 (0.1%)	0.94	22/6846 (0.3%)
21	R	0.42	0/557	0.69	0/750
22	S	0.45	1/4248 (0.0%)	0.69	1/5759 (0.0%)
23	T	0.49	1/5482 (0.0%)	0.77	6/7438 (0.1%)
24	W	0.44	0/1757	0.80	0/2372
26	Y	0.45	0/722	0.86	2/963 (0.2%)
27	Z	0.39	0/446	0.69	0/591
28	a	0.48	0/1154	0.72	0/1561
29	b	0.44	0/758	0.86	0/1018
29	k	0.50	1/836 (0.1%)	0.96	0/1120
30	c	0.39	0/295	0.65	0/386
31	d	0.50	0/642	0.81	0/868
31	n	0.56	0/642	0.90	0/868

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.45	0/616	0.84	0/835
32	p	0.51	0/616	0.88	0/835
33	f	0.46	0/614	0.74	0/830
33	q	0.46	0/614	0.79	0/830
34	g	0.49	0/562	0.95	2/756 (0.3%)
34	r	0.49	0/562	0.93	1/756 (0.1%)
35	h	0.48	0/828	0.80	2/1124 (0.2%)
35	l	0.59	2/828 (0.2%)	0.98	2/1124 (0.2%)
36	j	0.46	0/807	0.86	2/1083 (0.2%)
36	m	0.49	0/807	0.93	1/1083 (0.1%)
37	o	0.50	1/2737 (0.0%)	0.88	2/3696 (0.1%)
38	s	0.67	2/428 (0.5%)	0.95	3/577 (0.5%)
39	t	0.53	0/805	0.92	3/1094 (0.3%)
39	u	0.57	0/867	0.98	3/1178 (0.3%)
39	v	0.56	0/837	0.92	2/1137 (0.2%)
39	w	0.48	0/3469	0.88	11/4707 (0.2%)
40	y	0.38	0/1008	0.63	0/1350
All	All	0.50	19/111541 (0.0%)	0.93	455/153378 (0.3%)

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
5	B	0	1
6	C	0	1
20	Q	0	2
23	T	0	2
29	b	0	1
36	m	0	1
37	o	0	2
38	s	0	1
39	w	0	1
All	All	0	12

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	128	A	N9-C4	9.45	1.43	1.37
5	B	756	TRP	CB-CG	8.09	1.64	1.50
38	s	122	LYS	CB-CG	-7.31	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	906	CYS	CB-SG	-6.53	1.71	1.82
37	o	352	CYS	CB-SG	-6.51	1.71	1.82
1	2	77	U	C2-N3	-6.41	1.33	1.37
20	Q	580	PHE	CB-CG	-6.29	1.40	1.51
5	B	500	ASN	C-N	6.20	1.46	1.34
2	5	129	G	N9-C4	6.19	1.42	1.38
20	Q	862	CYS	CB-SG	-6.17	1.71	1.82
35	l	25	VAL	CB-CG1	-6.04	1.40	1.52
22	S	242	GLU	CB-CG	-5.75	1.41	1.52
23	T	149	ASP	C-N	5.61	1.45	1.34
13	J	327	CYS	CB-SG	-5.58	1.72	1.81
38	s	127	VAL	CB-CG2	-5.55	1.41	1.52
35	l	43	VAL	CB-CG1	-5.21	1.42	1.52
29	k	100	LYS	C-N	5.17	1.44	1.34
20	Q	580	PHE	CD2-CE2	-5.16	1.28	1.39
3	6	54	U	N1-C2	5.14	1.43	1.38

All (455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	77	U	N1-C2-O2	15.45	133.62	122.80
1	2	1103	C	N1-C2-O2	15.07	127.94	118.90
1	2	77	U	N3-C4-O4	-14.99	108.91	119.40
3	6	54	U	N1-C2-O2	14.34	132.84	122.80
1	2	77	U	N3-C2-O2	-14.29	112.20	122.20
3	6	54	U	N3-C2-O2	-13.41	112.81	122.20
2	5	54	C	N1-C2-O2	13.19	126.82	118.90
1	2	1105	C	N1-C2-O2	12.31	126.29	118.90
1	2	1103	C	N3-C2-O2	-12.23	113.34	121.90
1	2	1134	C	C6-N1-C2	-12.00	115.50	120.30
2	5	54	C	N3-C2-O2	-11.96	113.53	121.90
12	I	57	C	N1-C2-O2	11.91	126.04	118.90
2	5	79	C	N1-C2-O2	11.84	126.01	118.90
1	2	77	U	C5-C4-O4	11.77	132.96	125.90
1	2	37	G	O5'-P-OP1	-11.65	95.22	105.70
2	5	129	G	N3-C4-C5	-11.64	122.78	128.60
2	5	129	G	C2-N3-C4	11.57	117.68	111.90
1	2	1103	C	C6-N1-C2	-11.46	115.72	120.30
1	2	44	U	N3-C2-O2	-11.34	114.27	122.20
12	I	61	U	N3-C2-O2	-11.24	114.33	122.20
2	5	101	C	N1-C2-O2	10.86	125.42	118.90
2	5	79	C	C2-N1-C1'	10.78	130.66	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	61	U	N1-C2-O2	10.77	130.34	122.80
2	5	128	A	C2-N3-C4	10.73	115.96	110.60
2	5	60	U	N3-C2-O2	-10.64	114.75	122.20
1	2	1103	C	C2-N1-C1'	10.52	130.37	118.80
2	5	128	A	P-O3'-C3'	10.50	132.30	119.70
12	I	57	C	N3-C2-O2	-10.39	114.63	121.90
2	5	60	U	N1-C2-O2	10.32	130.03	122.80
3	6	16	C	C6-N1-C2	-10.32	116.17	120.30
2	5	63	C	N1-C2-O2	10.30	125.08	118.90
1	2	1105	C	N3-C2-O2	-10.21	114.75	121.90
12	I	90	A	O4'-C1'-N9	10.20	116.36	108.20
1	2	120	G	P-O3'-C3'	10.12	131.84	119.70
1	2	1102	C	C5-C6-N1	9.96	125.98	121.00
3	6	54	U	C2-N1-C1'	9.81	129.47	117.70
1	2	74	C	C6-N1-C2	-9.79	116.38	120.30
1	2	44	U	N1-C2-O2	9.74	129.62	122.80
1	2	74	C	C5-C6-N1	9.70	125.85	121.00
39	w	270	ASP	CB-CG-OD1	9.67	127.00	118.30
2	5	129	G	N3-C4-N9	9.47	131.68	126.00
2	5	61	U	N3-C2-O2	-9.44	115.59	122.20
1	2	1102	C	C6-N1-C2	-9.43	116.53	120.30
2	5	79	C	N3-C2-O2	-9.42	115.31	121.90
2	5	142	C	C6-N1-C2	-9.39	116.54	120.30
2	5	4	C	C6-N1-C2	-9.36	116.56	120.30
2	5	79	C	C6-N1-C2	-9.35	116.56	120.30
1	2	113	U	C5-C6-N1	9.25	127.33	122.70
8	E	-12	U	N3-C2-O2	-9.22	115.75	122.20
1	2	41	C	N1-C2-O2	9.19	124.41	118.90
3	6	16	C	N1-C2-O2	9.19	124.41	118.90
2	5	145	U	N3-C2-O2	-9.05	115.86	122.20
1	2	120	G	O4'-C1'-N9	-9.03	100.97	108.20
1	2	7	C	N1-C2-O2	9.02	124.31	118.90
1	2	1134	C	C5-C6-N1	8.95	125.48	121.00
13	J	148	ASP	CB-CG-OD1	8.94	126.35	118.30
2	5	178	C	N1-C2-O2	8.94	124.27	118.90
8	E	-12	U	C5-C6-N1	8.92	127.16	122.70
2	5	64	C	N1-C2-O2	8.91	124.25	118.90
1	2	1131	U	N3-C2-O2	-8.86	116.00	122.20
1	2	1103	C	C5-C6-N1	8.85	125.43	121.00
1	2	47	U	C5-C6-N1	8.78	127.09	122.70
1	2	1161	U	N3-C2-O2	-8.70	116.11	122.20
1	2	1119	C	C5-C6-N1	8.66	125.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1131	U	N1-C2-O2	8.63	128.84	122.80
2	5	63	C	N3-C2-O2	-8.62	115.86	121.90
2	5	153	U	N3-C2-O2	-8.61	116.17	122.20
2	5	130	A	OP2-P-O3'	8.57	124.05	105.20
3	6	16	C	C5-C6-N1	8.52	125.26	121.00
1	2	1105	C	C2-N1-C1'	8.52	128.17	118.80
2	5	61	U	N1-C2-O2	8.50	128.75	122.80
8	E	-12	U	N1-C2-O2	8.50	128.75	122.80
4	A	2287	ASP	CB-CG-OD1	8.47	125.92	118.30
20	Q	768	ASP	CB-CG-OD1	8.45	125.91	118.30
12	I	90	A	N9-C1'-C2'	-8.42	102.74	112.00
8	E	-12	U	C6-N1-C2	-8.42	115.95	121.00
1	2	121	C	O4'-C1'-N1	8.41	114.93	108.20
2	5	70	A	O5'-P-OP1	8.41	120.79	110.70
39	u	53	ILE	CG1-CB-CG2	-8.39	92.95	111.40
1	2	7	C	N3-C2-O2	-8.38	116.03	121.90
34	g	33	ASP	CB-CG-OD1	8.31	125.78	118.30
2	5	4	C	C5-C6-N1	8.31	125.15	121.00
3	6	43	C	N1-C2-O2	8.31	123.89	118.90
3	6	43	C	N3-C2-O2	-8.30	116.09	121.90
20	Q	712	TYR	CA-CB-CG	-8.28	97.68	113.40
2	5	108	C	N1-C2-O2	8.27	123.86	118.90
1	2	40	U	N3-C2-O2	-8.18	116.48	122.20
2	5	128	A	N3-C4-N9	8.15	133.92	127.40
1	2	1113	U	O4'-C1'-N1	8.12	114.69	108.20
39	w	451	ASP	CB-CG-OD1	8.06	125.55	118.30
2	5	79	C	C5-C6-N1	8.02	125.01	121.00
1	2	54	U	N3-C2-O2	-8.01	116.59	122.20
5	B	1689	ASP	CB-CG-OD1	8.00	125.50	118.30
1	2	1150	U	N3-C2-O2	-7.96	116.63	122.20
5	B	790	ASP	CB-CG-OD1	7.94	125.44	118.30
2	5	96	U	N3-C2-O2	-7.89	116.68	122.20
1	2	124	C	O4'-C1'-N1	7.87	114.49	108.20
2	5	60	U	C2-N1-C1'	7.83	127.10	117.70
2	5	146	C	C6-N1-C2	-7.83	117.17	120.30
37	o	244	LEU	CB-CG-CD2	-7.80	97.73	111.00
2	5	142	C	C5-C6-N1	7.78	124.89	121.00
36	m	62	ASP	CB-CG-OD1	7.76	125.29	118.30
1	2	1119	C	C6-N1-C2	-7.73	117.21	120.30
3	6	68	C	N1-C2-O2	7.72	123.53	118.90
12	I	12	G	C2-N3-C4	7.71	115.75	111.90
12	I	55	U	O4'-C1'-N1	7.68	114.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	96	U	N1-C2-O2	7.66	128.16	122.80
12	I	71	C	N1-C2-O2	7.66	123.50	118.90
3	6	16	C	N3-C2-O2	-7.64	116.56	121.90
3	6	67	C	C6-N1-C2	-7.62	117.25	120.30
2	5	163	C	C6-N1-C2	-7.58	117.27	120.30
2	5	178	C	N3-C2-O2	-7.53	116.63	121.90
1	2	1161	U	N1-C2-O2	7.52	128.06	122.80
2	5	145	U	N1-C2-O2	7.52	128.06	122.80
5	B	1229	ASP	CB-CG-OD1	7.50	125.05	118.30
1	2	1105	C	C6-N1-C2	-7.49	117.30	120.30
15	L	25	ASP	CB-CG-OD1	7.49	125.04	118.30
1	2	40	U	N1-C2-O2	7.49	128.04	122.80
12	I	77	C	P-O3'-C3'	7.48	128.67	119.70
2	5	101	C	P-O3'-C3'	7.46	128.66	119.70
3	6	66	C	C6-N1-C2	-7.45	117.32	120.30
2	5	70	A	OP1-P-OP2	-7.43	108.46	119.60
2	5	151	A	C2-N3-C4	7.43	114.31	110.60
2	5	153	U	N1-C2-O2	7.42	128.00	122.80
1	2	105	A	OP1-P-O3'	7.42	121.53	105.20
1	2	1113	U	OP1-P-OP2	-7.39	108.51	119.60
2	5	64	C	N3-C2-O2	-7.37	116.74	121.90
1	2	41	C	N3-C2-O2	-7.36	116.75	121.90
2	5	96	U	C5-C6-N1	7.35	126.37	122.70
1	2	1089	G	OP1-P-OP2	-7.34	108.59	119.60
1	2	1096	C	C6-N1-C2	-7.33	117.37	120.30
12	I	89	G	O4'-C1'-N9	7.33	114.07	108.20
2	5	101	C	N3-C2-O2	-7.33	116.77	121.90
5	B	1626	ASP	CB-CG-OD1	7.33	124.90	118.30
1	2	1144	U	OP1-P-OP2	-7.33	108.61	119.60
2	5	108	C	N3-C2-O2	-7.30	116.79	121.90
1	2	69	G	OP1-P-OP2	-7.28	108.67	119.60
13	J	294	ASP	CB-CG-OD1	7.27	124.84	118.30
1	2	1150	U	N1-C2-O2	7.26	127.88	122.80
3	6	1	G	OP1-P-OP2	-7.26	108.71	119.60
1	2	4	A	OP1-P-OP2	-7.25	108.72	119.60
12	I	67	C	N1-C2-O2	7.25	123.25	118.90
2	5	70	A	C2-N3-C4	7.23	114.22	110.60
1	2	154	U	N3-C2-O2	-7.21	117.15	122.20
1	2	1081	U	OP1-P-OP2	-7.16	108.85	119.60
35	1	52	LEU	CA-CB-CG	7.16	131.77	115.30
2	5	161	U	C5-C6-N1	7.16	126.28	122.70
1	2	1160	C	O4'-C1'-N1	7.15	113.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	s	168	LEU	CB-CG-CD2	-7.14	98.86	111.00
12	I	12	G	O5'-P-OP2	-7.12	99.30	105.70
23	T	483	ASP	CB-CG-OD1	7.11	124.70	118.30
39	w	401	ASP	CB-CG-OD1	7.09	124.68	118.30
2	5	11	A	N7-C8-N9	7.09	117.35	113.80
20	Q	461	ASP	CB-CG-OD1	7.09	124.68	118.30
1	2	79	A	N7-C8-N9	7.08	117.34	113.80
2	5	127	U	N3-C2-O2	-7.05	117.26	122.20
38	s	147	ILE	CG1-CB-CG2	-6.97	96.08	111.40
1	2	42	U	C5-C6-N1	6.95	126.18	122.70
23	T	537	VAL	CA-CB-CG1	6.94	121.31	110.90
19	P	159	ASP	CB-CG-OD1	6.93	124.54	118.30
5	B	1601	PHE	CB-CG-CD1	6.93	125.65	120.80
1	2	12	U	N3-C2-O2	-6.91	117.36	122.20
2	5	150	U	C5-C6-N1	6.89	126.14	122.70
5	B	990	ASP	CB-CG-OD1	6.88	124.50	118.30
36	j	62	ASP	CB-CG-OD1	6.88	124.50	118.30
1	2	123	C	C6-N1-C2	-6.88	117.55	120.30
20	Q	513	PHE	CB-CG-CD2	-6.88	115.99	120.80
20	Q	583	LEU	CB-CG-CD2	-6.86	99.34	111.00
3	6	16	C	C2-N1-C1'	6.85	126.33	118.80
1	2	4	A	O4'-C1'-N9	6.84	113.67	108.20
1	2	1160	C	OP1-P-OP2	-6.79	109.41	119.60
8	E	-14	A	OP1-P-OP2	-6.79	109.41	119.60
20	Q	465	ASP	CB-CG-OD1	6.79	124.41	118.30
1	2	1162	U	N3-C2-O2	-6.78	117.46	122.20
2	5	79	C	C6-N1-C1'	-6.77	112.68	120.80
1	2	44	U	O4'-C1'-N1	6.76	113.61	108.20
6	C	202	ASP	CB-CG-OD1	6.76	124.38	118.30
20	Q	513	PHE	CB-CG-CD1	6.76	125.53	120.80
39	w	227	ASP	CB-CG-OD1	6.73	124.36	118.30
5	B	474	ASP	CB-CG-OD1	6.73	124.36	118.30
1	2	47	U	C6-N1-C2	-6.70	116.98	121.00
2	5	128	A	C5-C6-N1	6.69	121.04	117.70
20	Q	543	ASP	CB-CG-OD1	6.68	124.32	118.30
13	J	161	ASP	CB-CG-OD1	6.68	124.31	118.30
3	6	68	C	N3-C2-O2	-6.66	117.23	121.90
2	5	96	U	C6-N1-C2	-6.66	117.00	121.00
2	5	60	U	C6-N1-C2	-6.65	117.01	121.00
12	I	87	U	OP1-P-OP2	-6.65	109.62	119.60
13	J	287	ASP	CB-CG-OD1	6.65	124.28	118.30
2	5	74	U	C5-C6-N1	6.64	126.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	67	C	N1-C2-O2	6.63	122.88	118.90
23	T	347	LEU	CA-CB-CG	6.63	130.55	115.30
8	E	-12	U	C2-N1-C1'	6.61	125.63	117.70
2	5	54	C	O4'-C1'-N1	6.60	113.48	108.20
2	5	55	U	O4'-C1'-N1	6.59	113.47	108.20
1	2	1164	C	C6-N1-C2	-6.58	117.67	120.30
5	B	774	ASP	CB-CG-OD1	6.55	124.20	118.30
12	I	71	C	N3-C2-O2	-6.52	117.33	121.90
2	5	127	U	N1-C2-O2	6.51	127.36	122.80
1	2	1136	U	OP1-P-O3'	6.50	119.51	105.20
1	2	22	C	O5'-P-OP1	-6.50	99.85	105.70
1	2	43	G	C2-N3-C4	6.48	115.14	111.90
1	2	1096	C	C2-N1-C1'	6.48	125.93	118.80
2	5	56	U	OP1-P-O3'	6.48	119.46	105.20
11	H	372	ASP	CB-CG-OD1	6.48	124.13	118.30
2	5	60	U	C5-C6-N1	6.47	125.94	122.70
2	5	7	C	C5-C6-N1	6.46	124.23	121.00
16	M	110	ASP	CB-CG-OD1	6.44	124.10	118.30
1	2	40	U	O4'-C1'-N1	6.44	113.35	108.20
12	I	62	A	OP1-P-O3'	6.43	119.36	105.20
3	6	15	C	N1-C2-O2	6.43	122.76	118.90
2	5	161	U	N3-C2-O2	-6.43	117.70	122.20
2	5	34	C	N1-C2-O2	6.41	122.75	118.90
2	5	129	G	C4-N9-C1'	6.41	134.83	126.50
1	2	98	U	OP1-P-OP2	-6.40	110.00	119.60
39	w	429	ASP	CB-CG-OD1	6.40	124.06	118.30
5	B	1601	PHE	CB-CG-CD2	-6.39	116.33	120.80
2	5	161	U	N1-C2-O2	6.38	127.26	122.80
12	I	89	G	C8-N9-C4	-6.38	103.85	106.40
1	2	15	C	P-O3'-C3'	6.37	127.34	119.70
1	2	106	A	OP1-P-OP2	-6.36	110.06	119.60
12	I	67	C	N3-C2-O2	-6.36	117.45	121.90
12	I	63	U	N3-C4-O4	-6.36	114.95	119.40
1	2	76	A	O4'-C1'-N9	6.35	113.28	108.20
5	B	1057	LEU	CB-CG-CD2	-6.35	100.21	111.00
2	5	58	U	C5-C6-N1	6.34	125.87	122.70
12	I	10	A	OP2-P-O3'	6.32	119.11	105.20
3	6	54	U	C5-C6-N1	6.31	125.86	122.70
5	B	1793	ASP	CB-CG-OD1	6.31	123.98	118.30
12	I	17	G	C8-N9-C4	-6.30	103.88	106.40
39	w	127	LEU	CA-CB-CG	6.29	129.78	115.30
3	6	54	U	C6-N1-C2	-6.25	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	14	C	C6-N1-C2	-6.25	117.80	120.30
1	2	54	U	N1-C2-O2	6.23	127.16	122.80
26	Y	99	LEU	CB-CG-CD1	-6.21	100.44	111.00
20	Q	480	LEU	CA-CB-CG	6.21	129.58	115.30
12	I	90	A	C1'-O4'-C4'	-6.20	104.94	109.90
3	6	66	C	N1-C2-O2	6.19	122.61	118.90
39	t	38	ASP	CB-CG-OD1	6.19	123.87	118.30
2	5	7	C	C6-N1-C2	-6.18	117.83	120.30
3	6	102	U	C5-C6-N1	6.16	125.78	122.70
10	G	28	ASP	CB-CG-OD1	6.16	123.85	118.30
20	Q	763	PHE	CB-CG-CD2	-6.16	116.49	120.80
2	5	43	G	C2-N3-C4	6.16	114.98	111.90
1	2	14	C	N1-C2-O2	6.15	122.59	118.90
1	2	1096	C	C5-C6-N1	6.14	124.07	121.00
39	w	124	ALA	N-CA-CB	6.14	118.70	110.10
1	2	12	U	N1-C2-O2	6.13	127.09	122.80
16	M	171	ASP	CB-CG-OD1	6.12	123.81	118.30
39	v	84	LEU	CB-CG-CD2	6.09	121.36	111.00
12	I	57	C	C6-N1-C2	-6.09	117.86	120.30
2	5	128	A	N3-C4-C5	-6.08	122.54	126.80
2	5	53	C	O4'-C1'-N1	6.08	113.06	108.20
1	2	121	C	C3'-C2'-C1'	-6.07	96.64	101.50
5	B	2147	ASP	CB-CG-OD1	6.07	123.76	118.30
1	2	154	U	N1-C2-O2	6.06	127.04	122.80
20	Q	401	VAL	CG1-CB-CG2	-6.05	101.22	110.90
38	s	132	LEU	N-CA-C	6.04	127.32	111.00
5	B	1673	PHE	CB-CG-CD1	6.04	125.03	120.80
12	I	62	A	P-O3'-C3'	6.01	126.92	119.70
3	6	36	U	O4'-C1'-N1	6.01	113.01	108.20
1	2	31	A	OP2-P-O3'	6.01	118.42	105.20
2	5	92	U	N3-C2-O2	-6.00	118.00	122.20
5	B	1673	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	2	111	C	C5-C6-N1	5.99	124.00	121.00
1	2	121	C	C5'-C4'-O4'	5.98	116.27	109.10
3	6	15	C	C6-N1-C2	-5.97	117.91	120.30
20	Q	575	ASP	CB-CG-OD1	5.97	123.67	118.30
1	2	44	U	C6-N1-C2	-5.96	117.42	121.00
1	2	45	U	O4'-C1'-N1	5.96	112.97	108.20
1	2	77	U	C4-C5-C6	-5.95	116.13	119.70
11	H	124	LEU	CA-CB-CG	5.95	128.98	115.30
1	2	19	U	O5'-P-OP1	-5.94	100.35	105.70
1	2	1131	U	C2-N1-C1'	5.94	124.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Q	751	LEU	CA-CB-CG	5.93	128.94	115.30
2	5	130	A	P-O3'-C3'	5.92	126.81	119.70
2	5	137	U	C5-C6-N1	5.92	125.66	122.70
1	2	112	A	O5'-P-OP1	-5.90	100.39	105.70
20	Q	846	LEU	CA-CB-CG	5.90	128.87	115.30
1	2	1164	C	C5-C6-N1	5.89	123.95	121.00
1	2	1151	U	N3-C2-O2	-5.89	118.08	122.20
4	A	289	ASP	CB-CG-OD1	5.89	123.60	118.30
2	5	56	U	P-O3'-C3'	5.87	126.75	119.70
3	6	72	C	N1-C2-O2	5.87	122.42	118.90
39	v	38	ASP	CB-CG-OD1	5.86	123.58	118.30
1	2	1162	U	N1-C2-O2	5.86	126.90	122.80
1	2	77	U	N3-C4-C5	5.86	118.11	114.60
3	6	67	C	N3-C2-O2	-5.85	117.80	121.90
5	B	1703	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	2	1140	U	N3-C2-O2	-5.83	118.12	122.20
5	B	1612	VAL	CG1-CB-CG2	-5.81	101.61	110.90
2	5	94	C	C6-N1-C2	-5.80	117.98	120.30
2	5	129	G	C8-N9-C4	-5.80	104.08	106.40
2	5	147	C	C6-N1-C2	-5.78	117.99	120.30
1	2	1103	C	C6-N1-C1'	-5.77	113.88	120.80
1	2	1093	C	O4'-C1'-N1	5.76	112.81	108.20
12	I	57	C	O4'-C1'-N1	5.76	112.81	108.20
2	5	102	C	N3-C2-O2	-5.75	117.87	121.90
2	5	150	U	C6-N1-C2	-5.75	117.55	121.00
1	2	76	A	OP1-P-O3'	5.75	117.85	105.20
1	2	1096	C	N1-C2-O2	5.73	122.34	118.90
3	6	4	C	C5-C6-N1	5.73	123.86	121.00
1	2	1151	U	N1-C2-O2	5.72	126.81	122.80
20	Q	486	LEU	CB-CG-CD1	5.71	120.71	111.00
16	M	222	LEU	CA-CB-CG	5.71	128.43	115.30
3	6	54	U	C6-N1-C1'	-5.71	113.21	121.20
39	w	125	GLN	CA-CB-CG	5.69	125.92	113.40
2	5	152	C	O5'-P-OP1	-5.69	100.58	105.70
1	2	1108	A	C2-N3-C4	5.69	113.44	110.60
5	B	1658	TYR	CA-CB-CG	5.69	124.21	113.40
11	H	110	ASP	CB-CG-OD1	5.69	123.42	118.30
12	I	63	U	C5-C4-O4	5.68	129.31	125.90
3	6	66	C	N3-C2-O2	-5.67	117.93	121.90
13	J	420	ASP	CB-CG-OD1	5.67	123.40	118.30
12	I	11	A	O4'-C1'-N9	5.66	112.73	108.20
2	5	128	A	N9-C4-C5	-5.65	103.54	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1605	ILE	CA-CB-CG2	5.64	122.19	110.90
12	I	88	U	OP1-P-O3'	5.64	117.61	105.20
12	I	70	A	C8-N9-C4	-5.64	103.55	105.80
3	6	70	U	N3-C2-O2	-5.63	118.25	122.20
1	2	41	C	P-O3'-C3'	5.63	126.45	119.70
1	2	43	G	N3-C4-C5	-5.63	125.78	128.60
2	5	172	U	N1-C2-O2	5.63	126.74	122.80
5	B	1071	ASP	CB-CG-OD1	5.62	123.36	118.30
1	2	22	C	N1-C2-O2	5.62	122.27	118.90
39	t	1	MET	CG-SD-CE	5.62	109.19	100.20
5	B	953	MET	CG-SD-CE	5.61	109.18	100.20
3	6	43	C	O4'-C1'-N1	5.61	112.69	108.20
2	5	147	C	C2-N1-C1'	5.60	124.96	118.80
12	I	62	A	O4'-C1'-N9	-5.59	103.72	108.20
2	5	52	G	C2-N3-C4	5.59	114.70	111.90
1	2	120	G	C8-N9-C4	-5.57	104.17	106.40
1	2	1103	C	C2-N3-C4	5.56	122.68	119.90
2	5	161	U	C6-N1-C2	-5.56	117.67	121.00
2	5	170	U	OP1-P-O3'	5.56	117.43	105.20
1	2	1114	G	C2-N3-C4	5.56	114.68	111.90
2	5	146	C	C2-N1-C1'	5.55	124.91	118.80
2	5	34	C	N3-C2-O2	-5.55	118.02	121.90
35	h	52	LEU	CA-CB-CG	5.55	128.06	115.30
2	5	128	A	N1-C2-N3	-5.54	126.53	129.30
1	2	155	U	N3-C2-O2	-5.53	118.33	122.20
35	l	52	LEU	CB-CG-CD2	5.53	120.39	111.00
2	5	11	A	C8-N9-C4	-5.53	103.59	105.80
3	6	66	C	C5-C6-N1	5.53	123.76	121.00
5	B	1633	LEU	CA-CB-CG	5.52	128.00	115.30
3	6	67	C	C5-C6-N1	5.52	123.76	121.00
1	2	113	U	C6-N1-C2	-5.52	117.69	121.00
3	6	48	C	C6-N1-C2	-5.52	118.09	120.30
1	2	78	G	N3-C4-N9	-5.50	122.70	126.00
2	5	178	C	O4'-C1'-N1	5.50	112.60	108.20
26	Y	50	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	2	19	U	O4'-C1'-C2'	-5.50	100.30	105.80
2	5	92	U	N1-C2-O2	5.49	126.64	122.80
2	5	64	C	O4'-C1'-N1	5.48	112.59	108.20
37	o	150	LEU	CA-CB-CG	5.46	127.87	115.30
1	2	6	U	N3-C2-O2	-5.45	118.38	122.20
2	5	146	C	C5-C6-N1	5.45	123.72	121.00
16	M	110	ASP	CB-CG-OD2	-5.44	113.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Q	454	LEU	CB-CG-CD2	5.44	120.25	111.00
20	Q	386	TYR	CA-CB-CG	5.44	123.73	113.40
2	5	45	A	N7-C8-N9	5.43	116.52	113.80
2	5	96	U	C2-N1-C1'	5.43	124.22	117.70
12	I	12	G	O4'-C1'-N9	5.43	112.54	108.20
1	2	6	U	N1-C2-O2	5.43	126.60	122.80
3	6	23	G	N1-C6-O6	-5.42	116.65	119.90
12	I	17	G	N7-C8-N9	5.41	115.81	113.10
2	5	116	U	N1-C2-O2	5.41	126.59	122.80
2	5	127	U	C6-N1-C2	-5.41	117.76	121.00
2	5	61	U	C6-N1-C2	-5.40	117.76	121.00
1	2	69	G	O4'-C1'-N9	5.39	112.51	108.20
2	5	128	A	C4-N9-C1'	5.39	136.00	126.30
5	B	1339	PHE	CB-CG-CD1	5.39	124.57	120.80
13	J	148	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	2	54	U	O4'-C1'-N1	5.38	112.50	108.20
1	2	1140	U	N1-C2-O2	5.38	126.56	122.80
1	2	1168	U	N3-C2-O2	-5.38	118.44	122.20
7	D	165	LEU	CA-CB-CG	5.37	127.64	115.30
1	2	42	U	C6-N1-C2	-5.37	117.78	121.00
1	2	1161	U	C6-N1-C2	-5.37	117.78	121.00
20	Q	660	LYS	CA-CB-CG	5.35	125.17	113.40
2	5	54	C	C6-N1-C2	-5.35	118.16	120.30
3	6	69	C	N1-C2-O2	5.34	122.11	118.90
2	5	62	G	N3-C4-C5	-5.34	125.93	128.60
1	2	1168	U	N1-C2-O2	5.34	126.54	122.80
23	T	512	LEU	CB-CG-CD2	-5.34	101.93	111.00
3	6	15	C	N3-C2-O2	-5.33	118.17	121.90
2	5	65	U	O4'-C1'-N1	5.33	112.46	108.20
20	Q	724	LEU	CB-CG-CD1	-5.32	101.96	111.00
2	5	172	U	N3-C2-O2	-5.32	118.48	122.20
1	2	1131	U	C6-N1-C2	-5.31	117.81	121.00
2	5	61	U	O4'-C1'-N1	5.31	112.45	108.20
5	B	613	ASP	CB-CG-OD1	5.29	123.06	118.30
5	B	1876	LEU	CB-CG-CD1	-5.29	102.00	111.00
39	w	92	MET	CB-CG-SD	5.29	128.27	112.40
39	t	105	LEU	CA-CB-CG	5.29	127.47	115.30
2	5	164	C	C6-N1-C2	-5.28	118.19	120.30
39	u	38	ASP	CB-CG-OD1	5.27	123.05	118.30
20	Q	388	TYR	CA-CB-CG	5.27	123.42	113.40
20	Q	713	LEU	CB-CG-CD1	5.27	119.96	111.00
12	I	89	G	N7-C8-N9	5.26	115.73	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	92	C	C5-C6-N1	5.26	123.63	121.00
35	h	50	PRO	CA-N-CD	-5.26	104.13	111.50
1	2	1105	C	C6-N1-C1'	-5.25	114.50	120.80
4	A	1166	ASP	CB-CG-OD1	5.25	123.02	118.30
1	2	1105	C	C5-C6-N1	5.24	123.62	121.00
1	2	1141	C	C6-N1-C2	-5.24	118.20	120.30
4	A	534	LEU	CB-CG-CD1	-5.23	102.11	111.00
5	B	684	LEU	CA-CB-CG	5.23	127.33	115.30
1	2	7	C	C6-N1-C2	-5.19	118.22	120.30
12	I	92	C	C6-N1-C2	-5.19	118.22	120.30
5	B	591	ASP	CB-CG-OD1	5.19	122.97	118.30
4	A	1035	LEU	CB-CG-CD1	-5.19	102.18	111.00
2	5	127	U	C5-C6-N1	5.18	125.29	122.70
22	S	269	ILE	CG1-CB-CG2	-5.18	100.00	111.40
2	5	102	C	N1-C2-O2	5.17	122.00	118.90
2	5	116	U	N3-C2-O2	-5.17	118.58	122.20
1	2	14	C	N3-C2-O2	-5.17	118.28	121.90
2	5	62	G	C2-N3-C4	5.16	114.48	111.90
1	2	78	G	N3-C4-C5	5.16	131.18	128.60
1	2	113	U	OP2-P-O3'	5.16	116.54	105.20
12	I	86	A	OP1-P-O3'	5.14	116.51	105.20
4	A	315	SER	CA-C-O	-5.14	109.31	120.10
34	r	33	ASP	CB-CG-OD1	5.14	122.92	118.30
2	5	116	U	O4'-C1'-N1	5.13	112.31	108.20
12	I	61	U	C6-N1-C2	-5.13	117.92	121.00
39	w	318	ASP	CB-CG-OD1	5.13	122.92	118.30
8	E	-13	G	O4'-C1'-N9	5.13	112.30	108.20
34	g	71	LEU	CA-CB-CG	5.12	127.07	115.30
39	w	306	ASP	CB-CA-C	-5.11	100.18	110.40
8	E	-11	G	OP1-P-OP2	-5.11	111.94	119.60
2	5	128	A	C8-N9-C1'	-5.10	118.52	127.70
39	u	91	ILE	CA-CB-CG1	5.10	120.69	111.00
1	2	120	G	C2'-C3'-O3'	5.10	121.85	113.70
2	5	45	A	C2-N3-C4	5.09	113.14	110.60
4	A	1495	PHE	CB-CG-CD2	5.09	124.36	120.80
36	j	99	ASP	CB-CG-OD1	5.09	122.88	118.30
1	2	59	C	O4'-C1'-N1	5.08	112.27	108.20
23	T	613	PRO	CA-N-CD	-5.08	104.39	111.50
2	5	142	C	C2-N1-C1'	5.07	124.38	118.80
23	T	358	LEU	CB-CG-CD2	5.07	119.61	111.00
1	2	7	C	O4'-C1'-N1	5.06	112.25	108.20
5	B	1058	LEU	CA-CB-CG	5.06	126.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	63	C	O4'-C1'-N1	5.05	112.24	108.20
2	5	70	A	OP2-P-O3'	5.05	116.31	105.20
3	6	43	C	C6-N1-C2	-5.05	118.28	120.30
1	2	78	G	N3-C2-N2	-5.05	116.37	119.90
2	5	141	G	C2-N3-C4	5.04	114.42	111.90
1	2	1161	U	C2-N1-C1'	5.04	123.75	117.70
5	B	872	LEU	CB-CG-CD1	5.04	119.57	111.00
1	2	47	U	C6-N1-C1'	5.04	128.25	121.20
12	I	9	A	O4'-C1'-N9	5.03	112.22	108.20
1	2	1151	U	C5-C6-N1	5.02	125.21	122.70
1	2	1143	C	OP1-P-O3'	5.01	116.23	105.20
3	6	36	U	C2'-C3'-O3'	5.01	121.72	113.70
20	Q	388	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	1519	ARG	Sidechain
6	C	132	ARG	Sidechain
20	Q	478	ARG	Sidechain
20	Q	496	ARG	Sidechain
23	T	546	SER	Mainchain
23	T	726	ARG	Mainchain
29	b	28	ARG	Sidechain
36	m	49	ARG	Sidechain
37	o	318	ARG	Sidechain
37	o	416	ARG	Sidechain
38	s	162	ARG	Sidechain
39	w	240	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4120	0	2095	2	0
2	5	3777	0	1908	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	6	2170	0	1095	0	0
4	A	18036	0	17967	5	0
5	B	13675	0	13679	8	0
6	C	7139	0	7304	1	0
7	D	1547	0	1503	0	0
8	E	304	0	151	0	0
9	F	505	0	485	0	0
10	G	1090	0	1000	0	0
11	H	3705	0	3777	2	0
12	I	1068	0	538	0	0
13	J	2926	0	2918	2	0
14	K	1455	0	1482	1	0
15	L	1283	0	1301	0	0
16	M	2048	0	2011	0	0
17	N	2092	0	2162	0	0
18	O	2143	0	2032	1	0
19	P	607	0	596	0	0
20	Q	4959	0	5070	3	0
21	R	555	0	491	0	0
22	S	4170	0	3705	3	0
23	T	5387	0	4887	4	0
24	W	1734	0	1787	2	0
25	X	355	0	79	0	0
26	Y	713	0	746	0	0
27	Z	446	0	486	0	0
28	a	1132	0	1166	0	0
29	b	752	0	811	0	0
29	k	830	0	905	0	0
30	c	293	0	290	0	0
31	d	633	0	660	0	0
31	n	633	0	660	0	0
32	e	606	0	630	0	0
32	p	606	0	630	0	0
33	f	601	0	600	0	0
33	q	601	0	600	0	0
34	g	557	0	575	0	0
34	r	557	0	575	0	0
35	h	819	0	866	0	0
35	l	819	0	866	0	0
36	j	795	0	830	0	0
36	m	795	0	830	0	0
37	o	2673	0	2614	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	s	426	0	385	0	0
39	t	794	0	784	0	0
39	u	856	0	827	0	0
39	v	827	0	807	0	0
39	w	3405	0	3303	0	0
40	y	1003	0	909	0	0
41	6	5	0	0	0	0
41	C	1	0	0	0	0
42	6	1	0	0	0	0
43	A	36	0	0	0	0
44	C	32	0	12	0	0
45	D	1	0	0	0	0
45	L	3	0	0	0	0
45	M	1	0	0	0	0
45	N	2	0	0	0	0
45	c	1	0	0	0	0
All	All	109105	0	102390	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:17:ASP:OD1	24:W:17:ASP:N	2.38	0.52
5:B:2011:ILE:HD12	5:B:2030:ILE:HD11	1.94	0.50
5:B:599:ILE:HG23	5:B:605:LEU:HD11	1.96	0.47
5:B:793:LEU:HD21	5:B:808:LEU:HD11	1.98	0.46
5:B:1759:ALA:HB2	5:B:1846:THR:HG21	1.99	0.45
23:T:340:ASP:O	23:T:344:ASN:ND2	2.50	0.45
20:Q:837:ILE:HG22	20:Q:839:LYS:H	1.82	0.45
23:T:320:ASP:N	23:T:320:ASP:OD1	2.50	0.44
2:5:159:C:O2'	2:5:161:U:OP2	2.32	0.43
11:H:10:ASP:OD1	11:H:10:ASP:N	2.49	0.43
20:Q:789:LEU:HA	20:Q:792:ILE:HG22	2.00	0.43
5:B:2013:VAL:HG13	5:B:2018:ASP:HB2	1.99	0.43
14:K:179:THR:HG23	18:O:26:GLN:HB3	2.01	0.43
5:B:478:LYS:HE2	5:B:507:PHE:CE2	2.53	0.43
6:C:88:THR:O	13:J:214:ASN:ND2	2.51	0.42
4:A:126:ASN:N	4:A:126:ASN:OD1	2.52	0.42
24:W:75:ASP:OD1	24:W:75:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:82:A:O3'	4:A:709:ARG:NH2	2.46	0.42
1:2:78:G:H2'	1:2:79:A:C8	2.54	0.42
5:B:1164:THR:HA	20:Q:497:ARG:HH22	1.84	0.42
2:5:26:A:OP2	2:5:141:G:N2	2.53	0.42
4:A:1785:ASP:OD1	4:A:1786:ALA:N	2.51	0.41
23:T:279:GLU:O	23:T:316:ARG:NH2	2.52	0.41
22:S:126:ILE:HD13	22:S:126:ILE:HG21	2.14	0.41
22:S:321:ASP:N	22:S:321:ASP:OD1	2.54	0.41
22:S:206:VAL:HG12	22:S:221:VAL:HG23	2.02	0.41
4:A:2189:LEU:HD13	4:A:2224:VAL:HG23	2.03	0.41
4:A:1286:TRP:CE2	4:A:1302:LEU:HD11	2.56	0.40
1:2:77:U:H1'	1:2:78:G:C4	2.56	0.40
13:J:200:VAL:HG12	13:J:206:VAL:HG22	2.02	0.40
11:H:100:LEU:HD13	11:H:100:LEU:HA	1.98	0.40
23:T:577:VAL:HG12	23:T:583:ILE:HG23	2.02	0.40
5:B:947:ARG:HD2	5:B:947:ARG:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	2185/2413 (91%)	2146 (98%)	38 (2%)	1 (0%)	100	100
5	B	1703/2163 (79%)	1657 (97%)	46 (3%)	0	100	100
6	C	888/1008 (88%)	873 (98%)	15 (2%)	0	100	100
7	D	171/291 (59%)	167 (98%)	4 (2%)	0	100	100
9	F	52/179 (29%)	52 (100%)	0	0	100	100
10	G	119/235 (51%)	119 (100%)	0	0	100	100
11	H	449/577 (78%)	440 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	366/451 (81%)	354 (97%)	12 (3%)	0	100	100
14	K	172/379 (45%)	170 (99%)	2 (1%)	0	100	100
15	L	154/157 (98%)	151 (98%)	3 (2%)	0	100	100
16	M	253/339 (75%)	249 (98%)	4 (2%)	0	100	100
17	N	256/364 (70%)	251 (98%)	5 (2%)	0	100	100
18	O	250/590 (42%)	245 (98%)	5 (2%)	0	100	100
19	P	68/175 (39%)	67 (98%)	1 (2%)	0	100	100
20	Q	618/1071 (58%)	589 (95%)	29 (5%)	0	100	100
21	R	77/135 (57%)	77 (100%)	0	0	100	100
22	S	525/687 (76%)	518 (99%)	7 (1%)	0	100	100
23	T	692/859 (81%)	663 (96%)	28 (4%)	1 (0%)	48	77
24	W	210/238 (88%)	199 (95%)	11 (5%)	0	100	100
26	Y	86/111 (78%)	83 (96%)	3 (4%)	0	100	100
27	Z	51/140 (36%)	51 (100%)	0	0	100	100
28	a	132/251 (53%)	131 (99%)	1 (1%)	0	100	100
29	b	89/196 (45%)	88 (99%)	1 (1%)	0	100	100
29	k	98/196 (50%)	94 (96%)	4 (4%)	0	100	100
30	c	33/382 (9%)	31 (94%)	2 (6%)	0	100	100
31	d	80/101 (79%)	80 (100%)	0	0	100	100
31	n	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
32	e	73/94 (78%)	71 (97%)	1 (1%)	1 (1%)	9	30
32	p	73/94 (78%)	71 (97%)	2 (3%)	0	100	100
33	f	73/86 (85%)	71 (97%)	2 (3%)	0	100	100
33	q	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
34	g	70/77 (91%)	64 (91%)	6 (9%)	0	100	100
34	r	70/77 (91%)	65 (93%)	5 (7%)	0	100	100
35	h	104/146 (71%)	98 (94%)	6 (6%)	0	100	100
35	l	104/146 (71%)	98 (94%)	6 (6%)	0	100	100
36	j	95/110 (86%)	89 (94%)	6 (6%)	0	100	100
36	m	95/110 (86%)	90 (95%)	5 (5%)	0	100	100
37	o	323/455 (71%)	308 (95%)	14 (4%)	1 (0%)	37	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	s	57/175 (33%)	55 (96%)	2 (4%)	0	100	100
39	t	103/503 (20%)	103 (100%)	0	0	100	100
39	u	113/503 (22%)	111 (98%)	2 (2%)	0	100	100
39	v	109/503 (22%)	105 (96%)	4 (4%)	0	100	100
39	w	426/503 (85%)	419 (98%)	5 (1%)	2 (0%)	25	56
40	y	124/215 (58%)	124 (100%)	0	0	100	100
All	All	11942/17672 (68%)	11636 (97%)	300 (2%)	6 (0%)	50	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	e	32	PHE
39	w	376	LYS
4	A	1347	ARG
37	o	348	GLN
39	w	351	ASP
23	T	441	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	
4	A	1987/2182 (91%)	1978 (100%)	9 (0%)	86	95
5	B	1536/1955 (79%)	1528 (100%)	8 (0%)	86	95
6	C	799/910 (88%)	795 (100%)	4 (0%)	86	95
7	D	165/252 (66%)	165 (100%)	0	100	100
9	F	52/154 (34%)	52 (100%)	0	100	100
10	G	102/206 (50%)	102 (100%)	0	100	100
11	H	422/538 (78%)	419 (99%)	3 (1%)	81	94
13	J	325/397 (82%)	323 (99%)	2 (1%)	84	95
14	K	164/328 (50%)	162 (99%)	2 (1%)	67	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	140/141 (99%)	140 (100%)	0	100	100
16	M	219/296 (74%)	218 (100%)	1 (0%)	86	95
17	N	243/332 (73%)	242 (100%)	1 (0%)	89	96
18	O	199/504 (40%)	198 (100%)	1 (0%)	86	95
19	P	61/151 (40%)	60 (98%)	1 (2%)	58	85
20	Q	557/969 (58%)	551 (99%)	6 (1%)	70	90
21	R	47/121 (39%)	45 (96%)	2 (4%)	25	57
22	S	369/633 (58%)	365 (99%)	4 (1%)	70	90
23	T	505/786 (64%)	502 (99%)	3 (1%)	84	95
24	W	201/219 (92%)	195 (97%)	6 (3%)	36	70
26	Y	79/100 (79%)	79 (100%)	0	100	100
27	Z	51/128 (40%)	51 (100%)	0	100	100
28	a	127/225 (56%)	126 (99%)	1 (1%)	79	93
29	b	86/176 (49%)	85 (99%)	1 (1%)	67	89
29	k	95/176 (54%)	95 (100%)	0	100	100
30	c	33/346 (10%)	33 (100%)	0	100	100
31	d	71/89 (80%)	71 (100%)	0	100	100
31	n	71/89 (80%)	70 (99%)	1 (1%)	62	87
32	e	70/83 (84%)	69 (99%)	1 (1%)	62	87
32	p	70/83 (84%)	68 (97%)	2 (3%)	37	71
33	f	67/77 (87%)	67 (100%)	0	100	100
33	q	67/77 (87%)	66 (98%)	1 (2%)	60	86
34	g	61/66 (92%)	59 (97%)	2 (3%)	33	67
34	r	61/66 (92%)	61 (100%)	0	100	100
35	h	95/129 (74%)	95 (100%)	0	100	100
35	l	95/129 (74%)	95 (100%)	0	100	100
36	j	90/103 (87%)	89 (99%)	1 (1%)	70	90
36	m	90/103 (87%)	89 (99%)	1 (1%)	70	90
37	o	298/412 (72%)	294 (99%)	4 (1%)	65	88
38	s	30/165 (18%)	30 (100%)	0	100	100
39	t	81/451 (18%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	u	83/451 (18%)	80 (96%)	3 (4%)	30	64
39	v	80/451 (18%)	80 (100%)	0	100	100
39	w	369/451 (82%)	368 (100%)	1 (0%)	91	97
40	y	91/193 (47%)	89 (98%)	2 (2%)	47	79
All	All	10504/15893 (66%)	10430 (99%)	74 (1%)	80	94

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	310	ASN
4	A	493	MET
4	A	908	ASP
4	A	928	ARG
4	A	1140	ASN
4	A	1196	GLU
4	A	1499	ARG
4	A	1907	GLN
4	A	2381	GLU
5	B	596	ARG
5	B	1056	GLN
5	B	1407	PHE
5	B	1654	ARG
5	B	1669	ASP
5	B	2009	LYS
5	B	2085	GLN
5	B	2125	GLN
6	C	222	MET
6	C	766	TRP
6	C	915	GLU
6	C	918	LEU
11	H	205	TYR
11	H	237	LYS
11	H	400	ASP
13	J	361	ASP
13	J	408	ASP
14	K	149	MET
14	K	222	LYS
16	M	96	GLU
17	N	145	ARG
18	O	202	LYS
19	P	20	TYR

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Mol	Chain	Res	Type
20	Q	388	TYR
20	Q	497	ARG
20	Q	511	LYS
20	Q	682	ASN
20	Q	710	ASP
20	Q	786	GLN
21	R	22	ARG
21	R	83	ARG
22	S	139	TYR
22	S	172	PHE
22	S	192	TYR
22	S	372	CYS
23	T	450	TRP
23	T	451	CYS
23	T	663	LYS
24	W	3	PHE
24	W	17	ASP
24	W	139	ASN
24	W	140	TYR
24	W	146	ARG
24	W	199	MET
28	a	227	ARG
29	b	52	ARG
32	e	46	PHE
34	g	40	LEU
34	g	74	LEU
36	j	71	ASN
36	m	71	ASN
31	n	60	ASP
37	o	195	ASP
37	o	201	ASP
37	o	277	ASP
37	o	389	LEU
32	p	46	PHE
32	p	89	LEU
33	q	83	GLU
39	u	20	ARG
39	u	96	PHE
39	u	106	THR
39	w	245	HIS
40	y	75	TYR
40	y	200	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
20	Q	942	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	187/1175 (15%)	42 (22%)	7 (3%)
12	I	53/95 (55%)	21 (39%)	4 (7%)
2	5	177/214 (82%)	33 (18%)	8 (4%)
3	6	101/112 (90%)	16 (15%)	1 (0%)
8	E	13/47 (27%)	1 (7%)	0
All	All	531/1643 (32%)	113 (21%)	20 (3%)

All (113) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	6	U
1	2	16	U
1	2	19	U
1	2	20	G
1	2	21	G
1	2	25	A
1	2	30	A
1	2	32	G
1	2	33	U
1	2	41	C
1	2	42	U
1	2	45	U
1	2	75	A
1	2	76	A
1	2	77	U
1	2	82	C
1	2	83	U
1	2	106	A
1	2	112	A
1	2	114	U
1	2	115	U
1	2	119	G
1	2	120	G
1	2	121	C
1	2	122	A

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Mol	Chain	Res	Type
1	2	123	C
1	2	124	C
1	2	147	A
1	2	1090	A
1	2	1102	C
1	2	1103	C
1	2	1104	U
1	2	1106	G
1	2	1119	C
1	2	1123	C
1	2	1135	U
1	2	1136	U
1	2	1137	U
1	2	1144	U
1	2	1145	U
1	2	1164	C
1	2	1170	G
2	5	9	U
2	5	10	U
2	5	12	C
2	5	18	A
2	5	20	U
2	5	27	G
2	5	46	C
2	5	56	U
2	5	57	U
2	5	60	U
2	5	70	A
2	5	75	A
2	5	77	A
2	5	79	C
2	5	80	G
2	5	102	C
2	5	128	A
2	5	129	G
2	5	131	A
2	5	132	A
2	5	139	A
2	5	141	G
2	5	151	A
2	5	154	G
2	5	160	U

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Mol	Chain	Res	Type
2	5	165	A
2	5	166	U
2	5	167	A
2	5	168	U
2	5	169	U
2	5	170	U
2	5	174	G
2	5	175	G
3	6	11	U
3	6	12	A
3	6	14	C
3	6	15	C
3	6	16	C
3	6	36	U
3	6	37	U
3	6	52	G
3	6	55	G
3	6	60	G
3	6	67	C
3	6	68	C
3	6	79	A
3	6	80	U
3	6	85	C
3	6	88	U
8	E	-11	G
12	I	3	A
12	I	10	A
12	I	11	A
12	I	12	G
12	I	56	G
12	I	57	C
12	I	62	A
12	I	63	U
12	I	65	U
12	I	70	A
12	I	74	A
12	I	76	U
12	I	77	C
12	I	78	A
12	I	79	A
12	I	81	A
12	I	82	U

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Mol	Chain	Res	Type
12	I	84	C
12	I	86	A
12	I	87	U
12	I	89	G

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	15	C
1	2	19	U
1	2	41	C
1	2	81	G
1	2	111	C
1	2	120	G
1	2	1101	C
2	5	17	C
2	5	56	U
2	5	69	G
2	5	101	C
2	5	128	A
2	5	130	A
2	5	138	A
2	5	166	U
3	6	36	U
12	I	56	G
12	I	62	A
12	I	76	U
12	I	88	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
37	SEP	o	73	37	8,9,10	1.53	1 (12%)	8,12,14	1.53	2 (25%)

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
37	SEP	o	73	37	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	o	73	SEP	P-O1P	3.36	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	o	73	SEP	P-OG-CB	-2.75	110.73	118.30
37	o	73	SEP	OG-CB-CA	2.70	110.77	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 15 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	$\# Z > 2$
43	KGN	A	2500	-	36,36,36	0.78	0	54,60,60	0.51	0
44	GTP	C	1101	41	26,34,34	1.13	1 (3%)	32,54,54	1.43	5 (15%)

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
43	KGN	A	2500	-	-	4/30/54/54	0/1/1/1
44	GTP	C	1101	41	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	1101	GTP	C5-C6	-3.98	1.39	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C	1101	GTP	PA-O3A-PB	-3.55	120.66	132.83
44	C	1101	GTP	C5-C6-N1	3.15	119.51	113.95
44	C	1101	GTP	C8-N7-C5	3.02	108.74	102.99
44	C	1101	GTP	C2-N1-C6	-2.85	119.86	125.10
44	C	1101	GTP	PB-O3B-PG	-2.78	123.29	132.83

There are no chirality outliers.

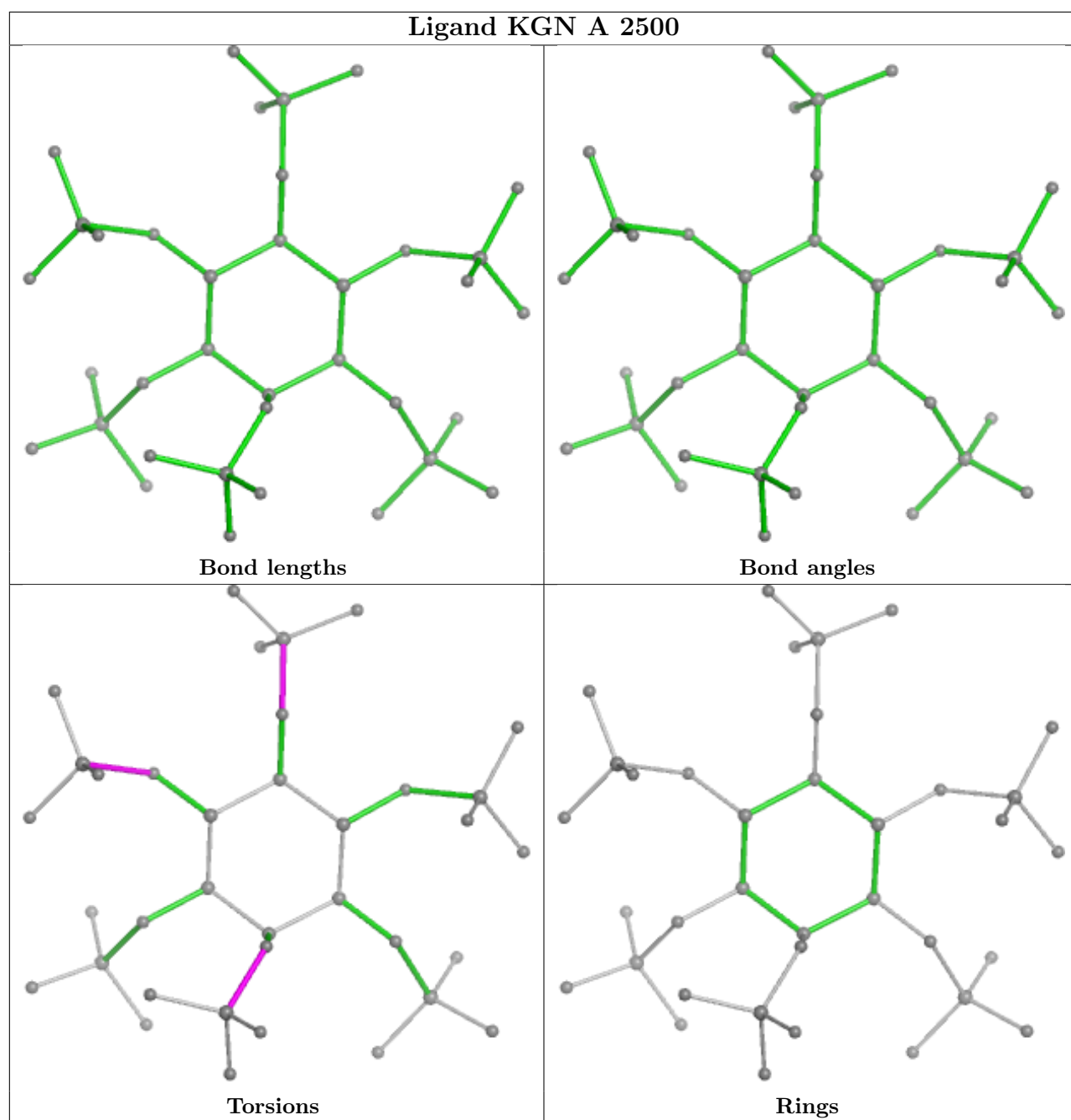
All (7) torsion outliers are listed below:

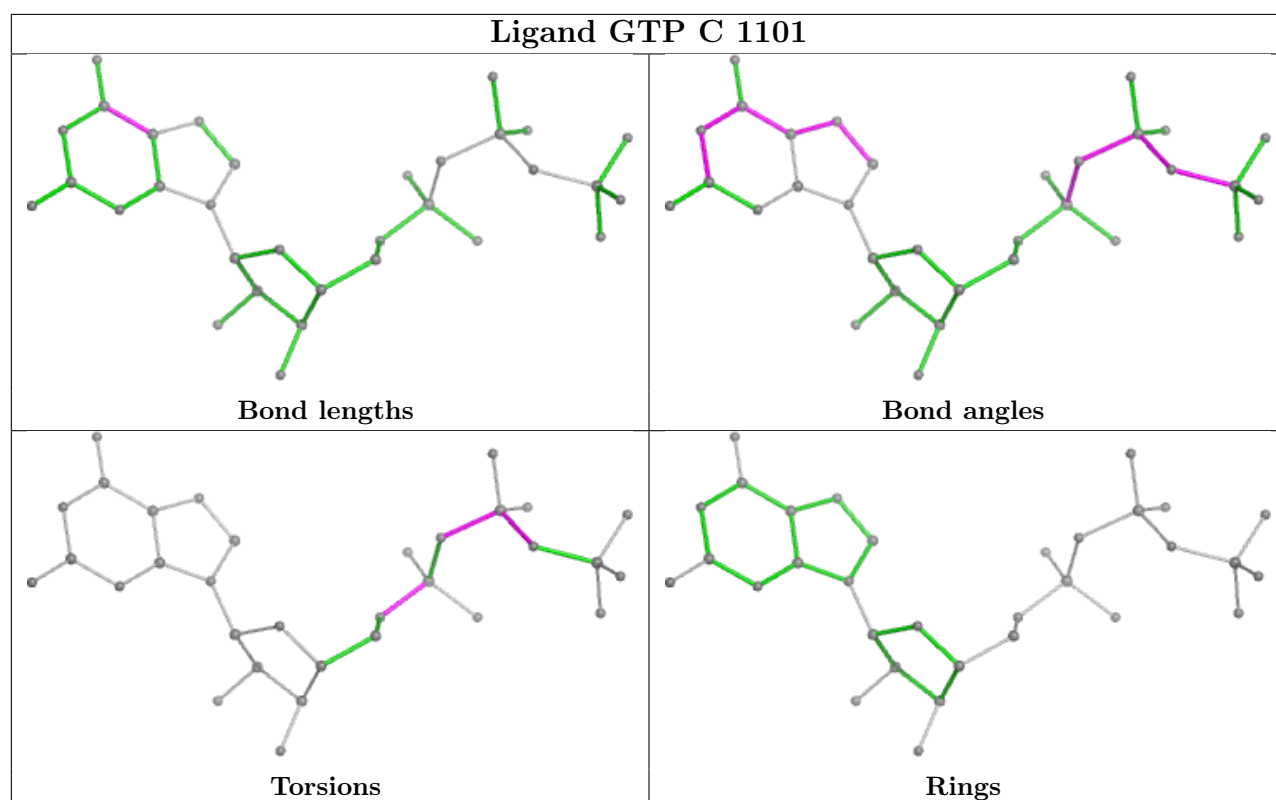
Mol	Chain	Res	Type	Atoms
43	A	2500	KGN	C3-O13-P3-O23
43	A	2500	KGN	C6-O16-P6-O46
44	C	1101	GTP	C5'-O5'-PA-O3A
44	C	1101	GTP	PA-O3A-PB-O1B
43	A	2500	KGN	C5-O15-P5-O45
43	A	2500	KGN	C6-O16-P6-O36
44	C	1101	GTP	PG-O3B-PB-O2B

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
25	X	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	18:UNK	C	35:UNK	N	201.98
1	X	51:UNK	C	200:UNK	N	106.75

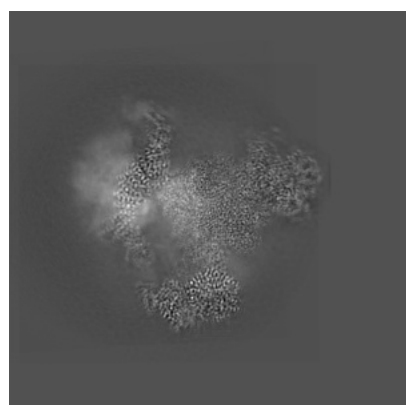
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12106. These allow visual inspection of the internal detail of the map and identification of artifacts.

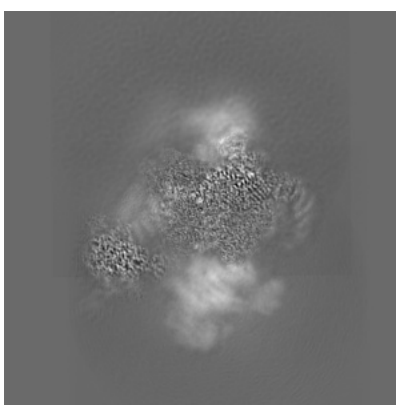
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

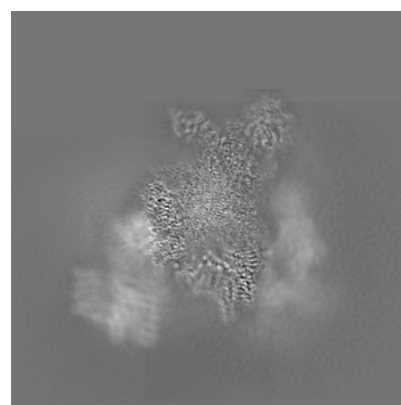
6.1.1 Primary map



X



Y

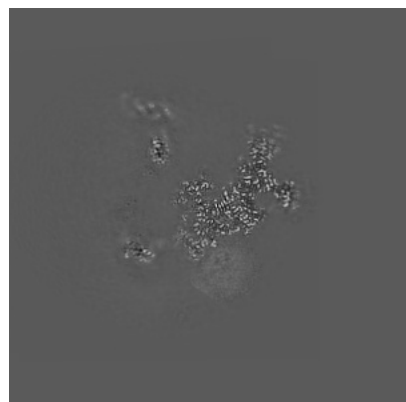


Z

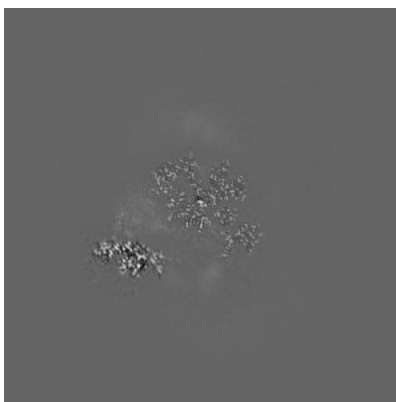
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

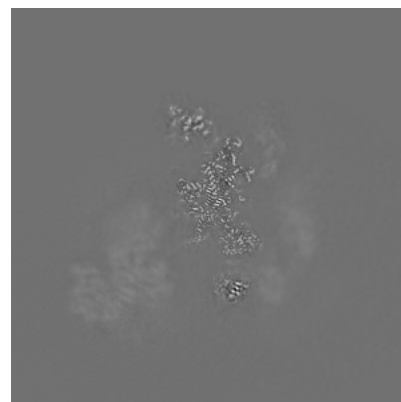
6.2.1 Primary map



X Index: 200



Y Index: 200

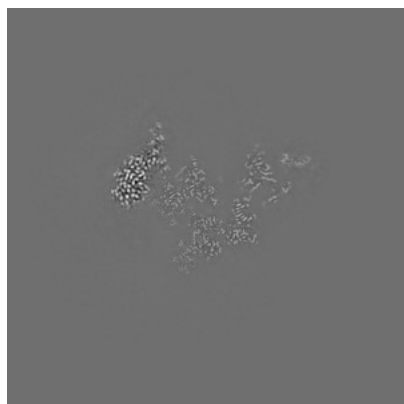


Z Index: 200

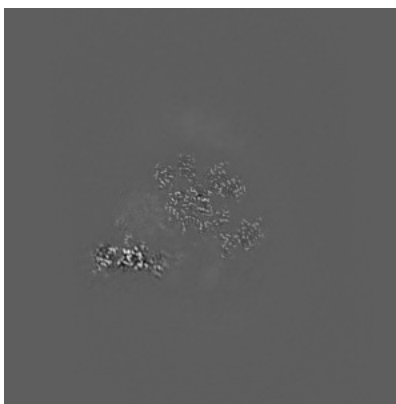
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

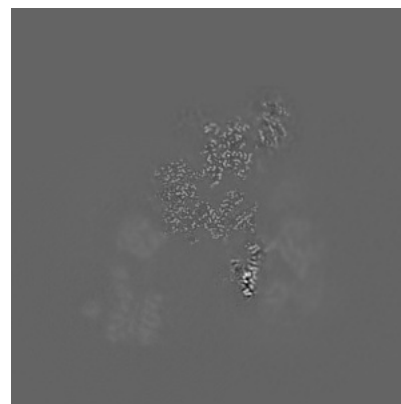
6.3.1 Primary map



X Index: 235



Y Index: 205

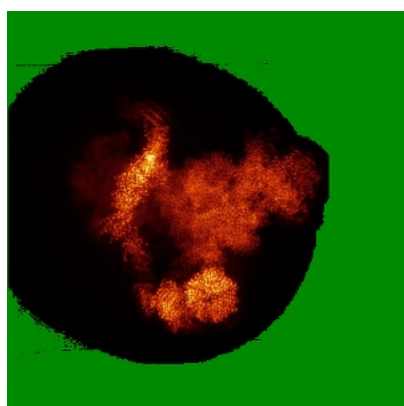


Z Index: 224

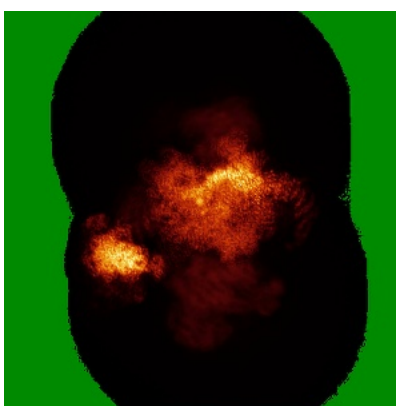
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

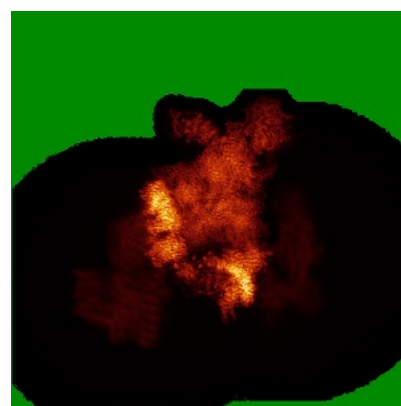
6.4.1 Primary map



X



Y

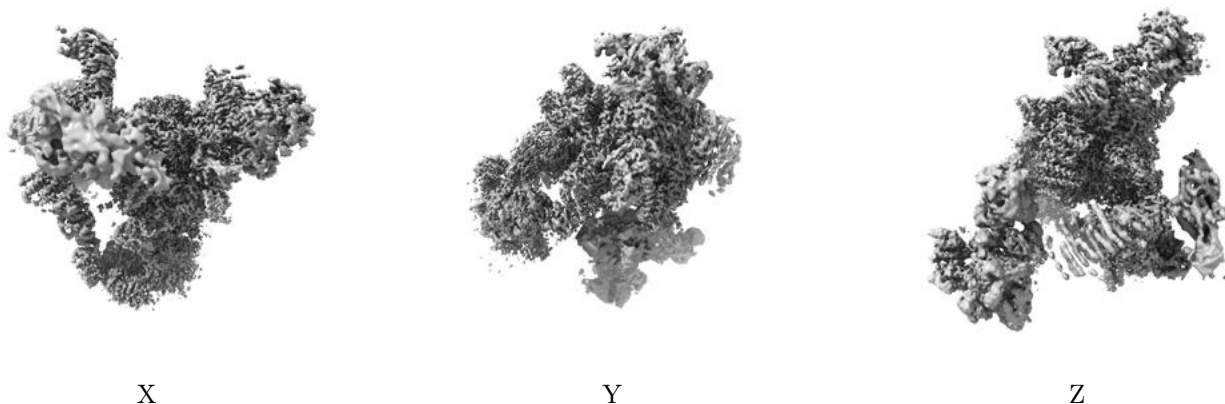


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

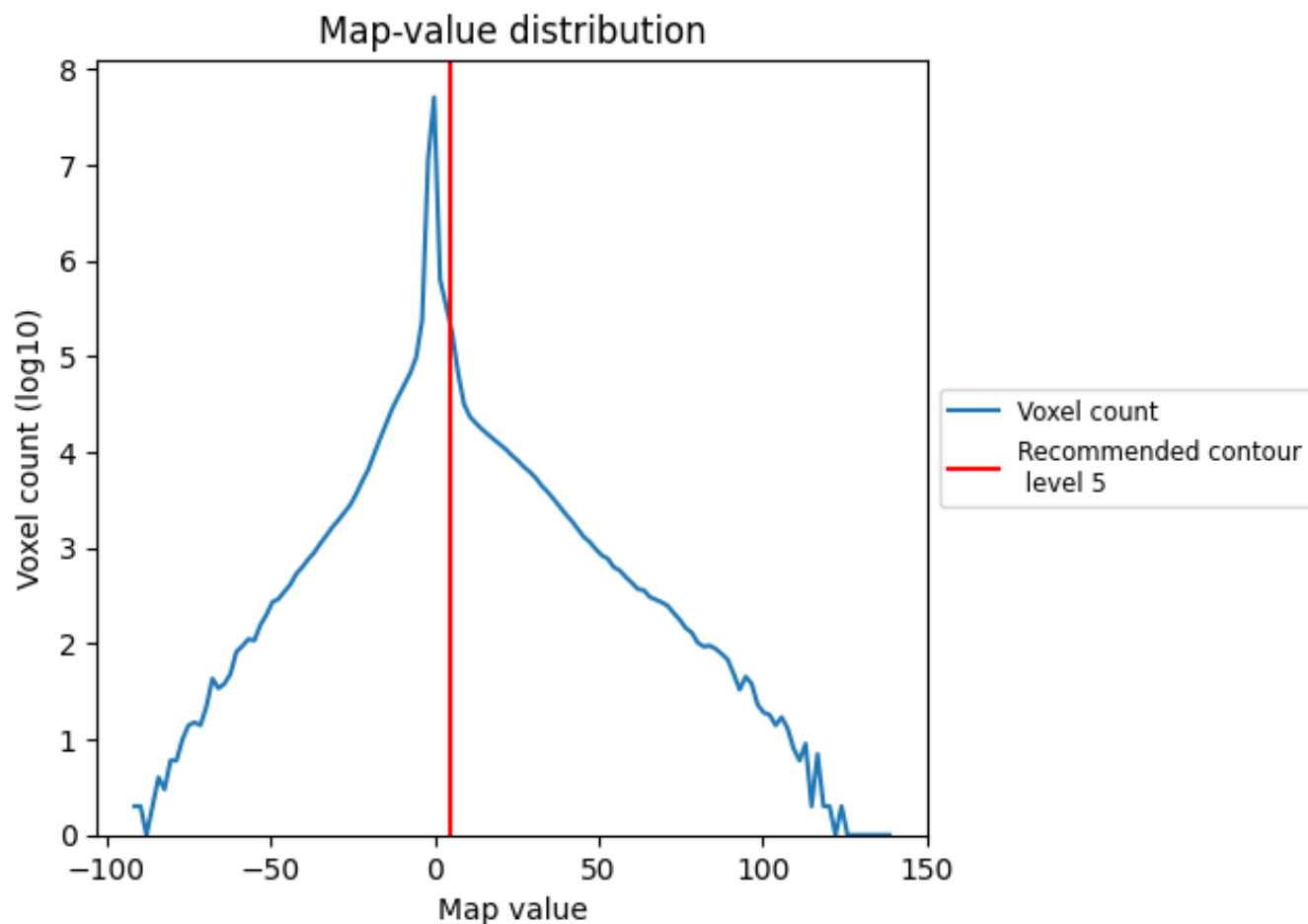
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

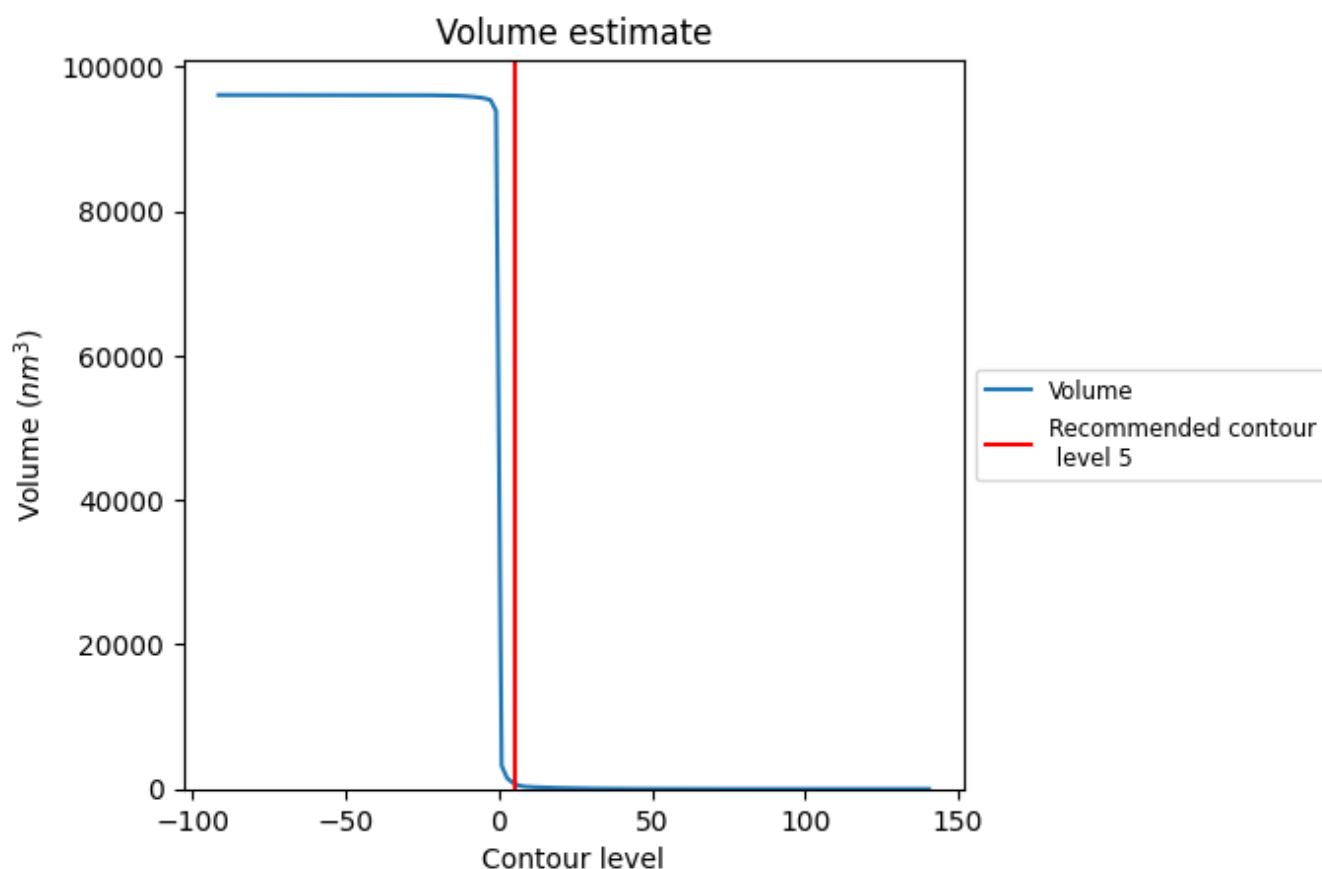
This section contains the results of statistical analysis of the map.

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.

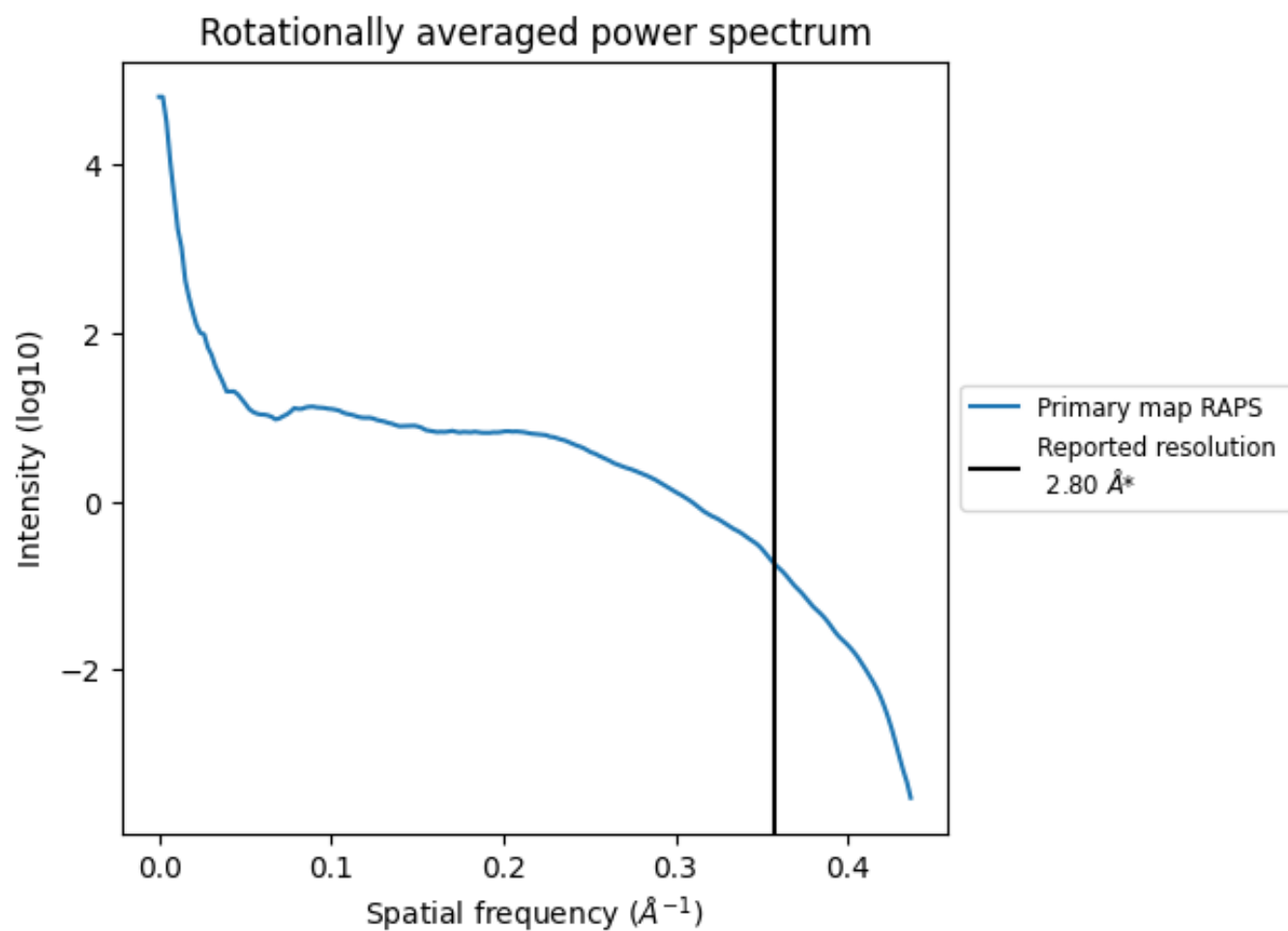
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 773 nm^3 ; this corresponds to an approximate mass of 699 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 0.357 Å⁻¹

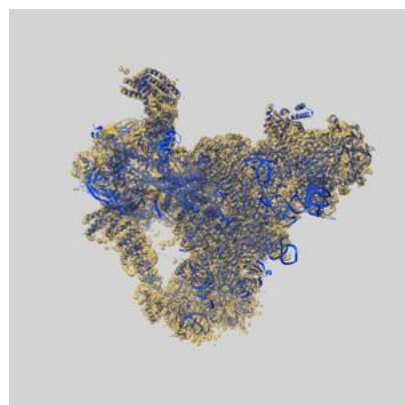
8 Fourier-Shell correlation

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

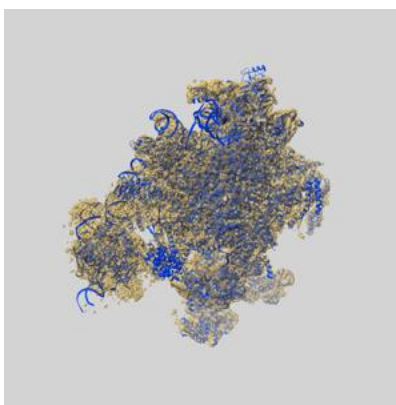
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12106 and PDB model 7B9V. Per-residue inclusion information can be found in section 3 on page 16.

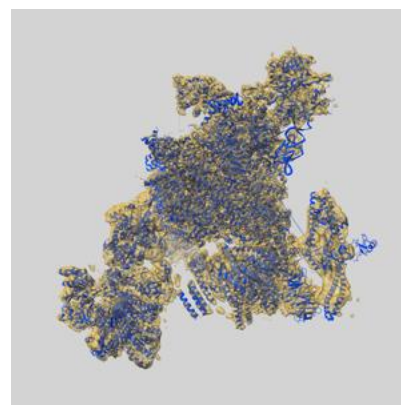
9.1 Map-model overlay [i](#)



X



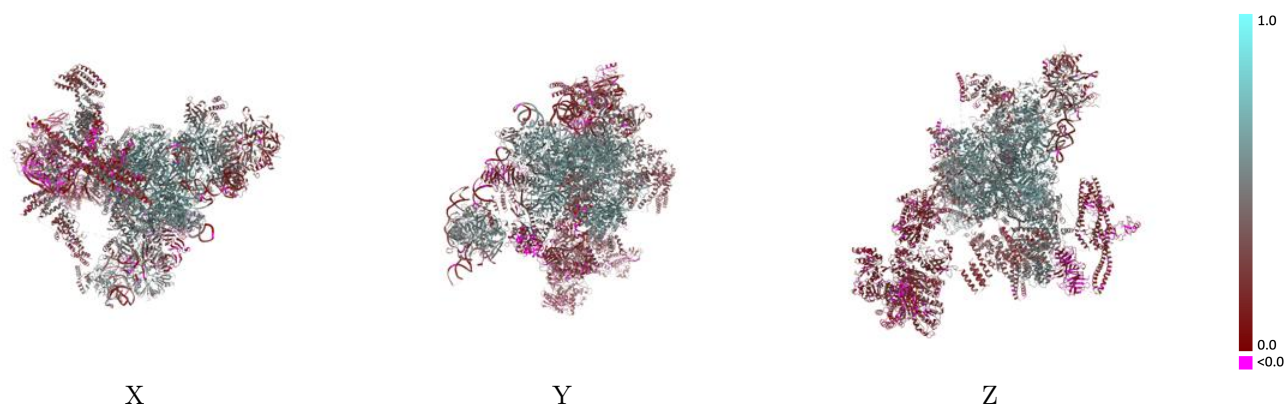
Y



Z

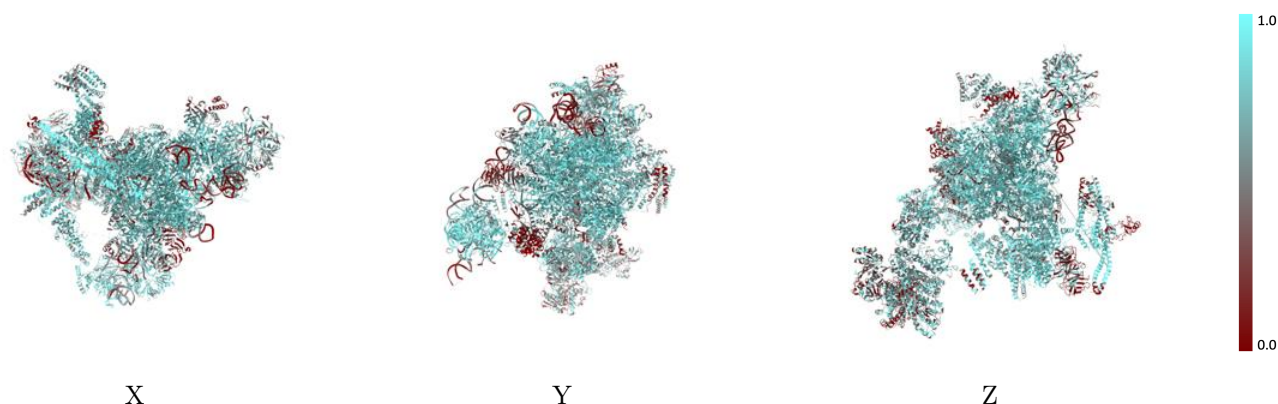
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



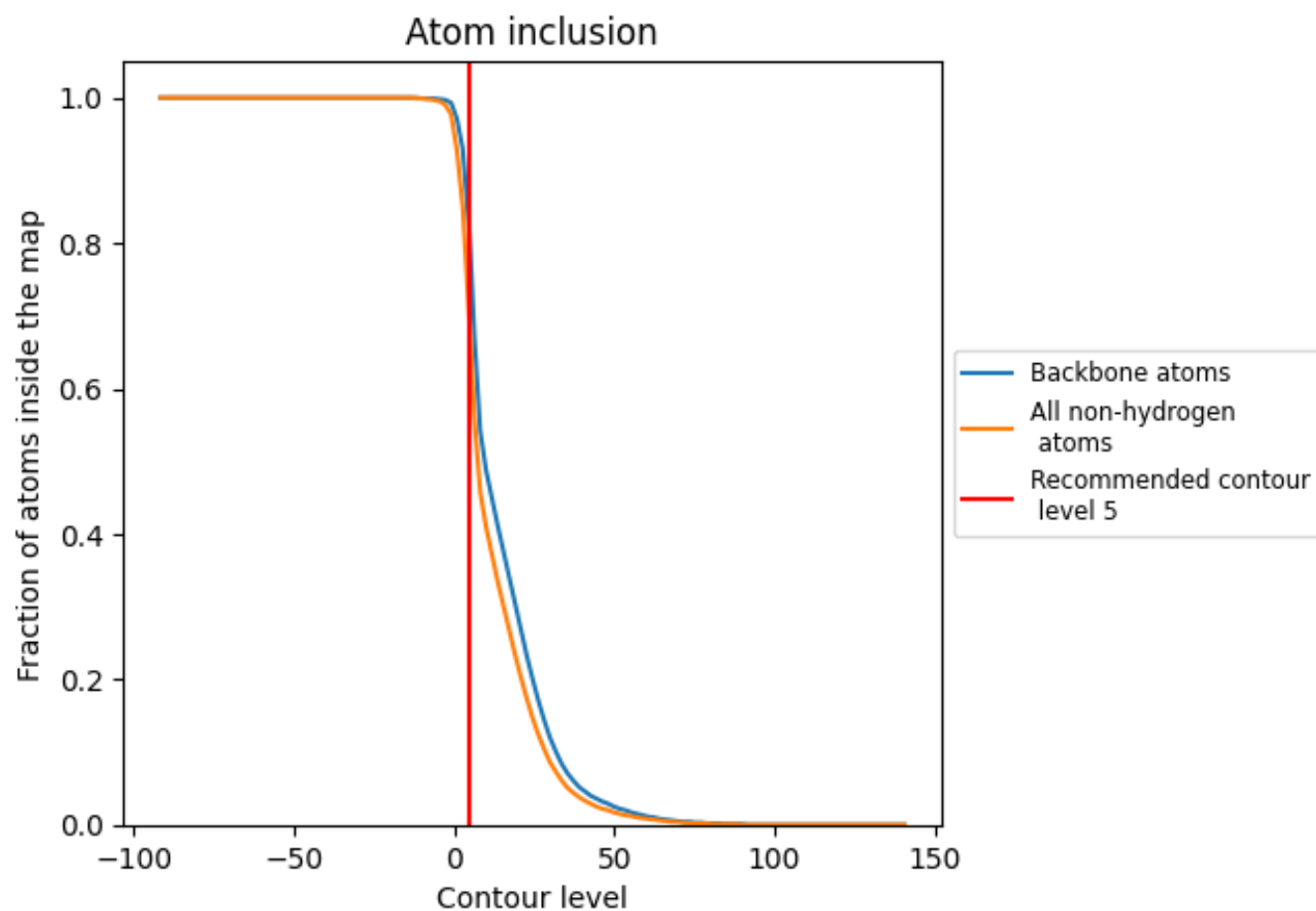
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6770	 0.3780
2	 0.5380	 0.2700
5	 0.5300	 0.3900
6	 0.7920	 0.5230
A	 0.7870	 0.5100
B	 0.5320	 0.1760
C	 0.7960	 0.5320
D	 0.7260	 0.4540
E	 0.8060	 0.5590
F	 0.6180	 0.4210
G	 0.7500	 0.4440
H	 0.6740	 0.3940
I	 0.6010	 0.3930
J	 0.8720	 0.5870
K	 0.7050	 0.5030
L	 0.8460	 0.5710
M	 0.8320	 0.5600
N	 0.6440	 0.4760
O	 0.7030	 0.4390
P	 0.7720	 0.5440
Q	 0.6890	 0.1520
R	 0.4060	 0.3950
S	 0.7910	 0.4500
T	 0.8050	 0.4100
W	 0.8300	 0.4660
X	 0.7180	 0.2720
Y	 0.8490	 0.4960
Z	 0.7120	 0.3900
a	 0.0000	 0.0600
b	 0.6440	 0.3770
c	 0.1320	 0.2090
d	 0.7510	 0.4440
e	 0.6090	 0.2880
f	 0.5980	 0.2340
g	 0.6540	 0.3420



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Chain	Atom inclusion	Q-score
h	 0.5790	 0.2710
j	 0.5370	 0.2290
k	 0.8750	 0.5160
l	 0.8870	 0.5170
m	 0.8380	 0.4800
n	 0.8450	 0.4850
o	 0.3000	 0.1940
p	 0.8440	 0.4680
q	 0.8710	 0.5020
r	 0.8230	 0.4780
s	 0.7270	 0.1840
t	 0.3380	 0.1080
u	 0.6010	 0.1290
v	 0.6780	 0.1380
w	 0.3620	 0.0630
y	 0.6880	 0.4420