



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:58 AM UTC

PDB ID : 7B9V / pdb_00007b9v
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:

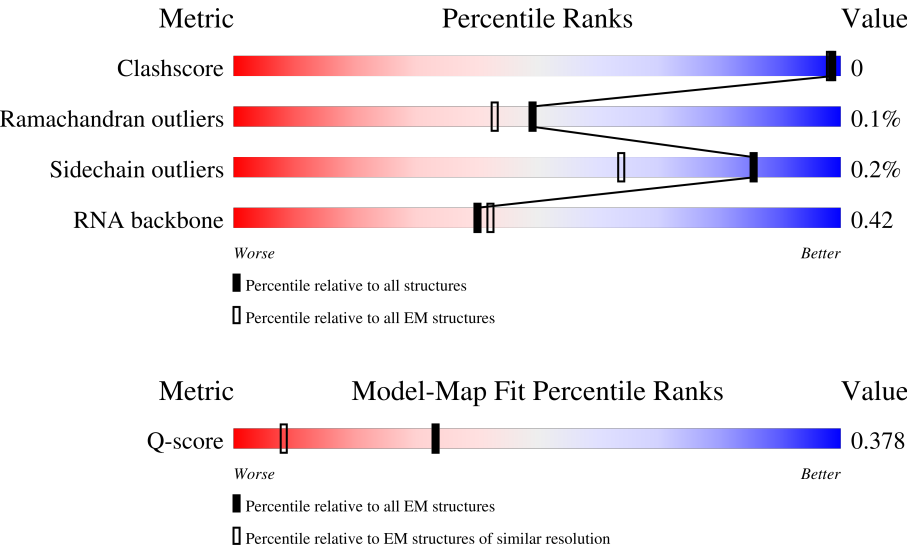
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	6% 13% 83%
2	5	214	39% 64% 17% 17%
3	6	112	16% 77% 13% 9%

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Mol	Chain	Length	Quality of chain
4	A	2413	
5	B	2163	
6	C	1008	
7	D	291	
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	

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Mol	Chain	Length	Quality of chain
29	b	196	
29	k	196	
30	c	382	
31	d	101	
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		

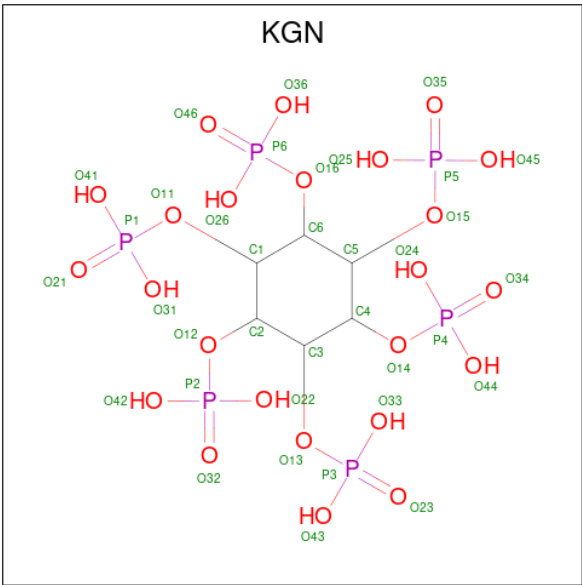
- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: K) (formula: K).

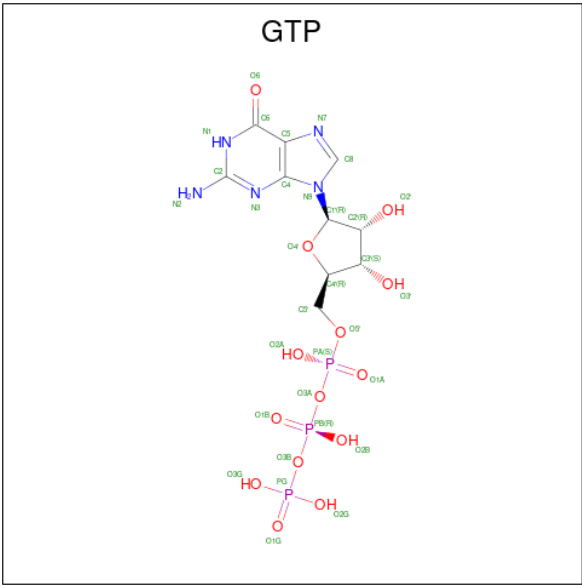
Mol	Chain	Residues	Atoms		AltConf
42	6	1	Total	K	0
			1	1	

- Molecule 43 is D-chiro inositol hexakisphosphate (CCD ID: 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 (CCD ID: 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	

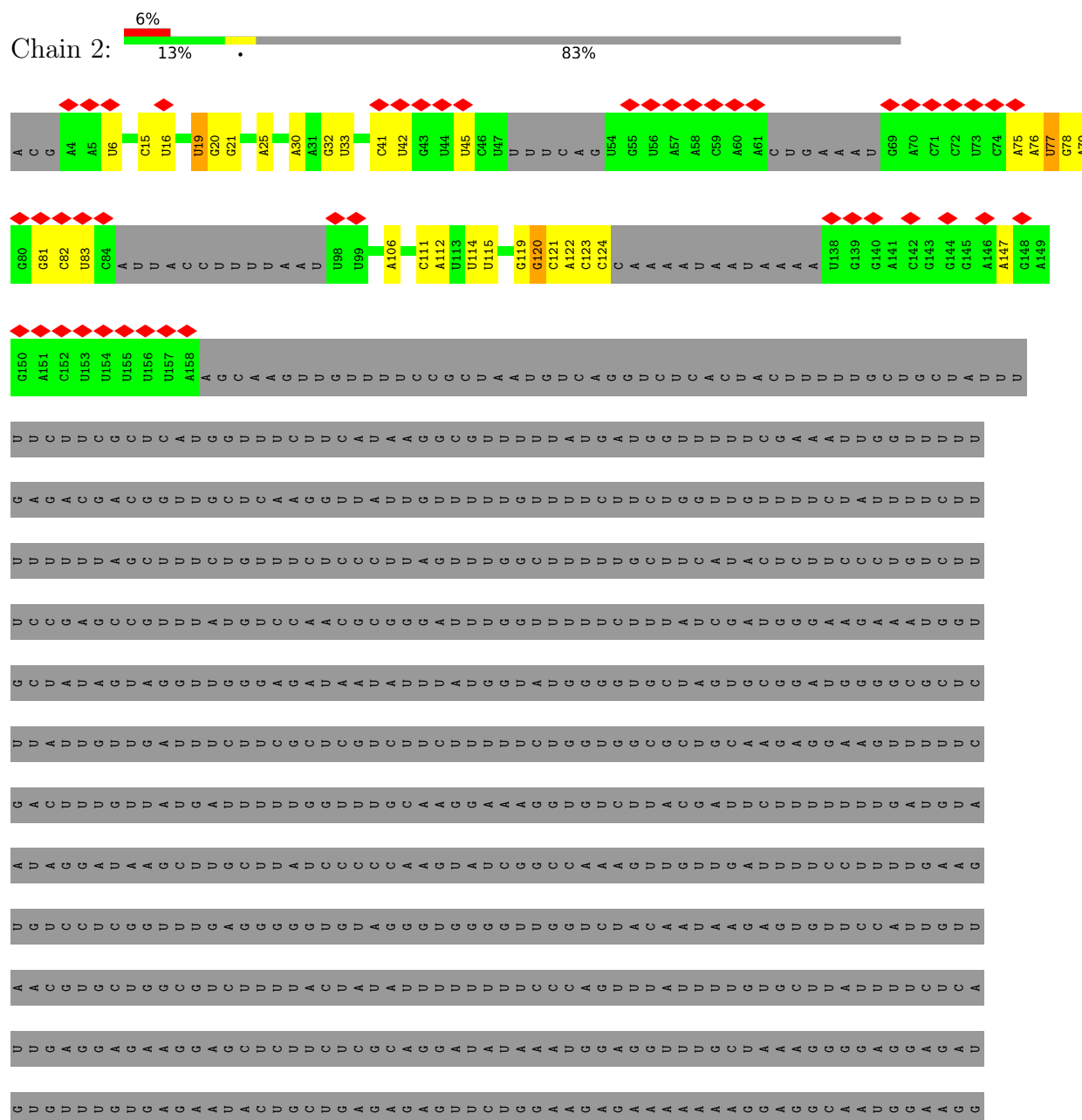
- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: U2 snRNA







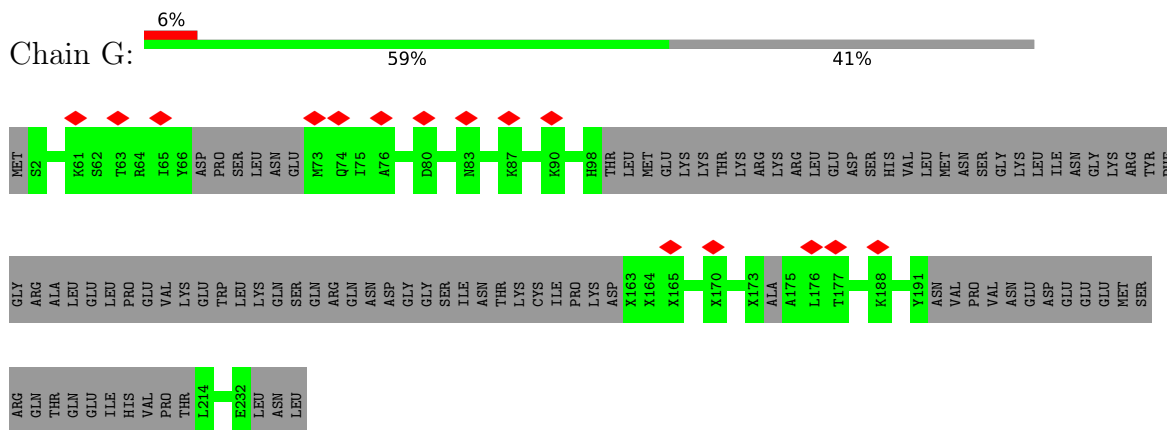
• Molecule 6: Pre-mRNA-splicing factor SNU114

- Molecule 7: Splicing factor YJU2

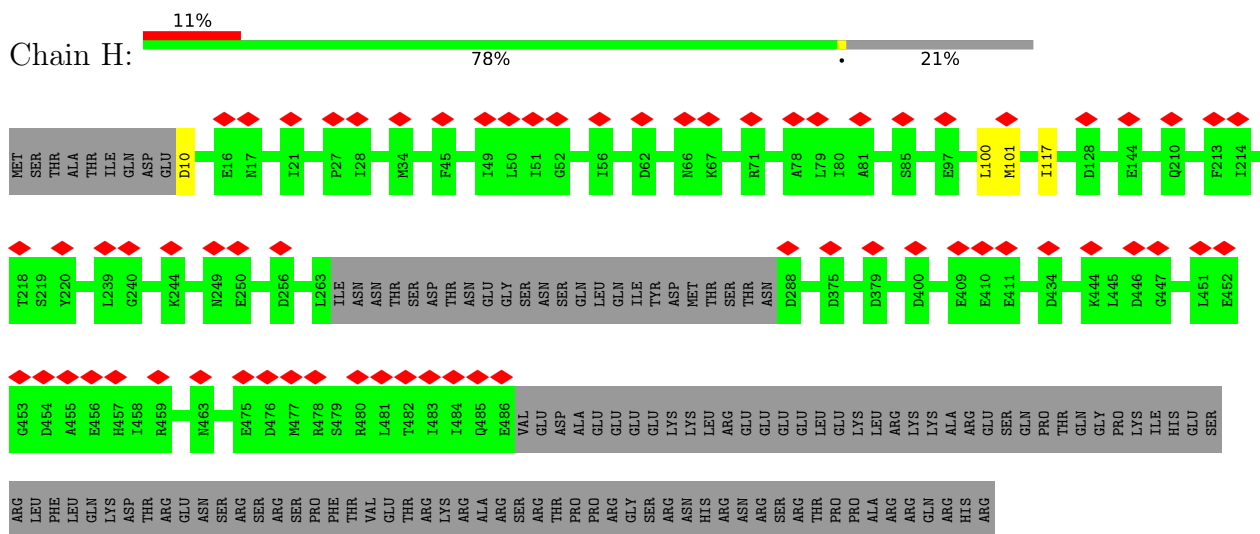
- Molecule 8: 5' exon of UBC4 mRNA

- Molecule 9: Pre-mRNA-splicing factor CWC25

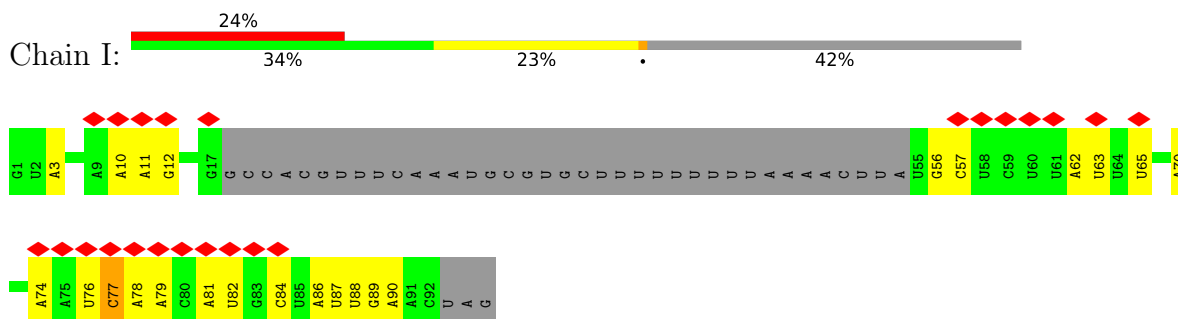
- Molecule 10: Pre-mRNA-splicing factor ISY1



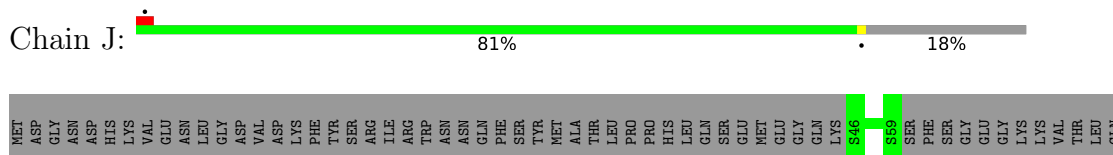
- Molecule 11: CWC22 isoform 1

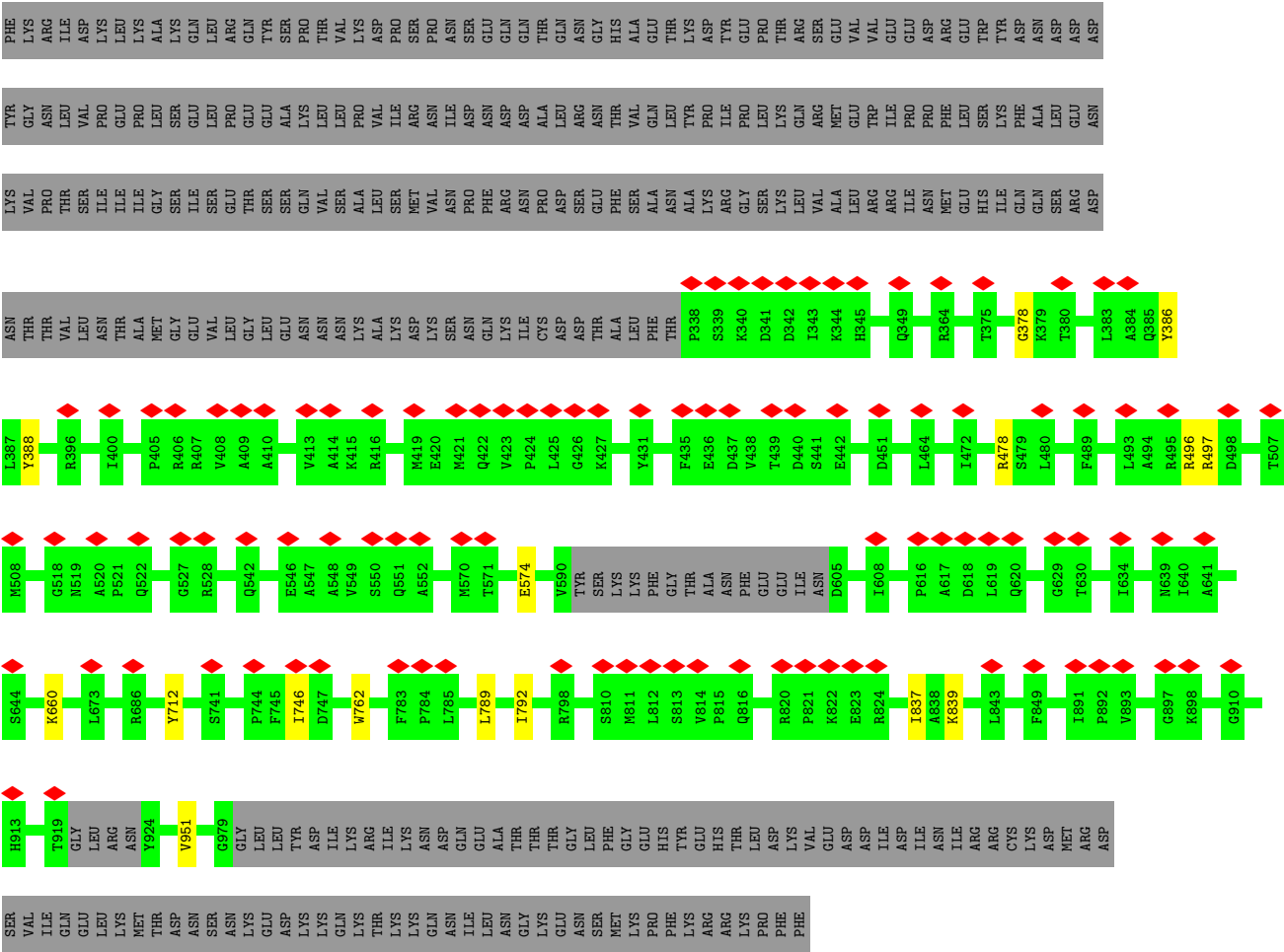


- Molecule 12: Branched intron and 3' exon of UBC4 pre-mRNA

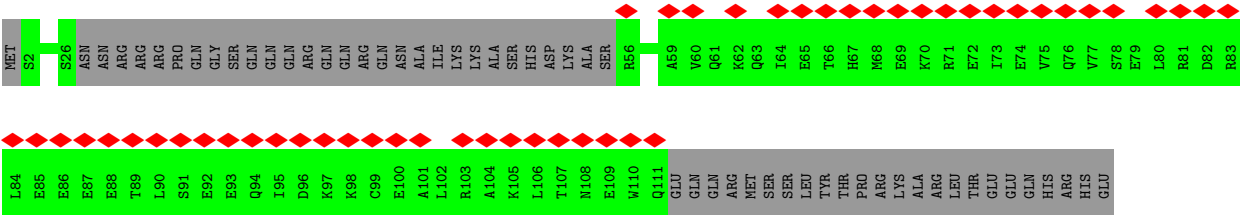


- Molecule 13: BJ4_G0054360.mRNA.1.CDS.1

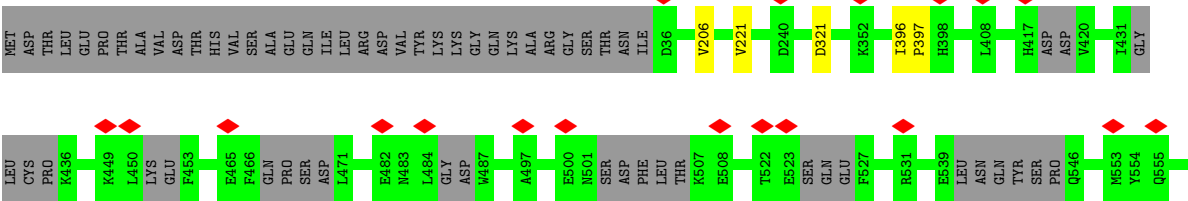
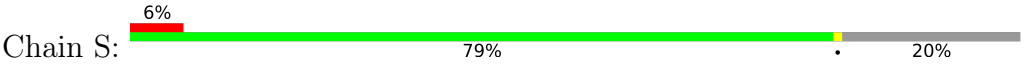


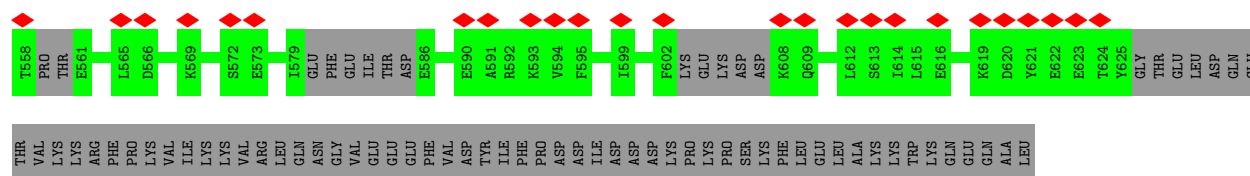


• Molecule 21: Pre-mRNA-splicing factor CWC21

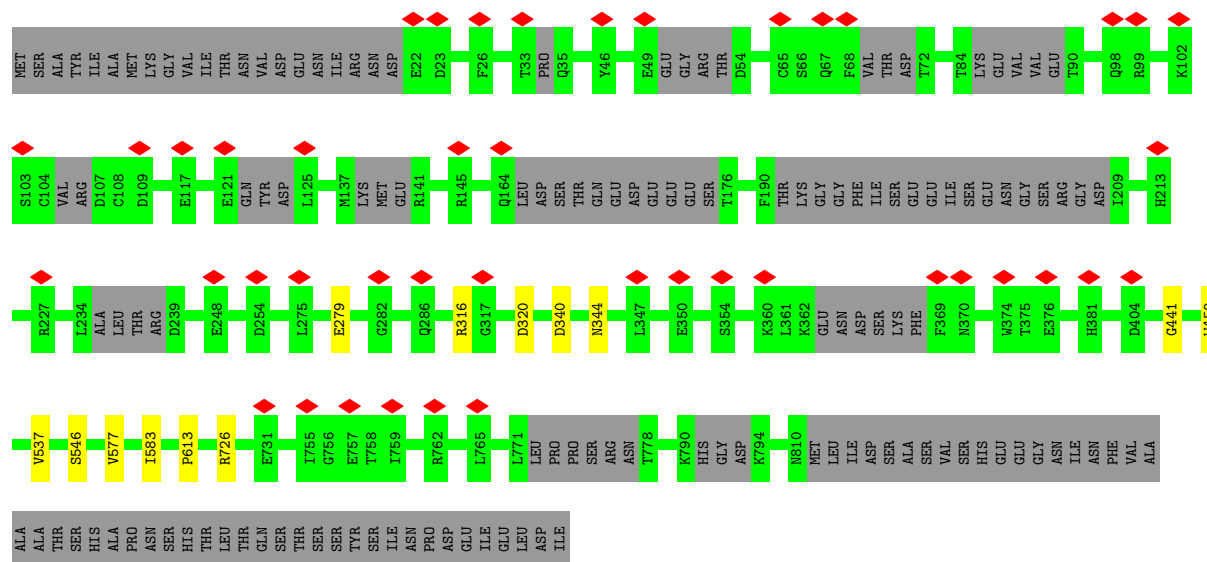
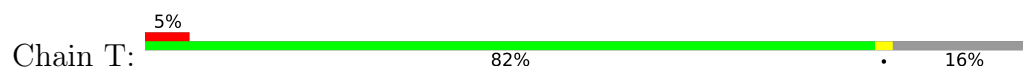


• Molecule 22: CLF1 isoform 1

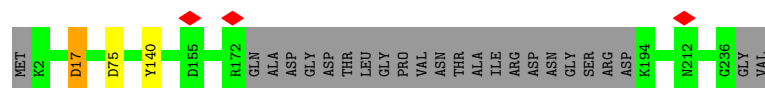
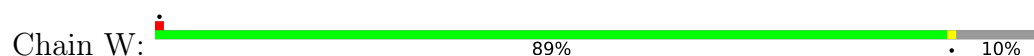




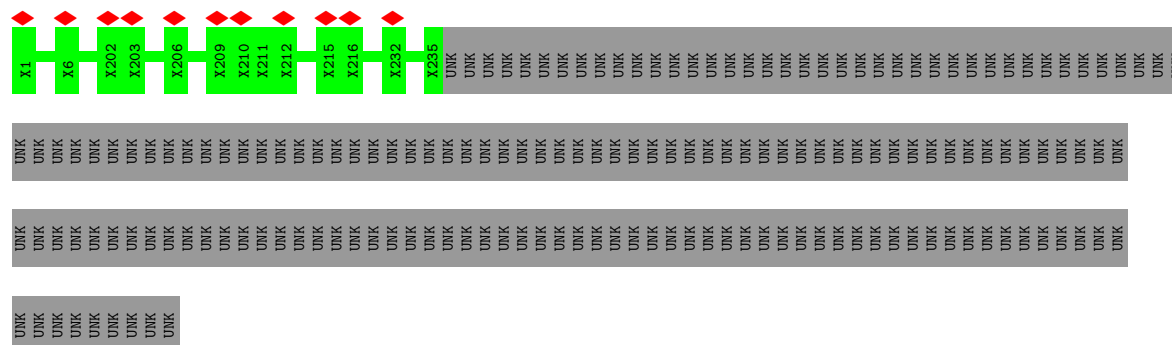
• Molecule 23: SYF1 isoform 1



• Molecule 24: HLJ1_G0053790.mRNA.1.CDS.1



• Molecule 25: Unassigned structure



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

Chain Y:  79% 21%

MET VAL GLU PRO GLN ARG LYS LYS GLN ARG ASP ARG ASP THR HIS THR VAL ALA GLU PRO VAL T24 L111

• Molecule 27: NTC20 isoform 1

Chain Z:  39% 61%

MET P2 N23 LEU GLY LYS THR GLN LYS THR GLU ALA LYS ASP THR VAL PHE ASP ASP THR ASN LEU VAL GLY ASN ILE SER SER PRO GLU VAL T24 L111

TYR ILE ILE PRO GLN LYS ASN GLU HIS ARG TYR ASP VAL C96 E110 G122 I123 I124 R125 K126 R127 V128 LEU GLN PRO CYS THR ARG ASP ASP ASP ASP ASP GLY

• Molecule 28: Pre-mRNA-splicing factor 18

Chain a:  55% 45%

MET ASP LEU ASP LEU ALA SER ILE LEU LYS GLU ILE SER LYS LYS LYS GLU LEU ALA ASN SER SER LYS VAL GLN PRO CYS THR GLU LYS PHE PRO HIS GLU SER ALA ILE ASP GLU THR PRO ARG GLN VAL GLU GLN THR ASP GLU ASN LEU SER

ASP ASN GLN SER ASP ASP ILE ARG THR THR ILE SER LEU N76 N77 P78 E79 R80 I81 Q82 E83 A84 I85 A86 Q87 D88 K89 T90 ILE S92 V93 I94 I95 D96 P97 S98 Q99 I100 G101 S102 T103 E104 G105 K106 P107 L108 L109 S110 M111 K112 G113 N114 L115 Y116 I117 H118 E119 I120

L121 S122 R123 V124 K125 A126 S127 L128 E129 A130 Y131 H132 P133 E134 L135 F136 D138 T139 K140 K141 A142 L143 F144 P145 L146 L147 L148 Q149 R151 R152 N153 Q154 L155 A156 P157 D158 L159 L160 I161 S162 L163 T165 V166 L167 Y168 H169 L170 Q171 Q172 P173 K174 E175 I176 N177 L178 A179 V180

Q181 S182 Y183 M184 K185 S187 I188 G189 VAL ALA THR PRO ILE GLY THR VAL GLY ILE HIS A182 ARG SER ALA HIS LYS ILE GLN GLY ARG ASN ILE D223 E224 R225 T226 R227 L228 W229 I230 T231 S232 I233 K234 R235 L236 T237 T238 F239 E240

E241 W242 Y243 T244 S245 N246 H247 ASP SER LEU ALA

• Molecule 29: Small nuclear ribonucleoprotein-associated protein B

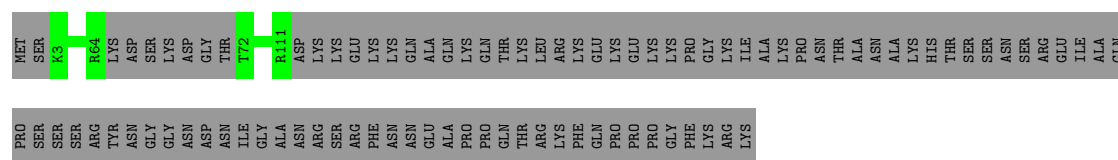
Chain b:  5% 47% 53%

MET SER K3 H5 S9 S10 R38 T56 D59 R62 P63 R64 LYS ASP ASP THR T72 L73 N74 L102 LEU SER LYS LYS GLU ARG LEU VAL ARG ASP ASP LYS LYS GLU LYS LYS GLN ALA PRO PRO GLN THR LYS LYS LEU ARG LYS PRO PRO GLU GLU LYS LYS PRO

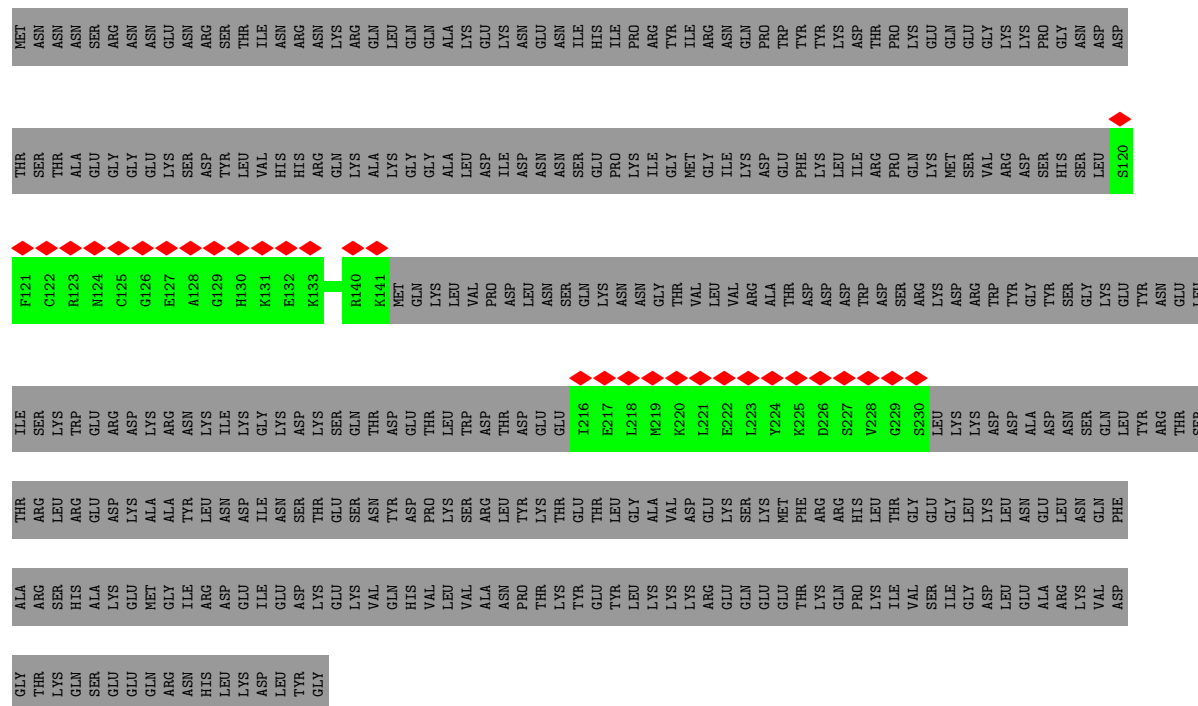
GLY LYS ILE ALA LYS PRO ASN THR ALA ASN ALA HIS THR SER SER ASN SER ARG GLU ILE GLN PRO SER SER SER TYR ASN GLY GLY ASN ASP ASP ILE GLY ALA ARG ARG ARG PHE ASN ASN LYS LYS ALA PRO PRO GLN THR ARG PHE GLN PRO PRO GLY PHE

LYS ARG LYS

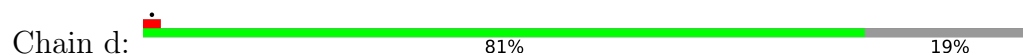
• Molecule 29: Small nuclear ribonucleoprotein-associated protein B



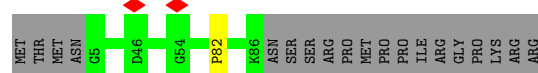
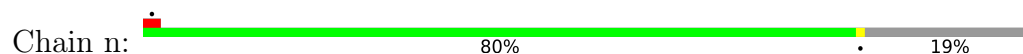
- Molecule 30: Pre-mRNA-splicing factor SLU7



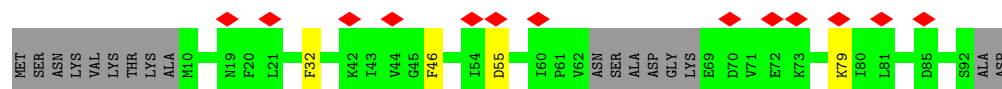
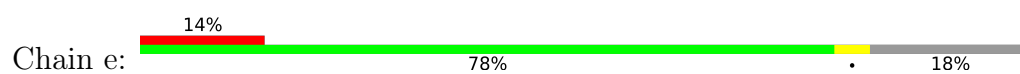
- Molecule 31: Small nuclear ribonucleoprotein Sm D3



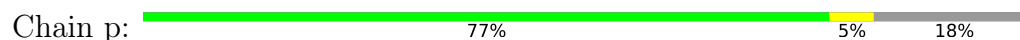
- Molecule 31: Small nuclear ribonucleoprotein Sm D3



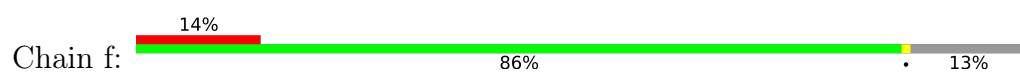
- Molecule 32: Small nuclear ribonucleoprotein E



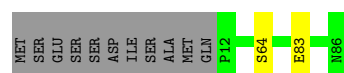
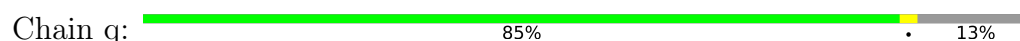
- Molecule 32: Small nuclear ribonucleoprotein E



- Molecule 33: Small nuclear ribonucleoprotein F



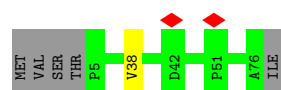
- Molecule 33: Small nuclear ribonucleoprotein F



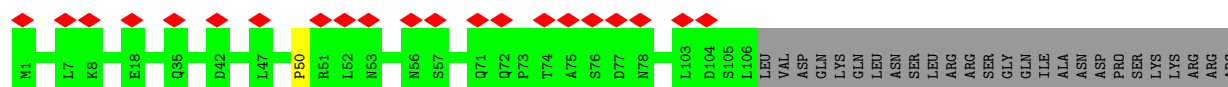
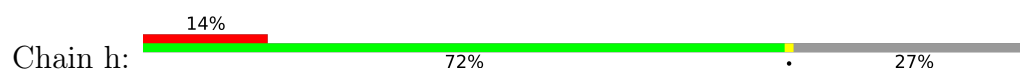
- Molecule 34: Small nuclear ribonucleoprotein G



- Molecule 34: Small nuclear ribonucleoprotein G



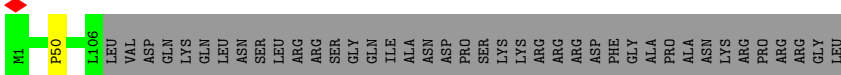
- Molecule 35: Small nuclear ribonucleoprotein Sm D1



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

- Molecule 35: Small nuclear ribonucleoprotein Sm D1

Chain l:  72% 27%

 M1 P50 L106

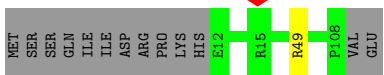
- Molecule 36: Small nuclear ribonucleoprotein Sm D2

Chain j:  20% 88% 12%

 MET SER GLN ILE ILE ASP ARG PRO LYS HIS E12 L13 S14 R15 A16 E17 L18 E19 E20 L21 E22 E23 G29 K73 E74 K80 G81 K82 N83 E88 R89 K93 D99 K106 T107 P108 VAL GLU

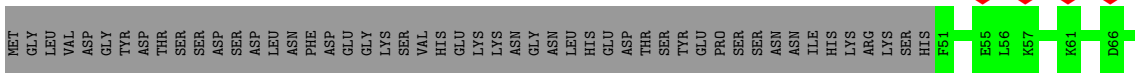
- Molecule 36: Small nuclear ribonucleoprotein Sm D2

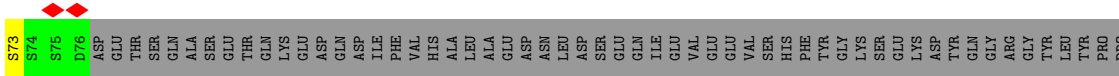
Chain m:  87% 12%

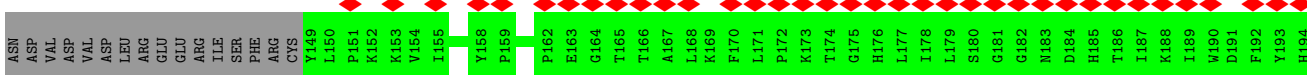
 MET SER GLN ILE ILE ASP ARG PRO LYS HIS E12 R15 R49 P108 VAL GLU

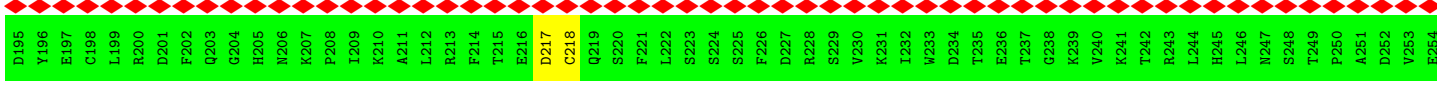
- Molecule 37: CDC40 isoform 1

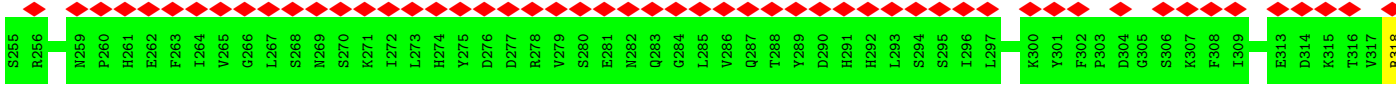
Chain o:  48% 71% 27%

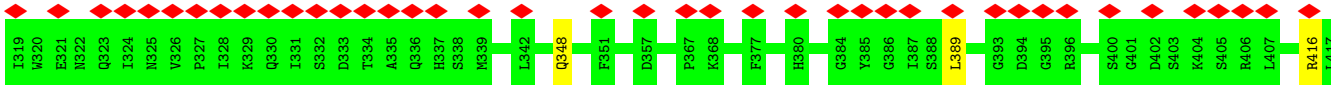
 MET GLY LEU VAL ASP GLY TYR ASP THR SER SER ASP ASP ASP LEU ASN CYS Y149 PHE ASP GLN GLY GLY LYS VAL SER HIS HIS GLU LYS ASN GLY ASN ASN LEU HIS GLU ASP THR SER THR TYR GLU PRO GLU SER ASN ASN ASN ILE HIS LYS ARG LYS SER HIS ASP P51 E55 L56 K57 K61 D66

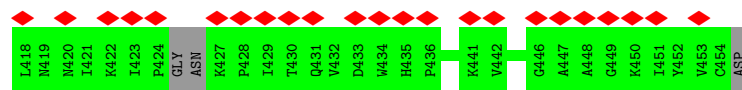
 S73 S74 S75 D76

 ASN ASP VAL ASP VAL ASP LEU ARG GLU GLU ARG ILE SER PHE ARG CYS Y149 L150 P151 K152 K153 V154 I155 Y158 P159 P162 E163 G164 T165 T166 A167 L168 K169 F170 S225 F226 D227 R228 S229 V230 K231 I232 W233 D234 T235 E236 G238 K239 V240 K241 T242 R243 I244 H245 L246 N247 S248 T249 P250 A251 D252 V253 E254

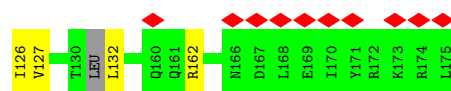
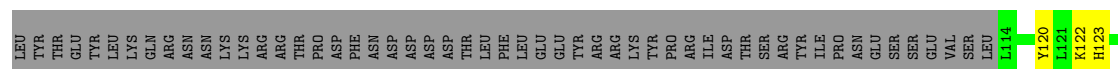
 D195 Y196 E197 C198 L199 R200 D201 F202 G203 Q204 H205 N206 K207 P208 I209 K210 A211 L212 R213 F214 T215 E216 D217 C218 Q219 S220 F221 L222 S223 S224 S225 F226 D227 R228 S229 V230 K231 I232 W233 D234 T235 E236 G238 K239 V240 K241 T242 R243 I244 H245 L246 N247 S248 T249 P250 A251 D252 V253 E254

 S255 R256 N259 P260 H261 E262 F263 I264 V265 G266 L267 S268 N269 S270 K271 I272 L273 H274 Y275 D276 D277 R278 V279 S280 E281 N282 Q283 G284 L285 V286 Q287 T288 Y289 D290 H291 H292 L293 S294 S295 I296 L297 K300 Y301 F302 P303 D304 G305 S306 K307 F308 I309 E313 D314 K315 T316 V317 R318

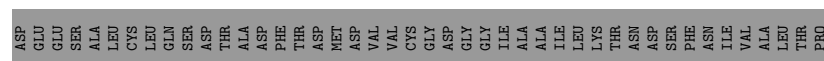
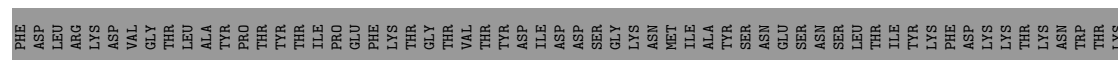
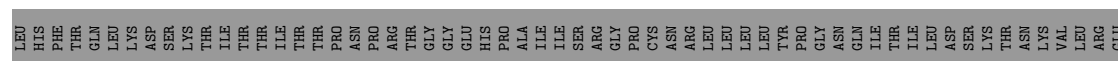
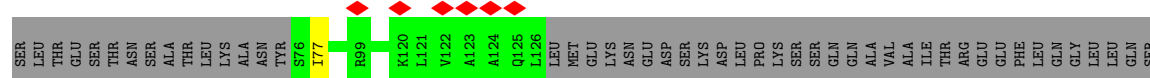
 I319 W320 E321 N322 Q323 T324 N325 V326 P327 T328 K329 Q330 I331 S332 D333 T334 A335 Q336 H337 S338 M339 L342 Q348 F351 D357 P357 K368 F377 H380 G384 Y385 G386 I387 S388 L389 G393 D394 G395 R396 S400 G401 D402 S403 K404 S405 R406 L407 R416 L417



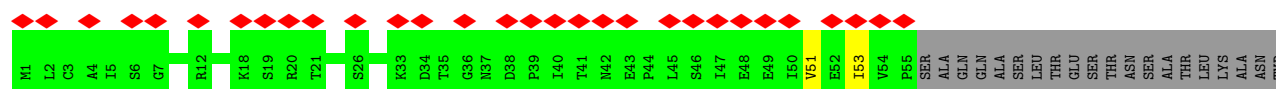
• Molecule 38: SNT309 isoform 1

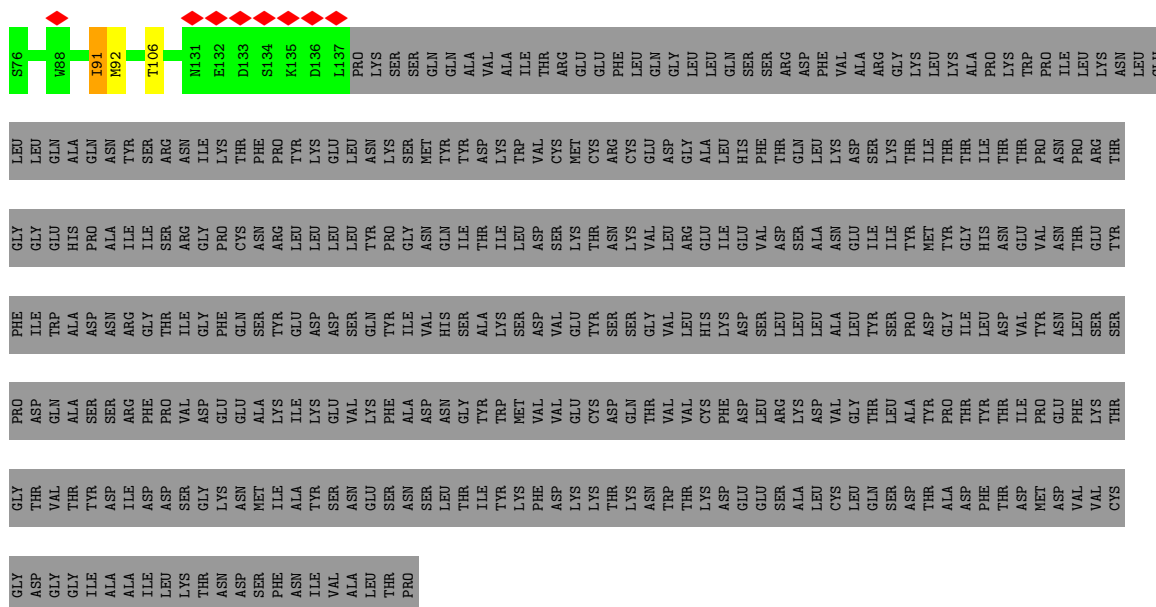


• Molecule 39: Pre-mRNA-processing factor 19

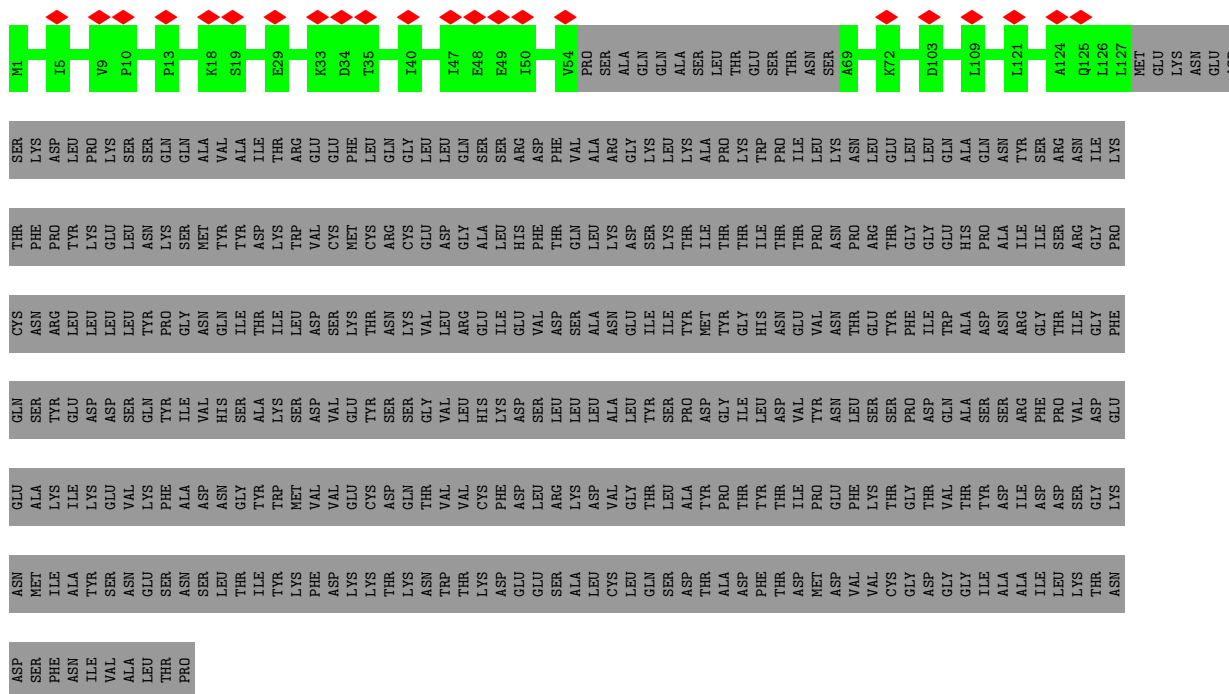


• Molecule 39: Pre-mRNA-processing factor 19

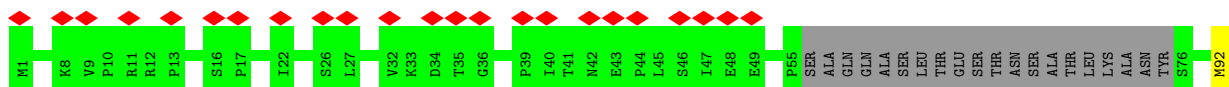
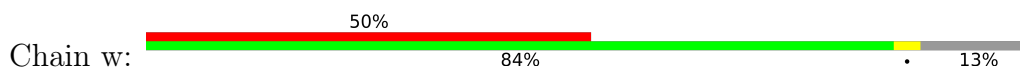


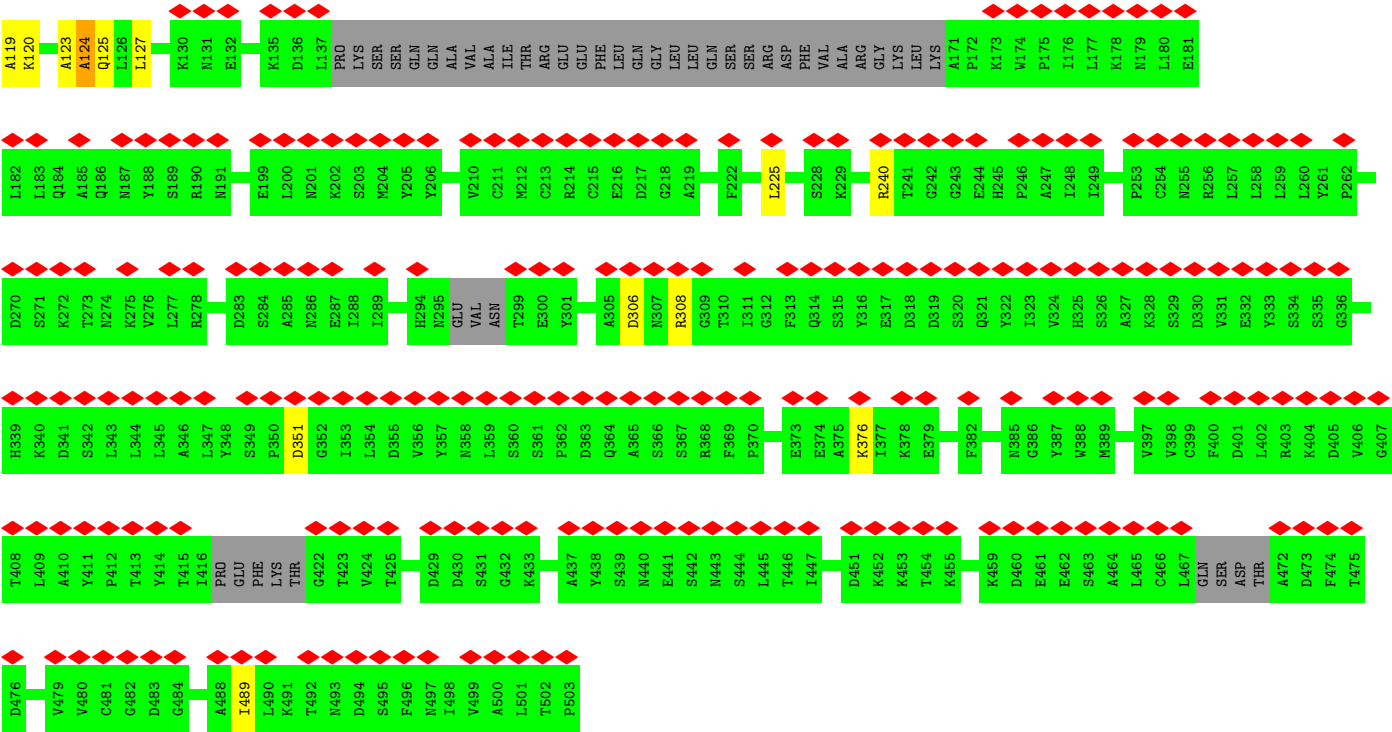


- Molecule 39: Pre-mRNA-processing factor 19

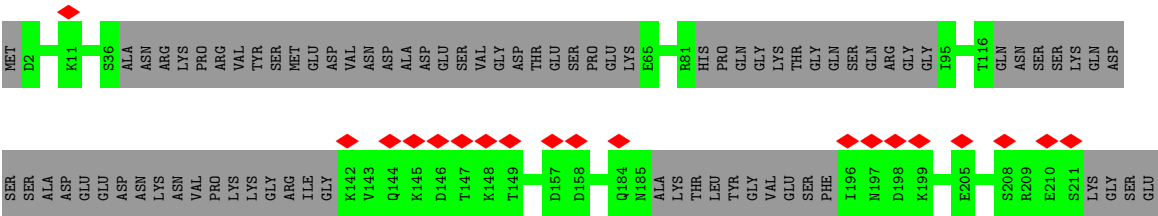


- Molecule 39: Pre-mRNA-processing factor 19





● Molecule 40: Pre-mRNA-splicing factor SYF2



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: KGN, K, GTP, ZN, SEP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.44	0/4585	0.76	3/7114 (0.0%)
2	5	0.41	0/4221	0.70	3/6573 (0.0%)
3	6	0.34	0/2427	0.61	1/3778 (0.0%)
4	A	0.45	0/18498	0.74	1/25078 (0.0%)
5	B	0.59	1/13971 (0.0%)	1.04	8/18941 (0.0%)
6	C	0.40	0/7291	0.66	1/9875 (0.0%)
7	D	0.45	0/1478	0.74	0/1967
8	E	0.35	0/341	0.69	0/530
9	F	0.44	0/459	0.64	0/613
10	G	0.41	0/1051	0.62	0/1406
11	H	0.46	0/3767	0.79	0/5076
12	I	0.49	0/1187	0.96	3/1839 (0.2%)
13	J	0.42	0/2989	0.75	0/4055
14	K	0.38	0/1479	0.64	0/1995
15	L	0.41	0/1307	0.67	0/1748
16	M	0.40	0/2094	0.76	1/2815 (0.0%)
17	N	0.46	0/2124	0.77	0/2860
18	O	0.51	0/2049	0.80	1/2748 (0.0%)
19	P	0.39	0/623	0.70	0/832
20	Q	0.63	0/5056	1.12	10/6846 (0.1%)
21	R	0.44	0/557	0.67	0/750
22	S	0.46	0/4248	0.74	3/5759 (0.1%)
23	T	0.51	0/5482	0.86	2/7438 (0.0%)
24	W	0.46	0/1757	0.80	0/2372
26	Y	0.45	0/722	0.90	0/963
27	Z	0.44	0/446	0.64	0/591
28	a	0.52	0/1154	0.69	0/1561
29	b	0.44	0/758	0.88	0/1018
29	k	0.49	0/836	0.97	0/1120
30	c	0.43	0/295	0.73	0/386
31	d	0.55	0/642	0.89	0/868
31	n	0.57	0/642	0.99	2/868 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.50	0/616	0.93	0/835
32	p	0.53	0/616	0.94	1/835 (0.1%)
33	f	0.48	0/614	0.80	0/830
33	q	0.48	0/614	0.83	0/830
34	g	0.54	0/562	0.99	0/756
34	r	0.53	0/562	1.04	0/756
35	h	0.49	0/828	0.84	1/1124 (0.1%)
35	l	0.62	0/828	1.09	1/1124 (0.1%)
36	j	0.47	0/807	0.80	0/1083
36	m	0.51	0/807	0.96	0/1083
37	o	0.55	0/2737	1.00	2/3696 (0.1%)
38	s	0.78	1/428 (0.2%)	1.32	1/577 (0.2%)
39	t	0.62	0/805	1.08	0/1094
39	u	0.69	0/867	1.15	2/1178 (0.2%)
39	v	0.64	0/837	1.06	0/1137
39	w	0.52	0/3469	0.95	5/4707 (0.1%)
40	y	0.40	0/1008	0.62	0/1350
All	All	0.49	2/111541 (0.0%)	0.85	52/153378 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	s	122	LYS	CB-CG	-6.55	1.32	1.52
5	B	500	ASN	C-N	5.21	1.46	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Q	712	TYR	CA-CB-CG	-9.01	97.68	113.90
1	2	120	G	C2'-C3'-O3'	8.24	121.85	109.50
2	5	128	A	P-O3'-C3'	8.06	132.30	120.20
1	2	120	G	P-O3'-C3'	7.76	131.84	120.20
5	B	1605	ILE	CA-CB-CG2	6.88	122.19	110.50
23	T	537	VAL	CA-CB-CG1	6.42	121.31	110.40
6	C	430	ARG	N-CA-C	6.23	118.80	111.02
12	I	90	A	N9-C1'-C2'	-6.17	102.74	112.00
22	S	397	PRO	CA-C-N	6.11	129.08	120.28
22	S	397	PRO	C-N-CA	6.11	129.08	120.28
39	u	91	ILE	CA-CB-CG1	6.06	120.69	110.40
32	p	89	LEU	CD1-CG-CD2	-5.95	97.72	110.80
39	u	53	ILE	CG1-CB-CG2	-5.92	92.95	110.70
39	w	125	GLN	CA-CB-CG	5.91	125.92	114.10
38	s	132	LEU	N-CA-C	5.83	127.32	111.00
5	B	1658	TYR	CA-CB-CG	5.73	124.21	113.90
20	Q	746	ILE	CB-CA-C	-5.70	104.68	111.97
12	I	77	C	P-O3'-C3'	5.65	128.67	120.20
2	5	101	C	P-O3'-C3'	5.64	128.66	120.20
35	h	50	PRO	CA-N-CD	-5.62	104.13	112.00
39	w	125	GLN	N-CA-CB	5.61	118.14	110.01
39	w	127	LEU	N-CA-CB	5.58	118.42	110.16
20	Q	660	LYS	CA-CB-CG	5.54	125.17	114.10
20	Q	378	GLY	CA-C-N	5.51	127.98	120.54
20	Q	378	GLY	C-N-CA	5.51	127.98	120.54
1	2	19	U	O4'-C1'-C2'	-5.50	100.30	105.80
37	o	218	CYS	N-CA-C	5.48	122.48	110.80
20	Q	386	TYR	CA-CB-CG	5.46	123.73	113.90
23	T	613	PRO	CA-N-CD	-5.44	104.39	112.00
37	o	217	ASP	N-CA-C	-5.41	99.70	108.52
2	5	130	A	OP2-P-O3'	5.35	124.05	108.00
3	6	36	U	C2'-C3'-O3'	5.34	121.72	113.70
18	O	505	PRO	CA-N-CD	-5.34	104.52	112.00
5	B	500	ASN	CA-CB-CG	5.33	117.93	112.60
20	Q	388	TYR	CA-CB-CG	5.29	123.42	113.90
16	M	159	ARG	CB-CG-CD	5.29	123.46	111.30
35	l	50	PRO	CA-N-CD	-5.26	104.64	112.00
5	B	1605	ILE	CA-C-N	5.24	129.07	120.63
5	B	1605	ILE	C-N-CA	5.24	129.07	120.63
12	I	90	A	O4'-C1'-N9	5.24	116.36	108.50
4	A	2389	PRO	CA-N-CD	-5.21	104.71	112.00
39	w	92	MET	CB-CG-SD	5.19	128.27	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	396	ILE	CA-CB-CG2	5.15	119.25	110.50
5	B	1484	TYR	CA-CB-CG	-5.12	104.69	113.90
5	B	1991	ASP	CA-C-N	5.10	128.13	120.83
5	B	1991	ASP	C-N-CA	5.10	128.13	120.83
20	Q	762	TRP	CA-CB-CG	5.05	123.19	113.60
20	Q	574	GLU	CA-C-N	5.04	126.99	120.44
20	Q	574	GLU	C-N-CA	5.04	126.99	120.44
31	n	82	PRO	CA-C-N	5.01	127.24	120.38
31	n	82	PRO	C-N-CA	5.01	127.24	120.38
39	w	124	ALA	N-CA-CB	5.01	118.70	110.39

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 [i](#)

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	4	0
3	6	2170	0	1095	0	0
4	A	18036	0	17967	6	0
5	B	13675	0	13679	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	2	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	1	0
32	p	606	0	630	1	0
33	f	601	0	600	1	0
33	q	601	0	600	1	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
38	s	426	0	385	5	0
39	t	794	0	784	2	0
39	u	856	0	827	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	v	827	0	807	0	0
39	w	3405	0	3303	5	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	51	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 (51) 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)
39:w:120:LYS:O	39:w:124:ALA:HB3	1.90	0.71
39:w:119:ALA:O	39:w:123:ALA:HB3	1.96	0.66
38:s:123:HIS:NE2	39:u:92:MET:HG2	2.23	0.53
24:W:17:ASP:OD1	24:W:17:ASP:N	2.38	0.52
32:e:55:ASP:OD2	32:e:79:LYS:NZ	2.42	0.50
39:t:77:ILE:HG13	39:u:91:ILE:HD11	1.93	0.50
39:w:119:ALA:O	39:w:123:ALA:N	2.44	0.50
5:B:2011:ILE:HD12	5:B:2030:ILE:HD11	1.94	0.50
5:B:1525:ALA:HB1	5:B:1527:MET:HE3	1.95	0.48
5:B:599:ILE:HG23	5:B:605:LEU:HD11	1.96	0.47
39:w:306:ASP:HB3	39:w:308:ARG:H	1.79	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
38:s:120:TYR:HA	38:s:123:HIS:ND1	2.32	0.45
23:T:340:ASP:O	23:T:344:ASN:ND2	2.50	0.45
38:s:123:HIS:CD2	39:u:92:MET:HG2	2.52	0.45
20:Q:837:ILE:HG22	20:Q:839:LYS:H	1.82	0.45
11:H:101:MET:HE3	11:H:117:ILE:HD11	1.98	0.44
23:T:320:ASP:OD1	23:T:320:ASP:N	2.50	0.44
2:5:159:C:O2'	2:5:161:U:OP2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
38:s:123:HIS:O	38:s:127:VAL:HG23	2.19	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
33:q:64:SER:O	33:q:64:SER:OG	2.33	0.43
4:A:1690:LYS:NZ	4:A:1735:ASP:OD1	2.52	0.42
39:w:225:LEU:HD21	39:w:489:ILE:HD11	2.01	0.42
6:C:88:THR:O	13:J:214:ASN:ND2	2.51	0.42
4:A:126:ASN:OD1	4:A:126:ASN:N	2.52	0.42
24:W:75:ASP:OD1	24:W:75:ASP:N	2.50	0.42
2:5:82:A:O3'	4:A:709:ARG:NH2	2.46	0.42
39:t:15:LEU:HD21	39:u:51:VAL:HG11	2.01	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
32:p:12:PRO:HA	32:p:13:PRO:HD3	1.93	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
38:s:126:ILE:HD13	38:s:126:ILE:HG21	1.92	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
2:5:175:G:C2	33:f:32:LYS:HE3	2.56	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	66
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%)	24	55
40	y	124/215 (58%)	124 (100%)	0	0	100	100
All	All	11942/17672 (68%)	11636 (97%)	300 (2%)	6 (0%)	49	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%)	1984 (100%)	3 (0%)	87	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	1536/1955 (79%)	1534 (100%)	2 (0%)	88	97
6	C	799/910 (88%)	799 (100%)	0	100	100
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%)	422 (100%)	0	100	100
13	J	325/397 (82%)	325 (100%)	0	100	100
14	K	164/328 (50%)	164 (100%)	0	100	100
15	L	140/141 (99%)	140 (100%)	0	100	100
16	M	219/296 (74%)	218 (100%)	1 (0%)	81	93
17	N	243/332 (73%)	243 (100%)	0	100	100
18	O	199/504 (40%)	199 (100%)	0	100	100
19	P	61/151 (40%)	60 (98%)	1 (2%)	55	83
20	Q	557/969 (58%)	556 (100%)	1 (0%)	87	96
21	R	47/121 (39%)	47 (100%)	0	100	100
22	S	369/633 (58%)	369 (100%)	0	100	100
23	T	505/786 (64%)	504 (100%)	1 (0%)	87	96
24	W	201/219 (92%)	199 (99%)	2 (1%)	68	88
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%)	127 (100%)	0	100	100
29	b	86/176 (49%)	86 (100%)	0	100	100
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%)	71 (100%)	0	100	100
32	e	70/83 (84%)	69 (99%)	1 (1%)	59	85
32	p	70/83 (84%)	68 (97%)	2 (3%)	37	73
33	f	67/77 (87%)	67 (100%)	0	100	100
33	q	67/77 (87%)	66 (98%)	1 (2%)	57	84
34	g	61/66 (92%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	r	61/66 (92%)	60 (98%)	1 (2%)	55	83
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%)	90 (100%)	0	100	100
36	m	90/103 (87%)	90 (100%)	0	100	100
37	o	298/412 (72%)	297 (100%)	1 (0%)	86	95
38	s	30/165 (18%)	30 (100%)	0	100	100
39	t	81/451 (18%)	81 (100%)	0	100	100
39	u	83/451 (18%)	82 (99%)	1 (1%)	63	87
39	v	80/451 (18%)	80 (100%)	0	100	100
39	w	369/451 (82%)	369 (100%)	0	100	100
40	y	91/193 (47%)	91 (100%)	0	100	100
All	All	10504/15893 (66%)	10486 (100%)	18 (0%)	85	96

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	908	ASP
4	A	1907	GLN
4	A	2381	GLU
5	B	668	ILE
5	B	1887	VAL
16	M	99	ILE
19	P	20	TYR
20	Q	951	VAL
23	T	450	TRP
24	W	17	ASP
24	W	140	TYR
32	e	46	PHE
37	o	389	LEU
32	p	46	PHE
32	p	60	ILE
33	q	83	GLU
34	r	38	VAL
39	u	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	233	HIS
4	A	433	HIS
4	A	509	HIS
4	A	576	HIS
4	A	592	HIS
4	A	617	ASN
4	A	866	GLN
4	A	952	ASN
4	A	1128	GLN
4	A	1295	GLN
4	A	1538	ASN
4	A	1600	GLN
4	A	1658	HIS
4	A	1677	GLN
4	A	1737	GLN
4	A	1863	HIS
4	A	2070	ASN
4	A	2076	GLN
4	A	2086	GLN
4	A	2168	ASN
4	A	2318	ASN
5	B	570	GLN
5	B	618	ASN
5	B	705	GLN
5	B	706	GLN
5	B	903	ASN
5	B	933	ASN
5	B	1281	GLN
5	B	1531	ASN
5	B	1628	HIS
5	B	2124	GLN
6	C	82	ASN
6	C	309	ASN
6	C	432	GLN
7	D	38	HIS
7	D	115	ASN
7	D	139	GLN
9	F	34	GLN
10	G	19	GLN
11	H	41	HIS
13	J	215	GLN
13	J	270	ASN
14	K	37	ASN

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Mol	Chain	Res	Type
15	L	54	GLN
15	L	58	GLN
16	M	39	GLN
16	M	189	GLN
17	N	30	GLN
18	O	31	HIS
20	Q	481	ASN
20	Q	509	ASN
20	Q	542	GLN
20	Q	682	ASN
20	Q	816	GLN
20	Q	889	GLN
22	S	61	ASN
22	S	79	HIS
22	S	214	ASN
22	S	290	GLN
22	S	400	HIS
23	T	240	ASN
23	T	418	GLN
23	T	730	GLN
24	W	24	ASN
24	W	49	HIS
26	Y	28	ASN
26	Y	68	GLN
26	Y	71	GLN
33	f	25	HIS
33	f	77	ASN
34	g	18	ASN
35	h	86	ASN
29	k	25	GLN
35	l	21	ASN
34	r	55	HIS
38	s	124	GLN
38	s	134	GLN
39	u	30	GLN
39	u	42	ASN
39	u	85	GLN
39	w	395	GLN

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
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

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Mol	Chain	Res	Type
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
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

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

All (20) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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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	1.59	1 (12%)	7,12,14	1.28	1 (14%)

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	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	o	73	SEP	P-O1P	3.51	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	0.79	0	60,60,60	0.58	0
44	GTP	C	1101	41	33,34,34	0.88	0	50,54,54	1.55	10 (20%)

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	-	-	3/30/54/54	0/1/1/1
44	GTP	C	1101	41	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C	1101	GTP	C5-C4-N3	-4.75	120.83	128.39
44	C	1101	GTP	C2-N3-C4	4.54	120.13	112.30
44	C	1101	GTP	C2-N1-C6	-2.90	119.86	125.11
44	C	1101	GTP	N9-C4-N3	2.78	131.51	125.95
44	C	1101	GTP	O2B-PB-O3B	2.68	114.52	107.27
44	C	1101	GTP	N9-C8-N7	-2.66	108.47	113.40
44	C	1101	GTP	C8-N7-C5	2.52	108.74	104.26
44	C	1101	GTP	C5-C6-N1	2.46	119.51	113.25
44	C	1101	GTP	O6-C6-C5	-2.30	120.47	126.53
44	C	1101	GTP	O2A-PA-O3A	2.06	112.84	107.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

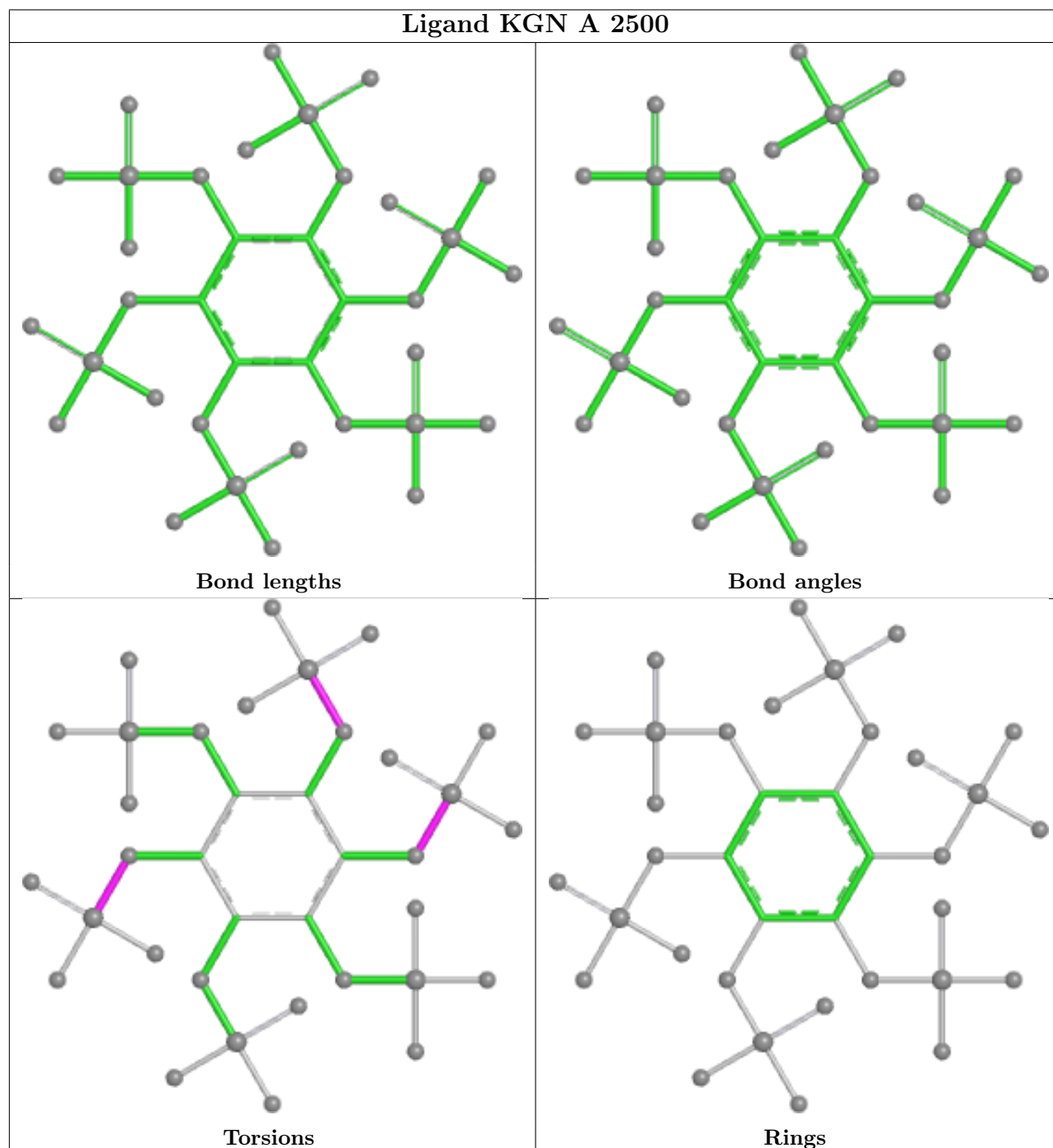
Mol	Chain	Res	Type	Atoms
43	A	2500	KGN	C6-O16-P6-O46
43	A	2500	KGN	C3-O13-P3-O23
44	C	1101	GTP	PA-O3A-PB-O1B
44	C	1101	GTP	PG-O3B-PB-O2B
43	A	2500	KGN	C5-O15-P5-O45

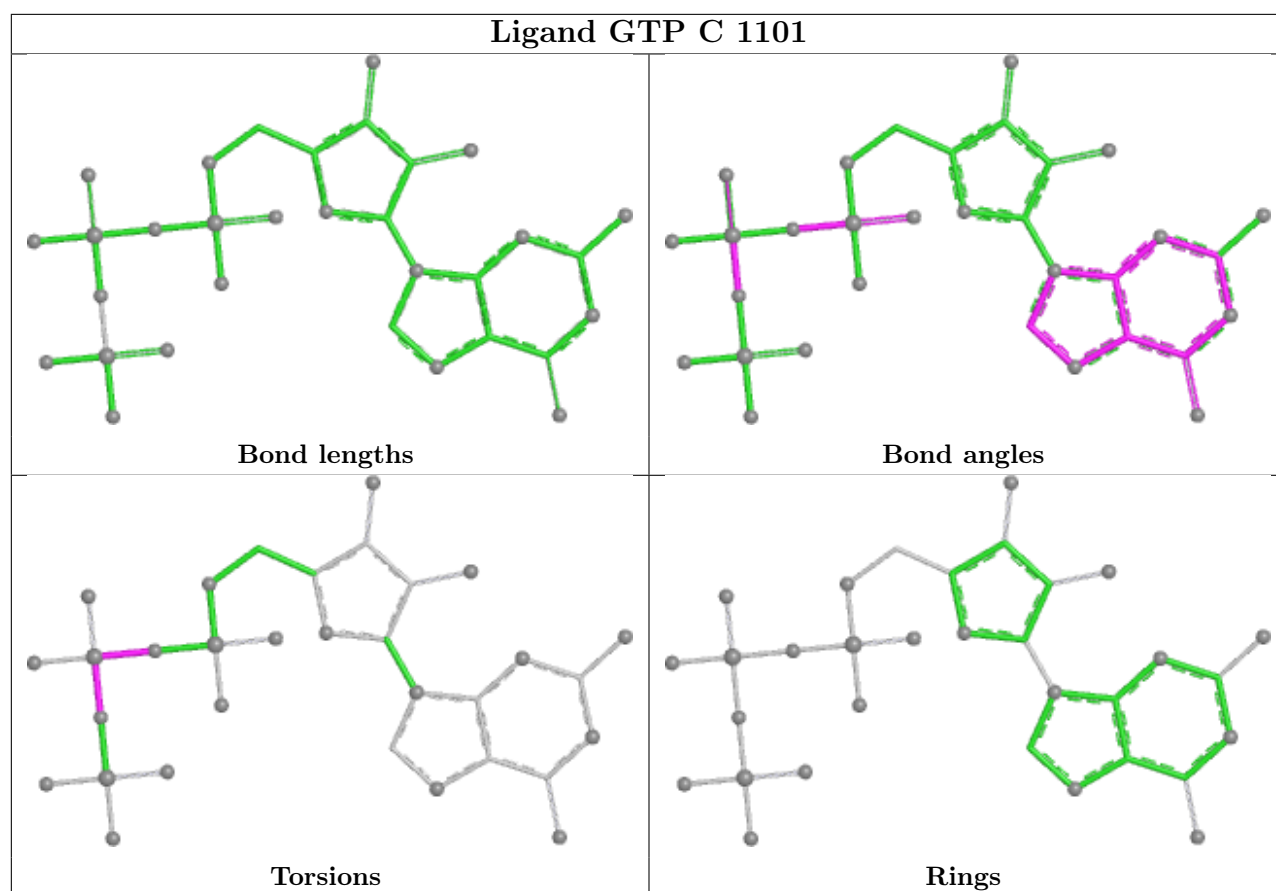
There are no ring outliers.

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

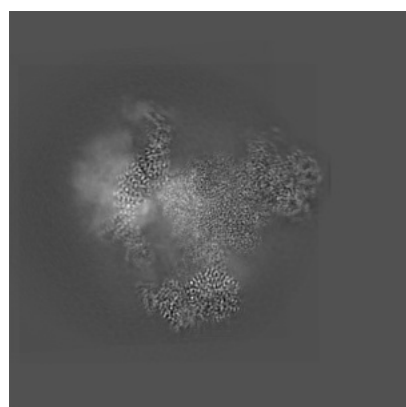
6 Map visualisation [i](#)

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.

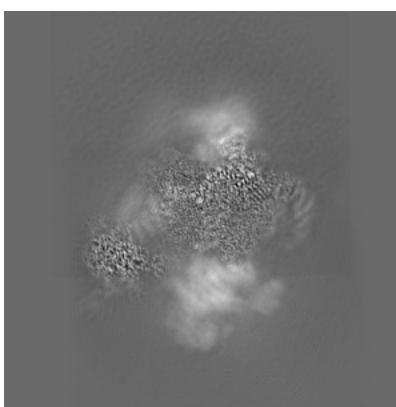
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

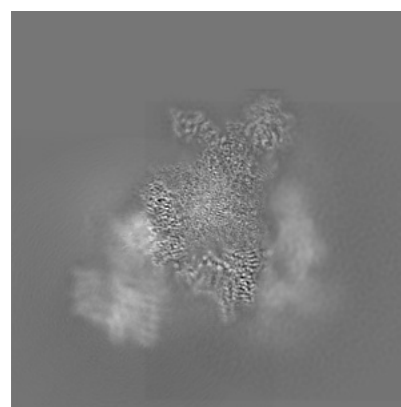
6.1.1 Primary map



X



Y

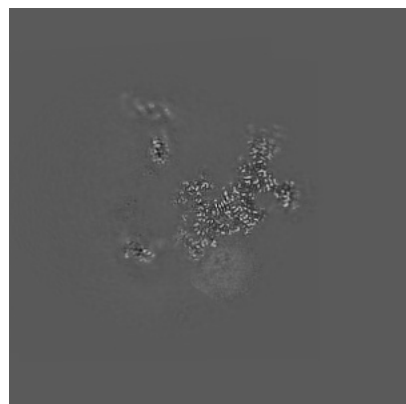


Z

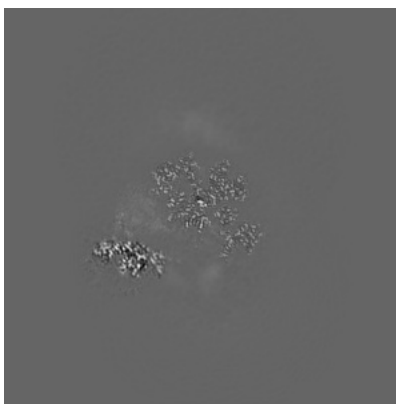
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

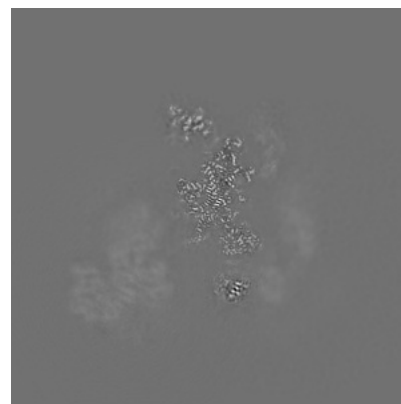
6.2.1 Primary map



X Index: 200



Y Index: 200

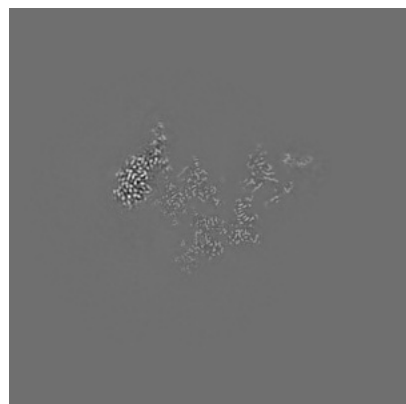


Z Index: 200

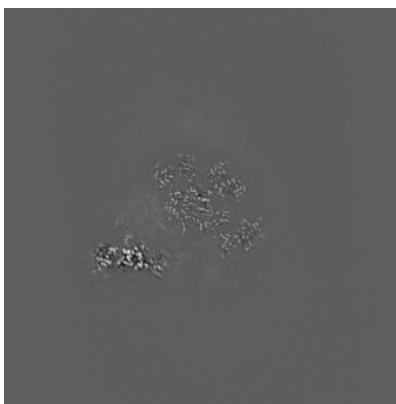
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

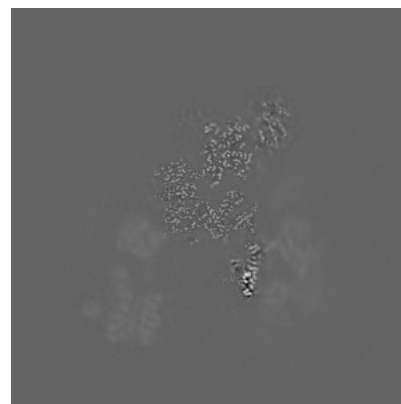
6.3.1 Primary map



X Index: 235



Y Index: 205

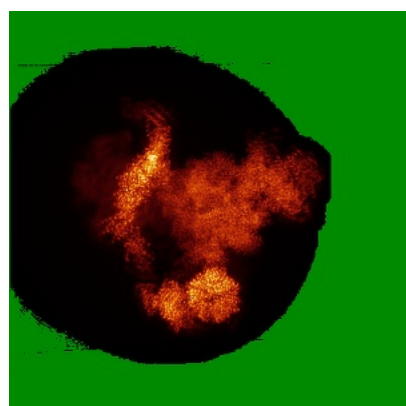


Z Index: 224

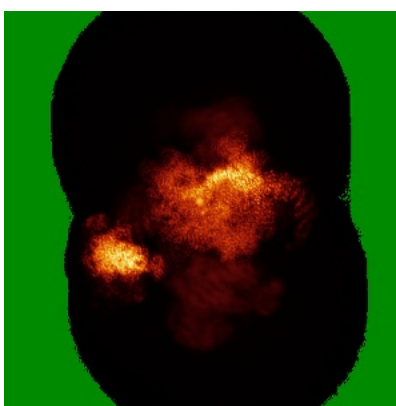
The images above show the largest variance slices of the map in three orthogonal directions.

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

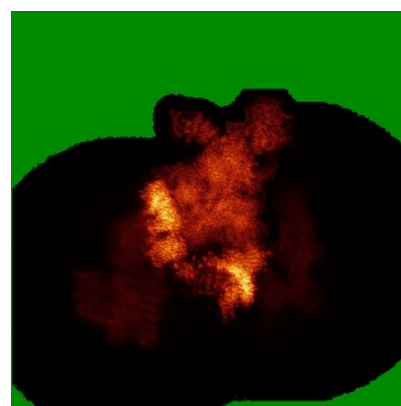
6.4.1 Primary map



X



Y

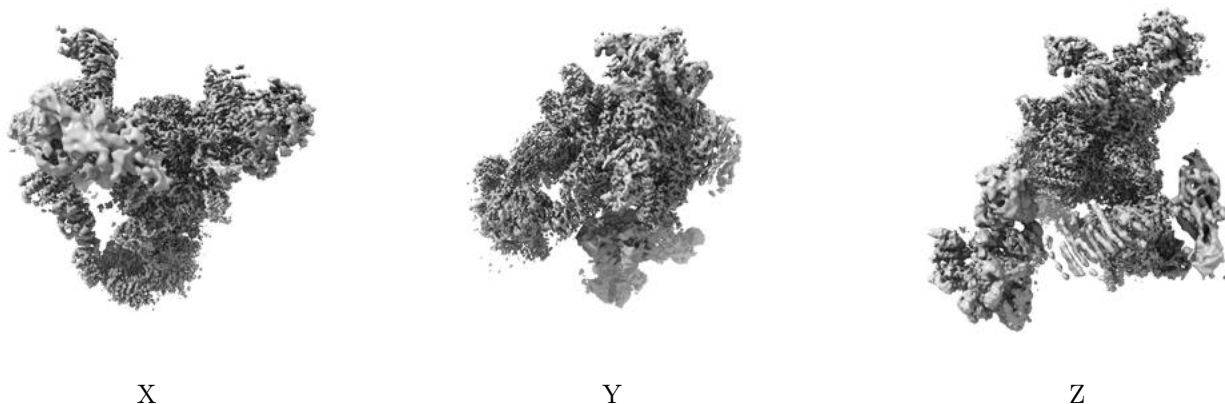


Z

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.

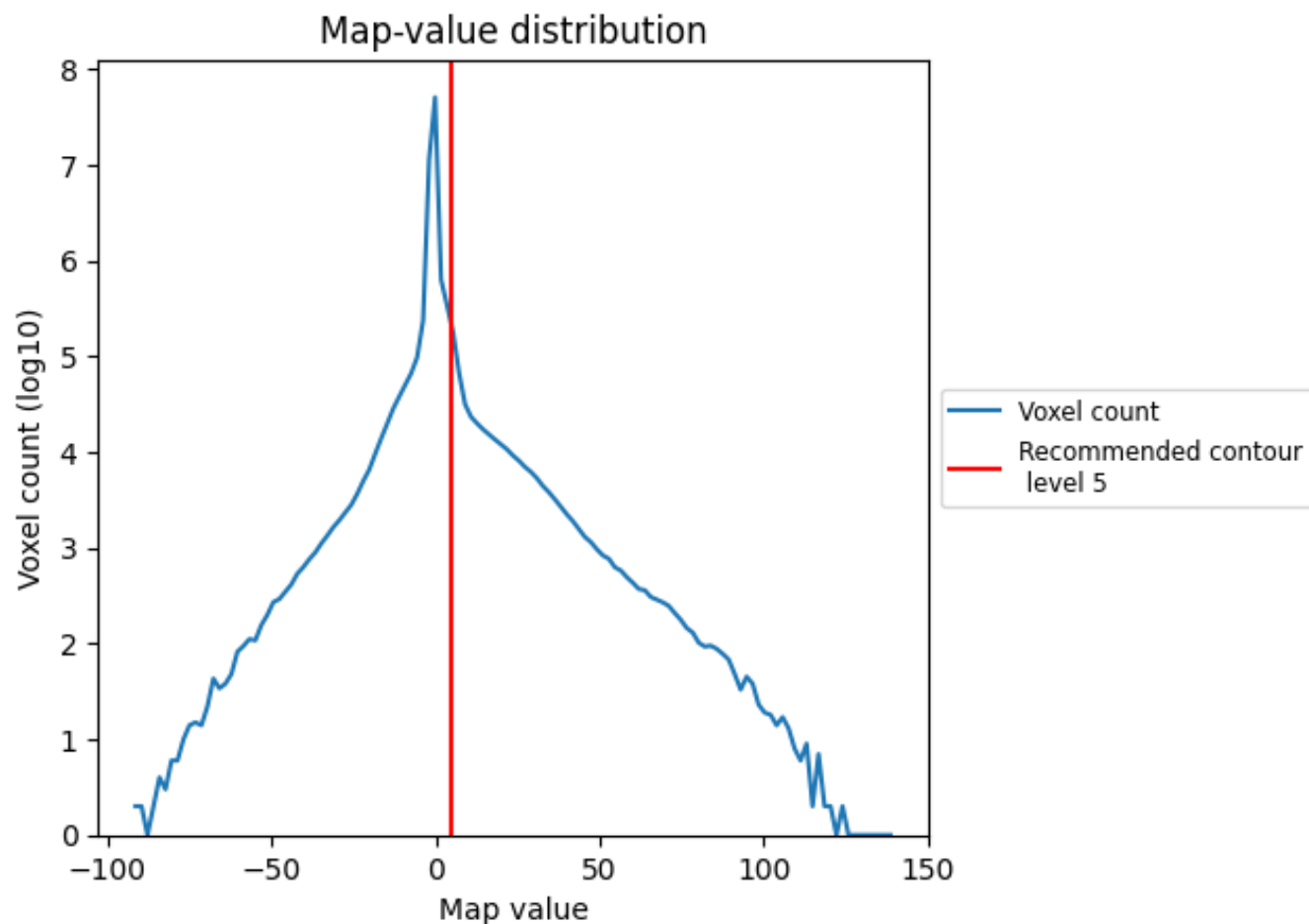
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

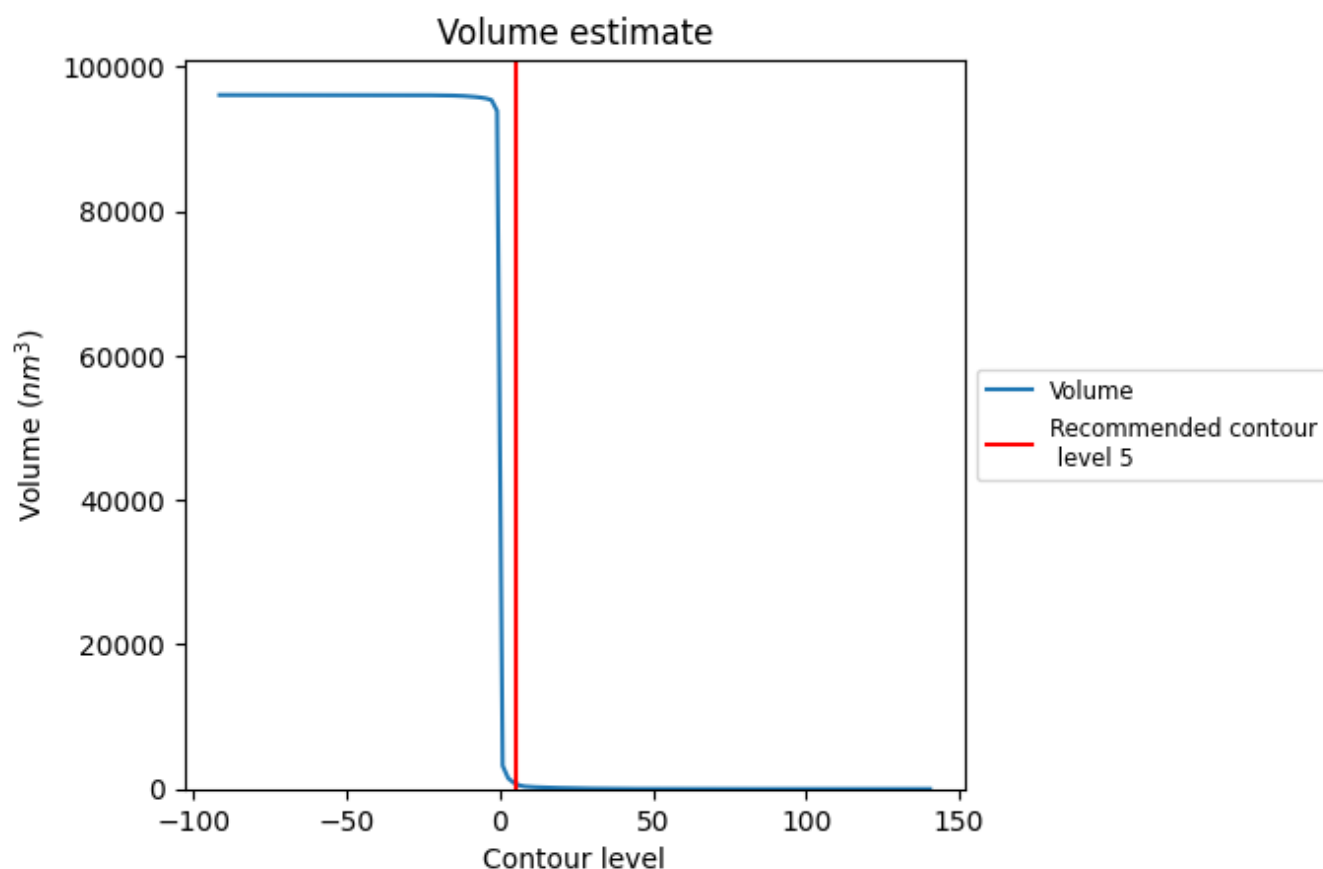
This section contains the results of statistical analysis of the map.

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.

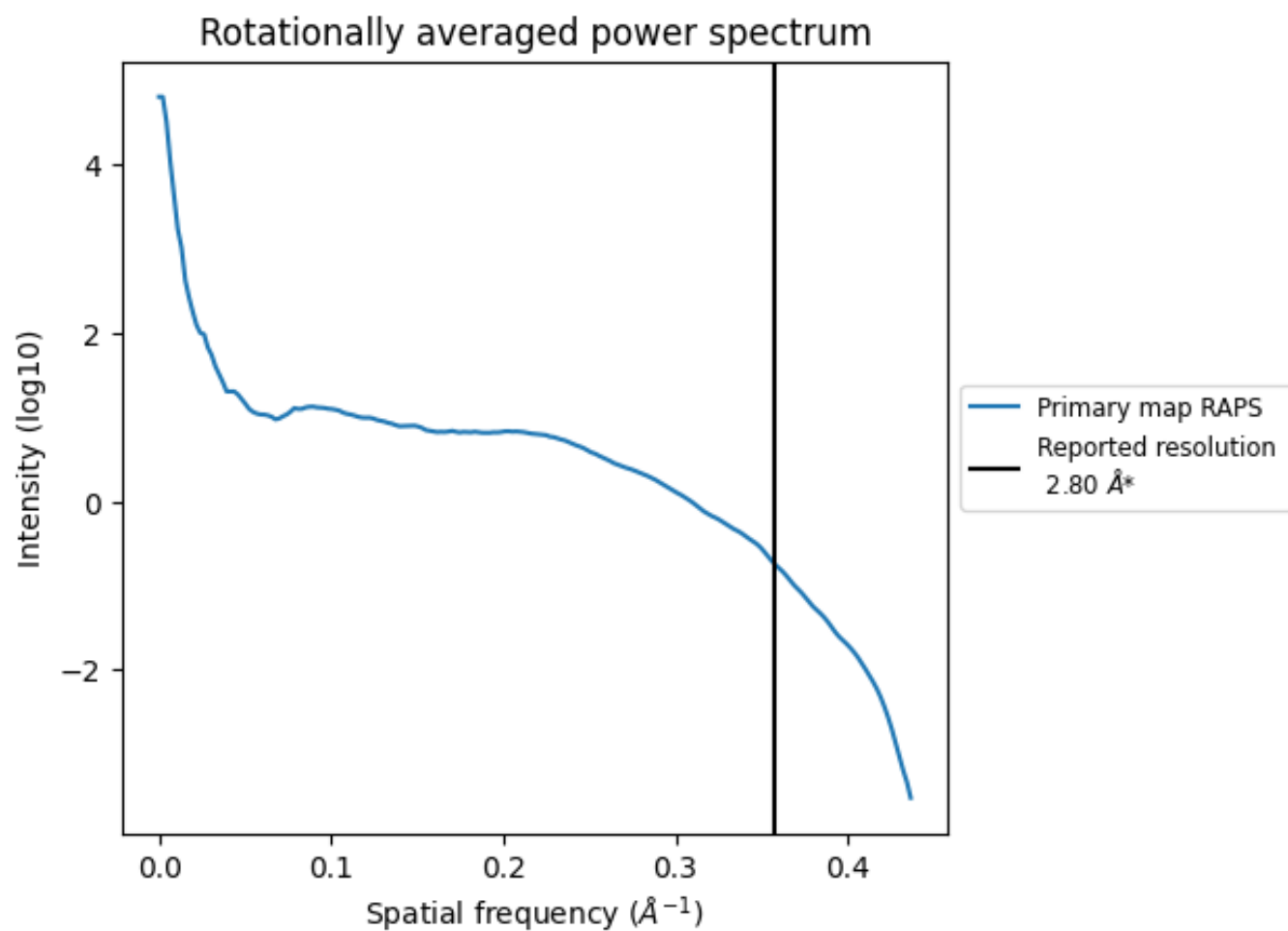
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 773 nm³; 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

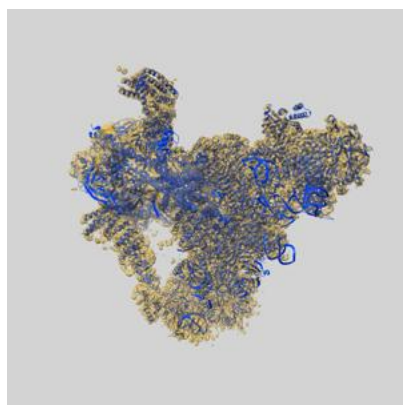
8 Fourier-Shell correlation

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

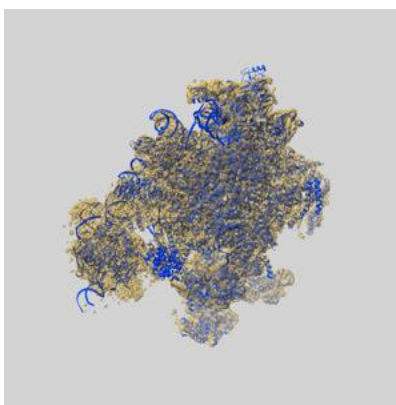
9 Map-model fit [i](#)

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](#).

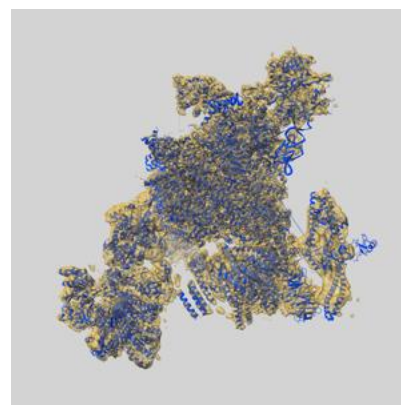
9.1 Map-model overlay [i](#)



X



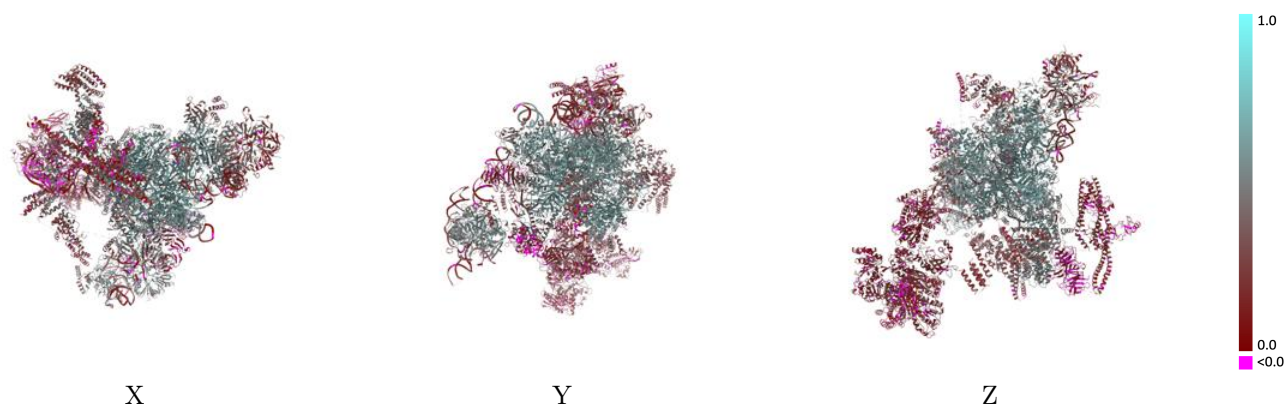
Y



Z

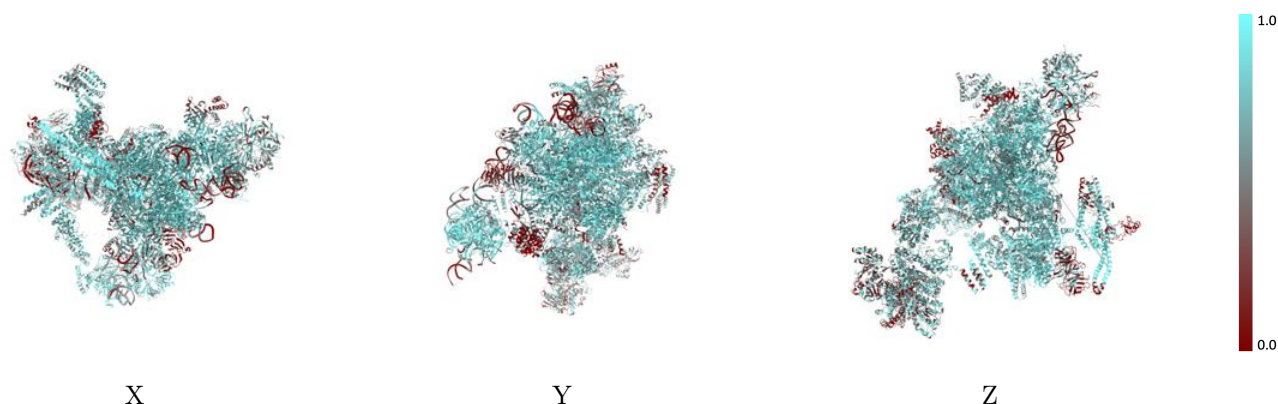
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



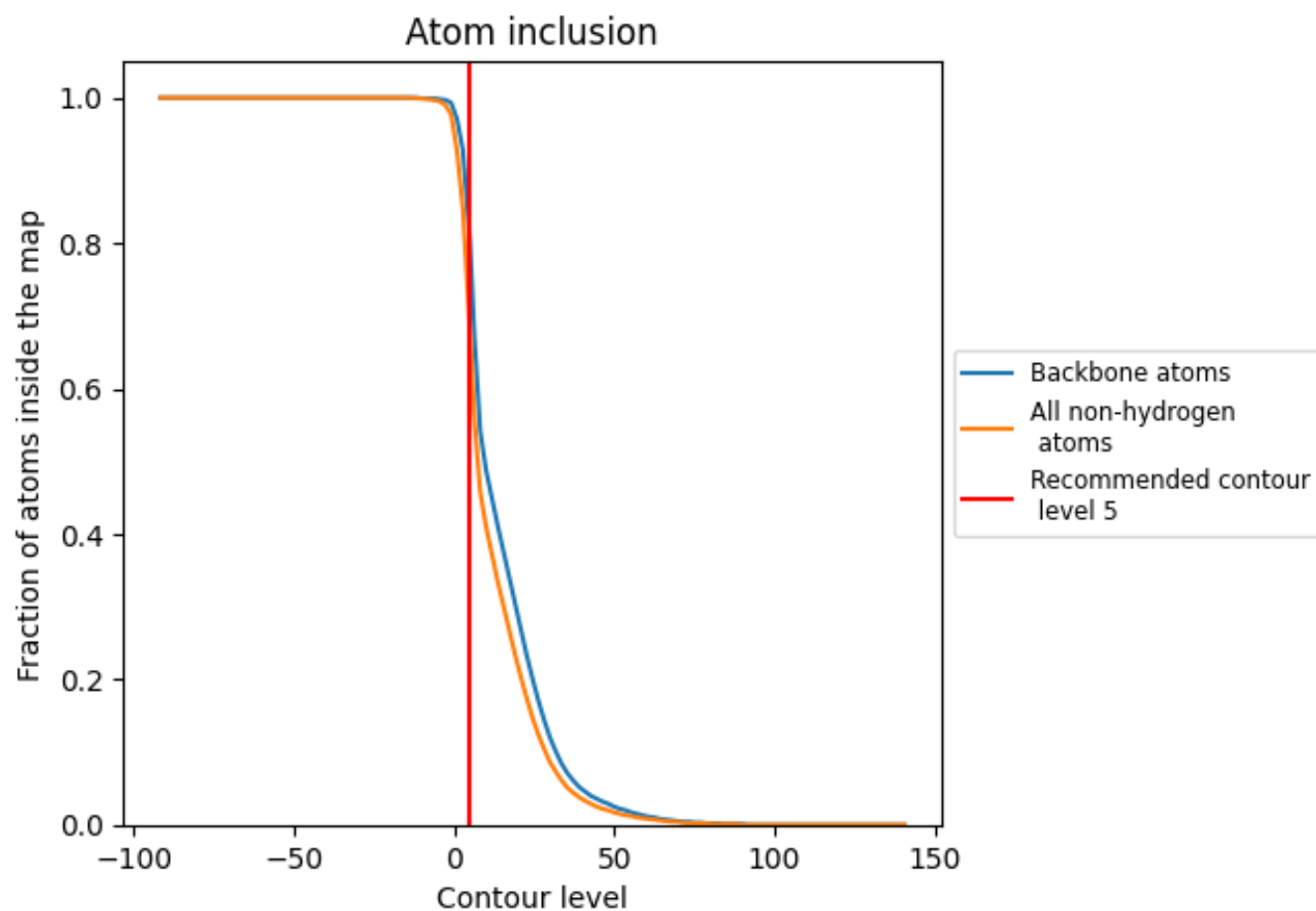
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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