



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:49 pm GMT

PDB ID : 6QDV
EMDB ID : EMD-4525
Title : Human post-catalytic P complex spliceosome
Authors : Fica, S.M.; Oubridge, C.; Wilkinson, M.E.; Newman, A.J.; Nagai, K.
Deposited on : 2019-01-03
Resolution : 3.30 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

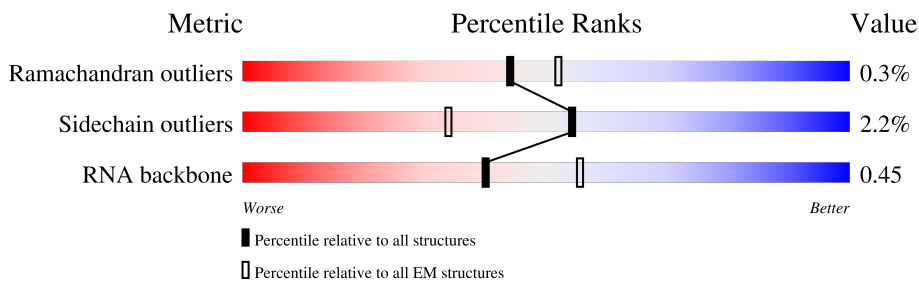
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	189	
2	5	116	
3	6	106	
4	7	390	
5	8	91	
6	9	144	
7	A	2335	
8	B	1722	

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Mol	Chain	Length	Quality of chain
9	C	899	12% 99%
10	D	123	54% 99%
11	E	14	7% 57% 29% 14%
12	F	122	18% 100%
13	G	60	17% 97%
14	H	908	30% 50% 49%
15	I	113	9% 19% 15% 63%
16	J	320	100%
17	K	295	26% 99%
18	L	144	6% 96%
19	M	289	39% 99%
20	N	306	15% 99%
21	O	802	27% 55% 45%
22	P	229	8% 46% 54%
23	R	26	92% 8%
24	S	848	37% 66% 33%
25	T	855	73% 73% 25%
26	U	1485	89% 86% 11%
27	V	1220	55% 55% 42%
28	W	162	99% 99%
29	Y	92	100% 100%
30	Z	30	7% 100%
31	b	82	59% 83% 17%
31	k	82	90% 100%
32	c	586	7% 46% 54%

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Mol	Chain	Length	Quality of chain
33	d	84	39% 100%
33	n	84	49% 99%
34	e	81	96% 98%
34	p	81	88% 100%
35	f	72	99% 99%
35	q	72	97% 100%
36	g	73	81% 100%
36	r	73	59% 99%
37	h	80	94% 100%
37	l	80	96% 100%
38	i	164	22% 100%
39	j	118	81% 81% 19%
39	m	118	81% 81% 19%
40	o	513	12% 99%
41	s	225	73% 74% 25%
42	t	504	25% 25% 75%
42	u	504	23% 23% 77%
42	v	504	25% 25% 75%
42	w	504	23% 23% 77%
43	y	144	20% 99%
44	z	34	100%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 121152 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
			Total	C	N	O	P		
1	2	120	2535	1135	428	852	120	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	75	1579	708	264	532	75	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	97	2075	928	381	669	97	0	0

- Molecule 4 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	7	390	3130	1976	546	589	19	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	?	-	GLU	deletion	UNP P38919
7	405	MET	-	expression tag	UNP P38919
7	406	ASN	-	expression tag	UNP P38919
7	407	VAL	-	expression tag	UNP P38919
7	408	ALA	-	expression tag	UNP P38919
7	409	ASP	-	expression tag	UNP P38919
7	410	LEU	-	expression tag	UNP P38919
7	411	ILE	-	expression tag	UNP P38919

- Molecule 5 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	8	91	730	463	122	142	3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	151	VAL	-	expression tag	UNP Q9Y5S9
8	152	ARG	-	expression tag	UNP Q9Y5S9
8	153	GLY	-	expression tag	UNP Q9Y5S9
8	154	PRO	-	expression tag	UNP Q9Y5S9

- Molecule 6 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	9	144	1196	772	200	221	3	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	146	LYS	-	expression tag	UNP Q96A72
9	147	PRO	-	expression tag	UNP Q96A72
9	148	ILE	-	expression tag	UNP Q96A72

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	2250	18655	12009	3256	3309	81	0	0

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	1722	13846	8848	2369	2557	72	0	0

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	899	7116	4553	1184	1345	34	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q15029

- Molecule 10 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	123	1013	635	193	180	5	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	140	LEU	-	expression tag	UNP Q9H875
D	141	ALA	-	expression tag	UNP Q9H875
D	142	LYS	-	expression tag	UNP Q9H875

- Molecule 11 is a RNA chain called Ligated exons: MINX mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	E	14	296	132	52	98	14	0	0

- Molecule 12 is a protein called Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	122	1084	712	197	173	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	654	ALA	GLU	conflict	UNP Q8WUQ7

- Molecule 13 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	60	Total	C	N	O	S	0	0
			504	314	96	92	2		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	459	Total	C	N	O	S	0	0
			3713	2380	634	678	21		

- Molecule 15 is a RNA chain called Intron lariat: MINX RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	42	Total	C	N	O	P	0	0
			872	390	148	292	42		

- Molecule 16 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	320	Total	C	N	O	S	0	0
			2523	1594	457	464	8		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	K	295	Total	C	N	O	P	S	0	0
			2360	1479	431	435	2	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	GLU	deletion	UNP Q13573
K	330	LYS	-	expression tag	UNP Q13573
K	331	ALA	-	expression tag	UNP Q13573
K	332	ARG	-	expression tag	UNP Q13573
K	333	GLU	-	expression tag	UNP Q13573
K	334	ARG	-	expression tag	UNP Q13573
K	335	ARG	-	expression tag	UNP Q13573

- Molecule 18 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	L	144	1188	748	218	210	12	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	M	289	2318	1455	416	428	19	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	143	ALA	THR	conflict	UNP Q9NW64
M	144	ALA	SER	conflict	UNP Q9NW64
M	145	ALA	ASP	conflict	UNP Q9NW64
M	146	ALA	MET	conflict	UNP Q9NW64

- Molecule 20 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	306	2394	1501	422	457	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ALA	deletion	UNP Q96DI7

- Molecule 21 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	O	441	3416	2116	648	639	13	0	0

- Molecule 22 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	P	106	888	544	174	168	2	0	0

- Molecule 23 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	R	26	193	120	36	36	1	0	0

- Molecule 24 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	570	3965	2482	740	737	6	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	T	639	4003	2479	748	763	13	0	0

- Molecule 26 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	1322	10885	6989	1879	1963	54	4	0

- Molecule 27 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	V	713	2995	1538	722	734	1	0	0

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	W	162	1282	820	219	240	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	163	LYS	-	expression tag	UNP P09661

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 30 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	30	Total	C	N	O	S	0	0
			230	140	43	45	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	68	Total	C	N	O	S	0	0
			545	347	95	96	7		
31	k	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 32 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	269	Total	C	N	O	S	0	0
			2215	1392	397	418	8		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
33	n	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	79	Total	C	N	O	S	0	0
			651	413	115	118	5		
34	p	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
35	q	72	Total	C	N	O	S	0	0
			562	364	93	100	5		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
36	r	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	80	Total	C	N	O	S	0	0
			634	404	111	115	4		
37	l	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	79	LEU	-	expression tag	UNP P62314
h	80	LEU	-	expression tag	UNP P62314
l	79	LEU	-	expression tag	UNP P62314
l	80	LEU	-	expression tag	UNP P62314

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	164	Total	C	N	O	S	0	0
			1270	810	220	233	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	165	SER	-	expression tag	UNP Q9Y3C6
i	166	GLY	-	expression tag	UNP Q9Y3C6

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	95	Total	C	N	O	S	0	0
			774	486	141	142	5		
39	m	95	Total	C	N	O	S	0	0
			774	486	141	142	5		

- Molecule 40 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	513	Total	C	N	O	S	0	0
			4157	2643	719	771	24		

- Molecule 41 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	169	Total	C	N	O	S	0	0
			1402	872	257	264	9		

- Molecule 42 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	125	Total	C	N	O	S	0	0
			988	618	176	190	4		
42	u	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
42	v	125	Total	C	N	O	S	0	0
			988	618	176	190	4		
42	w	118	Total	C	N	O	S	0	0
			938	586	167	181	4		

- Molecule 43 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	144	Total	C	N	O	S	0	0
			1218	758	225	233	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	240	GLY	-	expression tag	UNP O95926
y	241	THR	-	expression tag	UNP O95926
y	242	ALA	-	expression tag	UNP O95926
y	243	VAL	-	expression tag	UNP O95926

- Molecule 44 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	z	34	280	166	59	53	2	0	0

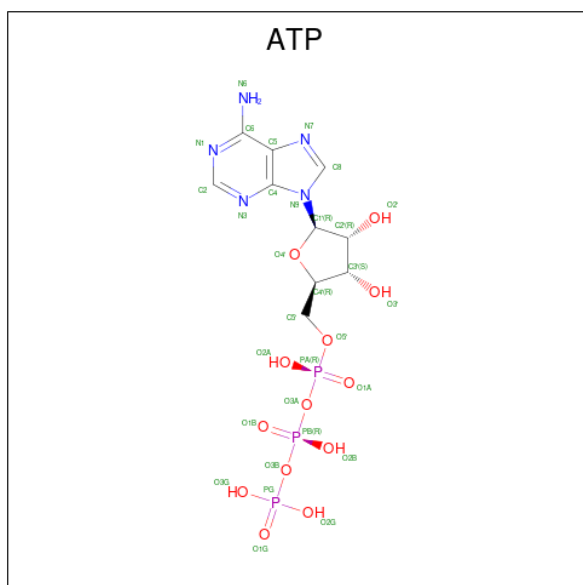
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	6	5	Total	Mg	0
			5	5	
45	7	1	Total	Mg	0
			1	1	
45	C	1	Total	Mg	0
			1	1	

- Molecule 46 is POTASSIUM ION (three-letter code: K) (formula: K).

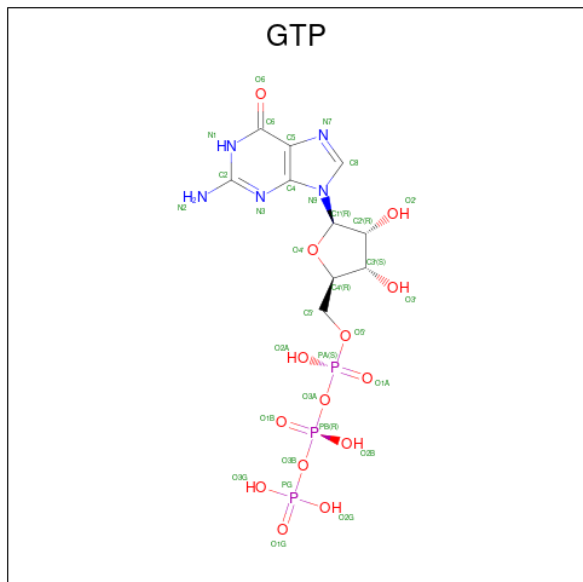
Mol	Chain	Residues	Atoms		AltConf
46	6	1	Total	K	0
			1	1	

- Molecule 47 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	7	1	31	10	5	13	3	0

- Molecule 48 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

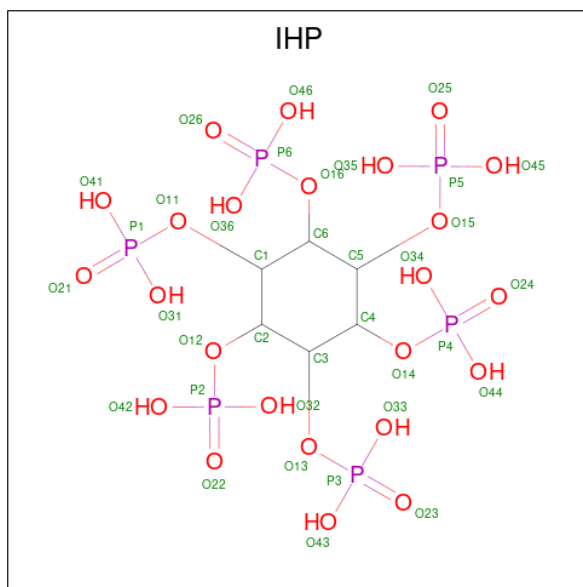


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	C	1	32	10	5	14	3	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
49	L	3	3	3	0
49	M	3	3	3	0
49	c	1	1	1	0

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

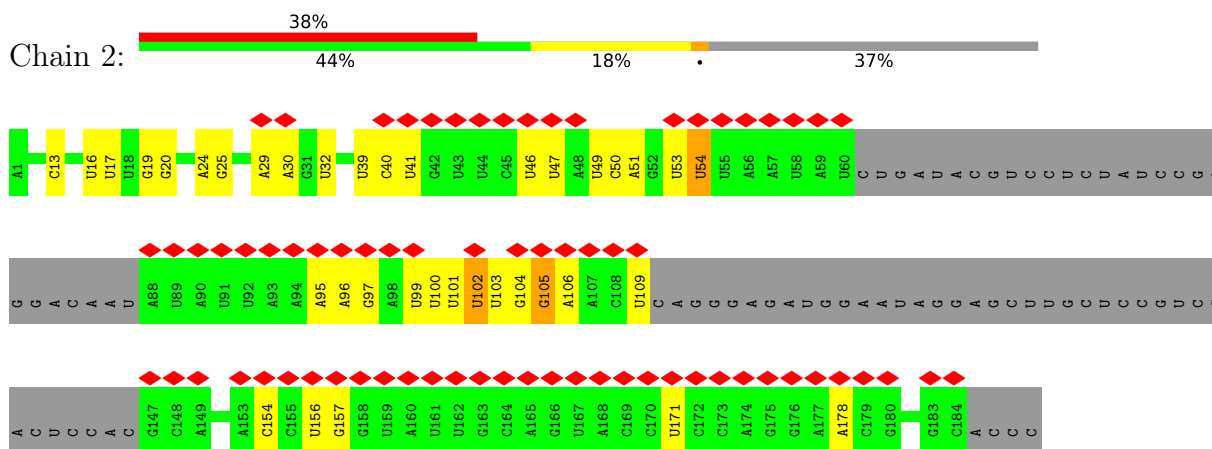


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
50	c	1	36	6	24	6	0

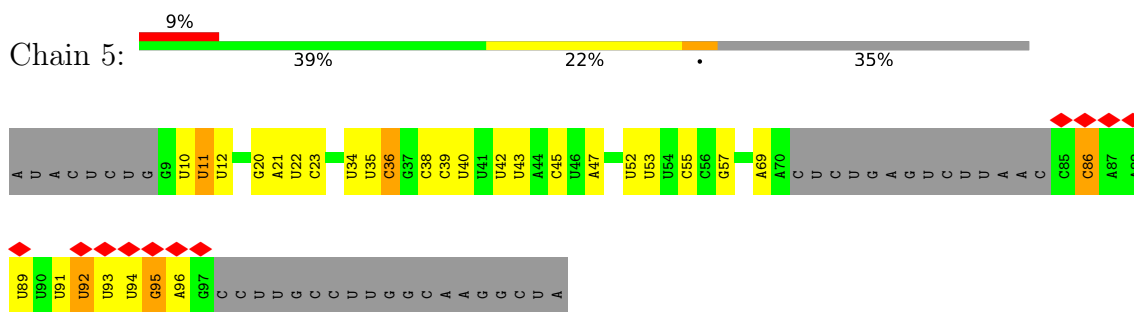
3 Residue-property plots [i](#)

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.

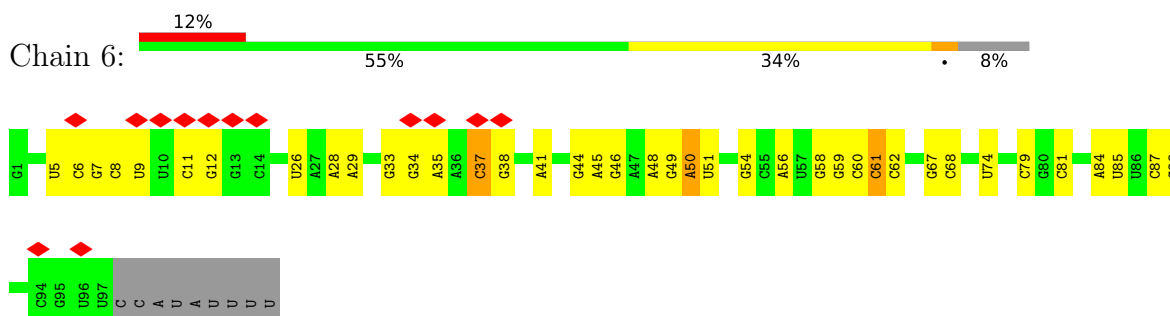
- Molecule 1: U2 snRNA



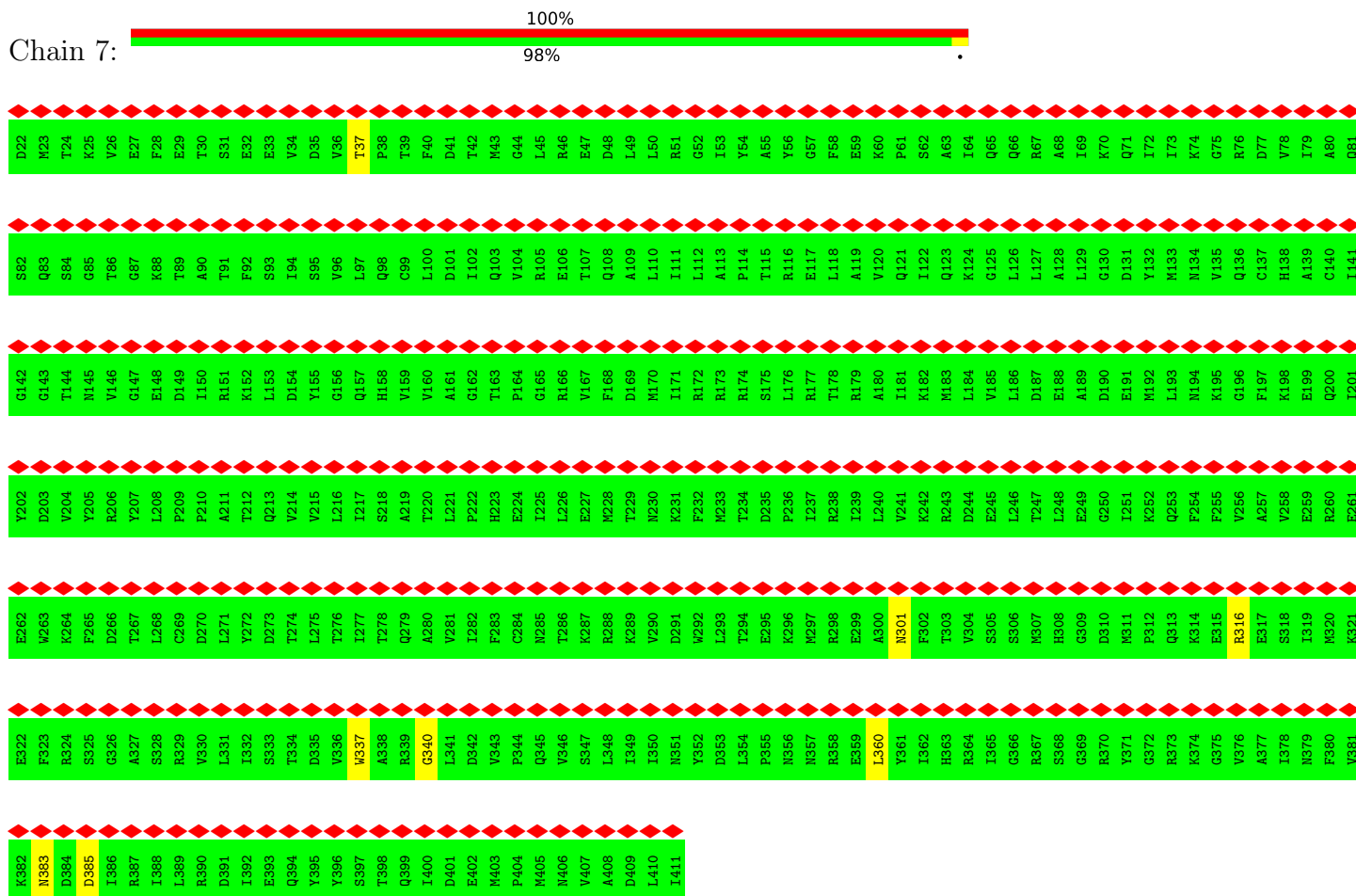
- Molecule 2: U5 snRNA



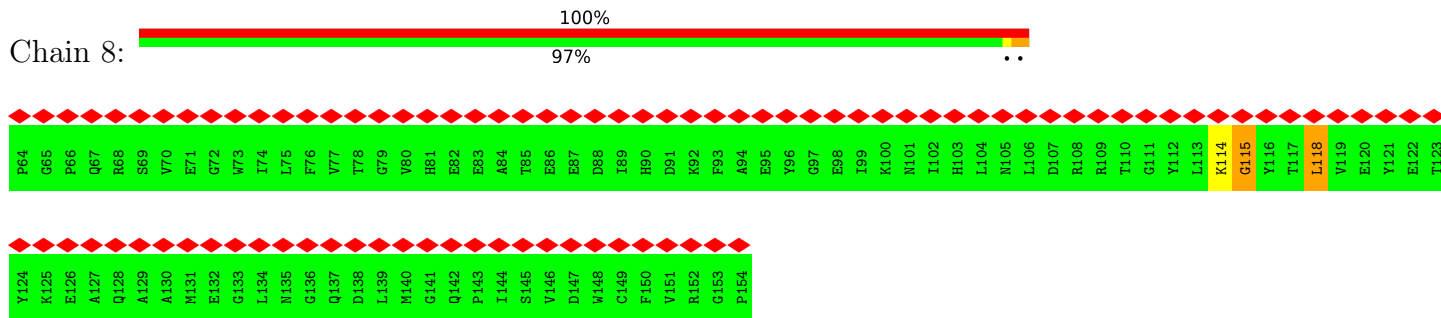
- Molecule 3: U6 snRNA



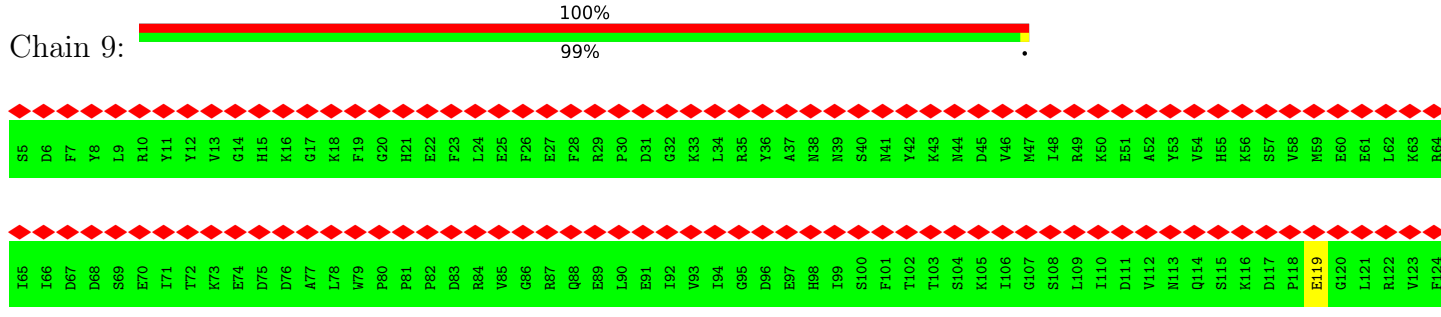
- Molecule 4: Eukaryotic initiation factor 4A-III



• Molecule 5: RNA-binding protein 8A

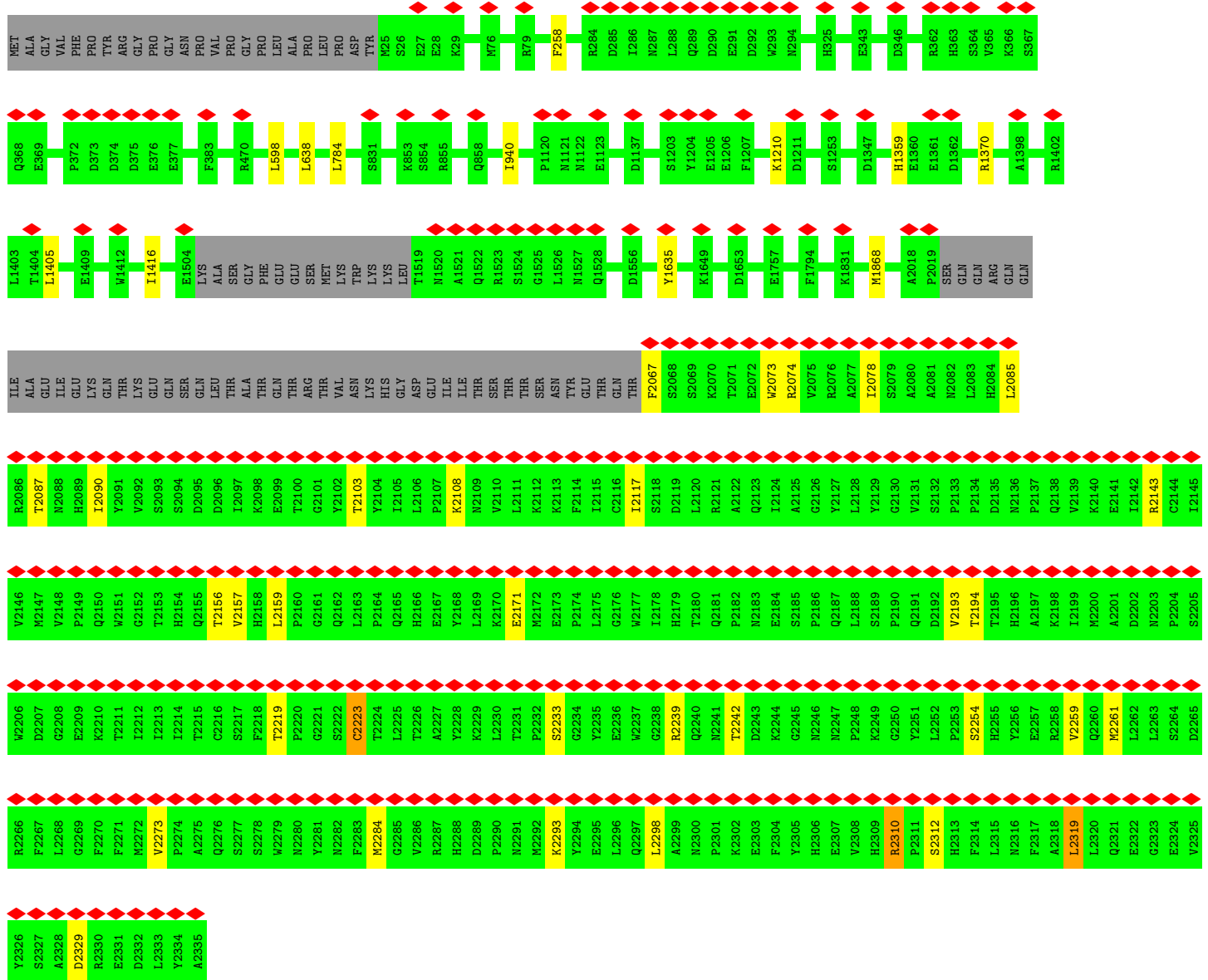
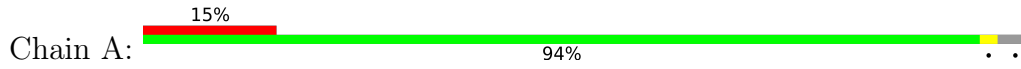


• Molecule 6: Protein mago nashi homolog 2

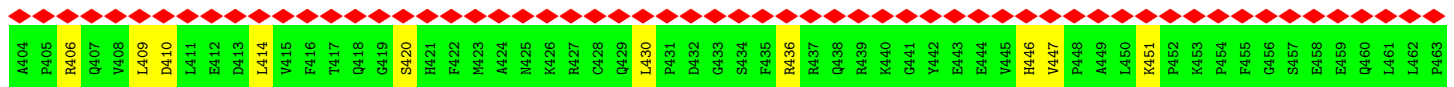
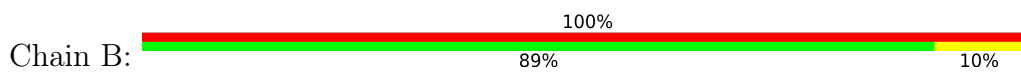




• Molecule 7: Pre-mRNA-processing-splicing factor 8

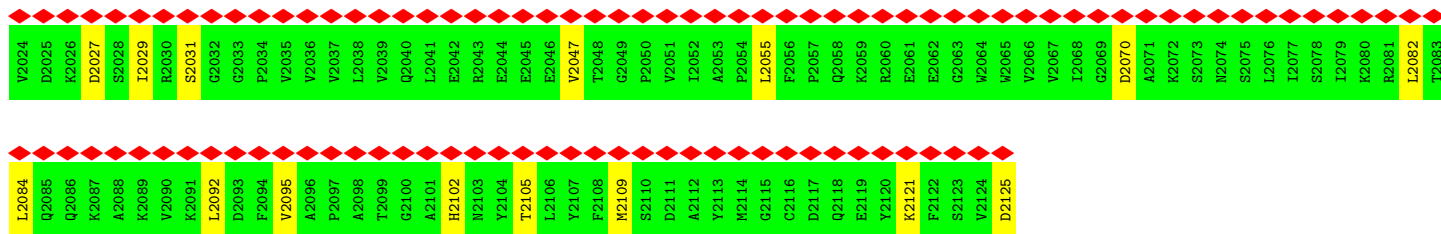


• Molecule 8: U5 small nuclear ribonucleoprotein 200 kDa helicase

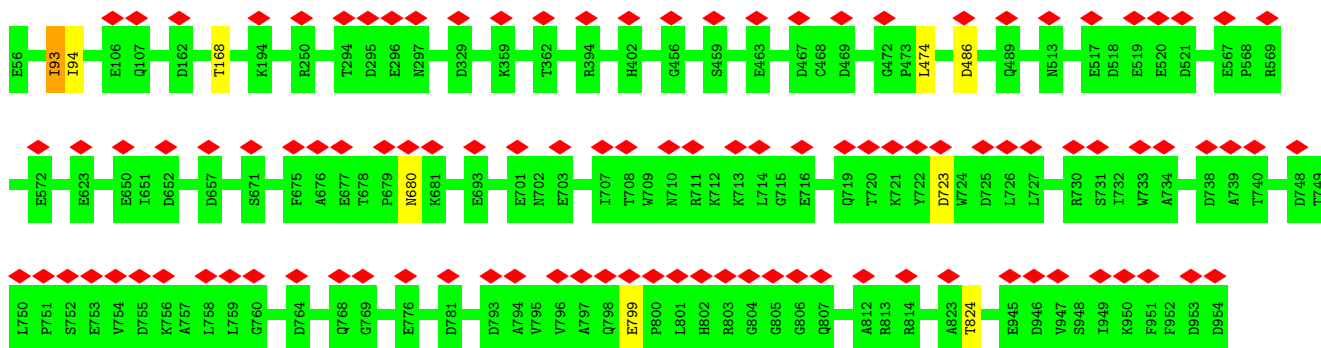


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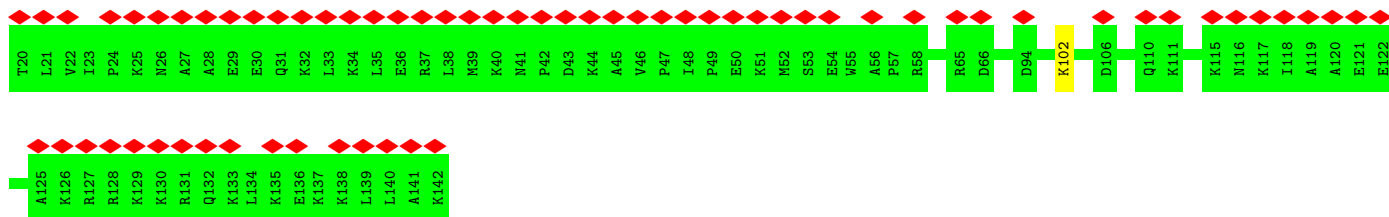
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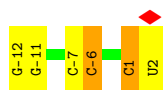
• Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component



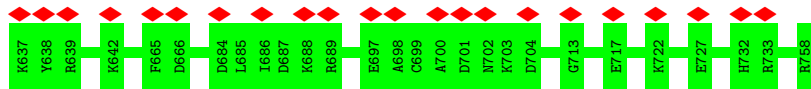
• Molecule 10: PRKR-interacting protein 1



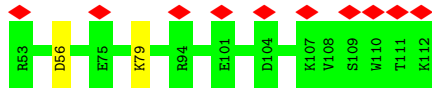
• Molecule 11: Ligated exons: MINX mRNA



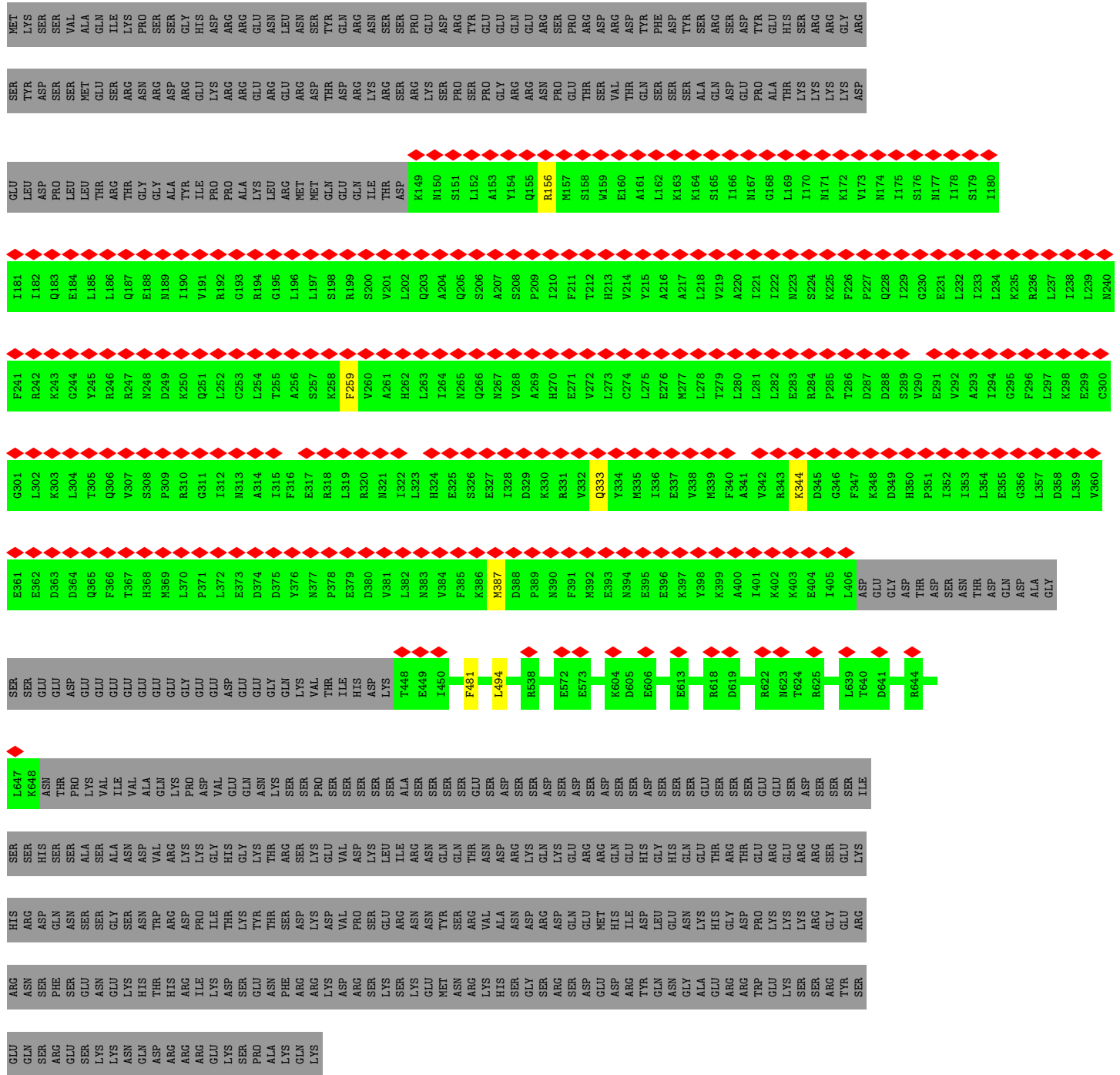
• Molecule 12: Cactin



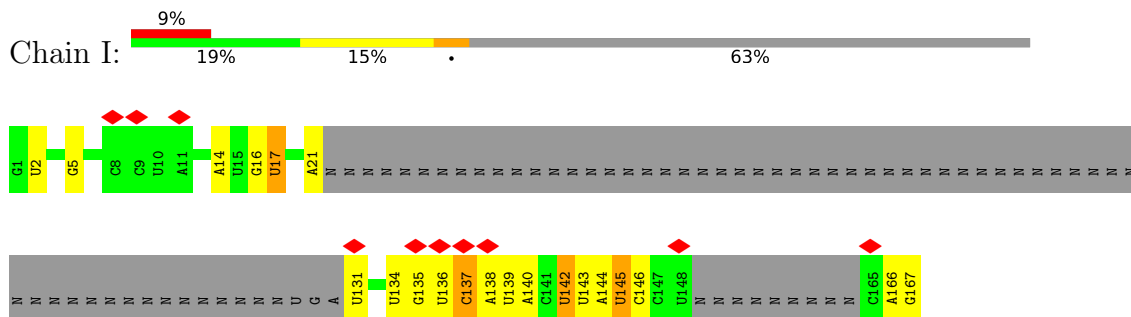
• Molecule 13: Protein FAM32A



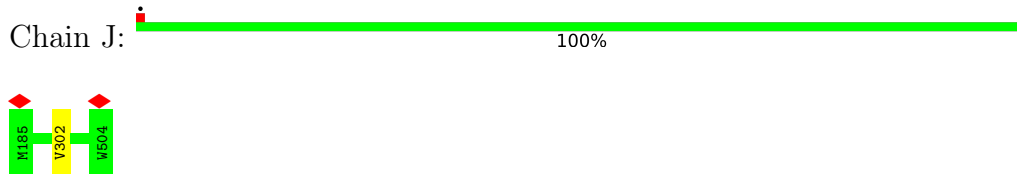
● Molecule 14: Pre-mRNA-splicing factor CWC22 homolog



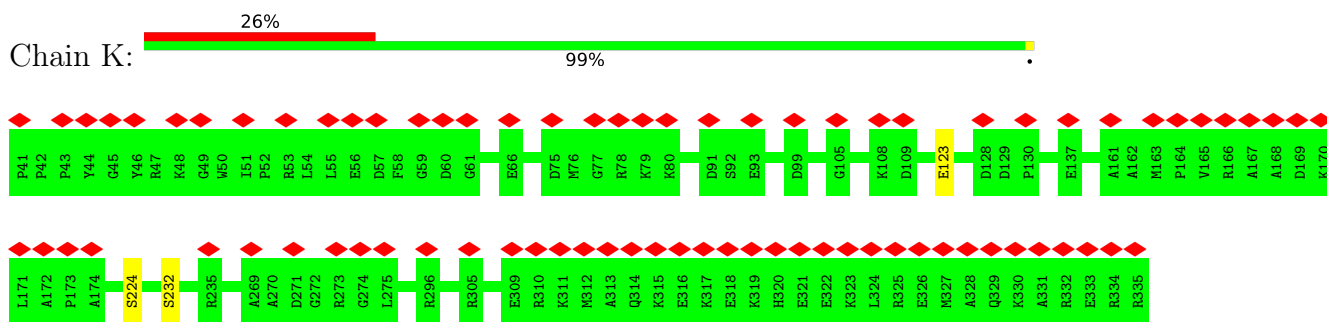
• Molecule 15: Intron lariat: MINX RNA



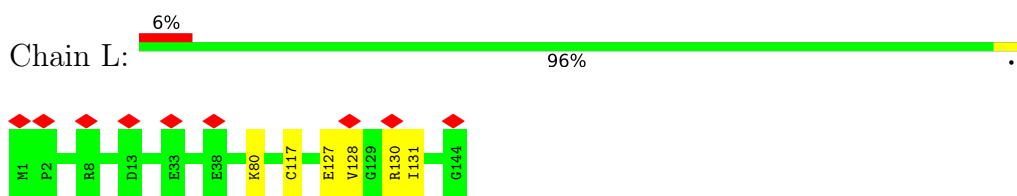
• Molecule 16: Pleiotropic regulator 1



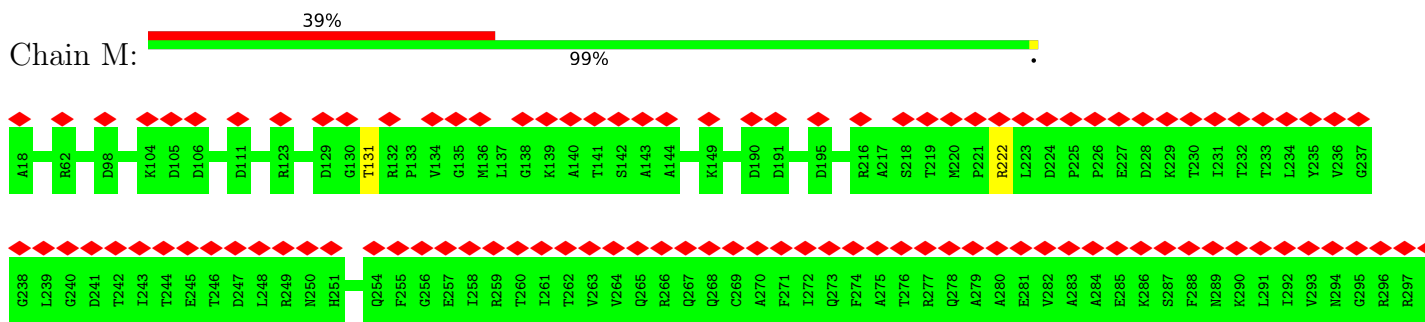
• Molecule 17: SNW domain-containing protein 1

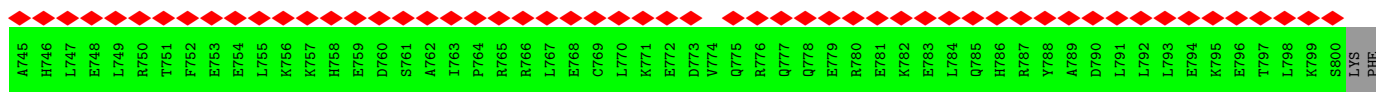


• Molecule 18: Protein BUD31 homolog

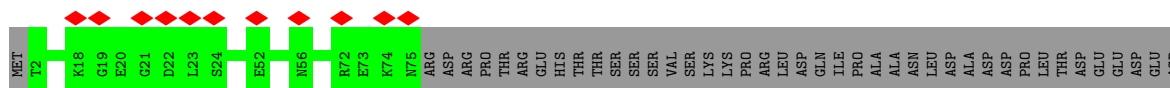


• Molecule 19: Pre-mRNA-splicing factor RBM22

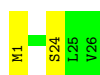




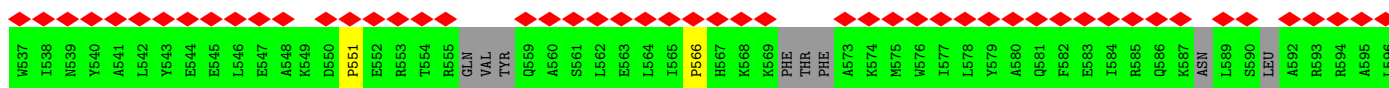
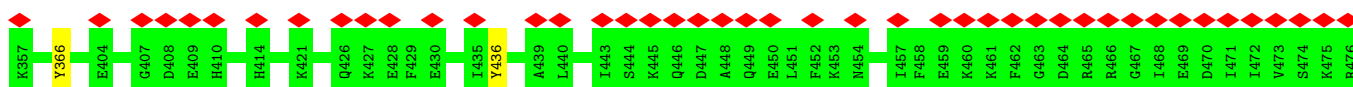
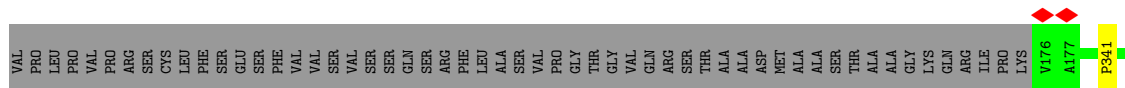
• Molecule 22: Spliceosome-associated protein CWC15 homolog

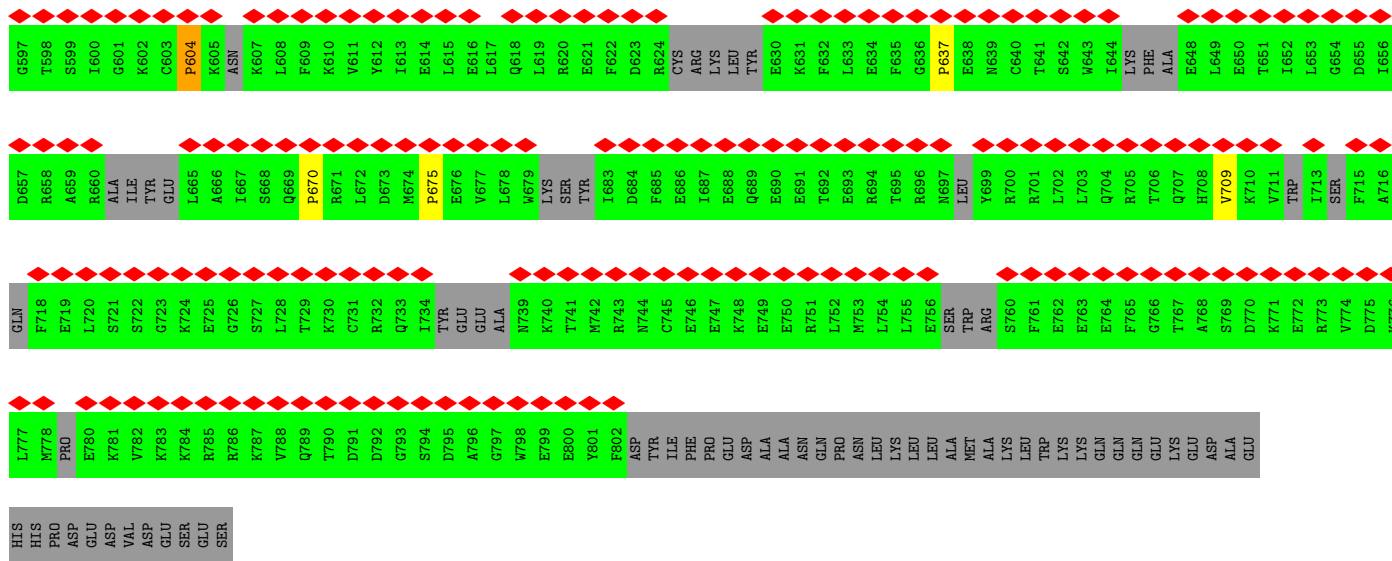


• Molecule 23: Serine/arginine repetitive matrix protein 2

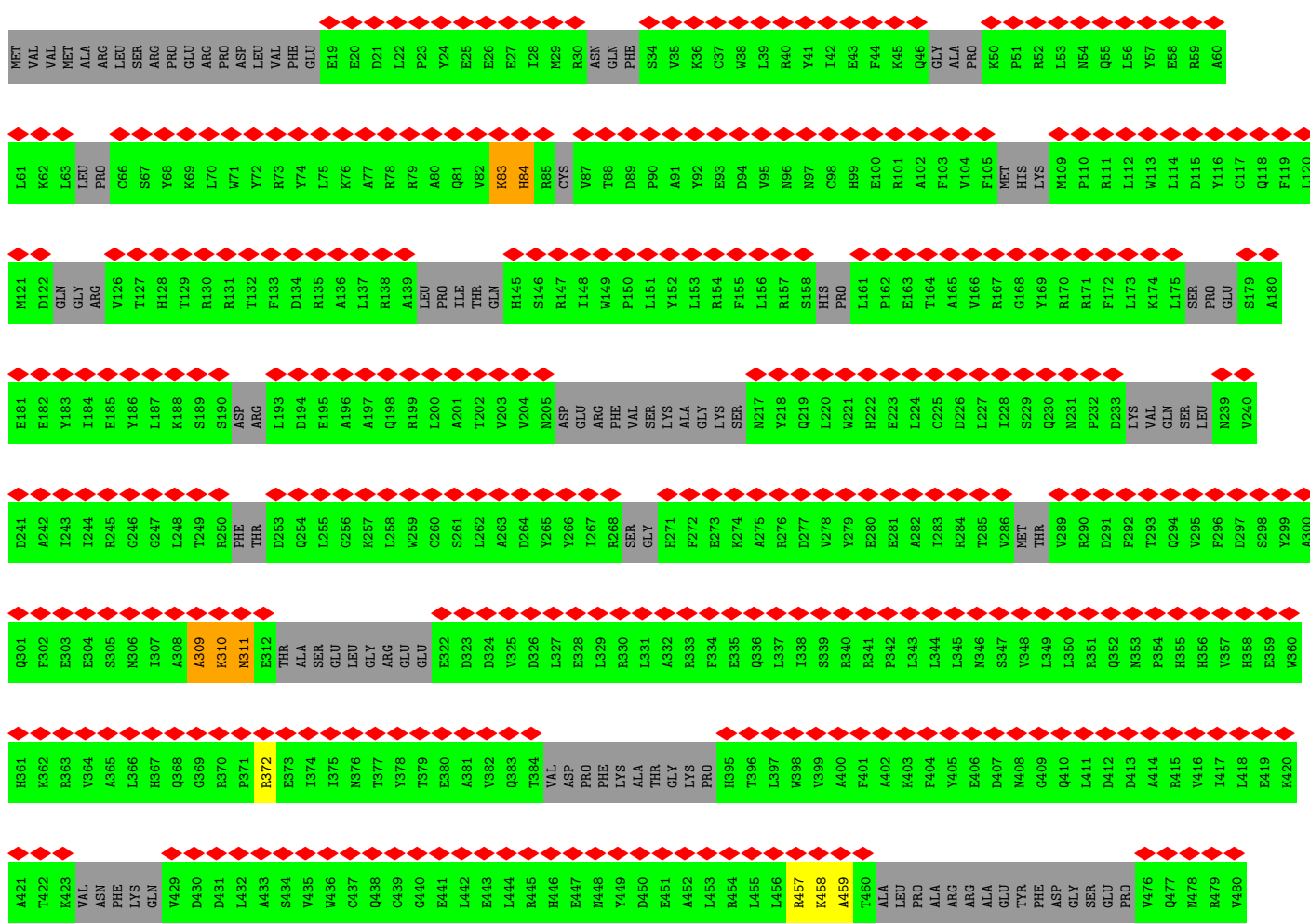
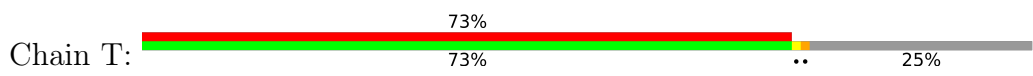


• Molecule 24: Crooked neck-like protein 1



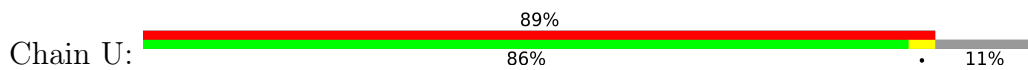


● Molecule 25: Pre-mRNA-splicing factor SYF1



Y481	K482	S483	L484	K485	V486	W487	S488	M489	L490	A491	D492	L493	E494	E495	S496	L497	GLY	THR	PHE	GLN	S502	T503	K504	A505	V506	Y507	D508	R509	I510	L511	D512	L513	R514	I515	A516	T517	P518	Q519	I520	V521	I522	N523	Y524	A525	M526	F527	L528	E529	E530	H531	K532	Y533	F534	E535	E536	S537	F538	K539	A540				
Y541	E542	R543	G544	I545	S546	L547	F548	K549	W550	V553	S554	D555	I556	W557	S558	T559	Y560	L561	T562	K563	F564	I565	A566	R567	Y568	G569	G570	R571	K572	L573	E574	R575	I576	A577	D578	L579	F580	E581	I582	A583	L584	D585	G586	C587	F588	P589	K590	Y591	A592	K593	T594	L595	Y596	L597	L598	Y599	A600	Q601					
L602	E603	E604	E605	W606	G607	L608	A609	R610	H611	A612	M613	V614	A615	Y616	E617	R618	A619	T620	R621	A622	V623	E624	P625	A626	Q627	Q628	Y629	D630	M631	F632	N633	I634	Y635	I636	K637	R638	A639	A640	E641	I642	Y643	G644	V645	F646	T647	T648	D649	G650	I651	Y652	Q653	K654	A655	I656	E657	V658	L659	S660	D661				
E662	H663	A664	R665	E666	M667	C668	L669	R670	F671	A672	D673	M674	E675	C676	K677	L678	G679	E680	I681	D682	R683	A684	R685	A686	I687	Y688	Y689	F690	C691	S692	Q693	I694	C695	D696	P697	R698	T699	T700	G701	A702	F703	W704	Q705	L706	T707	K708	D709	F710	I711	V712	Q713	H714	G715	N716	E717	D718	T719	I720	K721				
E722	M723	L724	R725	I726	R727	R728	S729	V730	Q731	A732	T733	Y734	N735	T736	Q737	V738	N739	F740	M741	A742	S743	Q744	M745	L746	K747	V748	S749	GLY	SER	ALA	THR	GLY	THR	THR	VAL	SER	ASP	GLU	ASP	GLU	LEU	LEU	GLY	ASP	ASN	GLY	PRO	MET	ASP	VAL	VAL	LYS	LEU	LEU	GLU	GLN	ARG	ALA	GLU	GLN	LEU	ALA	ALA
GLU	ALA	ARG	GLU	ASP	GLN	PRO	LEU	PRO	LYS	ARG	ALA	GLN	SER	LYS	LEU	GLN	SER	ASP	ALA	ALA	SER	ARG	GLU	GLU	VAL	GLY	GLY	ILE	GLN	LEU	LEU	GLY	GLY	THR	ASP	GLU	ASP	GLU	LEU	LEU	LEU	LEU	LEU	LEU	GLN	GLN	ARG	ALA	GLU	GLN	LEU	ALA	ALA										
GLN	SER	VAL	PRO	ALA	ALA	VAL	PHE	GLY	SER	VAL	ARG	VAL	ARG	ASP	ALA	GLU	ARG	GLU	LEU	ALA	GLU	ALA	GLN	GLN	VAL	ASN	PRO	GLU	ILE	GLN	LEU	THR	GLY	ASP	GLU	ASP	GLU	LEU	LEU	LEU	LEU	LEU	LEU	GLN	ARG	ALA	GLU	GLN	LEU	LEU	ALA	ALA											

• Molecule 26: Intron-binding protein aquarius



MET	ALA	ALA	PRO	ALA	GLN	PRO	LYS	LYS	ILE	VAL	ALA	PRO	THR	THR	VAL	VAL	GLN	ILE	M19	A20	E21	F22	V23	T24	Q25	L26	A27	C28	K29	Y30	Y31	W31	A32	P33	H34	I35	K36	K37	K38	S39	P40	F41	D42	I43	K44	V45	I46	E47	D48	I49	Y50	E51	K52	E53	I54	V55	K56	S57	R58	F59	A60
I61	R62	K63	I64	M65	L66	L67	E68	F69	K188	S189	T190	P191	L192	F193	L194	K195	F196	W197	M198	L199	T200	K201	M202	L203	D204	V145	S146	L147	K148	F149	L150	D151	H152	C153	M154	C155	S156	C157	V158	V159	D160	L161	L162	R163	S164	Q165	V166	Q167	Q168	L169	I170	S171	L172	P173	M174	W175	M176	G177	L178	Q179	L180
F121	F122	F123	K124	H125	I126	L127	K128	A129	A130	L131	A132	E133	T134	D135	G136	E137	F138	S139	L140	H141	E142	Q143	T144	V145	L146	L147	L148	F149	L150	D151	H152	C153	M154	C155	S156	C157	V158	V159	D160	L161	L162	R163	S164	Q165	V166	Q167	Q168	L169	I170	S171	L172	P173	M174	W175	M176	G177	L178	Q179	L180		
A181	R182	L183	E184	E185	L186	L187	K188	L189	T190	P191	K192	L193	R194	K195	F196	W197	M198	L199	T200	K201	M202	L203	D204	V205	K206	M207	D208	P209	E210	E211	R212	E213	F214	A215	Y216	Q217	Q218	R219	R220	F221	L222	S223	Q224	L225	L226	Q227	K228	F229	D230	S231	V232	L233	K234	S235	V236	P237	L238	S239	E240		
F241	V242	T243	W244	D245	K246	V247	H248	V249	C250	E251	R252	F253	L254	E255	L256	M257	D258	L259	L260	A320	E261	A262	L263	L264	F265	T266	R267	R268	F269	W270	M271	T272	L273	D274	D275	D276	Q277	H278	L279	L280	F281	H282	C283	Y284	L285	S286	M287	L288	V289	R290	R291	E292	L293	D294	G295	H296	L297	F298	S299	Q300	
L301	L302	D303	K304	L305	K306	F307	Y308	T309	G310	F311	E312	L313	N314	D315	Q316	T317	G318	N319	A320	L321	S322	E323	N324	E325	K326	T327	T328	L329	H330	Y331	D332	R333	L334	T335	S336	L337	Q338	R339	A340	F341	A342	A343	H344	F345	P346	E347	L348	Y349	D350	F351	A352	L353	S354	N355	V356	L357	E358	V359	D360		

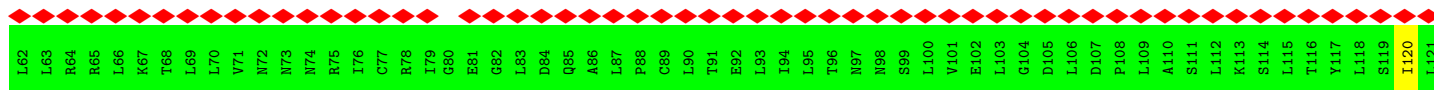
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L421	N422	Q423	M424	P425	L426	Y427	P428	T429	E430	K431	I432	I433	W434	D435	E436	N437	I438	V439	P440	T441	E442	Y443	Y444	S445	S446	E447	G448	C449	L450	A451	L452	P453	E454	L455	N456	L457	L458	F459	L460	T461	L462	H463	D464	Y465	L466	L467	R468	N469	M470	N471	L472	F473	R474	L475	E476	S477	T478	Y479	E480	
I481	R482	Q483	D484	I485	E486	D487	S488	F489	S490	R491	M492	K493	P494	W495	Q496	GLU	TYR	G500	G501	V502	V503	F504	G505	G506	W507	A508	R509	M510	A511	Q512	P513	I514	V515	A516	F517	T518	V519	V520	E521	V522	A523	K524	P525	N526	I527	G528	E529	N530	M531	P532	T533	R534	V535	E536	A537	D538	V539	T540		
I541	N542	L543	N544	V545	R546	D547	H548	I549	K550	D551	E552	M553	E554	G555	L556	R557	K558	H559	D560	G561	V562	F563	L564	I565	T566	V567	R568	P569	T570	K571	P572	Y573	G574	T575	K576	F577	T578	R579	R580	R581	V582	P582	F583	I584	E585	Q586	V587	G588	L589	V590	Y591	V592	R593	G594	C595	E596	I597	Q598	V599	M600
L601	D602	D603	K604	G605	R606	V607	I608	GLU	ASP	GLY	PRO	GLU	P614	R615	P616	N617	L618	R619	G620	E621	S622	G623	T624	F625	R626	V627	F628	L629	D630	P631	M632	Q633	Y634	Q635	Q636	M637	T639	M640	T641	I642	Q643	M644	G645	A646	Q647	D648	V649	R650	E651	V652	F653	M654	I655	M656	M657	R658	R659	G660		
P661	K662	E663	N664	N665	F666	K667	A668	V669	L670	E671	T672	I673	R674	N675	L676	M677	N678	T679	D680	C681	V682	F683	P684	D685	M686	L687	H688	D689	I690	I691	L692	G693	G694	G695	D696	P697	S698	S699	A700	H701	V702	S703	K704	M705	P706	N707	Q708	I709	A710	T711	L712	D713	F714	I656	M657	R658	R659	L719	S720	
I721	E722	H723	L724	K725	A726	S727	F728	P729	G730	H731	N732	K733	R734	N735	T736	E737	F738	D739	P740	A741	L742	Q743	I744	PRO	F746	F747	R748	I749	T750	F751	F752	V753	ARG	SER	GLY	LYS	LYS	ARG	LYS	ASP	ALA	ASP	VAL	GLU	ASP	GLU	THR	GLU	E773	A774	A775	T776	L777	I778	V779	E780				
P781	H782	V783	I784	P785	N786	R787	G788	P789	Y790	P791	Y792	N793	Q794	P795	K796	R797	N798	I799	I800	Q801	F802	T803	H804	T805	Q806	L807	E808	A809	I810	R811	A812	G813	M814	Q815	P816	G817	L818	T819	M820	V821	V822	G823	P824	P825	G826	T827	G828	K829	K830	D831	V832	A833	V834	Q835	I836	I837	S838	N839	I840	
H841	H842	N843	F844	P845	E846	R847	R848	T849	L850	I851	V852	T853	H854	S855	N856	Q857	A858	L859	N860	Q861	L862	F863	E864	K865	M866	M867	A868	L869	D870	I871	D872	E873	R874	H875	L876	L877	R878	L879	G880	H881	GLY	GLU	E884	E885	L886	E887	T888	E889	K890	D891	F892	S893	K894	Y895	G896	R897	V898	N899	Y900	
V901	L902	A903	R904	R905	I906	E907	L908	L909	E910	E911	V912	K913	R914	L915	Q916	K917	S918	L919	G920	V921	P922	G923	D924	A925	S926	Y927	T928	C929	E930	T931	A932	G933	Y934	F935	F936	L937	Y938	Q939	V940	M941	S942	R943	W944	E945	E946	E947	Y947	I948	S949	K950	V951	K952	N953	LYS	GLY	SER	THR	LEU	P959	D960
V961	T962	E963	V964	S965	T966	F967	F968	P969	F970	H971	E972	M1093	K1033	F974	A975	N976	A977	PRO	GLN	I981	F982	K983	G984	R985	S986	Y987	E988	E989	D990	M991	E992	I993	A994	E995	G996	C997	F998	R999	H1000	I1001	K1002	K1003	I1004	F1005	T1006	Q1007	L1008	E1009	I1010	F1011	F1012	A1013	S1014	E1015	A1016	L1017	R1018	S1019	G1020	
L1021	D1022	R1023	S1024	K1025	Y1026	L1027	L1028	V1029	K1030	E1031	A1032	K1033	F1034	I1035	A1036	M1037	T1038	C1039	T1040	H1041	A1042	A1043	L1044	K1045	R1046	H1047	D1048	L1049	Y1050	K1051	L1052	G1053	F1054	K1055	Y1056	D1057	I1058	I1059	L1060	M1061	E1062	E1063	A1064	R1065	Q1066	Q1067	I1067	L1068	E1069	I1070	E1071	T1072	F1073	I1074	P1075	L1076	L1077	L1078	Q1079	N1080
P1081	Q1082	D1083	G1084	F1085	S1086	R1087	L1088	K1089	R1090	W1091	I1092	M1093	I1094	G1095	D1096	H1097	H1098	Q1099	L1100	P1101	P1102	V1103	I1104	K1105	N1106	M1107	A1108	F1109	Q1110	K1111	Y1112	S1113	N1114	M1115	E1116	Q1117	S1118	L1119	F1120	T1121	R1122	F1123	V1124	R1125	V1126	G1127	V1128	P1129	T1130	V1131	D1132	L1133	L1134	A1135	Q1136	L1137	R1138	A1139	R1140	

L565	P566	S625	V626	D685	E745	P805	Y865	L925	L985	L1045	A1106	T1166
P567	I567	V627	A627	E686	I746	E806	N866	A926	E986	L1046	I1107	T1167
Y668	K628	K628	A627	H688	L747	L807	S867	S927	P987	A1047	C1108	I1168
K569	R629	R629	K628	H689	Y748	I808	K668	T928	M988	Y1048	S1109	D1169
L570	R630	R630	R629	E690	T749	I809	T869	V929	L989	Y1049	G1110	P1170
K571	V630	V630	R629	R690	K750	L810	G670	L930	C990	M1050	F1111	R1171
E572	S631	S631	V630	T691	E751	P811	I871	S931	K991	S1051	F1112	M1172
Q573	E632	E632	V630	I692	P752	V812	D872	L932	L993	M1052	R1113	L1173
L574	E633	E633	R634	H693	E753	Y813	Q873	K933	I994	K1053	M1114	V1174
V575	F634	F634	F634	T694	E754	S814	L874	A934	M995	M1054	A1115	E1175
Q576	G635	G635	G635	D695	T754	A815	V875	M935	S996	K1055	A1116	F1176
A577	C636	C636	C636	D696	Y756	L816	V876	G936	V997	K1056	K1117	A1177
V578	C637	C637	C637	L697	L757	P817	T877	I937	V998	F1057	K1118	P1178
H579	L638	L638	L638	F698	D758	S818	P878	N938	H998	S1058	D1119	A1179
D580	G639	G639	G639	G699	A759	E819	I879	D939	L999	N1059	P1120	F1180
N581	Q640	Q640	Q640	L700	S760	M820	S880	L940	G1000	P1060	Q1121	F1181
Q582	E641	E641	E641	L701	L761	Q821	Q881	L941	C1001	W1061	E1122	K1182
I583	T642	T642	T642	K702	I762	T822	A882	S942	S1002	C1062	G1123	V1183
L584	G643	G643	G643	K703	T763	R823	Q883	F943	E1003	Y1063	Y1124	S1184
I585	Y644	Y644	Y644	T704	V764	I824	A884	D944	M1004	E1064	R1125	D1185
I586	T645	T645	T645	V705	M765	F825	Q885	F945	M1005	N1065	T1126	P1186
I587	T646	T646	T646	Q706	Q766	D826	Q886	M946	L1006	F1066	L1127	T1187
E588	R647	R647	R647	K707	I767	P827	R887	D947	T1007	I1067	I1128	K1188
T590	F648	F648	F648	R708	H768	A828	A888	A948	I1008	Q1068	Q1129	LEU
G591	E649	E649	E649	Q709	L769	P829	G889	P949	V1009	A1069	Q1130	SER
S592	D650	D650	D650	D710	T770	R830	R890	P950	S1010	R1070	Q1131	LYS
G593	C651	C651	C651	M711	E771	G831	A891	M951	M1011	S1071	V1132	GLN
S594	T652	T652	T652	K712	P772	S832	G892	E952	L1012	L1072	V1133	LYS
K594	S653	S653	S653	L713	P773	R833	R893	T953	S1013	R1073	Y1134	GLN
T595	P654	P654	P654	I714	G774	K834	T894	L954	V1014	R1074	L1135	ARG
T596	E655	E655	E655	V715	D775	V835	G895	P955	Q1015	A1075	H1136	LEU
Q597	T656	T656	T656	T716	I776	V836	P896	T956	M1016	Q1076	P1137	GLU
I598	V657	V657	V657	A717	L777	I837	G897	A957	V1017	D1077	S1138	PRO
T599	I658	I658	I658	F718	S778	A838	K898	M958	F1018	I1078	S1139	LEU
Q600	K659	K659	K659	T719	F779	T839	C899	E959	Y1019	R1079	A1140	ASN
Y601	Q660	Q660	Q660	L720	T779	N840	Y900	Q960	R1020	K1080	L1141	ARG
A603	M661	M661	M661	D721	L781	I841	R901	L961	P1021	Q1081	F1142	TYR
E604	T662	T662	T662	A722	G782	A842	L902	Y962	K1022	M1082	N1143	GLU
A605	D663	D663	D663	V723	Q783	E843	Y903	T963	D1023	L1083	R1144	GLU
A606	G664	G664	G664	K724	E784	T844	T904	L964	K1024	G1084	Q1145	PRO
G606	M665	M665	M665	F725	E785	S845	E905	G965	Q1025	I1085	P1146	ALA
Y607	L666	L666	L666	S726	I786	L846	R906	A966	A1026	M1086	E1147	TRP
T608	L667	L667	L667	Q727	D787	T847	A907	L967	L1027	D1087	E1148	ARG
S609	R668	R668	R668	Y728	T788	I848	Y908	D968	A1028	H1088	V1149	ILE
G611	E669	E669	E669	F729	A789	D849	R909	D969	D1029	H1089	V1150	SER
K612	L671	L671	L671	Y731	E791	G850	D910	E970	Q1030	K1090	Y1151	ARG
I613	I672	I672	I672	A732	E792	I851	E911	E971	K1031	L1091	H1152	ARG
G614	D673	D673	D673	P733	I792	Y852	N912	L972	K1032	D1092	E1153	ARG
C615	E674	E674	E674	I734	L793	Y853	L913	L973	A1033	V1093	L1154	ARG
L616	P675	P675	P675	F735	Y794	V854	T914	R975	K1034	V1094	V1155	ARG
Q617	D676	D676	D676	T736	E795	V855	T915	R976	F1035	S1095	L1156	ALA
R618	L677	L677	L677	I737	R796	D856	N916	L976	H1036	C1096	T1157	ALA
R619	G678	G678	G678	P738	M797	P857	V917	G977	Q1037	G1097	T1158	PHE
R620	Y679	Y679	Y679	G739	K798	G858	P918	R978	T1038	K1098	K1159	ARG
V621	A680	A680	A680	R740	S799	F859	E919	R979	E1039	S1099	E1160	ARG
A622	I681	I681	I681	T741	L800	V860	I920	M980	G1040	V1100	Y1161	ARG
A623	I682	I682	I682	Y742	G801	K861	Q821	A981	D1041	W1101	M1162	ARG
M624	M683	M683	M683	P743	D803	K863	T923	F983	L1043	R1102	E1164	ARG
	L684	L684	L684	V744	V804	V864	N924	P984	T1044	V1103	V1165	ARG

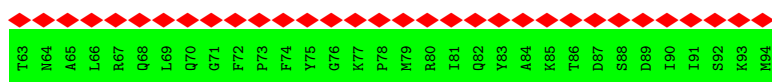
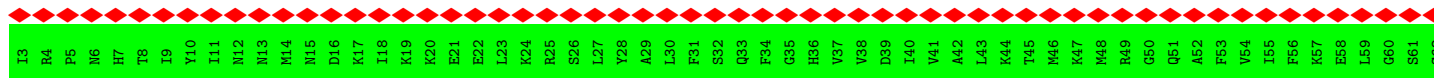
• Molecule 28: U2 small nuclear ribonucleoprotein A'



V2	K3	L4	T5	A6	E7	L8	I9	E10	Q11	A12	A13	Q14	Y15	T16	N17	A18	V19	R20	D21	R22	E23	L24	D25	R26	L27	G28	Y29	K30	I31	P32	V33	I34	E35	N36	L37	G38	A39	T40	L41	D42	Q43	F44	A45	A46	I47	D48	F49	S50	D51	M52	E53	I54	R55	K56	L57	D58	G59	F60	P61
----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



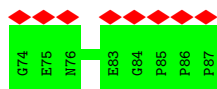
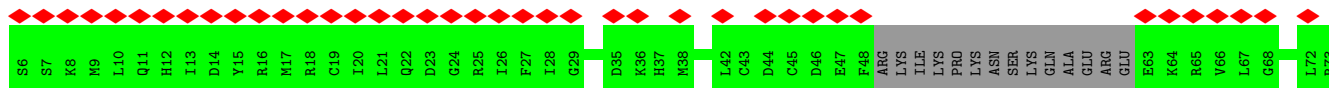
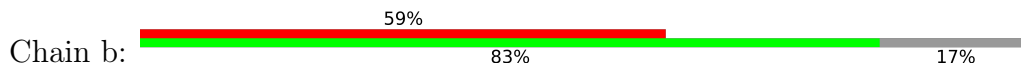
• Molecule 29: U2 small nuclear ribonucleoprotein B'



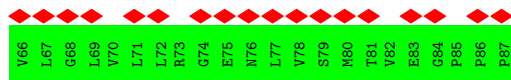
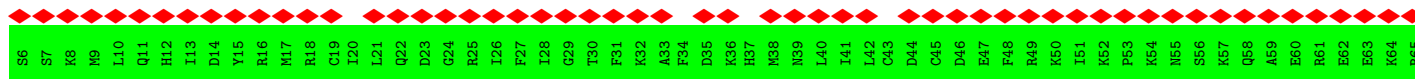
• Molecule 30: NF-kappa-B-activating protein



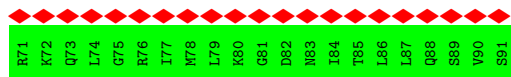
• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'



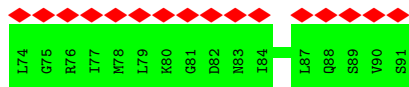
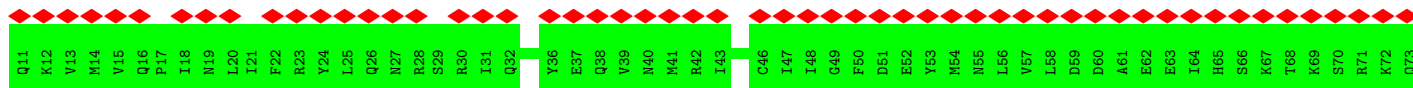
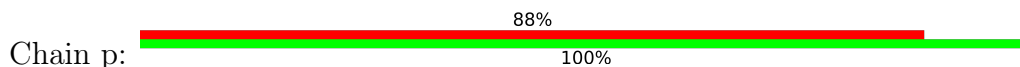
• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'



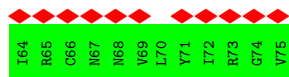
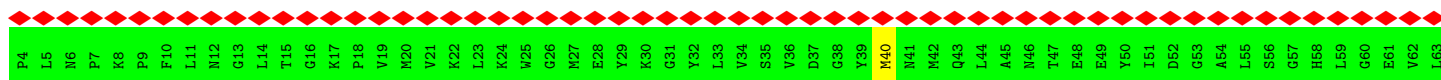
• Molecule 32: Pre-mRNA-splicing factor SLU7



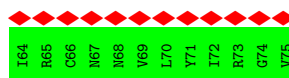
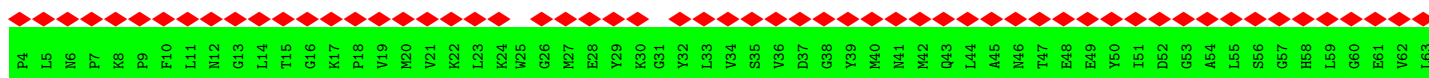
• Molecule 34: Small nuclear ribonucleoprotein E



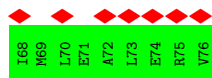
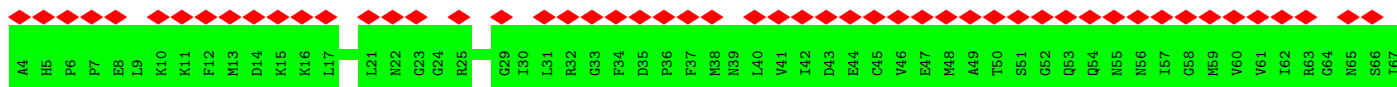
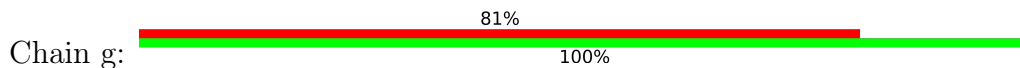
• Molecule 35: Small nuclear ribonucleoprotein F



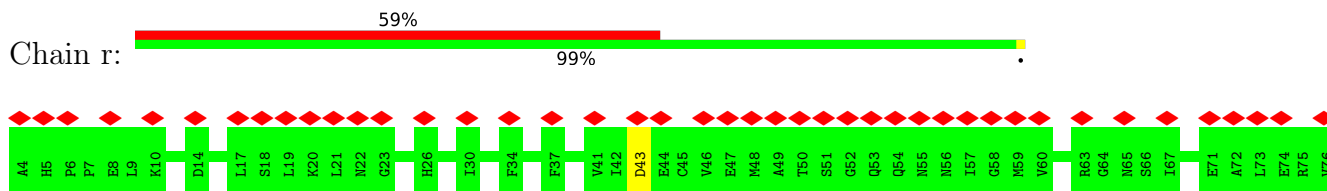
• Molecule 35: Small nuclear ribonucleoprotein F



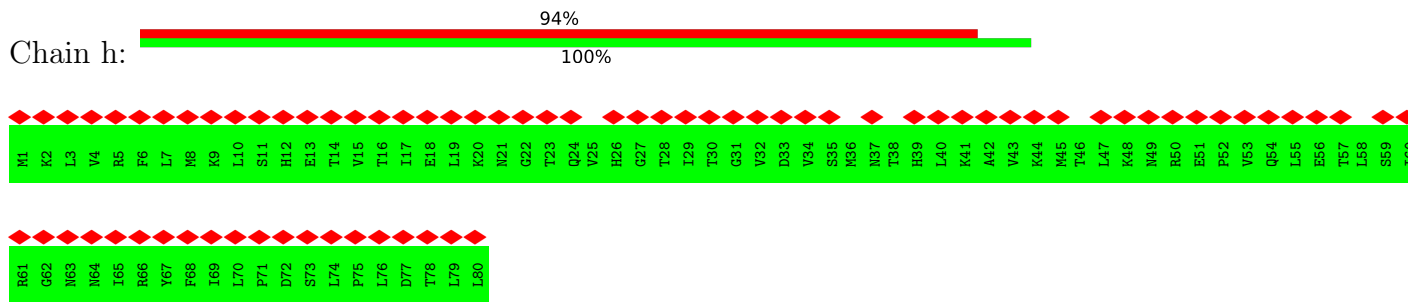
• Molecule 36: Small nuclear ribonucleoprotein G



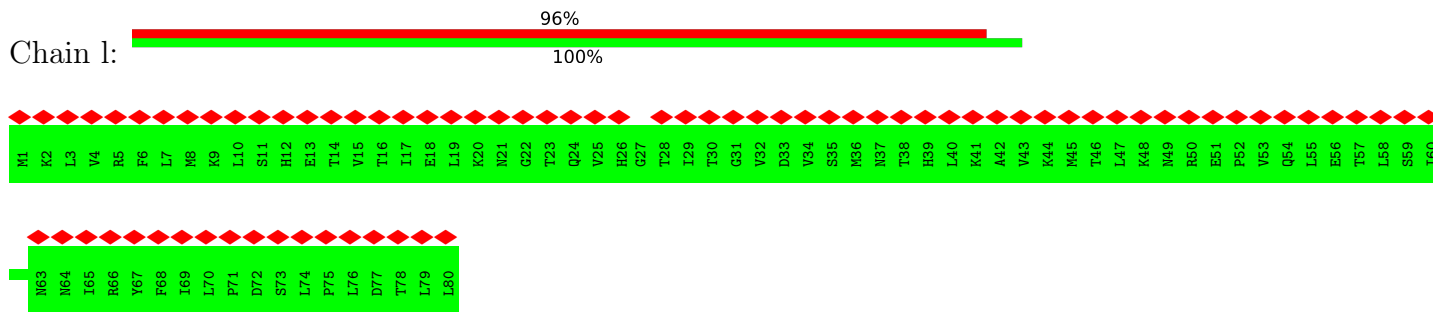
• Molecule 36: Small nuclear ribonucleoprotein G



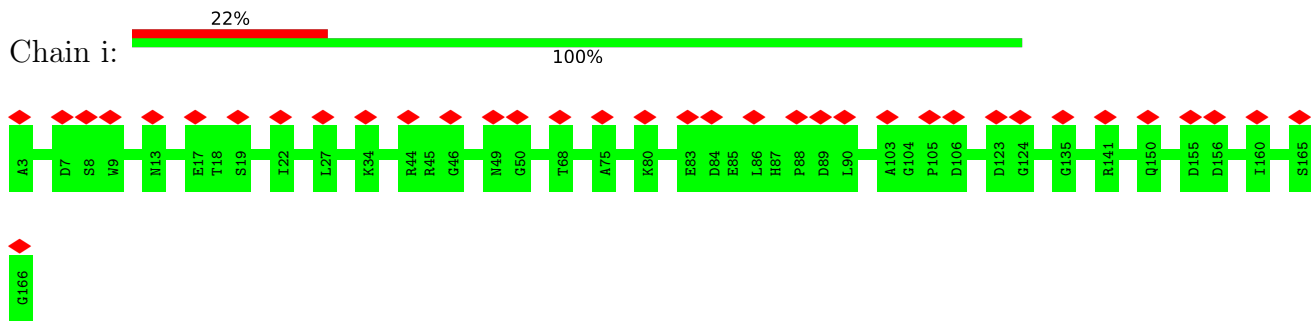
• Molecule 37: Small nuclear ribonucleoprotein Sm D1



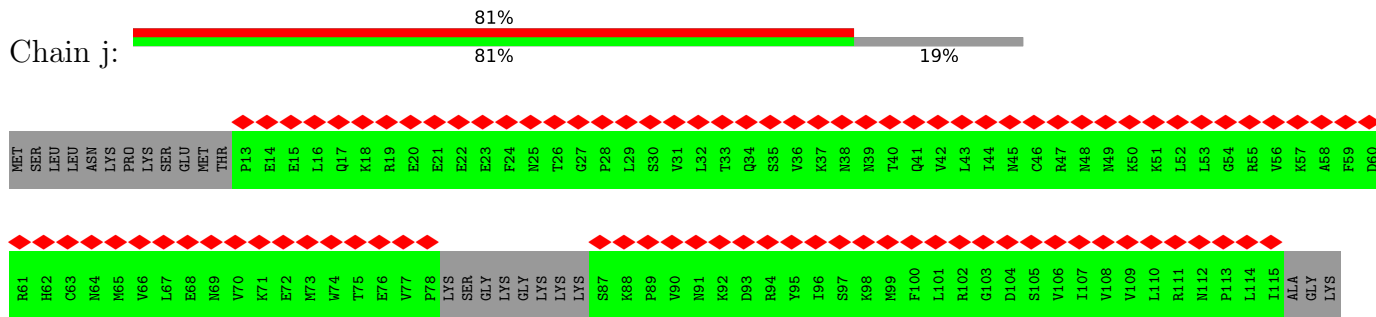
• Molecule 37: Small nuclear ribonucleoprotein Sm D1



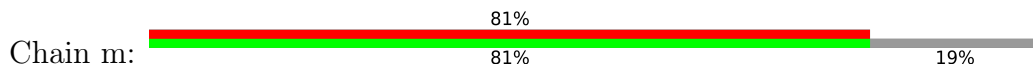
• Molecule 38: Peptidyl-prolyl cis-trans isomerase-like 1



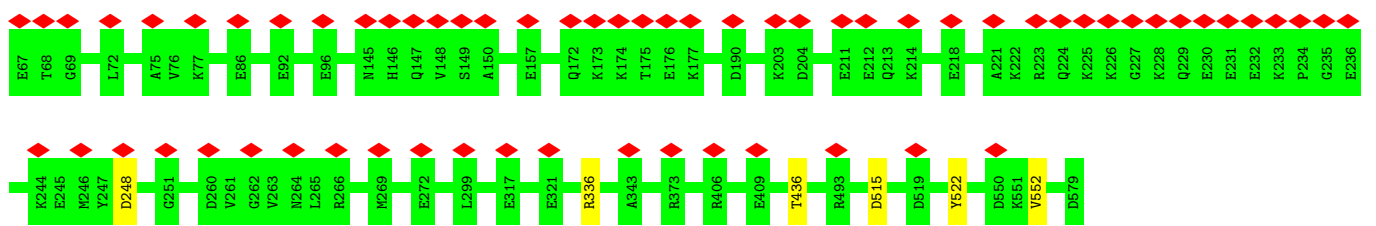
• Molecule 39: Small nuclear ribonucleoprotein Sm D2



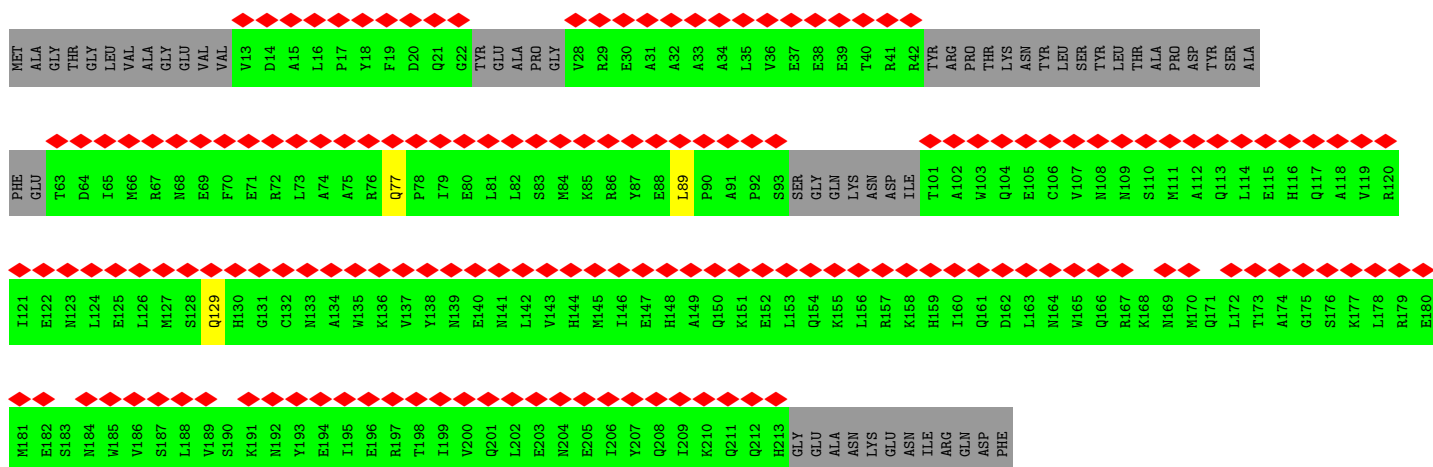
• Molecule 39: Small nuclear ribonucleoprotein Sm D2



• Molecule 40: Pre-mRNA-processing factor 17



• Molecule 41: Pre-mRNA-splicing factor SPF27



• Molecule 42: Pre-mRNA-processing factor 19

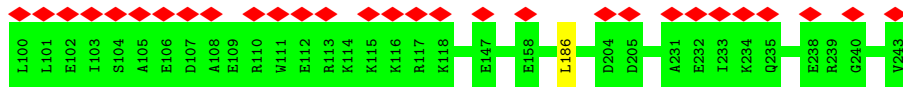


ASP GLY LEU LEU LEU ILE PHE HIS GLY THR GLY THR THR MET ILE ASP ASP SER SER GLN ILE ILE LYS LYS TRP ASP LEU LYS LEU GLU ARG THR THR ASP ASN VAL ALA ASP ASN GLY ASN PHE THR PRO TYR PRO GLY HIS SER SER GLY PRO ILE THR ASP THR THR ILE ILE ILE ALA PHE SER ILE SER GLU CYS GLU LYS ASN GLY TYR TYR THR TYR THR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

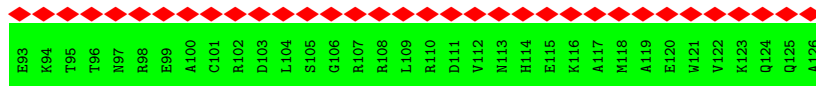
LEU ARG LYS LEU LYS PHE ASN PHE LYS ASP ASP ASN PHE ILE ASP VAL SER LYS LEU LEU ILE ARG THR THR ASP ASN VAL SER ALA ASN GLY PHE THR TYR LEU ALA LEU GLY PRO THR ASP VAL GLN ILE ALA TYR PHE ILE SER CYS LYS ASN GLN TRP THR TYR LEU ALA THR THR HIS PHE THR ASP ASP HIS SER SER SER VAL LYS LEU THR TRP TRP GLY ASP

VAL ALA PHE GLY HIS HIS ALA LYS PHE ILE ALA SER THR THR GLY MET ASP ARG SER SER LYS LEU PHE TYR SER SER LEU

• Molecule 43: Pre-mRNA-splicing factor SYF2



• Molecule 44: Replication stress response regulator SDE2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103860	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	135000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, GTP, ATP, SEP, IHP, ZN, 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	0.56	0/2827	1.12	16/4393 (0.4%)
2	5	0.58	0/1760	1.27	25/2733 (0.9%)
3	6	0.53	0/2323	0.98	3/3619 (0.1%)
4	7	0.38	0/3179	0.65	0/4291
5	8	0.36	0/748	0.71	3/1012 (0.3%)
6	9	0.38	0/1225	0.60	0/1648
7	A	0.43	1/19172 (0.0%)	0.58	7/26014 (0.0%)
8	B	0.37	0/14140	0.58	2/19159 (0.0%)
9	C	0.39	0/7277	0.62	4/9887 (0.0%)
10	D	0.34	0/1030	0.59	0/1371
11	E	0.60	0/329	1.18	4/510 (0.8%)
12	F	0.32	0/1129	0.53	0/1525
13	G	0.27	0/513	0.55	1/683 (0.1%)
14	H	0.33	0/3779	0.50	0/5087
15	I	0.41	0/971	1.20	10/1504 (0.7%)
16	J	0.46	0/2592	0.63	0/3535
17	K	0.35	0/2387	0.57	0/3205
18	L	0.45	1/1214 (0.1%)	0.58	0/1627
19	M	0.36	0/2366	0.57	1/3193 (0.0%)
20	N	0.31	0/2448	0.58	0/3316
21	O	0.32	0/3457	0.50	0/4627
22	P	0.34	0/902	0.54	0/1201
23	R	0.58	1/196 (0.5%)	0.53	0/265
24	S	0.38	0/4013	0.55	8/5432 (0.1%)
25	T	0.41	0/4031	0.81	8/5500 (0.1%)
26	U	0.43	35/11155 (0.3%)	0.41	0/15095
27	V	0.47	0/3000	0.93	0/3777
28	W	0.31	0/1299	0.62	0/1761
29	Y	0.38	0/759	0.50	0/1016
30	Z	0.32	0/232	0.48	0/307
31	b	0.33	0/553	0.53	0/739
31	k	0.45	0/674	0.55	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.36	0/2268	0.53	0/3052
33	d	0.39	0/666	0.55	0/897
33	n	0.47	0/660	0.61	0/889
34	e	0.29	0/659	0.54	0/885
34	p	0.47	0/677	0.60	0/908
35	f	0.30	0/574	0.55	0/775
35	q	0.49	0/574	0.59	0/775
36	g	0.34	0/575	0.59	0/768
36	r	0.47	0/575	0.62	0/768
37	h	0.28	0/642	0.53	0/867
37	l	0.41	0/642	0.55	0/867
38	i	0.31	0/1304	0.57	0/1767
39	j	0.28	0/784	0.51	0/1053
39	m	0.42	0/784	0.56	0/1053
40	o	0.37	0/4265	0.60	0/5761
41	s	0.35	0/1423	0.51	0/1914
42	t	0.32	0/1004	0.50	0/1365
42	u	0.34	0/953	0.49	0/1295
42	v	0.34	0/1004	0.51	0/1365
42	w	0.31	0/953	0.49	0/1295
43	y	0.33	0/1241	0.56	1/1662 (0.1%)
44	z	0.44	0/282	0.50	0/375
All	All	0.40	38/124189 (0.0%)	0.64	93/169287 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	4
8	B	0	1
9	C	0	2
17	K	0	1
18	L	0	2
25	T	0	5
27	V	0	15
35	f	0	1
41	s	0	3
All	All	0	34

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2223	CYS	CB-SG	-6.69	1.70	1.82
18	L	117	CYS	CB-SG	-6.56	1.71	1.82
23	R	24	SER	CA-CB	-5.95	1.44	1.52
26	U	1107	MET	CG-SD	5.78	1.96	1.81
26	U	244	MET	CG-SD	5.75	1.96	1.81

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	86	C	N1-C2-O2	14.03	127.32	118.90
2	5	86	C	C2-N1-C1'	11.76	131.73	118.80
2	5	86	C	N3-C2-O2	-11.61	113.78	121.90
1	2	50	C	N1-C2-O2	10.30	125.08	118.90
1	2	50	C	C2-N1-C1'	9.37	129.10	118.80

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	1210	LYS	Peptide
7	A	1416	ILE	Peptide
7	A	1635	TYR	Peptide
7	A	940	ILE	Peptide
8	B	430	LEU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	7	388/390 (100%)	376 (97%)	9 (2%)	3 (1%)	19	51
5	8	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	14	45
6	9	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
7	A	2244/2335 (96%)	2105 (94%)	139 (6%)	0	100	100
8	B	1720/1722 (100%)	1633 (95%)	84 (5%)	3 (0%)	47	77
9	C	897/899 (100%)	828 (92%)	67 (8%)	2 (0%)	47	77
10	D	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
12	F	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
13	G	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
14	H	455/908 (50%)	440 (97%)	15 (3%)	0	100	100
16	J	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
17	K	291/295 (99%)	271 (93%)	20 (7%)	0	100	100
18	L	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
19	M	287/289 (99%)	271 (94%)	16 (6%)	0	100	100
20	N	304/306 (99%)	283 (93%)	19 (6%)	2 (1%)	22	54
21	O	429/802 (54%)	416 (97%)	12 (3%)	1 (0%)	47	77
22	P	100/229 (44%)	97 (97%)	3 (3%)	0	100	100
23	R	24/26 (92%)	17 (71%)	7 (29%)	0	100	100
24	S	531/848 (63%)	500 (94%)	28 (5%)	3 (1%)	25	57
25	T	597/855 (70%)	584 (98%)	12 (2%)	1 (0%)	47	77
26	U	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
27	V	709/1220 (58%)	617 (87%)	60 (8%)	32 (4%)	2	15
28	W	160/162 (99%)	147 (92%)	13 (8%)	0	100	100
29	Y	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
30	Z	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
31	b	64/82 (78%)	62 (97%)	2 (3%)	0	100	100
31	k	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
32	c	265/586 (45%)	248 (94%)	17 (6%)	0	100	100
33	d	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
33	n	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	e	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
34	p	79/81 (98%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	f	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
35	q	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
36	g	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
36	r	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
37	h	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
37	l	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
38	i	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
39	j	91/118 (77%)	87 (96%)	4 (4%)	0	100	100
39	m	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
40	o	511/513 (100%)	465 (91%)	45 (9%)	1 (0%)	47	77
41	s	161/225 (72%)	148 (92%)	13 (8%)	0	100	100
42	t	121/504 (24%)	118 (98%)	3 (2%)	0	100	100
42	u	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
42	v	121/504 (24%)	119 (98%)	2 (2%)	0	100	100
42	w	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
43	y	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
44	z	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
All	All	14378/18759 (77%)	13605 (95%)	724 (5%)	49 (0%)	44	71

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	383	ASN
8	B	957	VAL
8	B	1584	ILE
20	N	59	ILE
27	V	531	MET

5.3.2 Protein sidechains [i](#)

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	7	345/345 (100%)	340 (99%)	5 (1%)	67	82
5	8	76/76 (100%)	75 (99%)	1 (1%)	69	82
6	9	132/132 (100%)	131 (99%)	1 (1%)	81	89
7	A	2033/2108 (96%)	1996 (98%)	37 (2%)	59	78
8	B	1541/1541 (100%)	1363 (88%)	178 (12%)	5	22
9	C	799/799 (100%)	797 (100%)	2 (0%)	92	96
10	D	106/106 (100%)	105 (99%)	1 (1%)	78	87
12	F	110/110 (100%)	110 (100%)	0	100	100
13	G	54/55 (98%)	53 (98%)	1 (2%)	57	77
14	H	410/838 (49%)	403 (98%)	7 (2%)	60	78
16	J	276/276 (100%)	275 (100%)	1 (0%)	91	95
17	K	246/247 (100%)	246 (100%)	0	100	100
18	L	130/130 (100%)	127 (98%)	3 (2%)	50	73
19	M	254/254 (100%)	253 (100%)	1 (0%)	91	95
20	N	263/263 (100%)	263 (100%)	0	100	100
21	O	322/709 (45%)	321 (100%)	1 (0%)	92	96
22	P	94/203 (46%)	94 (100%)	0	100	100
23	R	21/21 (100%)	20 (95%)	1 (5%)	25	56
24	S	275/751 (37%)	273 (99%)	2 (1%)	84	90
25	T	213/749 (28%)	210 (99%)	3 (1%)	67	82
26	U	1202/1336 (90%)	1193 (99%)	9 (1%)	84	90
27	V	31/1085 (3%)	31 (100%)	0	100	100
28	W	139/147 (95%)	138 (99%)	1 (1%)	84	90
29	Y	81/82 (99%)	81 (100%)	0	100	100
30	Z	25/25 (100%)	25 (100%)	0	100	100
31	b	62/75 (83%)	62 (100%)	0	100	100
31	k	75/75 (100%)	75 (100%)	0	100	100
32	c	236/520 (45%)	235 (100%)	1 (0%)	91	95
33	d	74/74 (100%)	74 (100%)	0	100	100
33	n	73/74 (99%)	73 (100%)	0	100	100
34	e	74/76 (97%)	74 (100%)	0	100	100
34	p	76/76 (100%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	f	61/61 (100%)	61 (100%)	0	100	100
35	q	61/61 (100%)	61 (100%)	0	100	100
36	g	63/63 (100%)	63 (100%)	0	100	100
36	r	63/63 (100%)	62 (98%)	1 (2%)	62	79
37	h	75/75 (100%)	75 (100%)	0	100	100
37	l	75/75 (100%)	75 (100%)	0	100	100
38	i	133/133 (100%)	133 (100%)	0	100	100
39	j	91/110 (83%)	91 (100%)	0	100	100
39	m	91/110 (83%)	91 (100%)	0	100	100
40	o	451/451 (100%)	446 (99%)	5 (1%)	73	85
41	s	152/196 (78%)	152 (100%)	0	100	100
42	t	111/435 (26%)	111 (100%)	0	100	100
42	u	106/435 (24%)	106 (100%)	0	100	100
42	v	111/435 (26%)	111 (100%)	0	100	100
42	w	106/435 (24%)	105 (99%)	1 (1%)	78	87
43	y	129/129 (100%)	129 (100%)	0	100	100
44	z	29/29 (100%)	29 (100%)	0	100	100
All	All	11756/16654 (71%)	11493 (98%)	263 (2%)	54	74

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	H	481	PHE
21	O	261	LYS
40	o	552	VAL
8	B	855	ARG
8	B	837	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
20	N	101	ASN
42	v	79	GLN
28	W	72	ASN
42	v	43	ASN

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Mol	Chain	Res	Type
34	p	88	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	117/189 (61%)	30 (25%)	5 (4%)
11	E	14/14 (100%)	5 (35%)	1 (7%)
15	I	39/113 (34%)	19 (48%)	2 (5%)
2	5	73/116 (62%)	24 (32%)	2 (2%)
3	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	339/538 (63%)	115 (33%)	15 (4%)

5 of 115 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	U
1	2	17	U
1	2	19	G
1	2	20	G
1	2	24	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	6	5	U
15	I	137	C
3	6	33	G
15	I	142	U
3	6	58	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are 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
17	SEP	K	232	-	8,9,10	1.57	1 (12%)	8,12,14	1.47	2 (25%)
17	SEP	K	224	-	8,9,10	1.54	1 (12%)	8,12,14	1.58	1 (12%)

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
17	SEP	K	232	-	-	3/5/8/10	-
17	SEP	K	224	-	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	232	SEP	P-O1P	3.39	1.61	1.50
17	K	224	SEP	P-O1P	3.34	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	224	SEP	P-OG-CB	-3.83	107.75	118.30
17	K	232	SEP	P-OG-CB	-2.85	110.45	118.30
17	K	232	SEP	OG-CB-CA	2.46	110.54	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	232	SEP	CB-OG-P-O2P
17	K	232	SEP	CB-OG-P-O3P
17	K	232	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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
47	ATP	7	702	45	26,33,33	0.92	1 (3%)	31,52,52	1.55	5 (16%)
48	GTP	C	1500	45	26,34,34	1.24	1 (3%)	32,54,54	1.70	7 (21%)
50	IHP	c	601	-	36,36,36	0.74	0	54,60,60	0.91	3 (5%)

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
47	ATP	7	702	45	-	0/18/38/38	0/3/3/3
48	GTP	C	1500	45	-	5/18/38/38	0/3/3/3
50	IHP	c	601	-	-	6/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	1500	GTP	C5-C6	-4.41	1.38	1.47
47	7	702	ATP	O4'-C1'	2.08	1.44	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	C	1500	GTP	PA-O3A-PB	-4.43	117.62	132.83
47	7	702	ATP	PB-O3B-PG	-4.34	117.95	132.83
47	7	702	ATP	N3-C2-N1	-4.09	122.29	128.68
48	C	1500	GTP	PB-O3B-PG	-3.51	120.78	132.83
48	C	1500	GTP	C5-C6-N1	3.47	120.07	113.95

There are no chirality outliers.

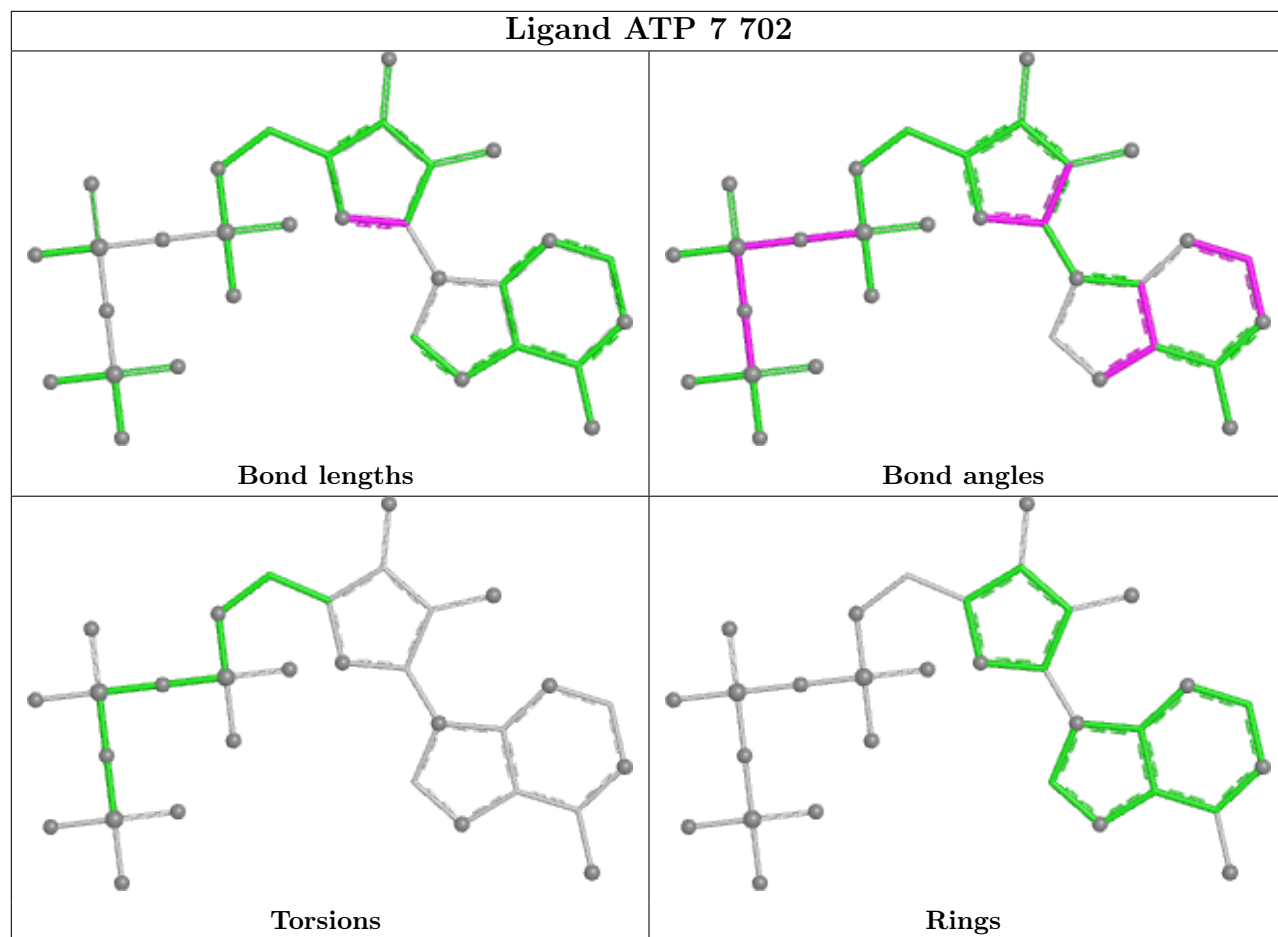
5 of 11 torsion outliers are listed below:

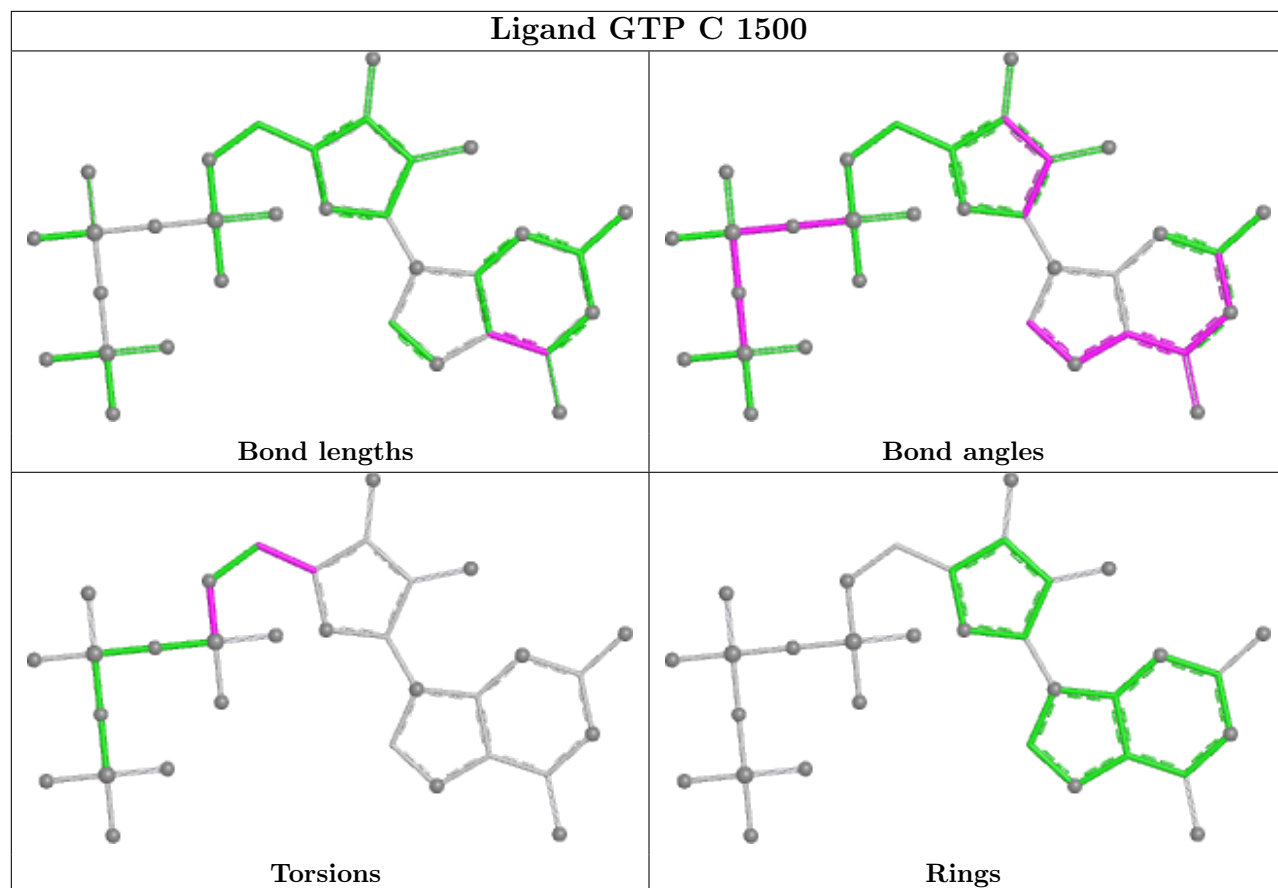
Mol	Chain	Res	Type	Atoms
48	C	1500	GTP	C5'-O5'-PA-O3A
48	C	1500	GTP	C5'-O5'-PA-O1A
48	C	1500	GTP	C5'-O5'-PA-O2A
50	c	601	IHP	C2-O12-P2-O42
50	c	601	IHP	C5-O15-P5-O25

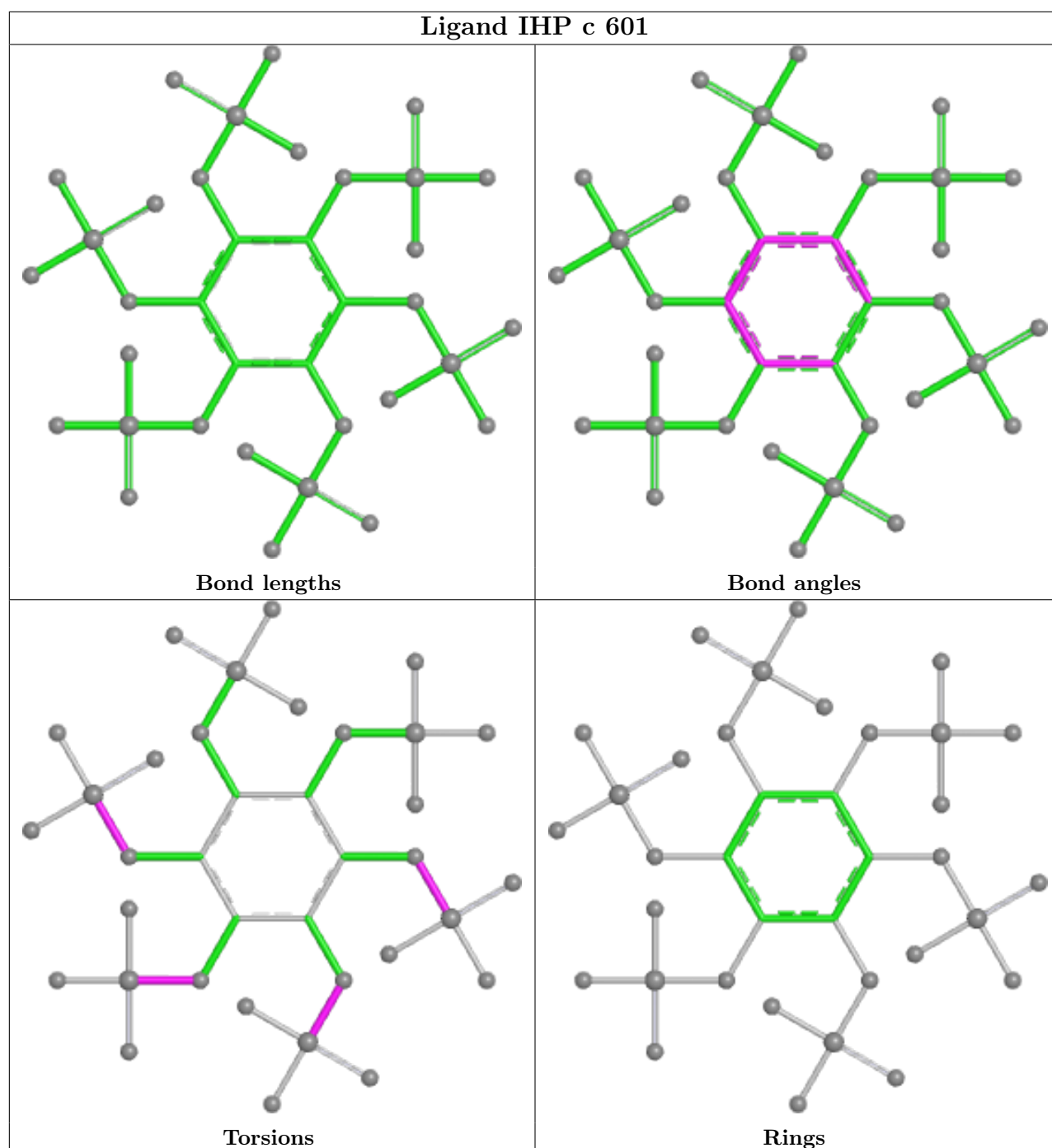
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

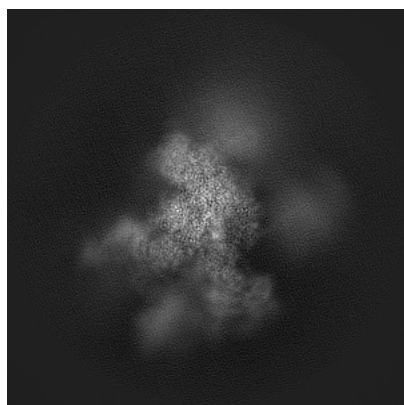
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

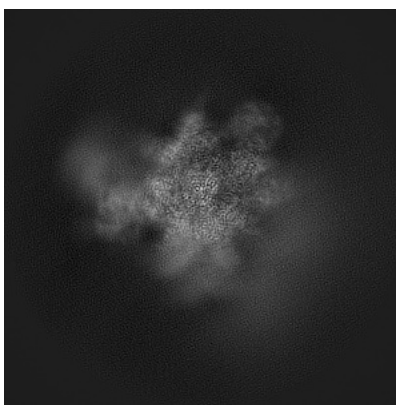
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

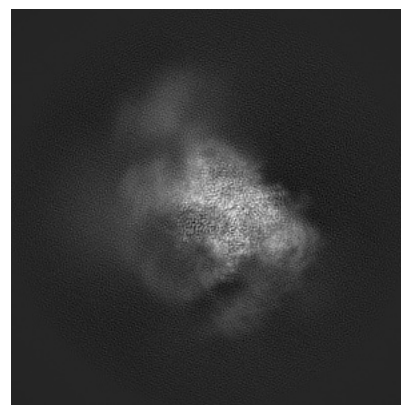
6.1.1 Primary map



X



Y

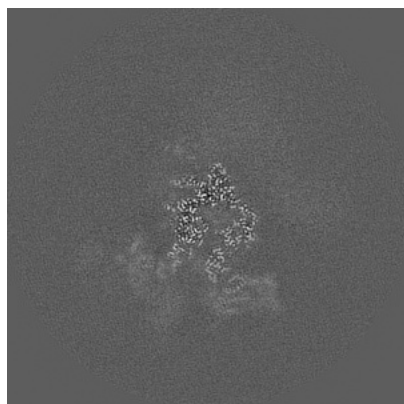


Z

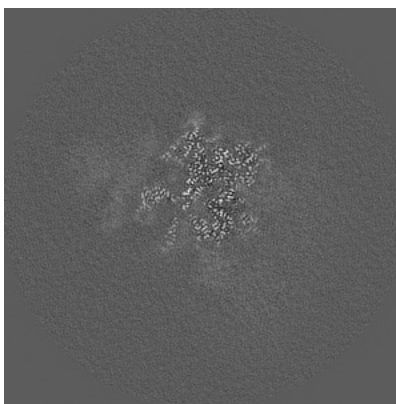
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

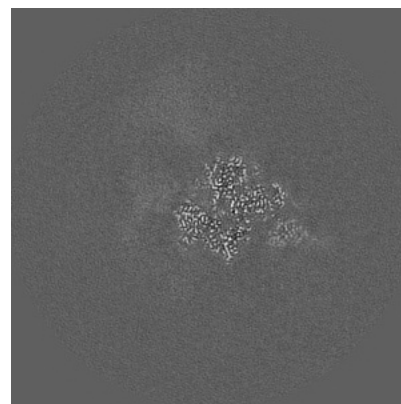
6.2.1 Primary map



X Index: 205



Y Index: 205

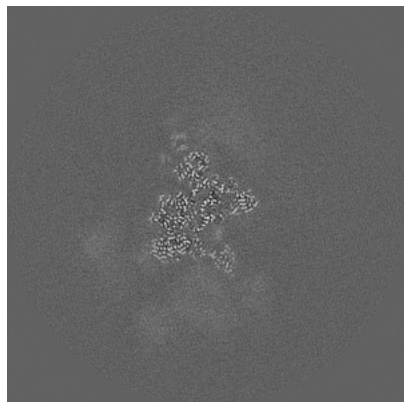


Z Index: 205

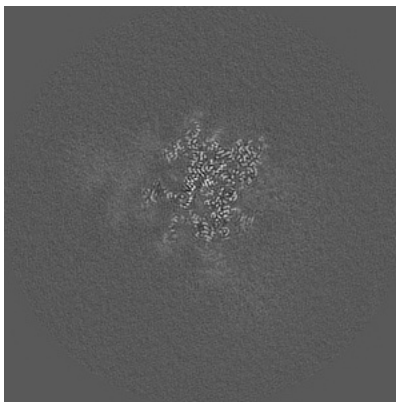
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

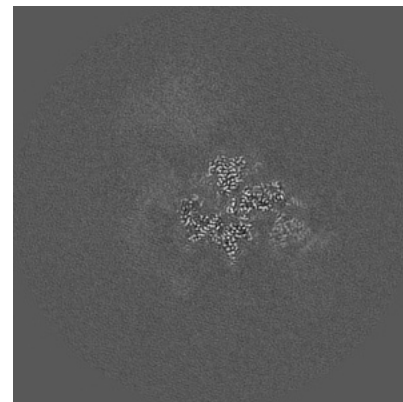
6.3.1 Primary map



X Index: 231



Y Index: 203



Z Index: 202

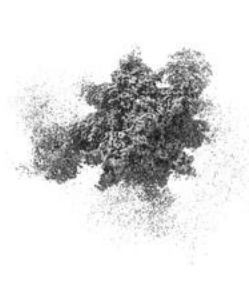
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

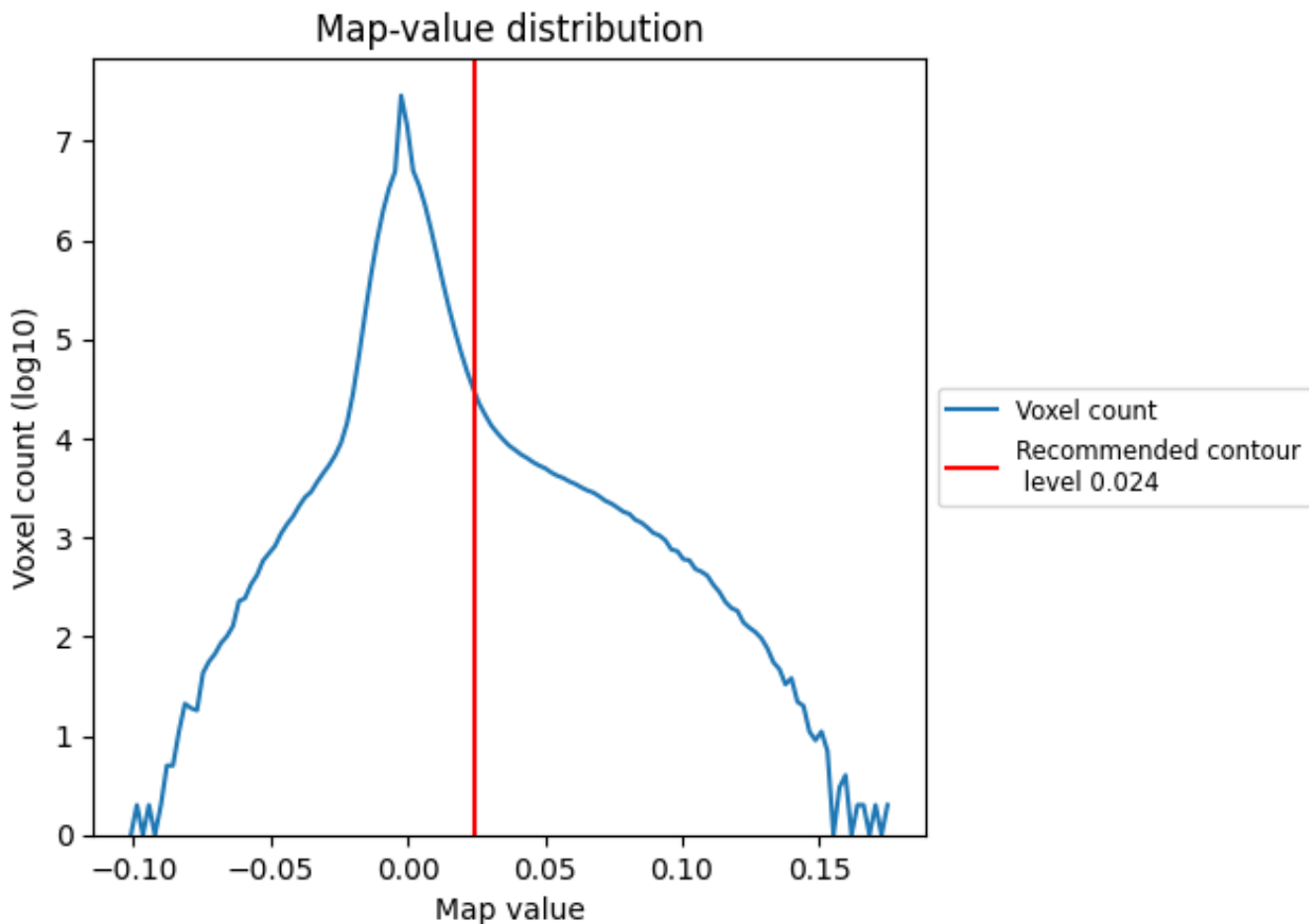
6.5 Mask visualisation

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

7 Map analysis [i](#)

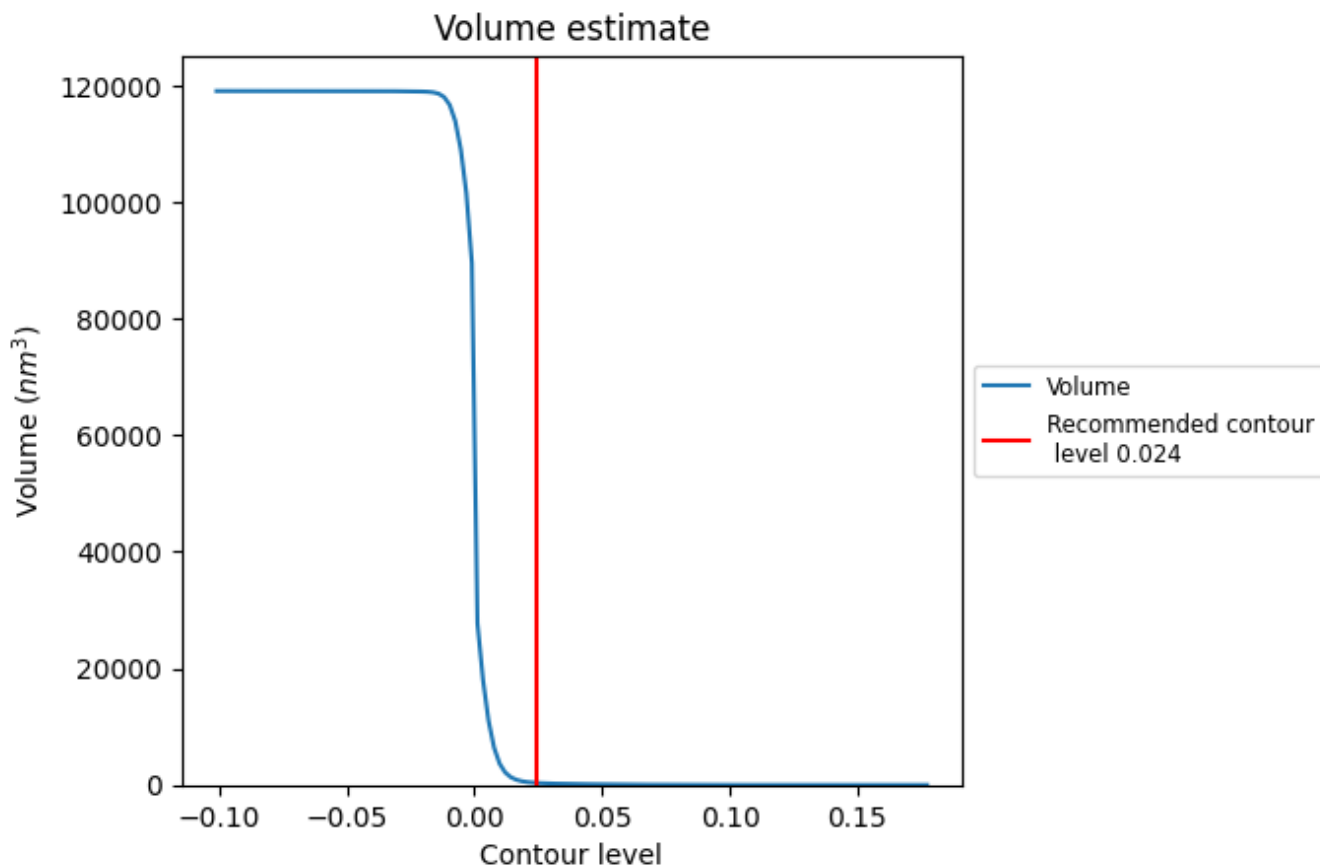
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

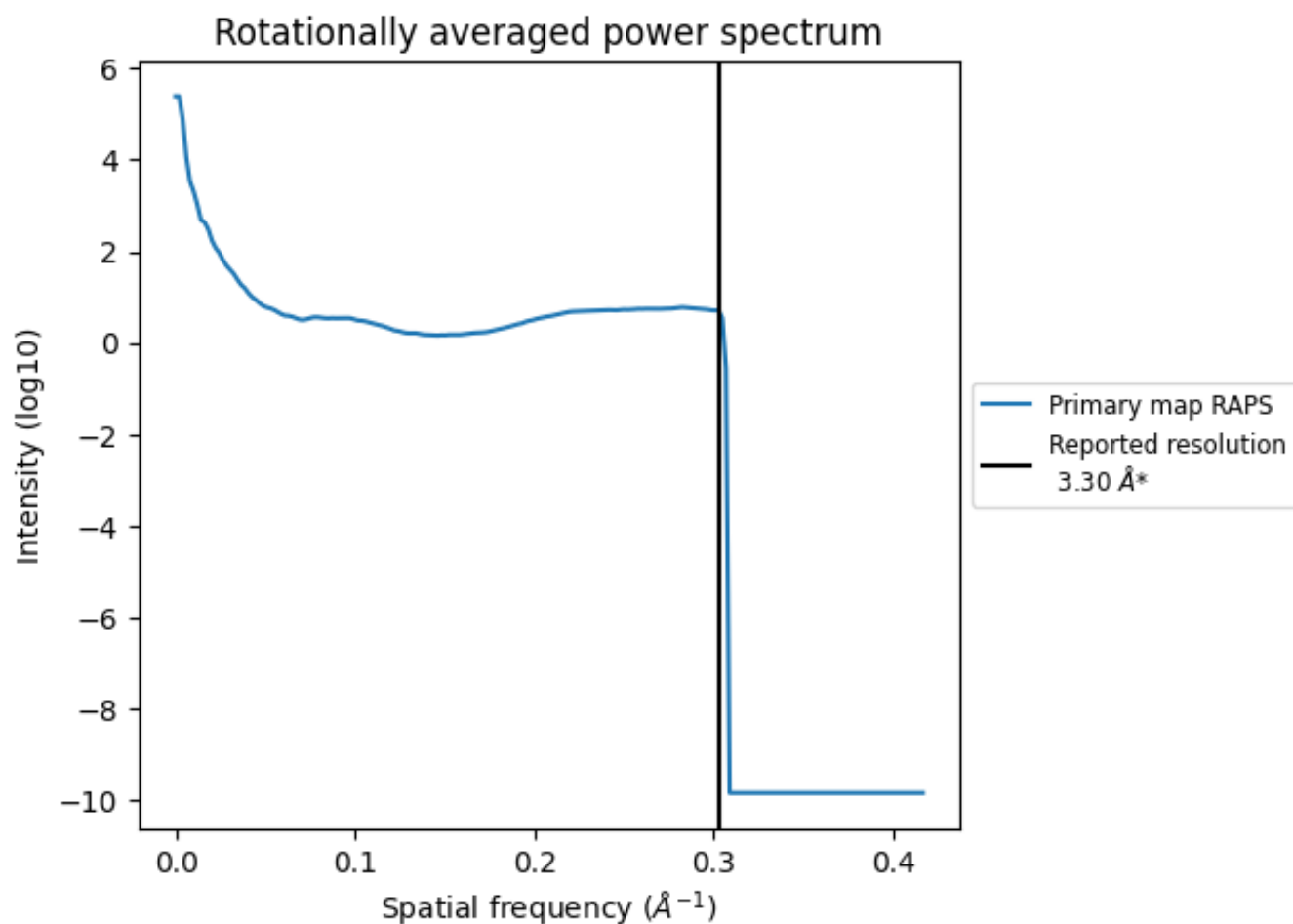
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 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 [\(i\)](#)

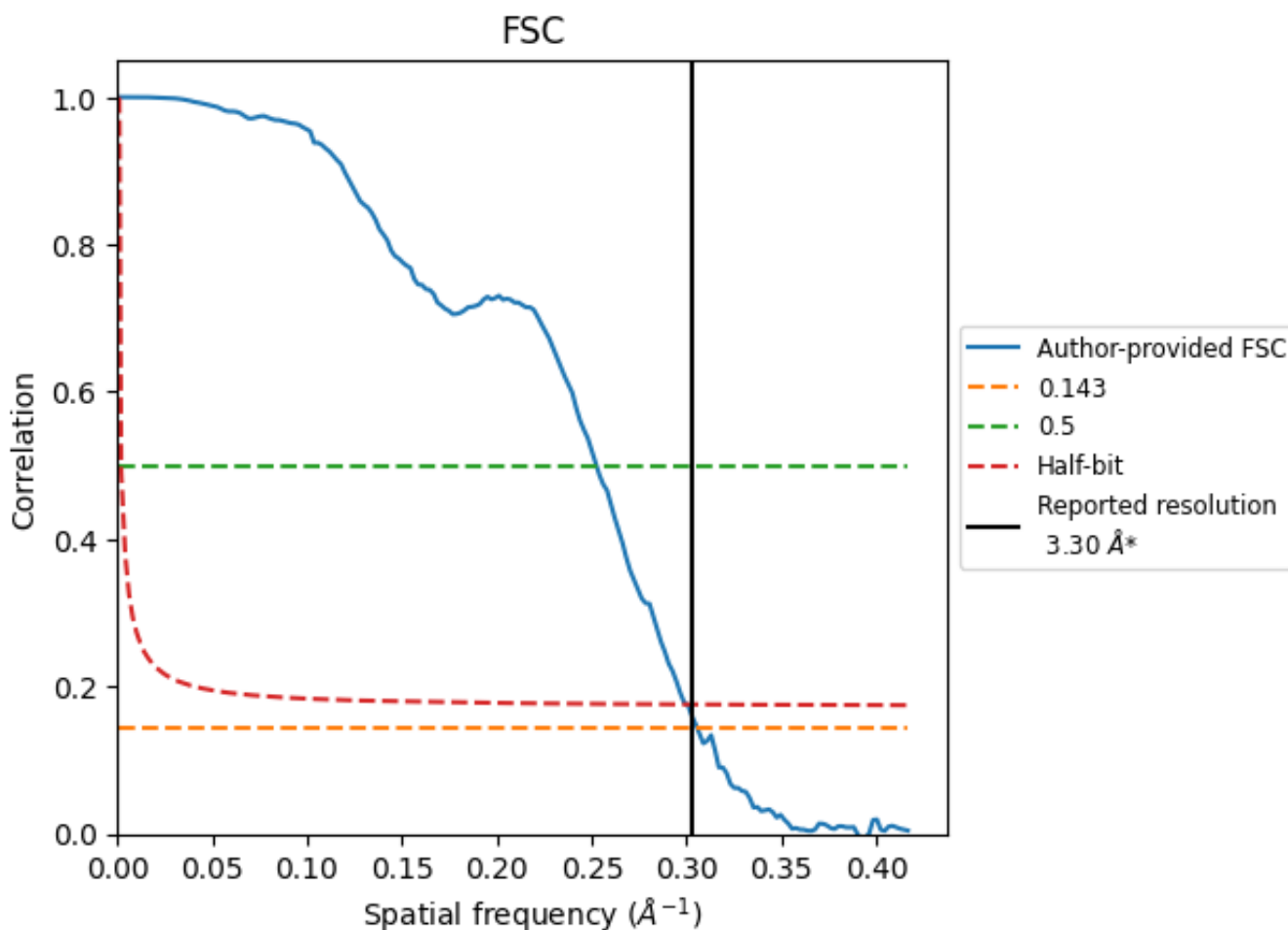


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

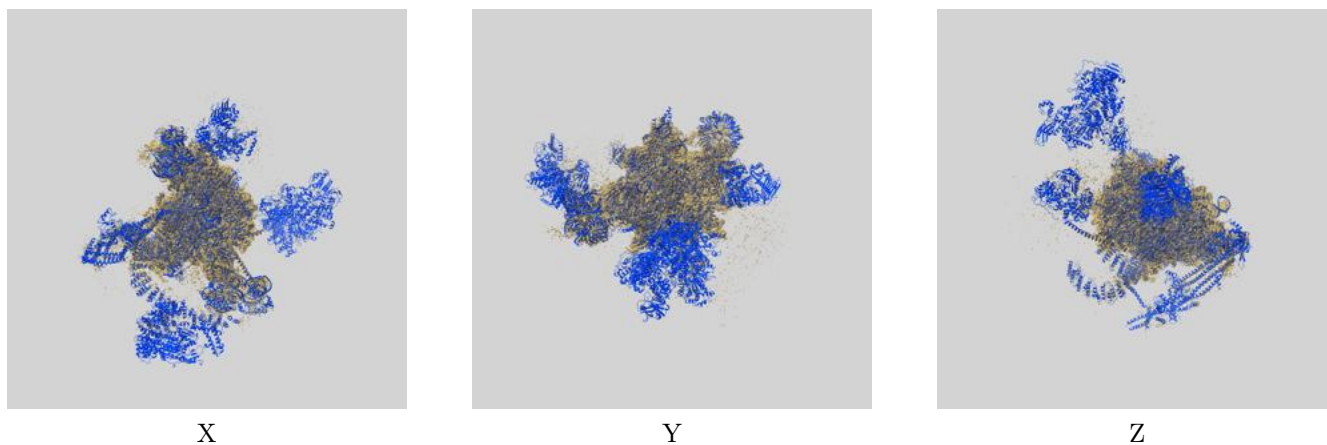
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

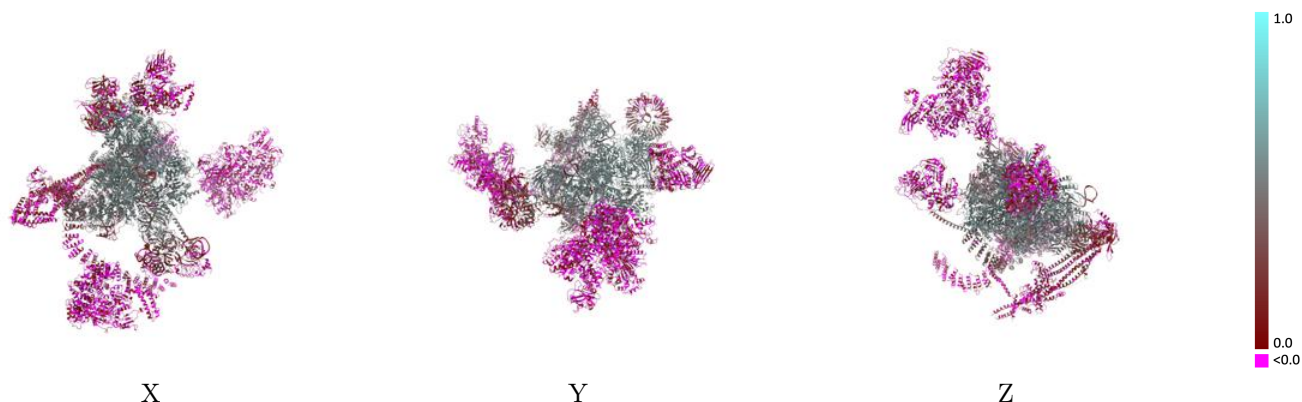
This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 6QDV. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



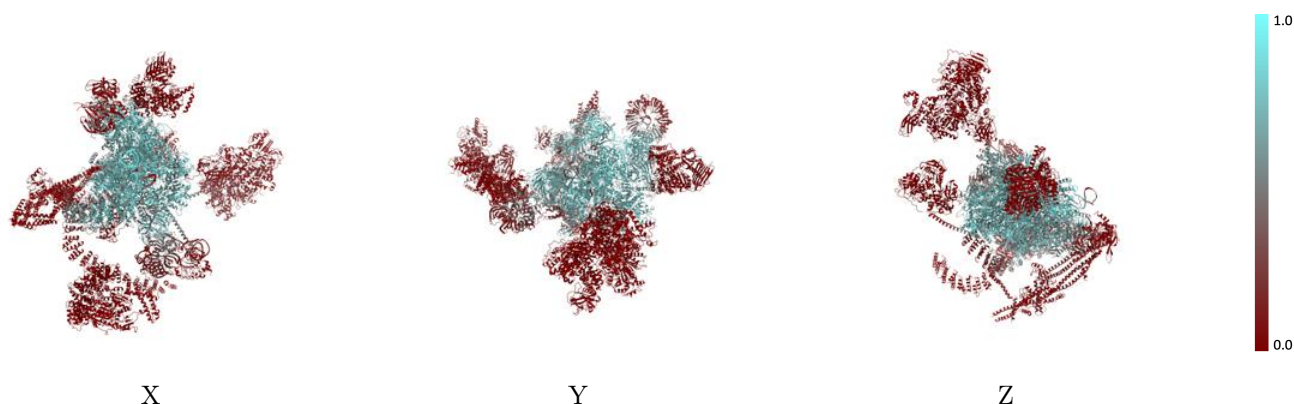
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



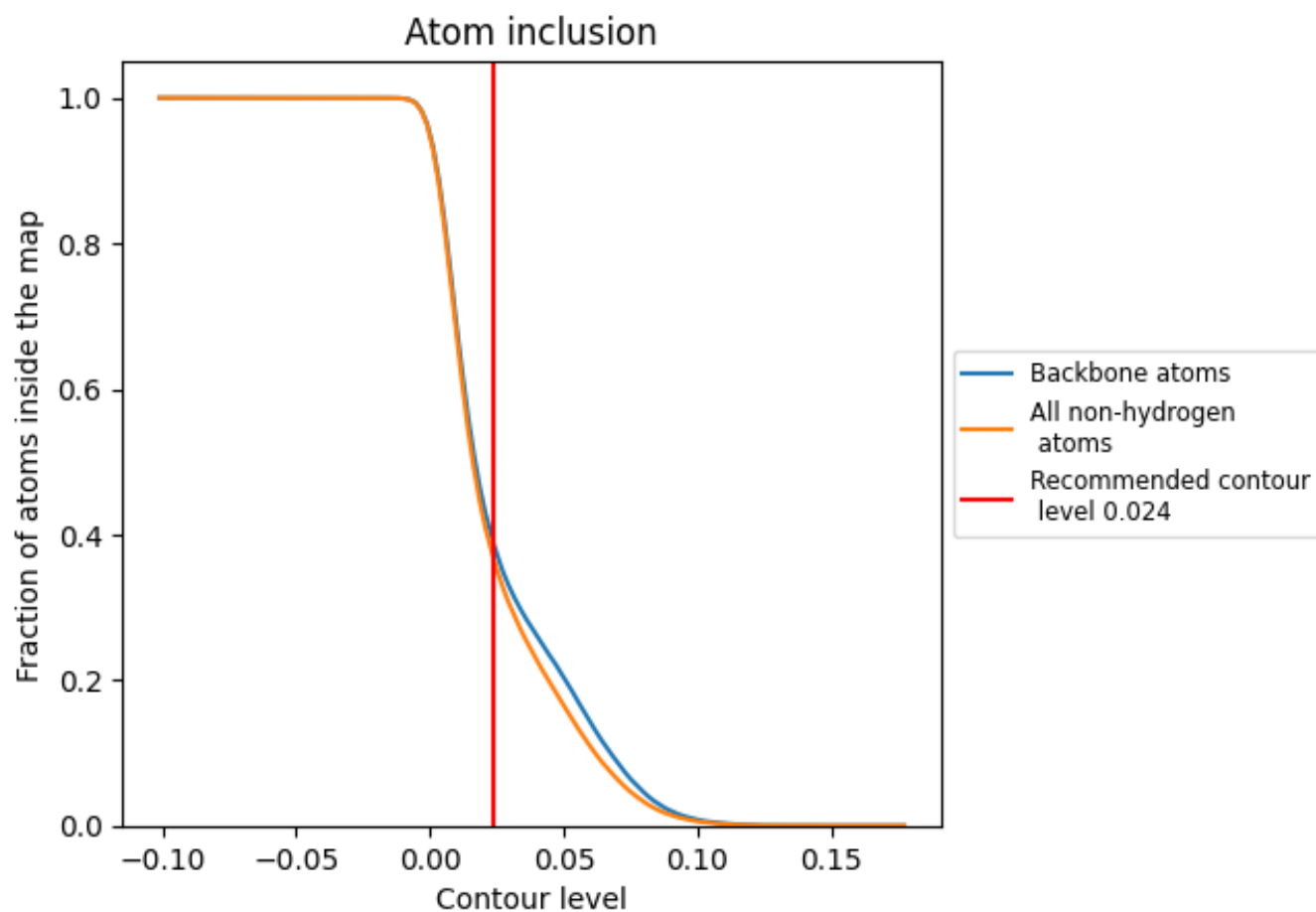
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary









































The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3639	 0.2780
2	 0.4154	 0.2640
5	 0.7511	 0.4540
6	 0.7381	 0.4570
7	 0.0049	 0.0600
8	 0.0000	 -0.0230
9	 0.0000	 0.0230
A	 0.6844	 0.4780
B	 0.0007	 0.0020
C	 0.6848	 0.5010
D	 0.4081	 0.3490
E	 0.8412	 0.5300
F	 0.6278	 0.4670
G	 0.5772	 0.5060
H	 0.3249	 0.2530
I	 0.6044	 0.3950
J	 0.8354	 0.5600
K	 0.5775	 0.4700
L	 0.7396	 0.5240
M	 0.5155	 0.4410
N	 0.6243	 0.4720
O	 0.4296	 0.3550
P	 0.6534	 0.5150
R	 0.8342	 0.5500
S	 0.4421	 0.3340
T	 0.0662	 0.1560
U	 0.0014	 -0.0010
V	 0.0732	 0.0630
W	 0.0215	 0.0440
Y	 0.0479	 0.0930
Z	 0.6516	 0.5040
b	 0.2809	 0.2660
c	 0.6516	 0.4960
d	 0.4341	 0.3790
e	 0.0740	 0.1380



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Chain	Atom inclusion	Q-score
f	 0.0417	 0.1010
g	 0.2161	 0.2880
h	 0.1072	 0.1720
i	 0.5726	 0.4500
j	 0.0501	 0.0950
k	 0.2065	 0.2370
l	 0.1232	 0.1500
m	 0.0607	 0.0830
n	 0.3693	 0.3190
o	 0.6617	 0.4960
p	 0.2236	 0.2290
q	 0.1141	 0.1190
r	 0.3482	 0.3330
s	 0.0730	 0.1200
t	 0.0258	 0.0690
u	 0.0163	 0.0240
v	 0.0237	 0.1160
w	 0.0098	 0.0760
y	 0.6404	 0.4890
z	 0.0112	 0.1960