



wwPDB EM Validation Summary Report ⓘ

Dec 21, 2024 – 01:11 PM EST

PDB ID : 9DTR
EMDB ID : EMD-47157
Title : Structure of the yeast post-catalytic P complex spliceosome at 2.3 Angstrom resolution
Authors : Wilkinson, M.E.; Hoskins, A.A.
Deposited on : 2024-10-01
Resolution : 2.31 Å(reported)
Based on initial model : 6EXN

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:

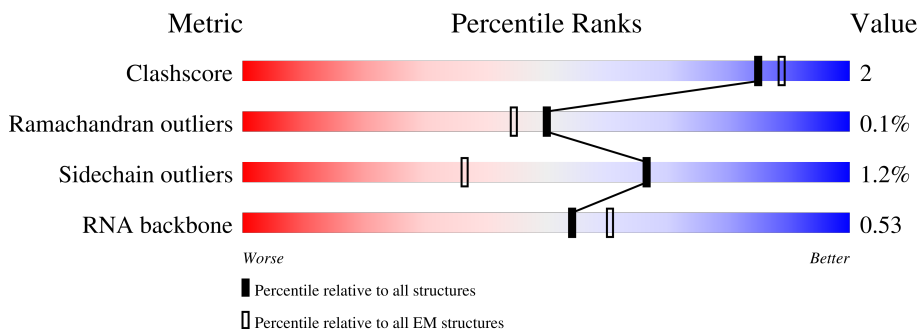
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.31 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	1175	
2	5	214	
3	6	112	
4	A	2413	
5	C	1008	
6	D	173	
7	E	42	

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Mol	Chain	Length	Quality of chain
8	G	235	12% 12% 88%
9	H	577	58% 70% 9% 20%
10	I	95	23% 28% 17% 49%
11	J	451	15% 80% 5% 14%
12	K	379	12% 42% 55%
13	L	157	11% 99%
14	M	339	28% 72% 25%
15	N	364	45% 69% 27%
16	O	590	42% 69% 28%
17	P	175	10% 41% 58%
18	R	135	49% 61% 6% 33%
19	S	687	61% 79% 9% 12%
20	T	859	82% 74% 8% 18%
21	V	1145	64% 64% 33%
22	W	238	71% 67% 29%
23	Y	111	77% 73% 5% 23%
24	Z	140	38% 35% 62%
25	a	251	29% 68% 31%
26	b	196	46% 45% 54%
26	k	196	53% 53% 47%
27	c	382	30% 57% 42%
28	d	101	80% 80% 20%
28	n	101	79% 79% 21%
29	e	94	91% 85% 6% 9%
29	p	94	88% 88% 12%

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Mol	Chain	Length	Quality of chain
30	f	86	86% 83% 14%
30	q	86	86% 85% 14%
31	g	77	92% 91% 8%
31	r	77	91% 91% 9%
32	h	146	73% 73% 27%
32	l	146	73% 72% 27%
33	j	110	83% 83% 17%
33	m	110	83% 81% 17%
34	o	455	43% 76% 24%
35	s	175	100% 100%
36	t	503	26% 26% 74%
36	u	503	26% 26% 74%
36	v	503	26% 26% 74%
36	w	503	26% 26% 74%
37	y	215	37% 66% 34%

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 91230 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	132	2779	1242	456	949	132	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	173	3671	1642	638	1218	173	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1950	16079	10335	2766	2919	59	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	879	7040	4551	1173	1289	27	0	0

- Molecule 6 is a protein called Protein FYV6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	108	914	573	168	172	1	0	0

- Molecule 7 is a RNA chain called UBC4 mRNA spliced exons.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	E	33	703	315	126	229	33	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	21	G	C	conflict	GB NM_001178430
E	22	C	A	conflict	GB NM_001178430

- Molecule 8 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	G	28	139	83	28	28	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	460	3762	2415	622	707	18	0	0

- Molecule 10 is a RNA chain called UBC4 lariat-intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	I	48	1012	455	172	337	48	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	386	2990	1887	530	562	11	0	0

- Molecule 12 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	170	1355	847	249	254	5	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC2.

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

- Molecule 15 is a protein called Pre-mRNA-splicing factor SLT11.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	424	2918	1805	546	560	7	0	0

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

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

- Molecule 18 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	91	510	305	101	103	1	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	604	4683	2996	818	855	14	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	707	5543	3563	922	1038	20	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	764	6096	3860	1061	1145	30	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	635	ALA	SER	engineered mutation	UNP P24384

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	170	1383	866	253	257	7	0	0

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	86	697	448	122	124	3	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor NTC20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	53	424	262	77	82	3	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	172	1380	884	245	247	4	0	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	90	Total	C	N	O	S	0	0
			725	461	131	130	3		
26	k	104	Total	C	N	O	S	0	0
			843	533	157	150	3		

- Molecule 27 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	223	Total	C	N	O	S	0	0
			1893	1183	344	358	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	81	Total	C	N	O	S	0	0
			624	398	107	117	2		
28	n	80	Total	C	N	O	S	0	0
			615	392	105	116	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	86	Total	C	N	O	S	0	0
			665	432	106	124	3		
29	p	83	Total	C	N	O	S	0	0
			646	420	102	121	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	74	Total	C	N	O	S	0	0
			592	381	103	107	1		
30	q	74	Total	C	N	O	S	0	0
			592	381	103	107	1		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	71	Total	C	N	O	S	0	0
			551	348	96	105	2		
31	r	70	Total	C	N	O	S	0	0
			544	344	95	103	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	107	Total	C	N	O	S	0	0
			826	522	145	157	2		
32	l	107	Total	C	N	O	S	0	0
			826	522	145	157	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	91	Total	C	N	O	S	0	0
			747	478	135	130	4		
33	m	91	Total	C	N	O	S	0	0
			747	478	135	130	4		

- Molecule 34 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	348	Total	C	N	O	S	0	0
			2821	1794	501	517	9		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	s	175	Total	C	N	O	0	0
			870	519	175	176		

- Molecule 36 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	t	132	Total	C	N	O	0	0
			658	394	132	132		
36	u	132	Total	C	N	O	0	0
			658	394	132	132		
36	v	132	Total	C	N	O	0	0
			658	394	132	132		
36	w	132	Total	C	N	O	0	0
			658	394	132	132		

- Molecule 37 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	141	Total	C	N	O	S	0	0
			1075	667	198	209	1		

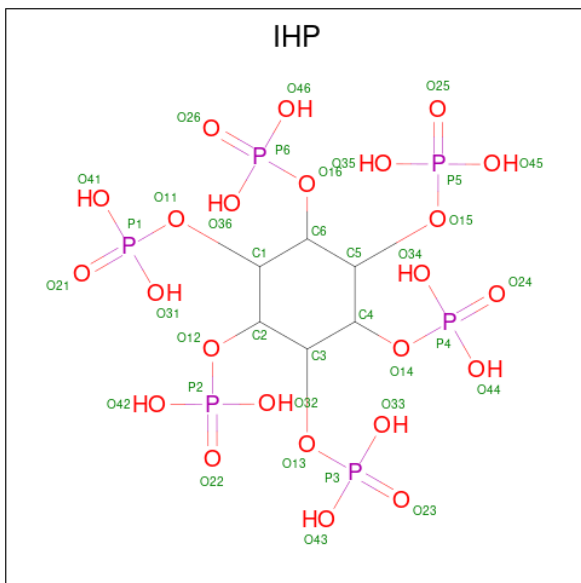
- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	6	1	Total	Mg	0
			1	1	
38	C	1	Total	Mg	0
			1	1	

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

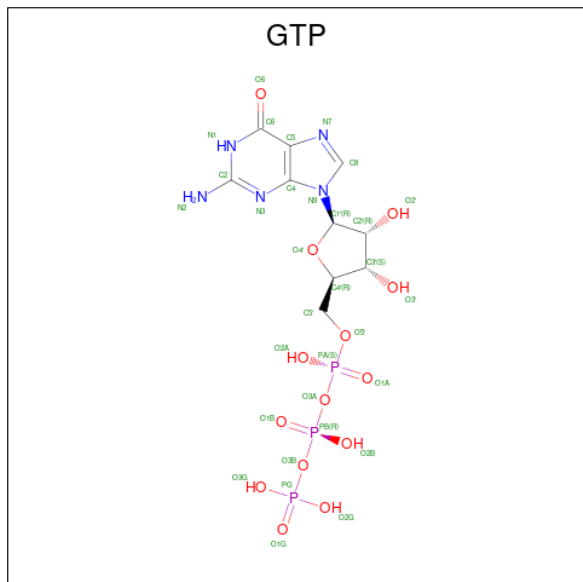
Mol	Chain	Residues	Atoms		AltConf
39	6	3	Total	K	0
			3	3	
39	E	1	Total	K	0
			1	1	

- Molecule 40 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 41 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	
41	C	1	32	10	5	14	3	0

- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

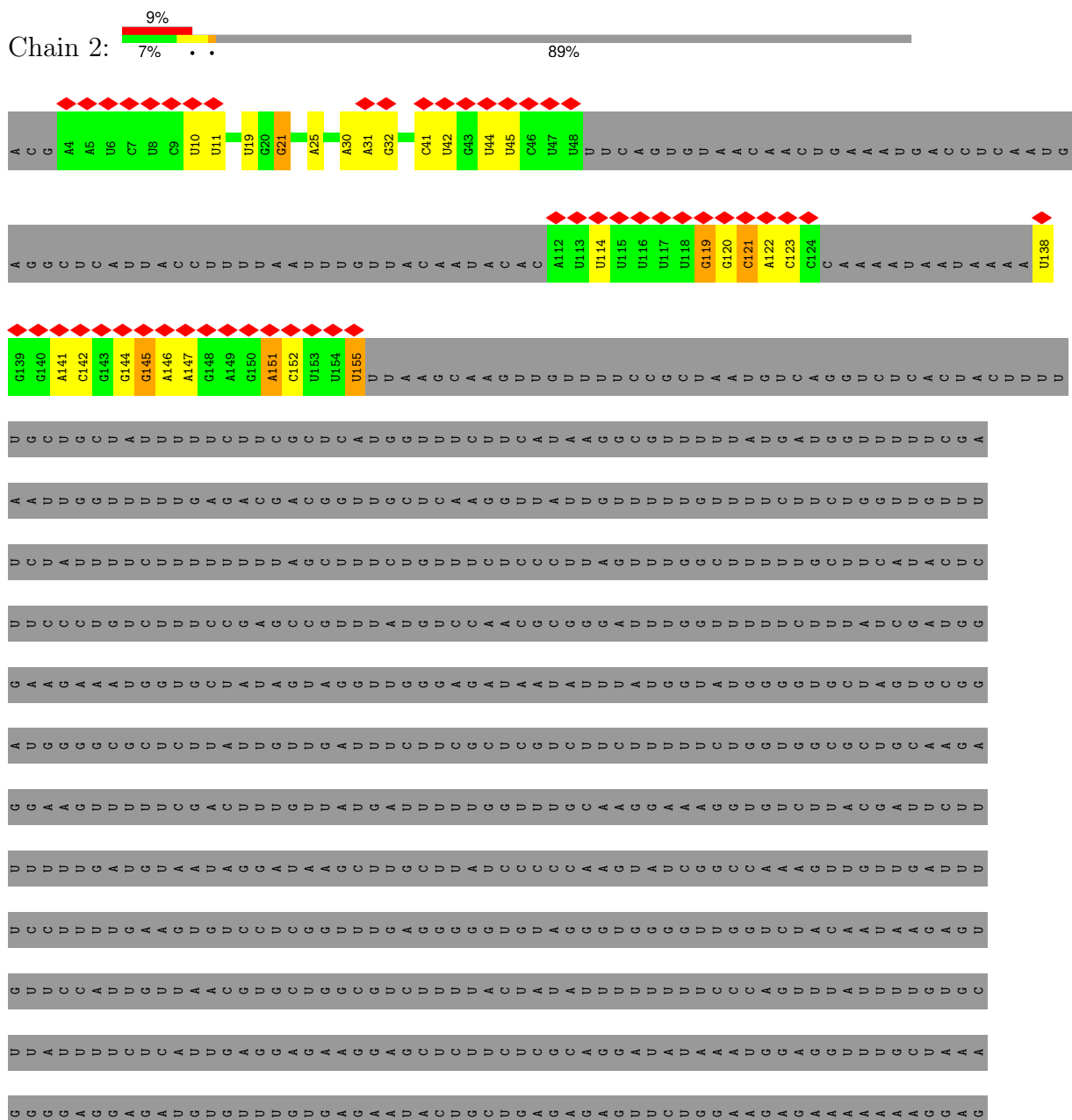
- Molecule 43 is water.

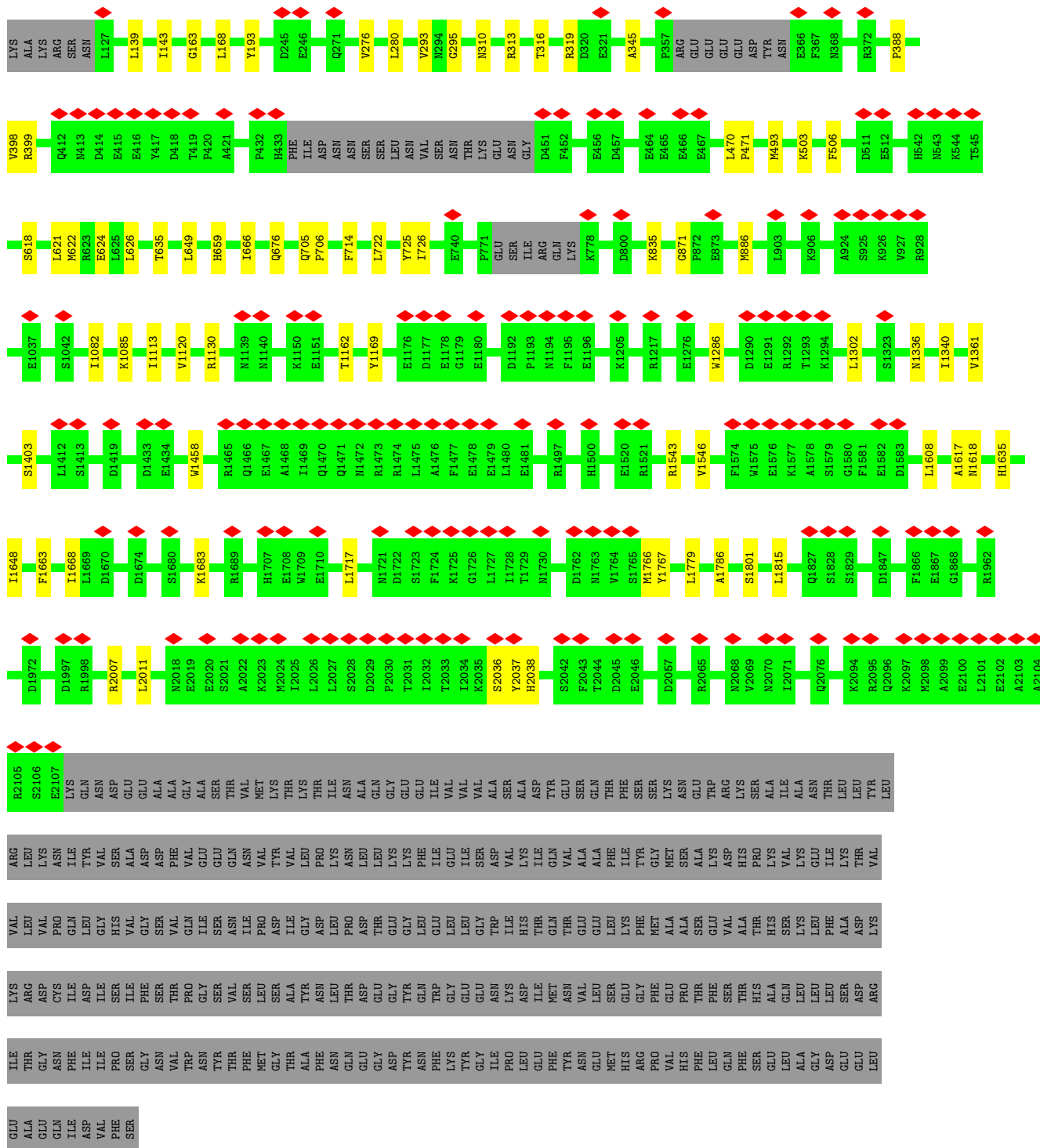
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	6	1	1	1	0

3 Residue-property plots

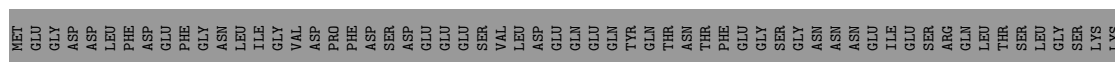
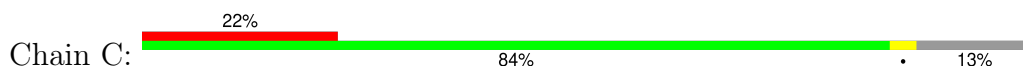
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

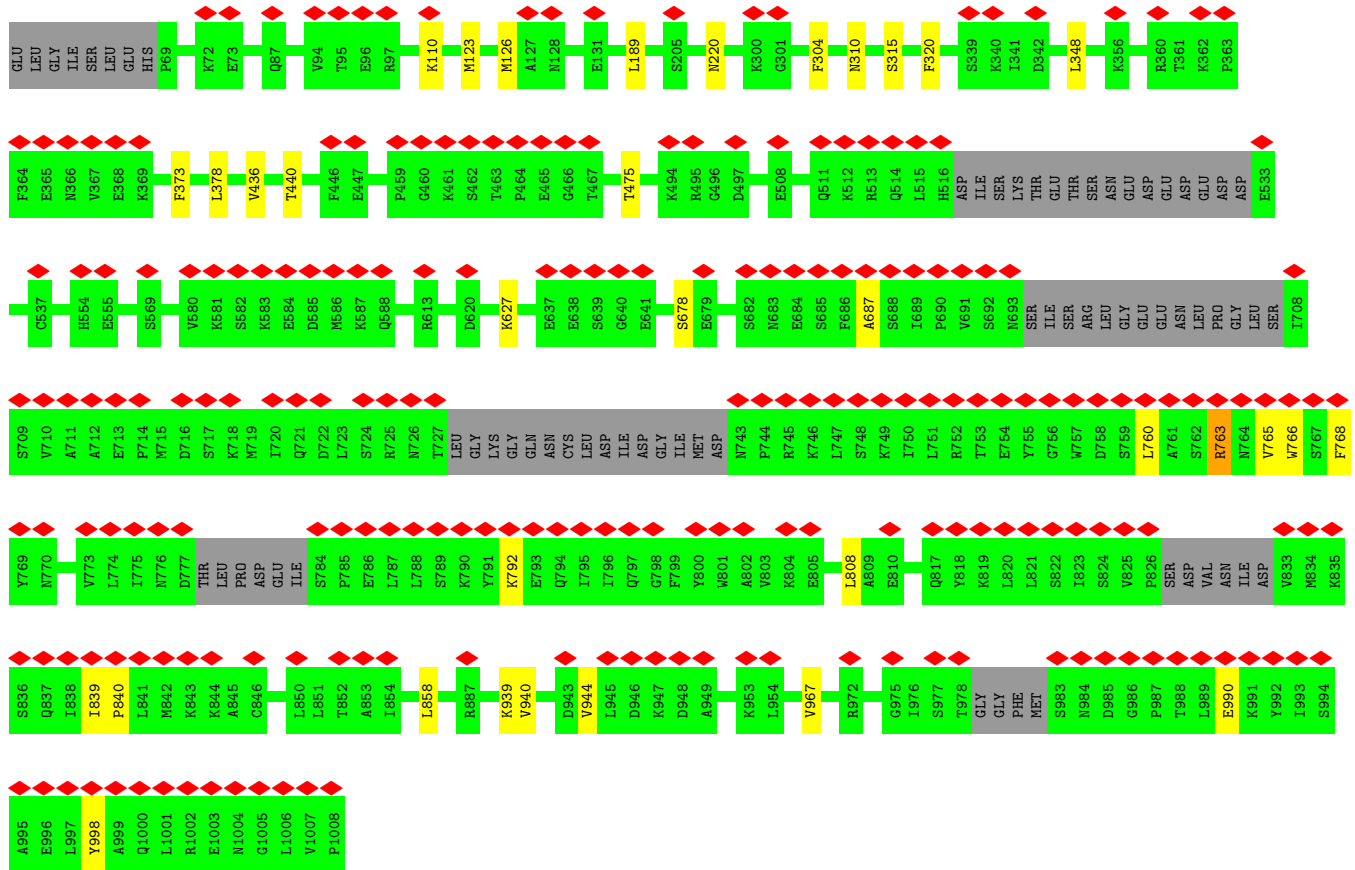
- Molecule 1: U2 snRNA



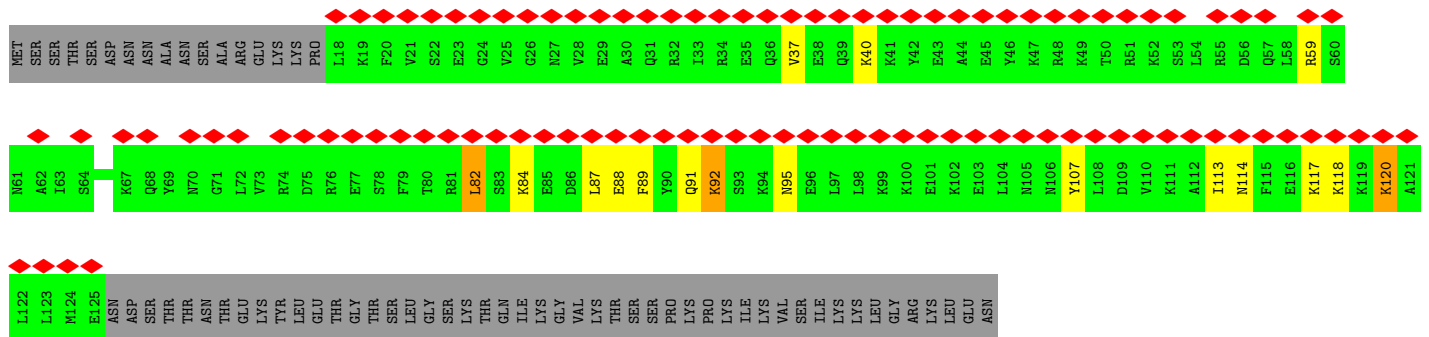


• Molecule 5: Pre-mRNA-splicing factor SNU114

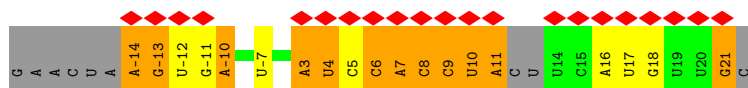
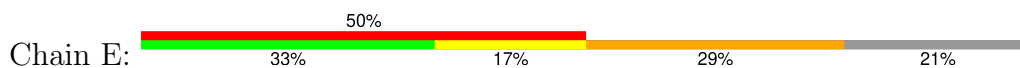




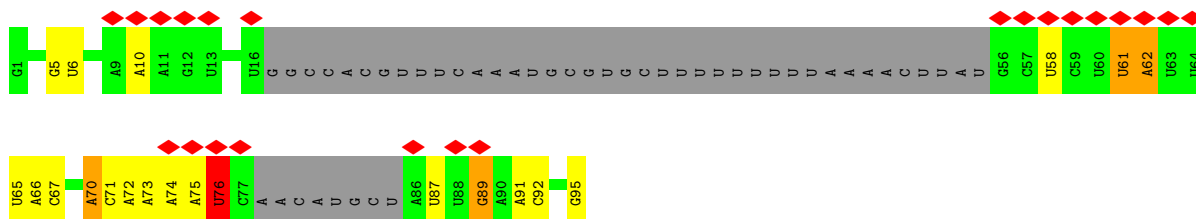
• Molecule 6: Protein FYV6



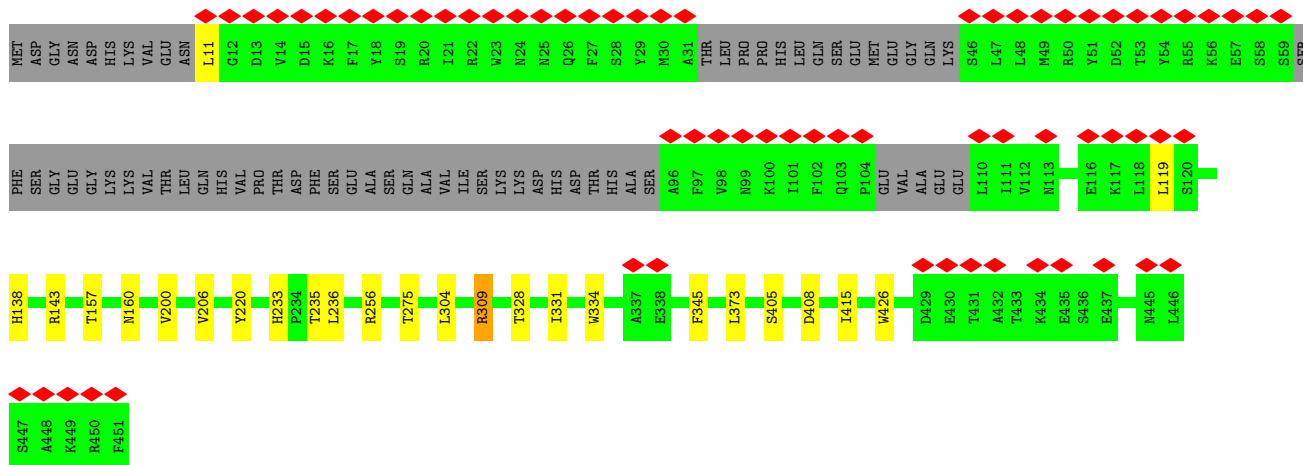
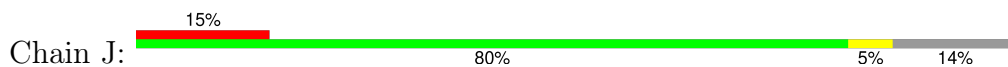
• Molecule 7: UBC4 mRNA spliced exons



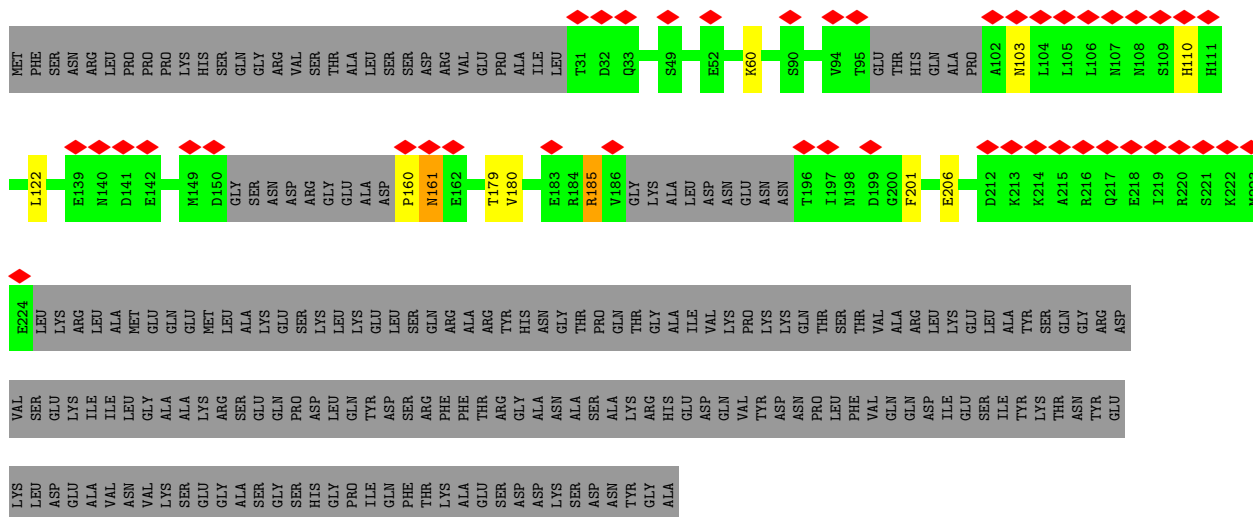
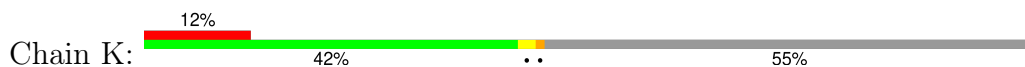
• Molecule 8: Pre-mRNA-splicing factor ISY1



• Molecule 11: Pre-mRNA-splicing factor PRP46

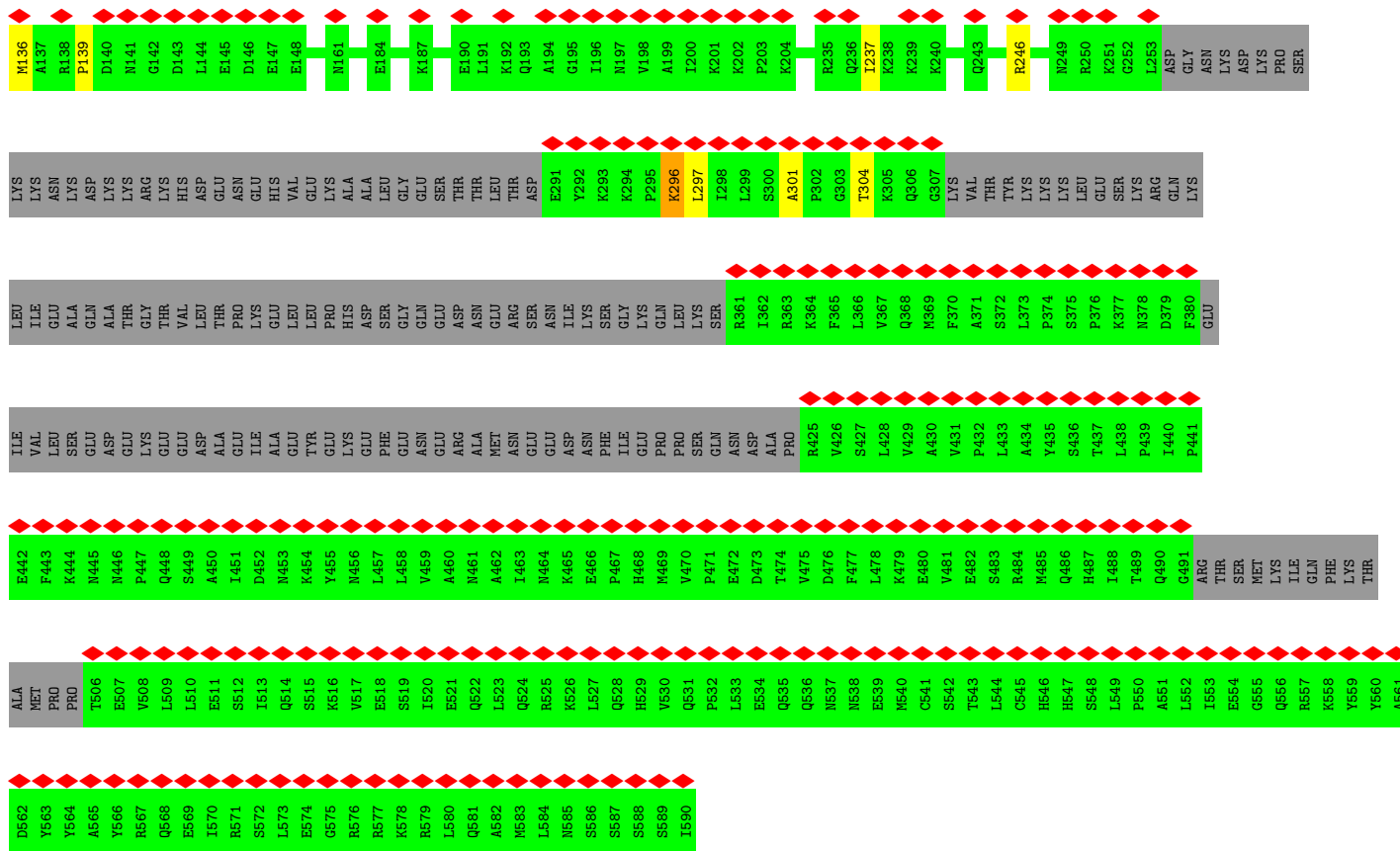


• Molecule 12: Pre-mRNA-processing protein 45

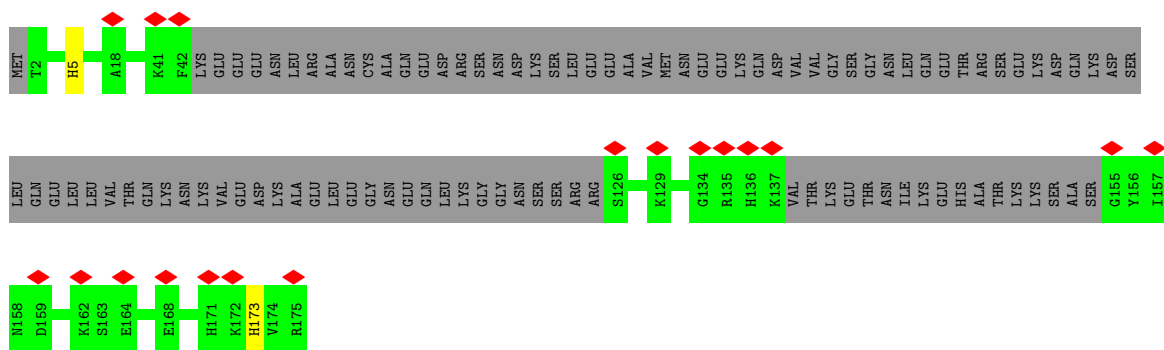


• Molecule 13: Pre-mRNA-splicing factor BUD31



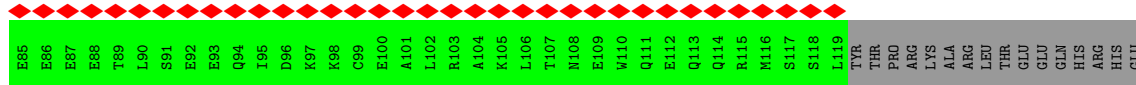


• Molecule 17: Pre-mRNA-splicing factor CWC15

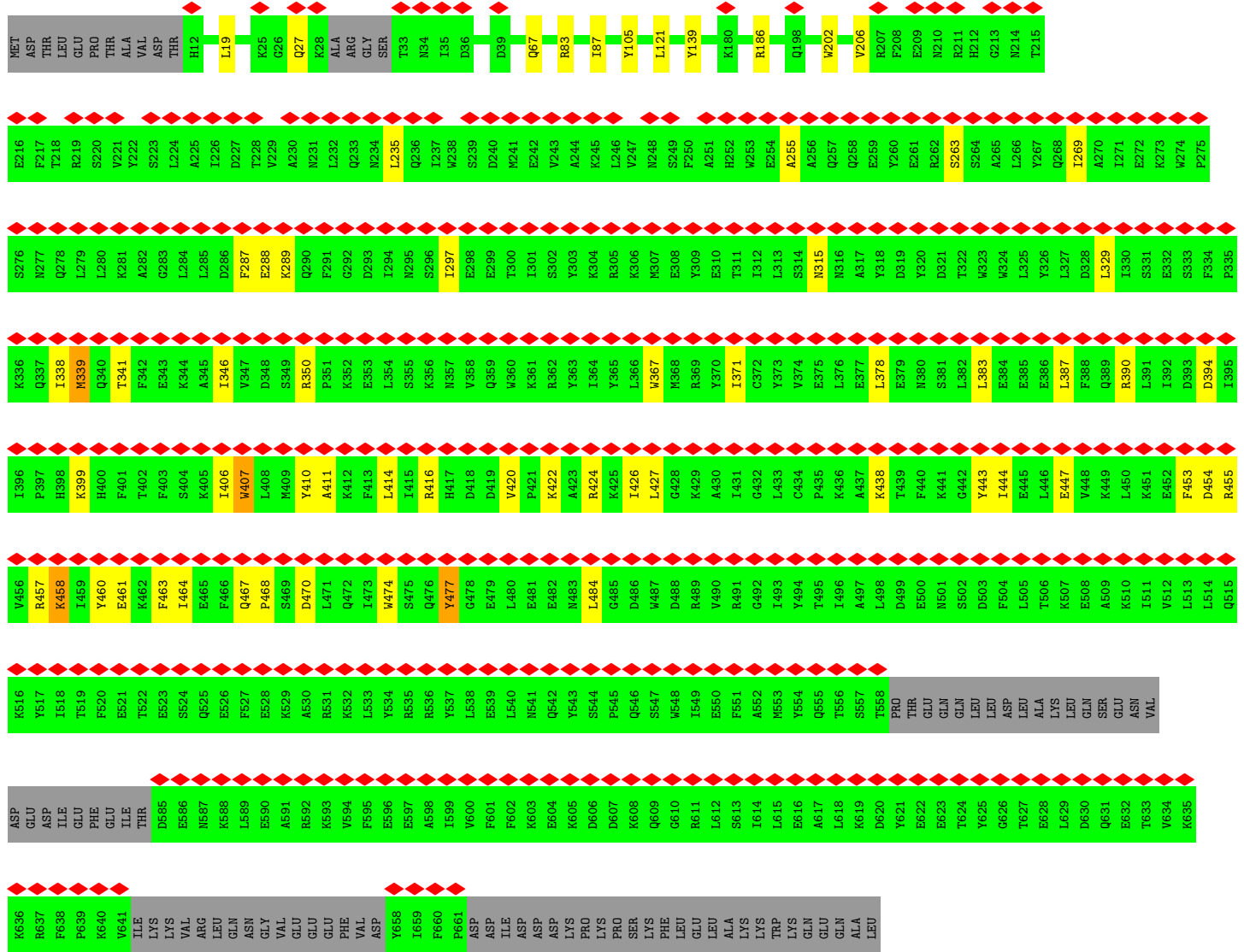
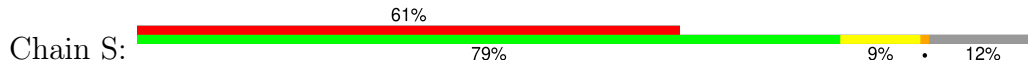


• Molecule 18: Pre-mRNA-splicing factor CWC21

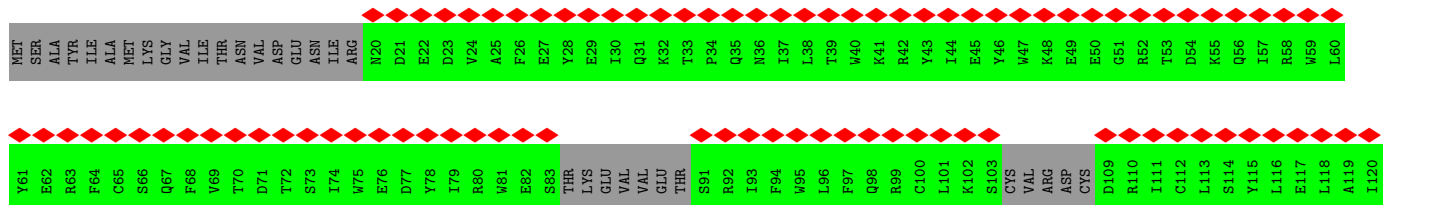
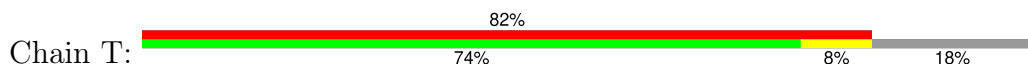




• Molecule 19: Pre-mRNA-splicing factor CLF1



• Molecule 20: Pre-mRNA-splicing factor SYF1

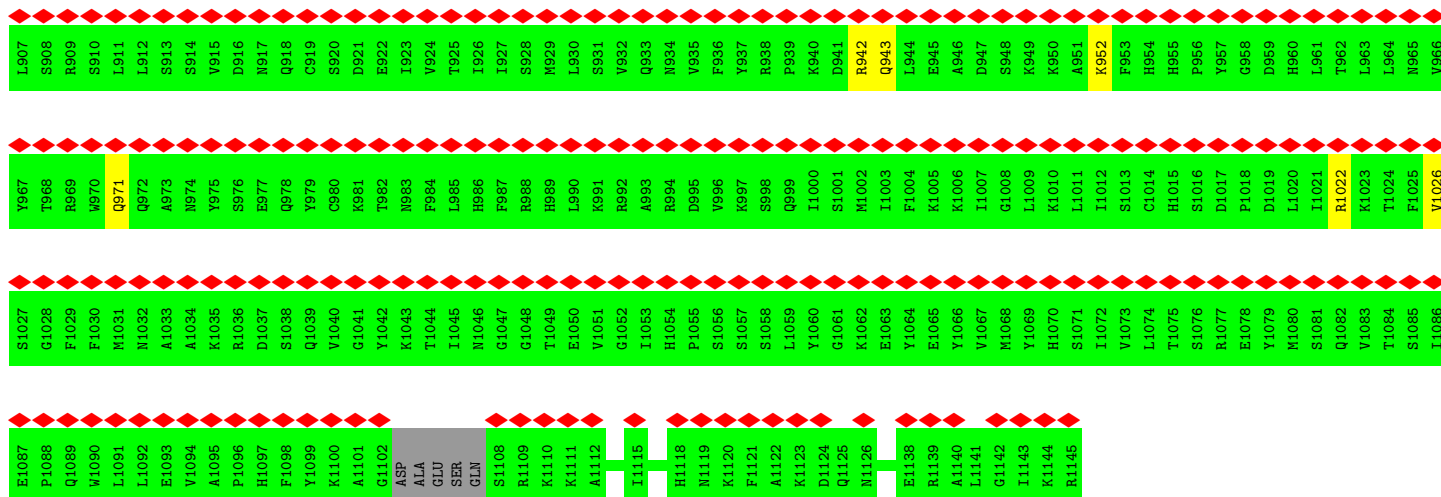


E121	Q122	Y123	D124	L125	A126	M127	I128	R129	H130	A131	L132	A133	S134	S135	L136	M137	K138	M139	GLU	ARG	GLY	ASN	ARG	HIS	R145	K146	V147	W148	D149	P150	V151	I152	K153	F154	V155	E156	E157	K158	V159	L160	P161	L162	T163	Q164	LEU	ASP	SER	THR	GLN	GLU	ASP	GLU	GLU	L234	A235	L236	T237	R238	D239	N240
L181	I182	N183	V184	L185	L186	V187	K188	G189	F190	T191	LYS	GLY	GLY	PHE	ILE	SER	GLU	GLU	SER	GLY	ASN	ARG	GLY	ASP	I209	W210	S211	S212	H213	L214	L215	E216	R217	Y218	L219	K220	V221	A222	P223	Q224	Q225	R226	R227	E228	E229	S230	L231	A232	T233	L234	A235	L236	T237	R238	D239	N240				
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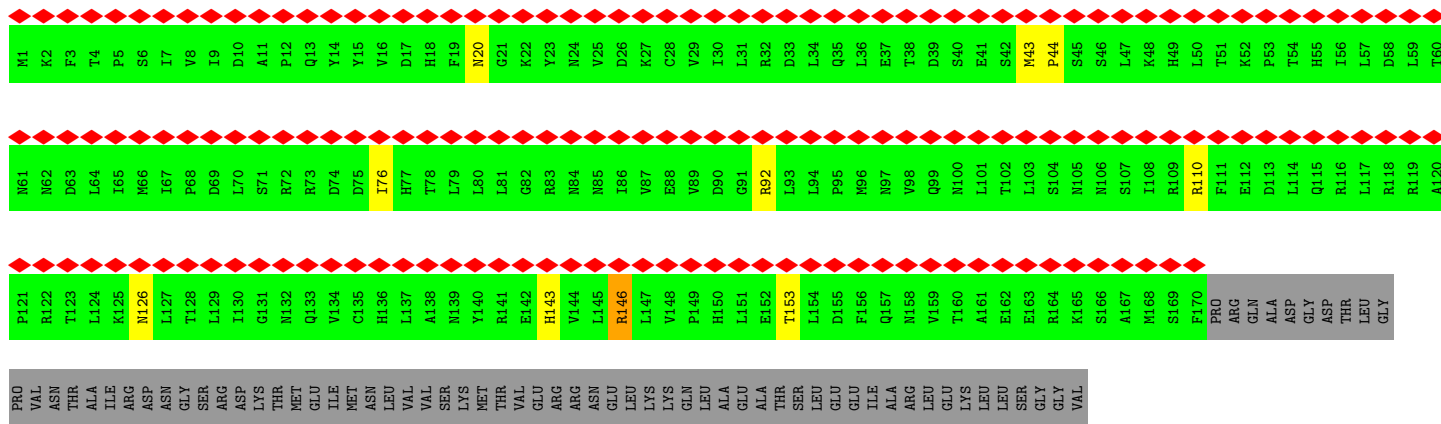
• Molecule 21: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22



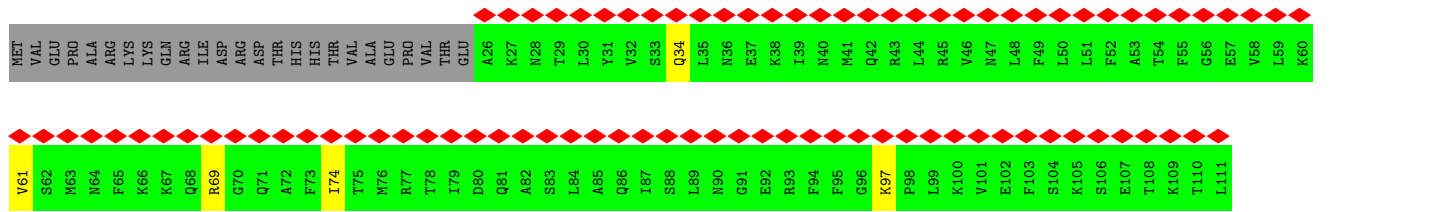
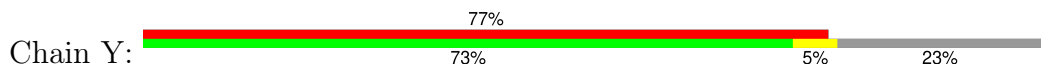
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M849	I789	P729	T669	T609	A549	R489	Q429	P369	A309	LYS	LYS	LYS	GLY	GLN	ASP
L850	E790	V730	P670	V610	E650	S490	S430	K370	I310	ILE	ILE	VAL	ASN	GLU	ILE
K851	Q791	W731	A671	A611	E551	E491	F431	F371	D311	SER	SER	ARG	ASN	GLY	LYS
A852	L792	S732	M672	T612	G652	L492	D432	L372	D312	LEU	LEU	ILE	ASN	VAL	ILE
M853	I793	A733	D673	D613	G553	I493	D433	K373	F313	MET	MET	THR	THR	ARG	GLY
G854	V794	L734	Y674	V614	C654	Q494	P434	D374	P314	LYS	LYS	PHE	PHE	ILE	ALA
I855	S795	P735	I675	L615	K555	A495	T435	Q375	E315	ILE	ILE	GLY	GLY	VAL	ILE
N856	P796	S736	E676	F616	V656	V496	K436	Q376	L316	ASP	ASP	CYS	TYR	VAL	GLY
D857	I797	E737	A677	A617	G557	R497	ASN	VAL	K317	VAL	GLN	PHE	GLN	SER	SER
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K860	A800	S740	D680	K620	V660	Q500	SER	ALA	ILE	GLY	GLY	VAL	PRO	LEU	PRO
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F863	N803	F743	T563	V503	I504	I504	ILE	MET	THR	THR	LYS	ARG	VAL	ASN	PHE
M864	Q804	E744	I664	V505	V505	V505	GLN	TYR	THR	TYR	ASN	ARG	GLN	VAL	VAL
D865	R805	P745	R565	V506	G506	G506	LEU	K387	LEU	THR	THR	THR	VAL	VAL	LEU
P866	K806	T746	F566	G507	E507	E507	LYS	I388	ALA	SER	SER	CYS	VAL	LEU	ASN
P867	G807	P747	E567	T508	T508	T508	ASN	T389	VAL	VAL	VAL	ASN	VAL	ASP	ILE
K868	R808	K748	D568	L508	L508	L508	GLN	K390	ARG	GLY	GLY	LEU	GLN	VAL	VAL
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G810	G810	S750	T570	S510	S510	S510	VAL	P392	ARG	ARG	ASN	HIS	PRO	ASN	ASN
R811	R811	K751	G571	G511	G511	G511	THR	R393	GLY	GLY	LYS	ILE	THR	GLY	GLY
T812	T812	R752	P572	K512	K512	K512	GLU	R394	SER	ARG	ARG	GLU	ILE	ASP	ASN
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L882	T822	T762	G582	E522	E522	E522	GLY	G403	LYS	LYS	LYS	ASP	VAL	ASN	ALA
Q883	E823	S763	F583	E523	E523	E523	LYS	S404	GLU	GLU	VAL	ARG	VAL	GLN	LYS
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E888	N828	G768	E588	N528	N528	N528	ILE	D409	GLU	GLU	GLU	ILE	ASP	GLU	GLU
G889	E829	I769	L589	G529	G529	G529	SER	H410	THR	THR	THR	PHE	PRO	PRO	PRO
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L894	T834	D774	E593	C533	C533	C533	T482	K414	V361	V361	V361	GLN	GLN	GLN	GLN
G895	V835	V775	M594	T534	T534	T534	L483	L415	E382	E382	E382	GLY	GLY	GLY	GLY
K896	P836	G776	S595	Q535	Q535	Q535	P484	R416	E382	E382	E382	THR	THR	THR	THR
E897	E837	F777	K596	K596	K596	K596	V485	K417	T365	T365	T365	HIS	HIS	HIS	HIS
M898	I838	A778	Y597	R537	R537	R537	Y486	R419	D366	D366	D366	ASP	ASP	ASP	ASP
S899	Q839	K779	G598	R538	R538	R538	E486	R419	E420	E420	E420	LEU	LEU	LEU	LEU
L900	R840	I780	V599	V539	V539	V539	R480	I421	I421	I421	I421	GLN	GLN	GLN	GLN
F901	Q841	N781	I600	A540	A540	A540	E412	E422	E422	E422	E422	ILE	ILE	ILE	ILE
P902	N842	I782	M601	A541	A541	A541	Q423	Q423	Q423	Q423	Q423	LYS	LYS	LYS	LYS
M903	L843	G723	D603	V542	V542	V542	I425	I425	I425	I425	I425	ILE	ILE	ILE	ILE
G904	S844	E724	E604	V544	V544	V544	R426	R426	R426	R426	R426	GLN	GLN	GLN	GLN
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T906	T846	R786	H606	K546	K546	K546									



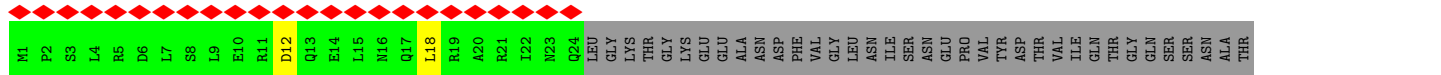
• Molecule 22: U2 small nuclear ribonucleoprotein A''

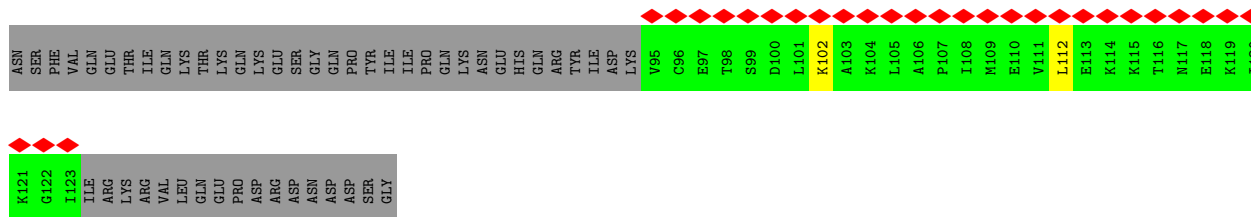


• Molecule 23: U2 small nuclear ribonucleoprotein B''

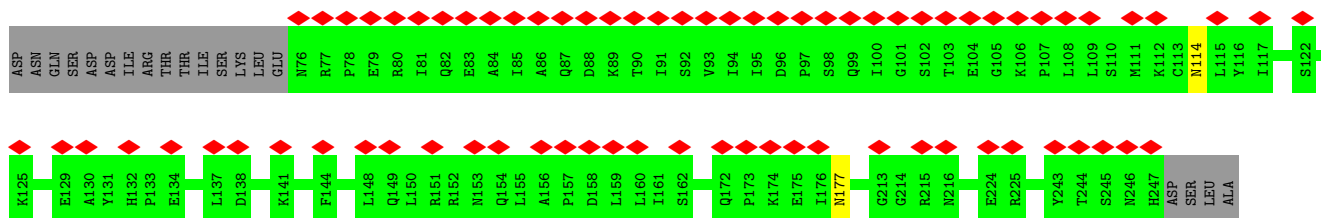
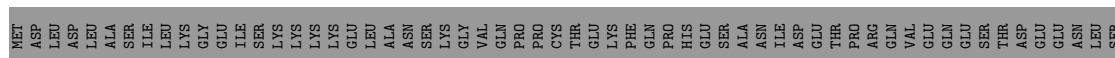


• Molecule 24: Pre-mRNA-splicing factor NTC20

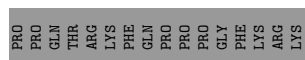
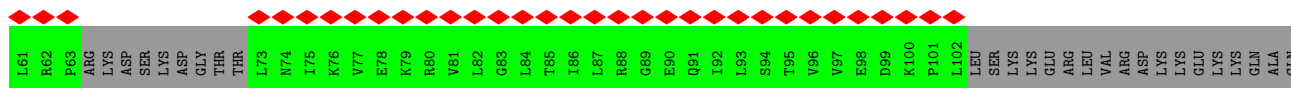
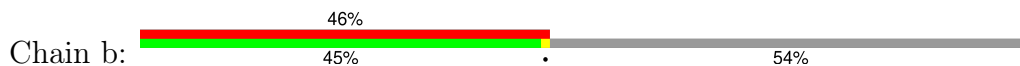




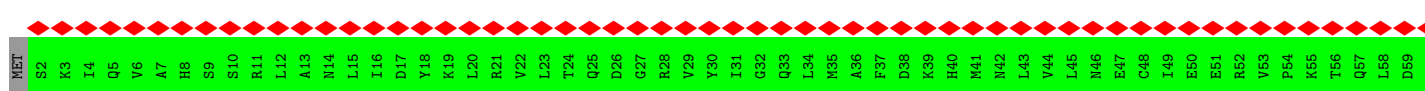
• Molecule 25: Pre-mRNA-splicing factor 18



• Molecule 26: Small nuclear ribonucleoprotein-associated protein B

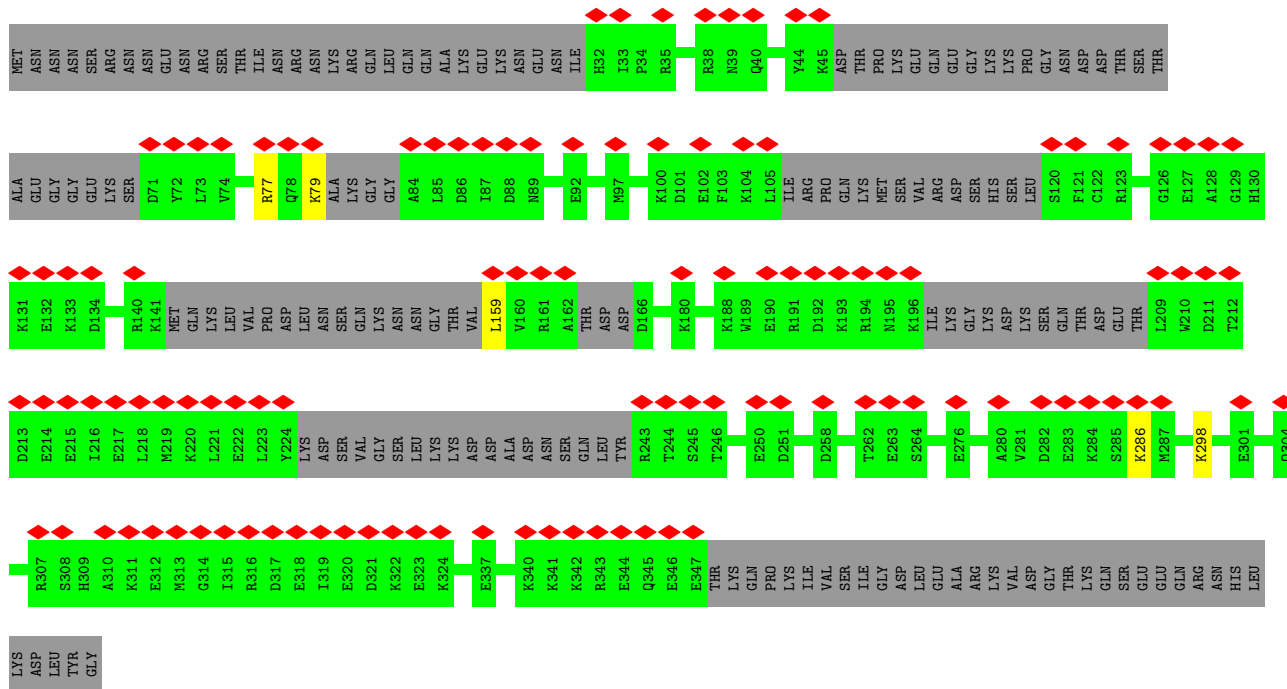


• Molecule 26: Small nuclear ribonucleoprotein-associated protein B

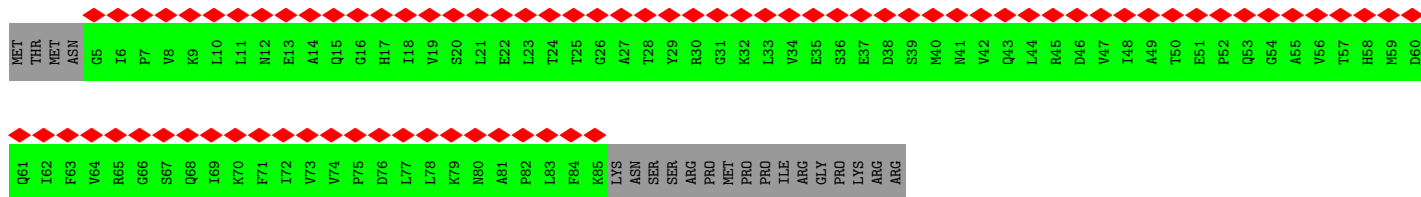
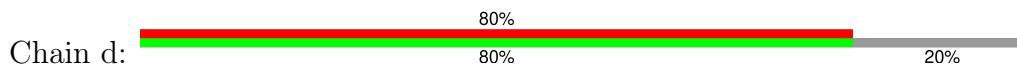


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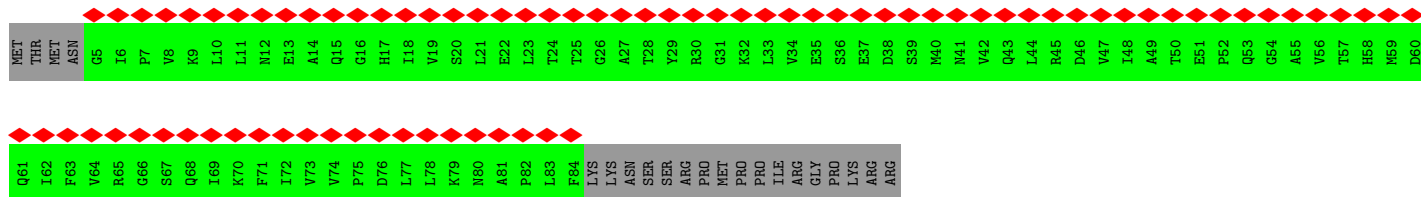
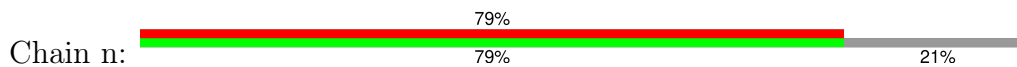
• Molecule 27: Pre-mRNA-splicing factor SLU7



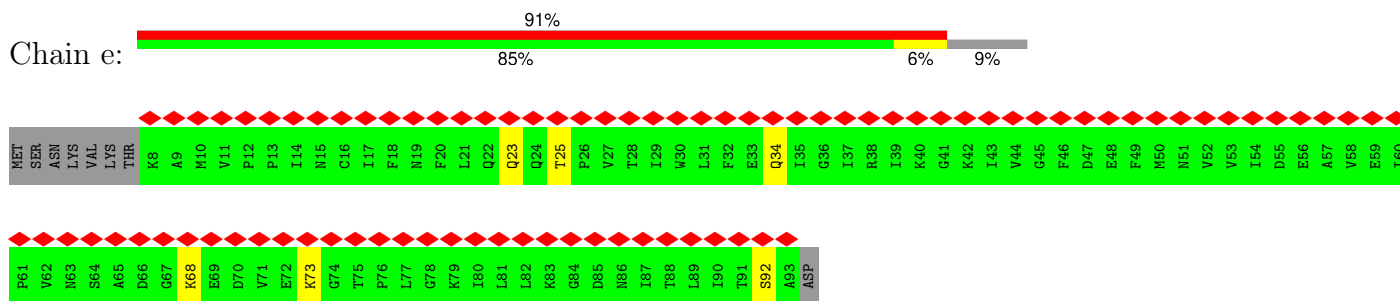
• Molecule 28: Small nuclear ribonucleoprotein Sm D3



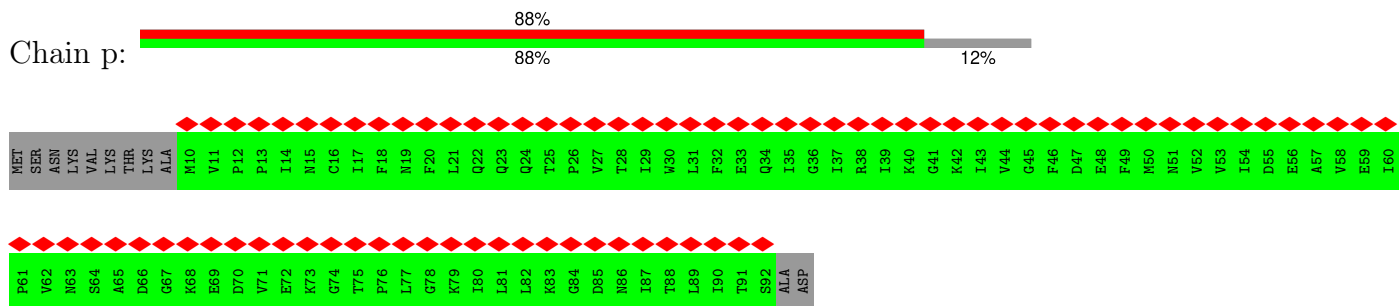
• Molecule 28: Small nuclear ribonucleoprotein Sm D3



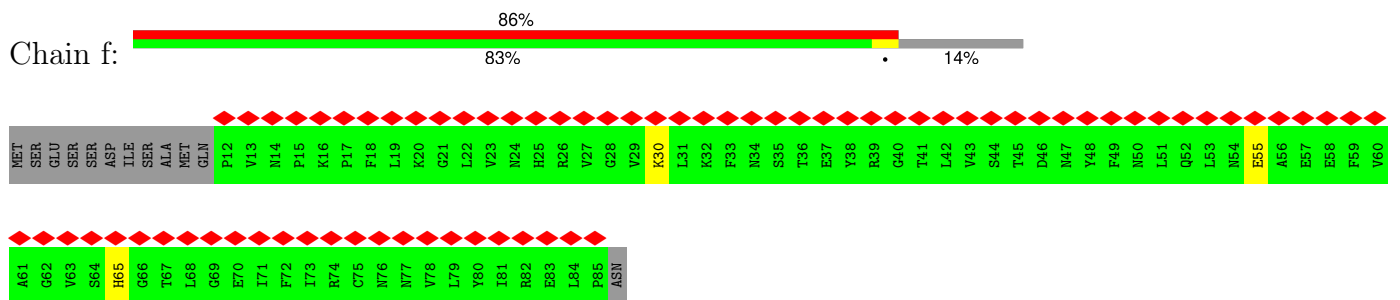
• Molecule 29: Small nuclear ribonucleoprotein E



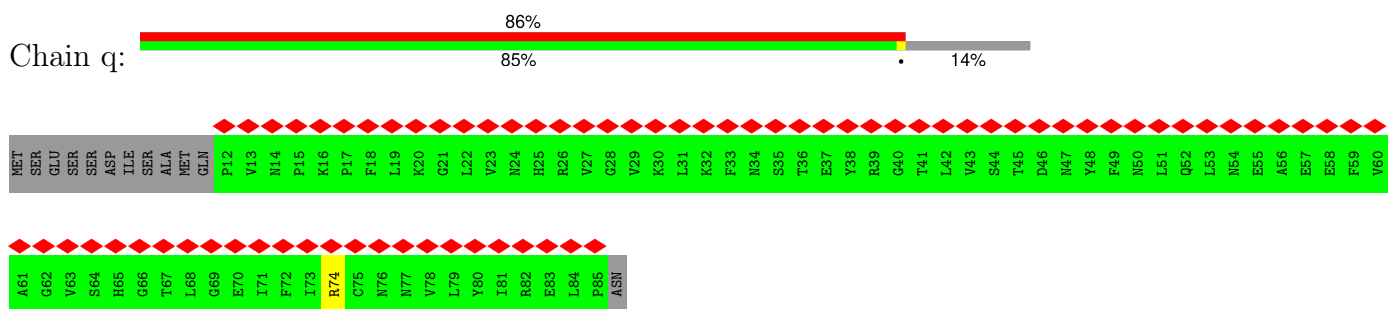
• Molecule 29: Small nuclear ribonucleoprotein E



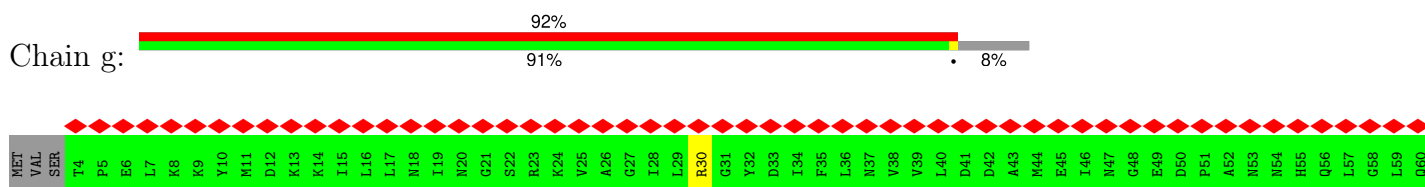
• Molecule 30: Small nuclear ribonucleoprotein F

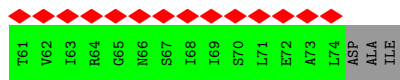


• Molecule 30: Small nuclear ribonucleoprotein F

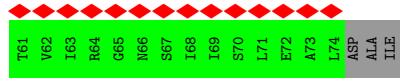
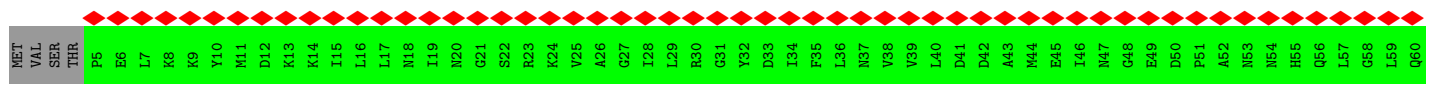
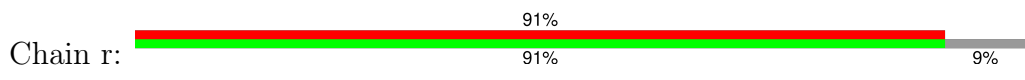


• Molecule 31: Small nuclear ribonucleoprotein G

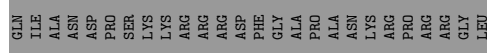
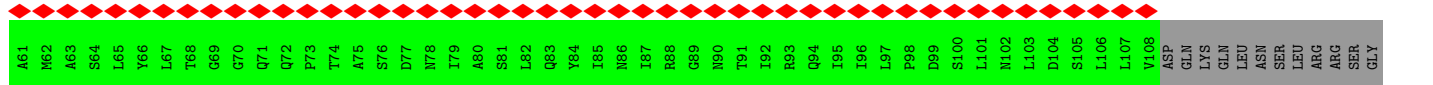
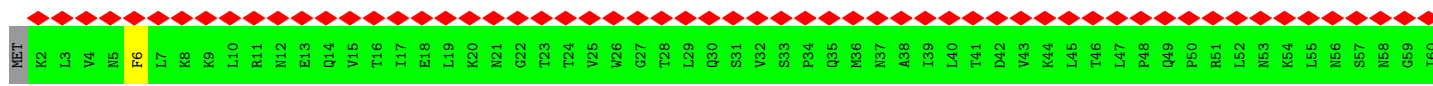




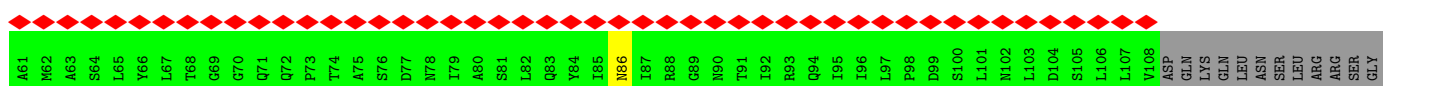
• Molecule 31: Small nuclear ribonucleoprotein G



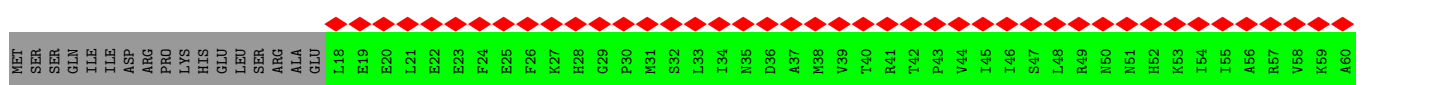
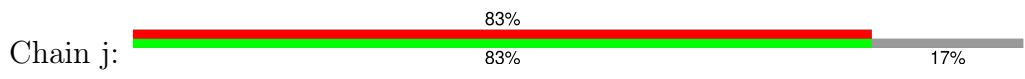
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

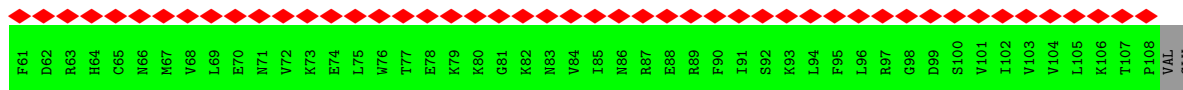


• Molecule 32: Small nuclear ribonucleoprotein Sm D1

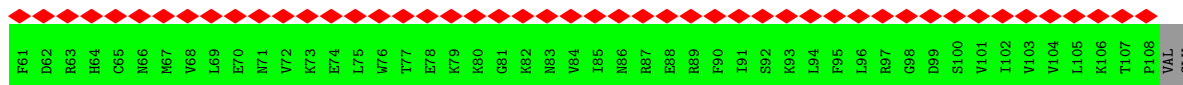
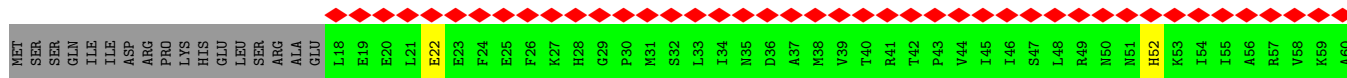
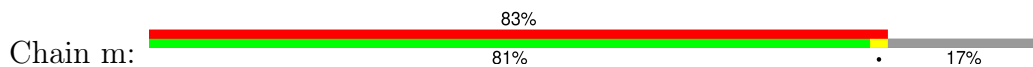


• Molecule 33: Small nuclear ribonucleoprotein Sm D2

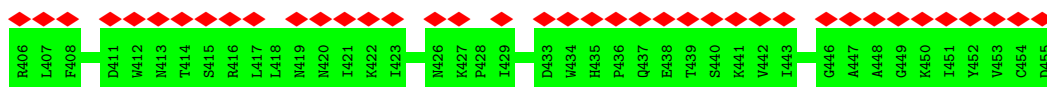
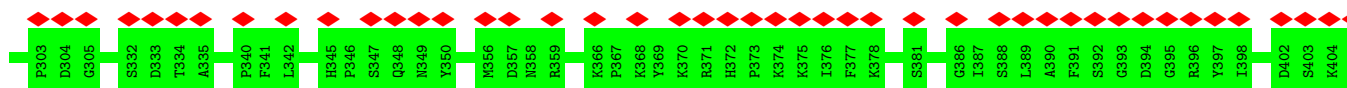
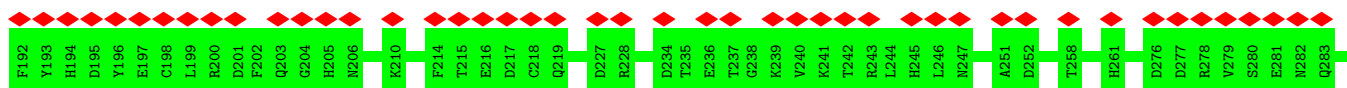
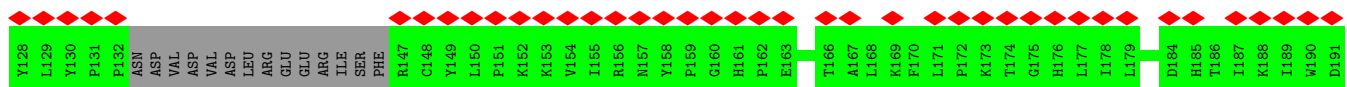
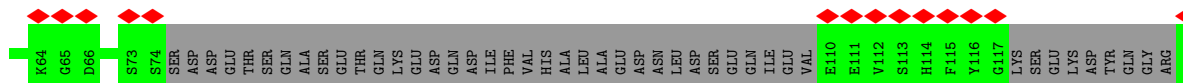
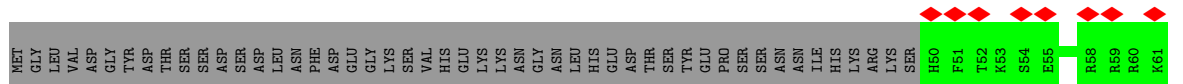
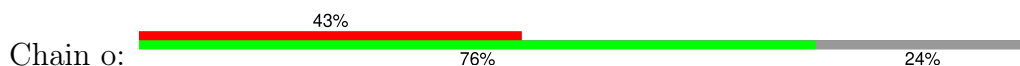




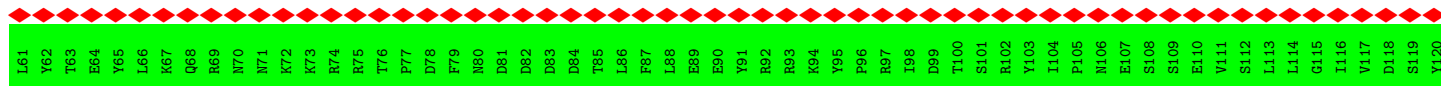
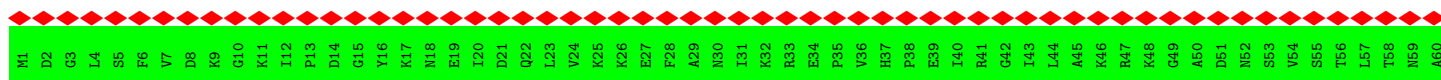
• Molecule 33: Small nuclear ribonucleoprotein Sm D2

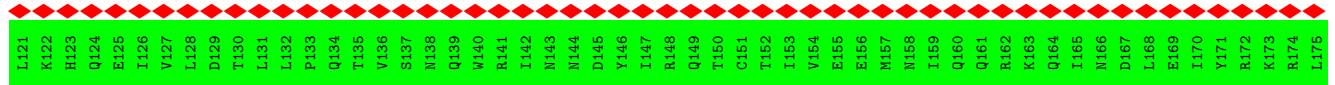


• Molecule 34: Pre-mRNA-processing factor 17

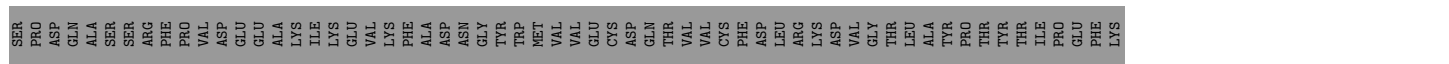
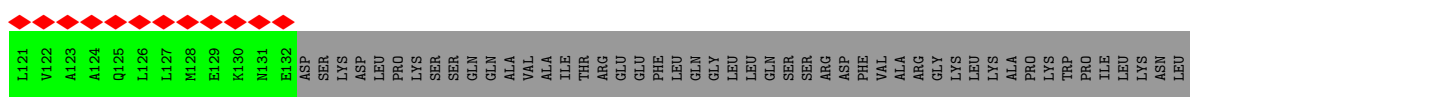


• Molecule 35: Pre-mRNA-splicing factor SNT309

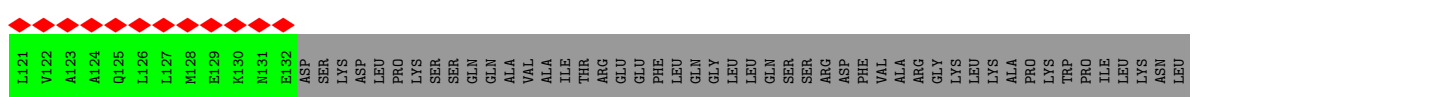


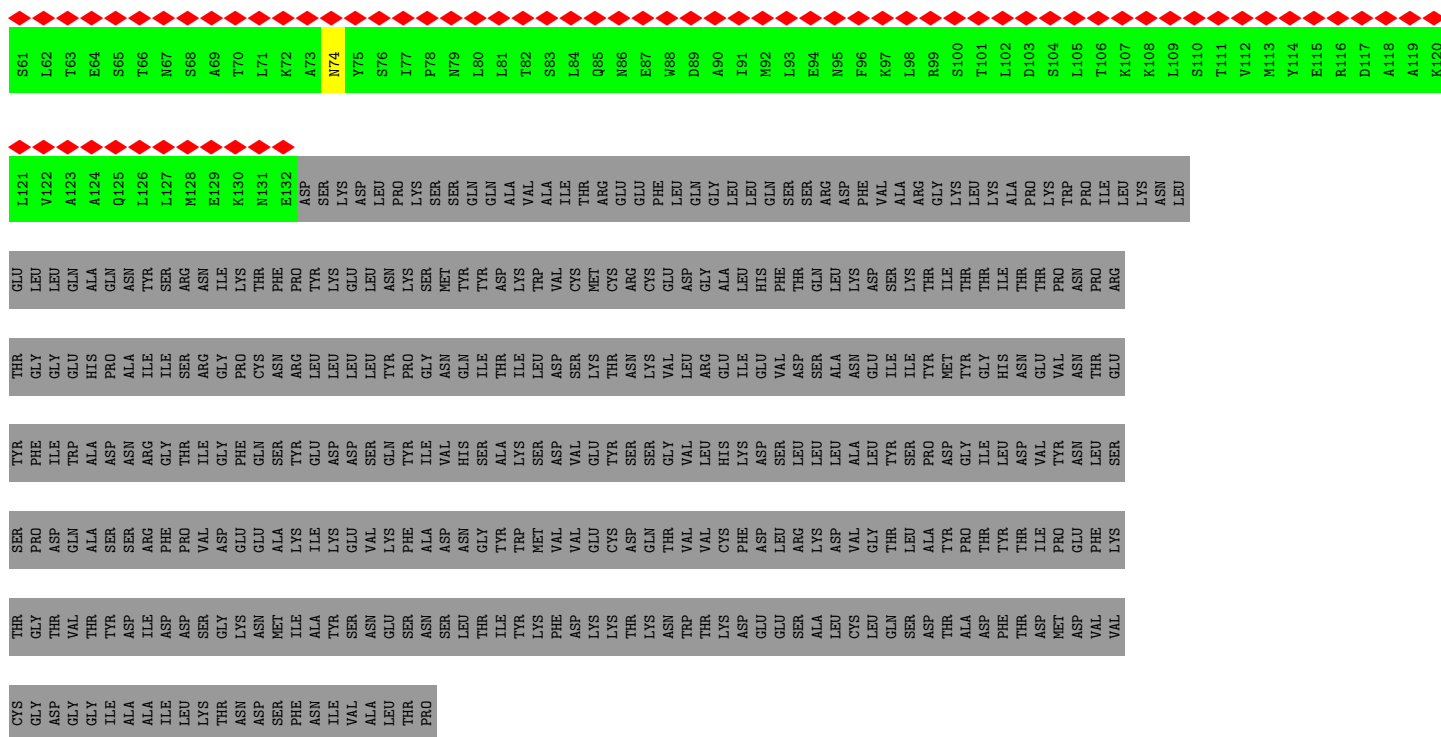


• Molecule 36: Pre-mRNA-processing factor 19

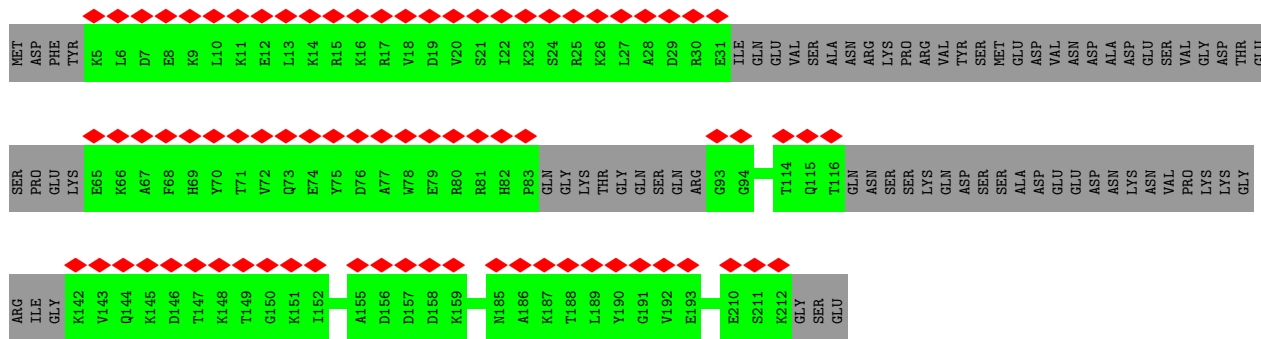


• Molecule 36: Pre-mRNA-processing factor 19





• Molecule 37: Pre-mRNA-splicing factor SYF2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	209005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.054	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	464.63998, 464.63998, 464.63998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.968, 0.968, 0.968	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.59	0/3090	1.14	10/4792 (0.2%)
2	5	0.73	0/4098	1.05	6/6373 (0.1%)
3	6	0.82	0/2405	0.98	0/3744
4	A	0.38	0/16489	0.59	0/22348
5	C	0.47	0/7189	0.62	0/9728
6	D	0.35	0/922	0.63	0/1220
7	E	0.68	0/785	1.39	17/1218 (1.4%)
8	G	0.24	0/137	0.52	0/188
9	H	0.46	0/3824	0.58	0/5154
10	I	0.66	0/1128	1.13	7/1747 (0.4%)
11	J	0.37	0/3052	0.64	0/4143
12	K	0.34	0/1375	0.60	0/1854
13	L	0.37	0/1307	0.60	0/1748
14	M	0.34	0/2094	0.61	0/2815
15	N	0.30	0/2124	0.57	0/2860
16	O	0.33	0/2945	0.54	0/3992
17	P	0.35	0/623	0.66	0/832
18	R	0.31	0/510	0.50	0/698
19	S	0.36	0/4780	0.54	0/6483
20	T	0.36	0/5658	0.52	0/7669
21	V	0.43	0/6210	0.61	0/8377
22	W	0.31	0/1406	0.62	0/1905
23	Y	0.31	0/706	0.62	0/941
24	Z	0.31	0/424	0.58	0/564
25	a	0.31	0/1409	0.57	0/1911
26	b	0.36	0/731	0.63	0/983
26	k	0.33	0/849	0.63	0/1138
27	c	0.37	0/1925	0.63	0/2565
28	d	0.40	0/633	0.61	0/857
28	n	0.33	0/624	0.57	0/846
29	e	0.36	0/676	0.59	0/916
29	p	0.32	0/657	0.60	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	f	0.37	0/605	0.60	0/819
30	q	0.35	0/605	0.60	0/819
31	g	0.35	0/556	0.60	0/749
31	r	0.32	0/549	0.62	0/738
32	h	0.33	0/835	0.59	0/1135
32	l	0.31	0/835	0.59	0/1135
33	j	0.36	0/759	0.62	0/1019
33	m	0.31	0/759	0.60	0/1019
34	o	0.31	0/2903	0.62	0/3921
35	s	0.25	0/869	0.40	0/1210
36	t	0.25	0/657	0.43	0/917
36	u	0.25	0/657	0.41	0/917
36	v	0.25	0/657	0.40	0/917
36	w	0.25	0/657	0.40	0/917
37	y	0.33	0/1085	0.52	0/1453
All	All	0.43	0/93773	0.68	40/129185 (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
11	J	0	1
12	K	0	1
19	S	0	1
21	V	0	1
22	W	0	1
27	c	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1082	A	N1-C2-N3	9.71	134.15	129.30
7	E	6	C	OP1-P-OP2	-9.25	105.73	119.60
1	2	1082	A	C2-N3-C4	-8.11	106.54	110.60
7	E	3	A	OP1-P-O3'	8.05	122.92	105.20
1	2	155	U	N1-C2-O2	-7.95	117.23	122.80

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	309	ARG	Sidechain
12	K	185	ARG	Sidechain
19	S	186	ARG	Sidechain
21	V	840	ARG	Sidechain
22	W	92	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	2779	0	1411	24	0
2	5	3671	0	1856	6	0
3	6	2170	0	1095	14	0
4	A	16079	0	16079	43	0
5	C	7040	0	7241	21	0
6	D	914	0	953	19	0
7	E	703	0	356	2	0
8	G	139	0	67	0	0
9	H	3762	0	3825	38	0
10	I	1012	0	510	5	0
11	J	2990	0	2906	12	0
12	K	1355	0	1383	7	0
13	L	1283	0	1301	0	0
14	M	2048	0	2011	9	0
15	N	2092	0	2162	9	0
16	O	2918	0	2467	15	0
17	P	607	0	596	2	0
18	R	510	0	327	6	0
19	S	4683	0	4267	39	0
20	T	5543	0	5182	41	0
21	V	6096	0	6158	10	0
22	W	1383	0	1407	2	0
23	Y	697	0	733	2	0
24	Z	424	0	455	2	0
25	a	1380	0	1425	0	0
26	b	725	0	778	0	0
26	k	843	0	917	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	c	1893	0	1849	0	0
28	d	624	0	647	0	0
28	n	615	0	634	0	0
29	e	665	0	690	0	0
29	p	646	0	667	0	0
30	f	592	0	594	0	0
30	q	592	0	594	0	0
31	g	551	0	572	0	0
31	r	544	0	566	0	0
32	h	826	0	874	0	0
32	l	826	0	874	0	0
33	j	747	0	784	0	0
33	m	747	0	784	0	0
34	o	2821	0	2743	0	0
35	s	870	0	363	0	0
36	t	658	0	291	0	0
36	u	658	0	291	0	0
36	v	658	0	291	0	0
36	w	658	0	291	0	0
37	y	1075	0	1004	0	0
38	6	1	0	0	0	0
38	C	1	0	0	0	0
39	6	3	0	0	0	0
39	E	1	0	0	0	0
40	A	36	0	6	1	0
40	S	36	0	6	1	0
41	C	32	0	12	0	0
42	L	3	0	0	0	0
42	M	1	0	0	0	0
42	N	2	0	0	0	0
42	c	1	0	0	0	0
43	6	1	0	0	0	0
All	All	91230	0	83295	296	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 2.

The worst 5 of 296 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)
6:D:84:LYS:HA	6:D:87:LEU:HD12	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:161:ARG:HH21	15:N:299:ALA:HB2	1.40	0.86
1:2:1141:C:H2'	1:2:1142:G:C8	2.20	0.76
11:J:143:ARG:HH11	11:J:160:ASN:HD21	1.35	0.74
5:C:763:ARG:HH22	18:R:82:ASP:CB	2.01	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1942/2413 (80%)	1888 (97%)	54 (3%)	0	100	100
5	C	865/1008 (86%)	833 (96%)	32 (4%)	0	100	100
6	D	106/173 (61%)	106 (100%)	0	0	100	100
8	G	24/235 (10%)	24 (100%)	0	0	100	100
9	H	456/577 (79%)	449 (98%)	7 (2%)	0	100	100
11	J	378/451 (84%)	360 (95%)	18 (5%)	0	100	100
12	K	162/379 (43%)	157 (97%)	5 (3%)	0	100	100
13	L	154/157 (98%)	152 (99%)	2 (1%)	0	100	100
14	M	253/339 (75%)	248 (98%)	5 (2%)	0	100	100
15	N	256/364 (70%)	247 (96%)	9 (4%)	0	100	100
16	O	412/590 (70%)	407 (99%)	5 (1%)	0	100	100
17	P	68/175 (39%)	67 (98%)	1 (2%)	0	100	100
18	R	87/135 (64%)	82 (94%)	3 (3%)	2 (2%)	5	4
19	S	596/687 (87%)	586 (98%)	10 (2%)	0	100	100
20	T	689/859 (80%)	671 (97%)	18 (3%)	0	100	100
21	V	754/1145 (66%)	722 (96%)	31 (4%)	1 (0%)	48	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	168/238 (71%)	152 (90%)	15 (9%)	1 (1%)	22	26
23	Y	84/111 (76%)	81 (96%)	3 (4%)	0	100	100
24	Z	49/140 (35%)	48 (98%)	1 (2%)	0	100	100
25	a	170/251 (68%)	165 (97%)	5 (3%)	0	100	100
26	b	86/196 (44%)	85 (99%)	1 (1%)	0	100	100
26	k	100/196 (51%)	97 (97%)	3 (3%)	0	100	100
27	c	207/382 (54%)	196 (95%)	11 (5%)	0	100	100
28	d	79/101 (78%)	78 (99%)	1 (1%)	0	100	100
28	n	78/101 (77%)	77 (99%)	1 (1%)	0	100	100
29	e	84/94 (89%)	81 (96%)	3 (4%)	0	100	100
29	p	81/94 (86%)	80 (99%)	1 (1%)	0	100	100
30	f	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
30	q	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
31	g	69/77 (90%)	65 (94%)	4 (6%)	0	100	100
31	r	68/77 (88%)	66 (97%)	2 (3%)	0	100	100
32	h	105/146 (72%)	104 (99%)	1 (1%)	0	100	100
32	l	105/146 (72%)	102 (97%)	3 (3%)	0	100	100
33	j	89/110 (81%)	88 (99%)	1 (1%)	0	100	100
33	m	89/110 (81%)	88 (99%)	1 (1%)	0	100	100
34	o	340/455 (75%)	323 (95%)	17 (5%)	0	100	100
35	s	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
36	t	130/503 (26%)	127 (98%)	2 (2%)	1 (1%)	16	20
36	u	130/503 (26%)	129 (99%)	1 (1%)	0	100	100
36	v	130/503 (26%)	129 (99%)	1 (1%)	0	100	100
36	w	130/503 (26%)	124 (95%)	5 (4%)	1 (1%)	16	20
37	y	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
All	All	10223/15286 (67%)	9922 (97%)	295 (3%)	6 (0%)	50	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	R	59	ALA
21	V	943	GLN

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Mol	Chain	Res	Type
18	R	57	PRO
36	t	74	ASN
36	w	74	ASN

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	A	1770/2182 (81%)	1765 (100%)	5 (0%)	91	95
5	C	795/910 (87%)	792 (100%)	3 (0%)	89	94
6	D	100/159 (63%)	97 (97%)	3 (3%)	36	51
9	H	429/538 (80%)	421 (98%)	8 (2%)	52	68
11	J	318/397 (80%)	315 (99%)	3 (1%)	75	86
12	K	152/328 (46%)	147 (97%)	5 (3%)	33	47
13	L	140/141 (99%)	140 (100%)	0	100	100
14	M	219/296 (74%)	218 (100%)	1 (0%)	86	93
15	N	243/332 (73%)	241 (99%)	2 (1%)	79	88
16	O	219/525 (42%)	214 (98%)	5 (2%)	45	62
17	P	61/151 (40%)	61 (100%)	0	100	100
18	R	21/121 (17%)	21 (100%)	0	100	100
19	S	433/633 (68%)	422 (98%)	11 (2%)	42	59
20	T	551/786 (70%)	541 (98%)	10 (2%)	54	70
21	V	675/1028 (66%)	666 (99%)	9 (1%)	65	78
22	W	161/219 (74%)	156 (97%)	5 (3%)	35	50
23	Y	77/100 (77%)	76 (99%)	1 (1%)	65	78
24	Z	49/128 (38%)	47 (96%)	2 (4%)	26	38
25	a	152/225 (68%)	150 (99%)	2 (1%)	65	78
26	b	83/176 (47%)	81 (98%)	2 (2%)	44	60
26	k	97/176 (55%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	c	204/346 (59%)	200 (98%)	4 (2%)	50	67
28	d	70/89 (79%)	70 (100%)	0	100	100
28	n	69/89 (78%)	69 (100%)	0	100	100
29	e	75/83 (90%)	69 (92%)	6 (8%)	10	12
29	p	74/83 (89%)	74 (100%)	0	100	100
30	f	66/77 (86%)	63 (96%)	3 (4%)	23	34
30	q	66/77 (86%)	65 (98%)	1 (2%)	60	75
31	g	61/66 (92%)	60 (98%)	1 (2%)	58	73
31	r	60/66 (91%)	60 (100%)	0	100	100
32	h	96/129 (74%)	95 (99%)	1 (1%)	73	84
32	l	96/129 (74%)	94 (98%)	2 (2%)	48	65
33	j	85/103 (82%)	85 (100%)	0	100	100
33	m	85/103 (82%)	83 (98%)	2 (2%)	44	60
34	o	314/413 (76%)	314 (100%)	0	100	100
37	y	102/193 (53%)	102 (100%)	0	100	100
All	All	8268/11597 (71%)	8171 (99%)	97 (1%)	66	80

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	V	388	ILE
24	Z	12	ASP
21	V	575	ARG
22	W	20	ASN
26	b	26	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
11	J	306	HIS
32	l	86	ASN
16	O	82	ASN
32	l	78	ASN
37	y	200	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	126/1175 (10%)	26 (20%)	5 (3%)
10	I	45/95 (47%)	13 (28%)	6 (13%)
2	5	169/214 (78%)	16 (9%)	4 (2%)
3	6	101/112 (90%)	9 (8%)	0
7	E	32/42 (76%)	14 (43%)	6 (18%)
All	All	473/1638 (28%)	78 (16%)	21 (4%)

5 of 78 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	19	U
1	2	21	G
1	2	25	A
1	2	31	A
1	2	32	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	E	16	A
10	I	70	A
10	I	91	A
10	I	71	C
10	I	61	U

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

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	$\# Z > 2$
3	PSU	6	28	3	18,21,22	1.06	1 (5%)	21,30,33	2.08	5 (23%)

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
3	PSU	6	28	3	-	1/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	28	PSU	C6-C5	3.01	1.38	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	28	PSU	N1-C2-N3	5.26	120.72	115.17
3	6	28	PSU	C4-N3-C2	-5.09	119.36	126.37
3	6	28	PSU	C6-C5-C4	3.07	120.25	118.17
3	6	28	PSU	O2-C2-N1	-2.79	119.91	122.79
3	6	28	PSU	C6-N1-C2	-2.56	120.32	122.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	6	28	PSU	O4'-C1'-C5-C4

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 16 ligands modelled in this entry, 13 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
41	GTP	C	2501	38	29,34,34	1.28	2 (6%)	35,54,54	1.44	5 (14%)
40	IHP	S	701	-	36,36,36	0.69	0	60,60,60	0.85	2 (3%)
40	IHP	A	2500	-	36,36,36	0.82	0	60,60,60	0.60	0

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
41	GTP	C	2501	38	-	2/18/38/38	0/3/3/3
40	IHP	S	701	-	-	2/30/54/54	0/1/1/1
40	IHP	A	2500	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	C	2501	GTP	C5-C6	-4.53	1.38	1.47
41	C	2501	GTP	C5-C4	-2.17	1.37	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	C	2501	GTP	C8-N7-C5	3.84	109.09	102.55
41	C	2501	GTP	C5-C6-N1	3.10	119.99	114.07
41	C	2501	GTP	C2-N1-C6	-2.94	119.73	125.11
41	C	2501	GTP	O2B-PB-O3A	2.81	114.88	107.27
40	S	701	IHP	C6-C1-C2	2.78	116.53	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	S	701	IHP	C1-O11-P1-O21
40	A	2500	IHP	C3-O13-P3-O43
40	S	701	IHP	C4-O14-P4-O34

Continued on next page...

Continued from previous page...

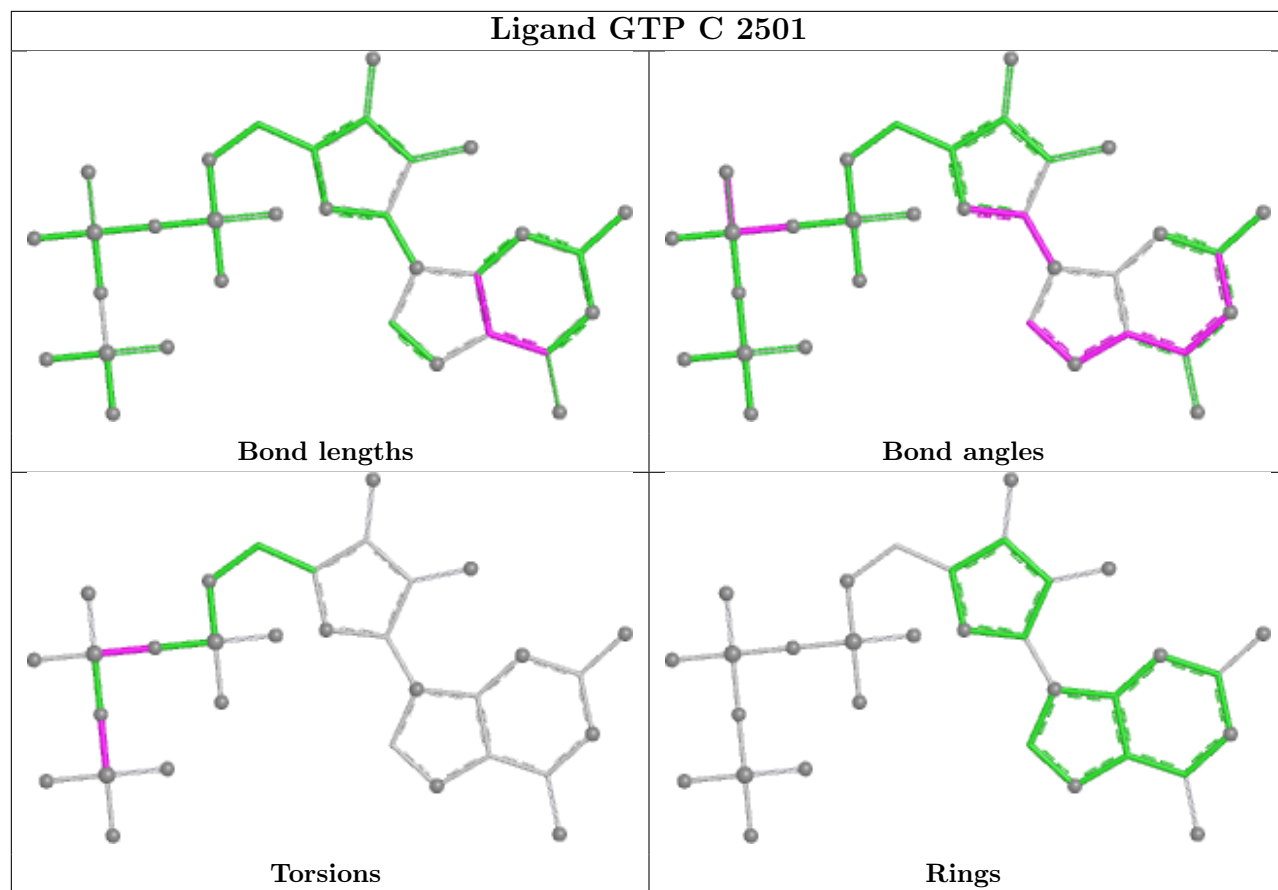
Mol	Chain	Res	Type	Atoms
41	C	2501	GTP	PA-O3A-PB-O1B
41	C	2501	GTP	PB-O3B-PG-O3G

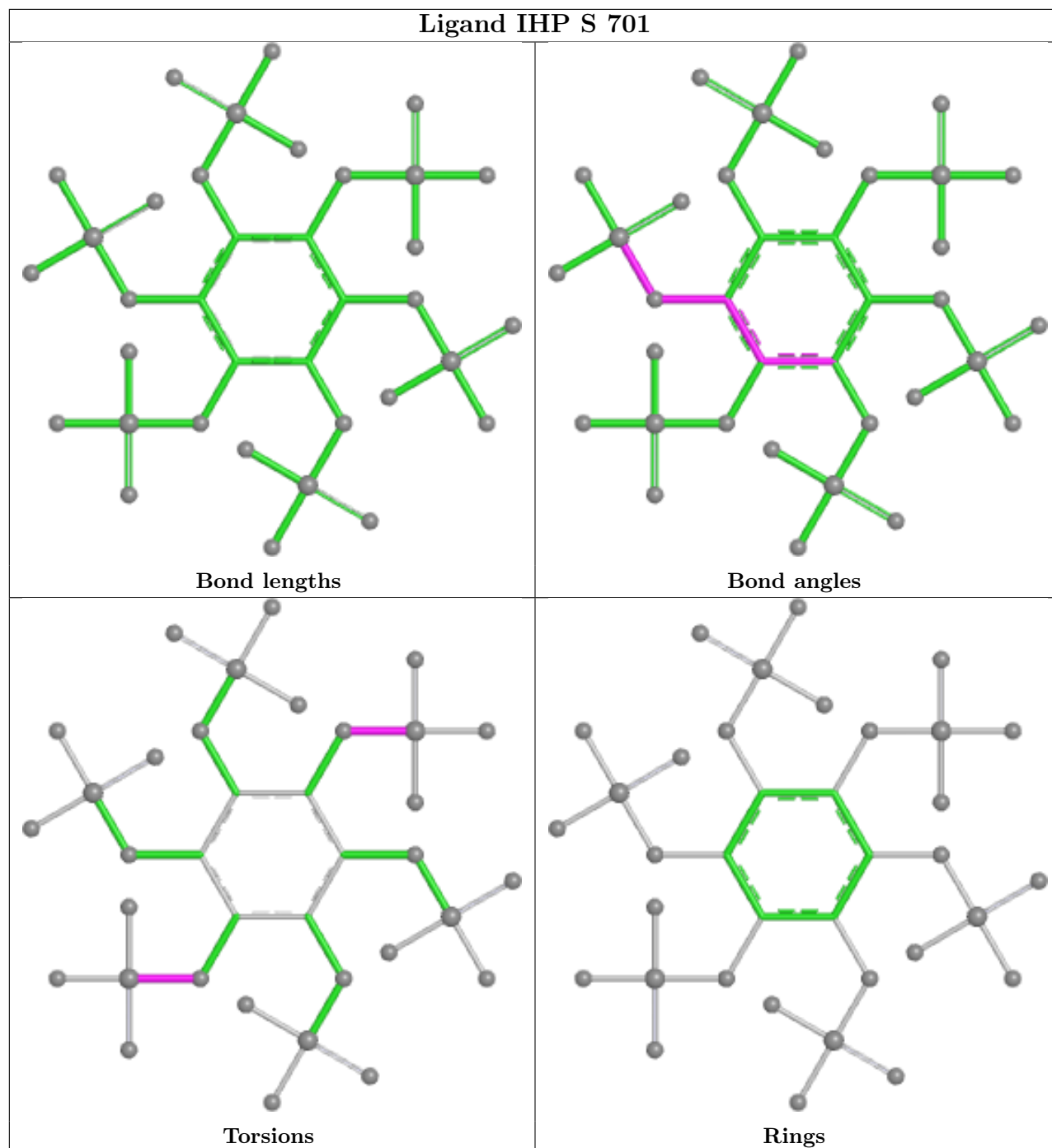
There are no ring outliers.

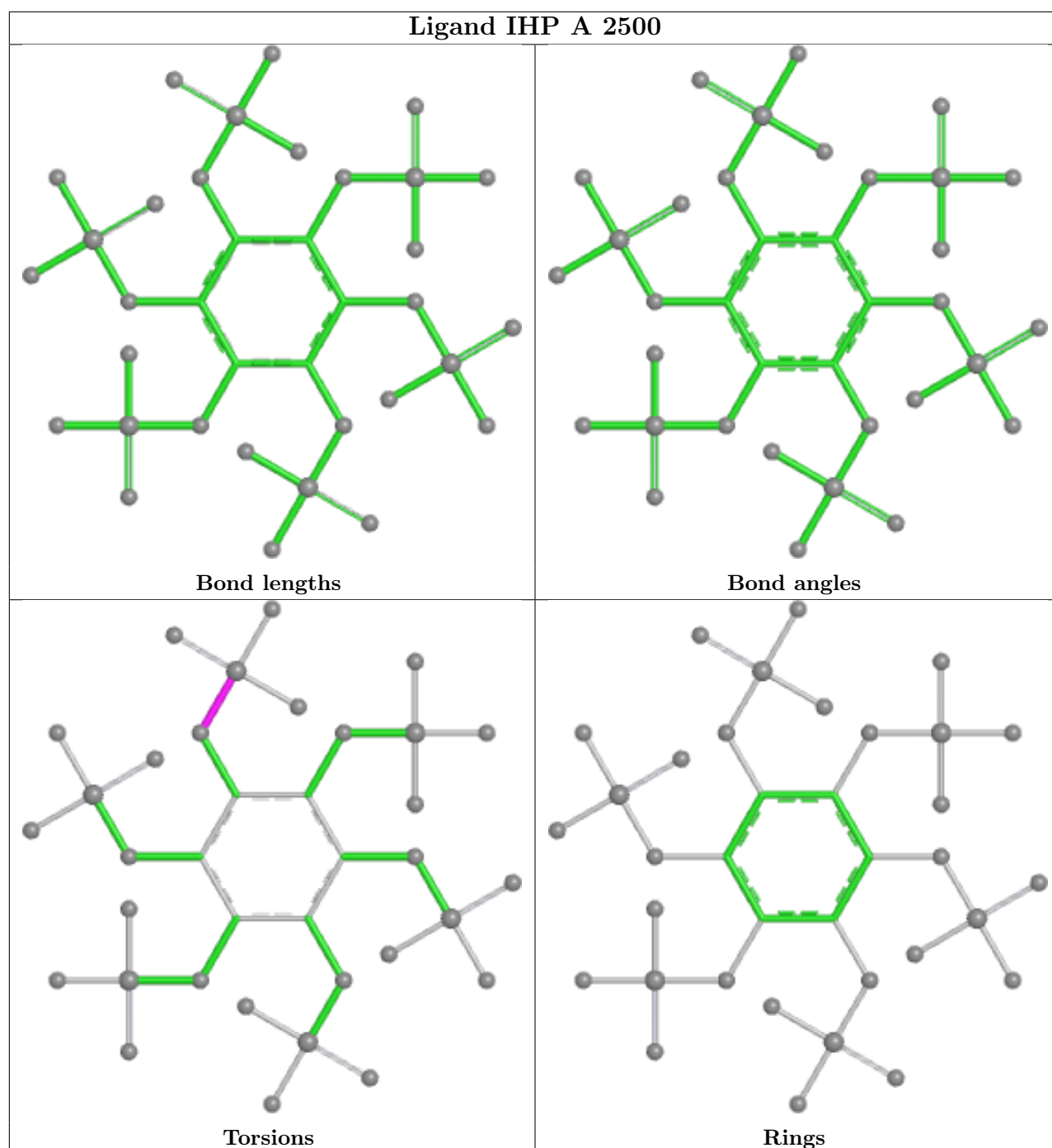
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	S	701	IHP	1	0
40	A	2500	IHP	1	0

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.

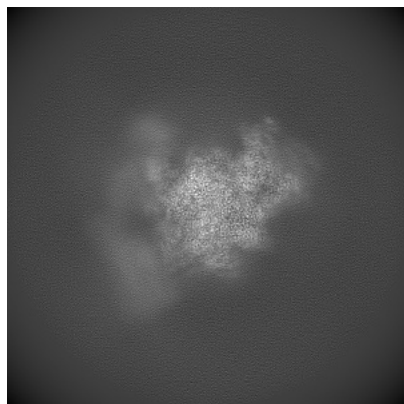
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47157. These allow visual inspection of the internal detail of the map and identification of artifacts.

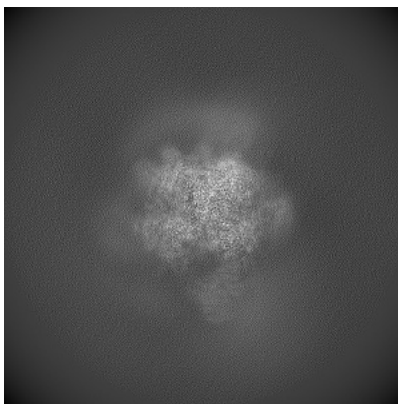
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

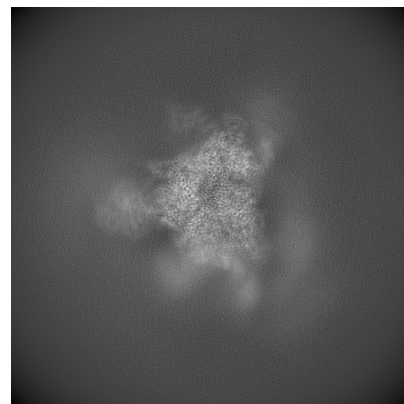
6.1.1 Primary map



X

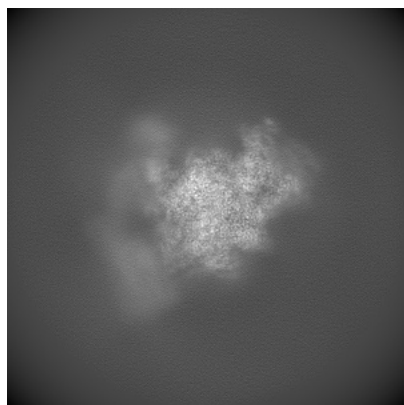


Y

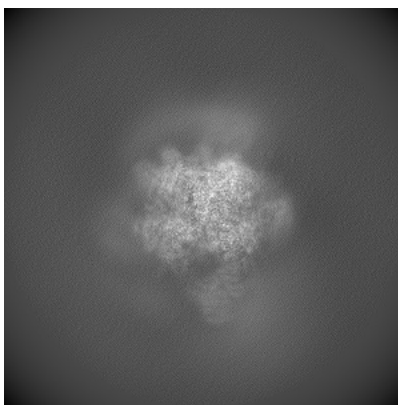


Z

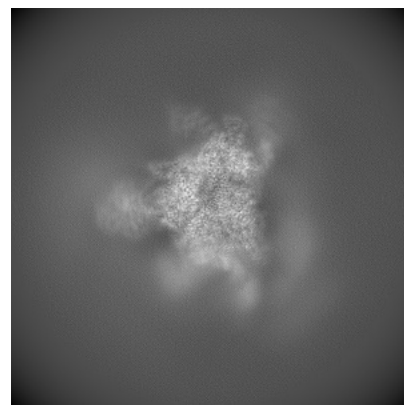
6.1.2 Raw map



X



Y

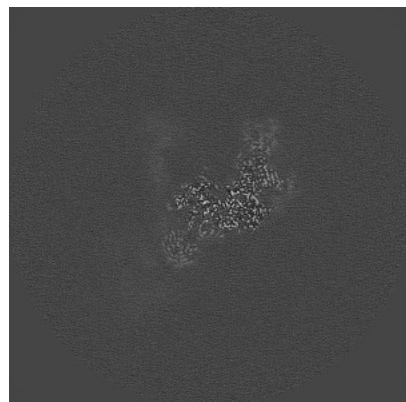


Z

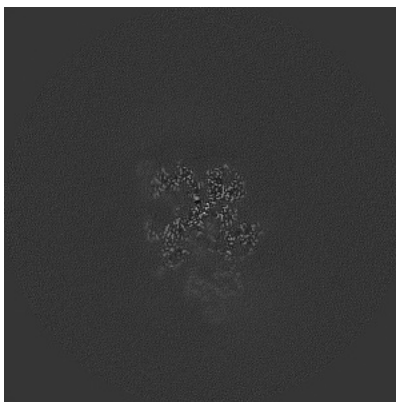
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

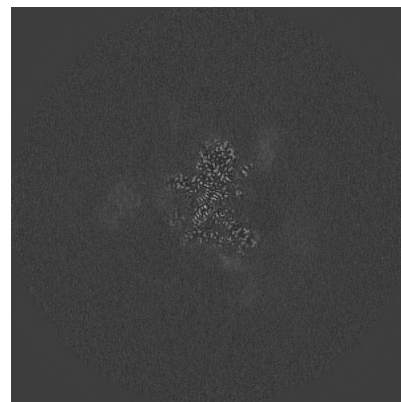
6.2.1 Primary map



X Index: 240

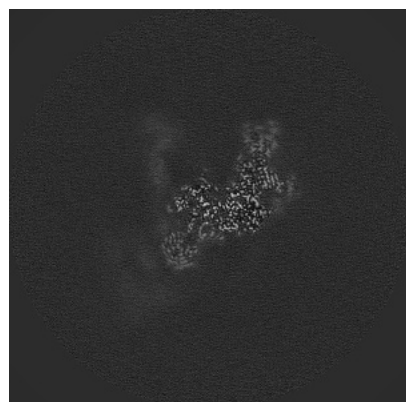


Y Index: 240

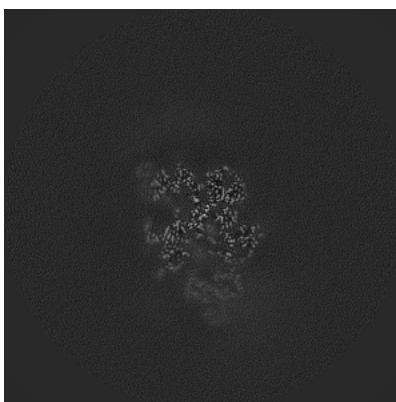


Z Index: 240

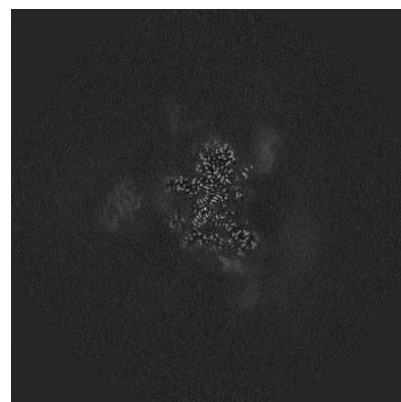
6.2.2 Raw map



X Index: 240



Y Index: 240

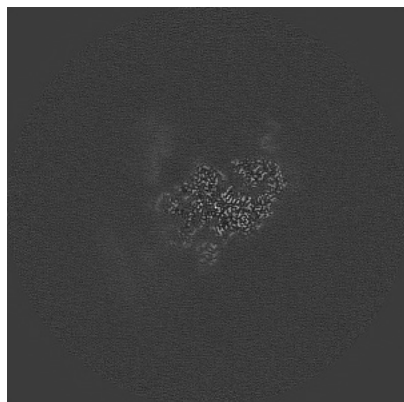


Z Index: 240

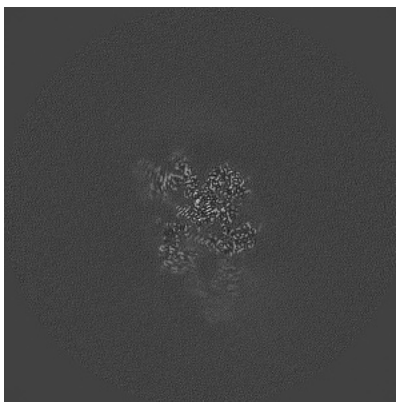
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

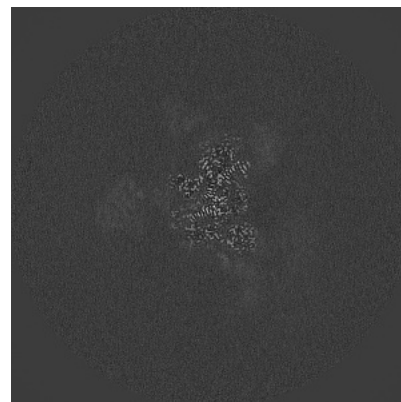
6.3.1 Primary map



X Index: 253

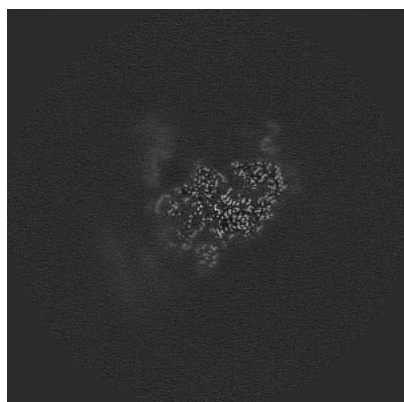


Y Index: 234

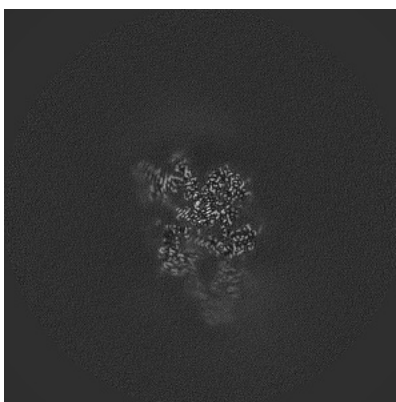


Z Index: 244

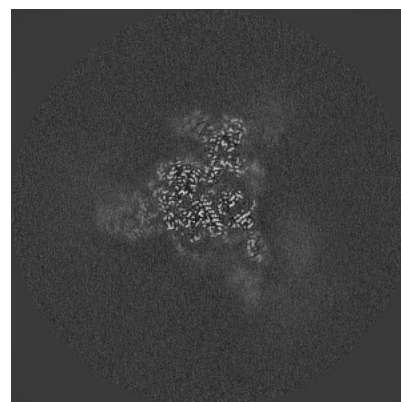
6.3.2 Raw map



X Index: 253



Y Index: 234

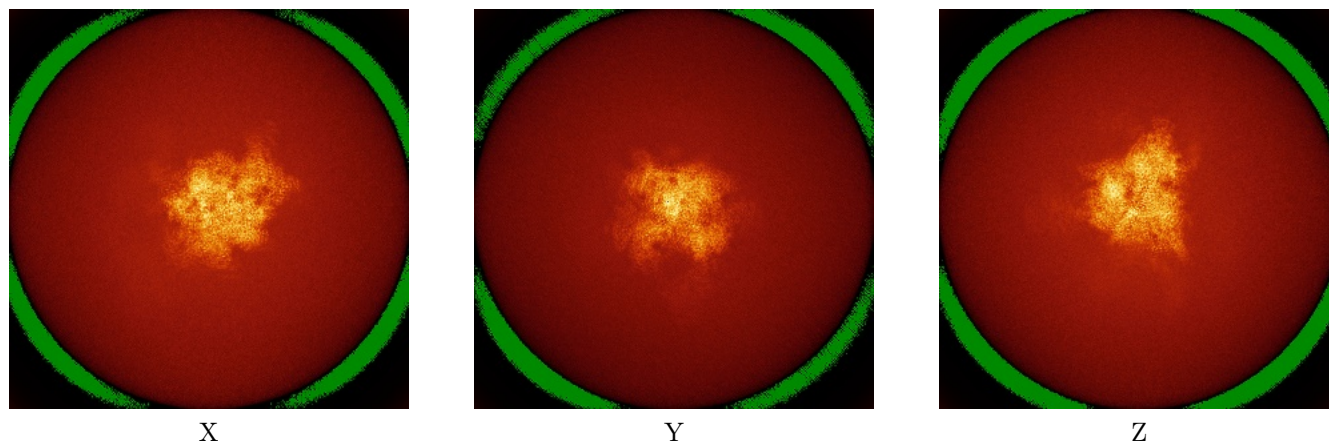


Z Index: 265

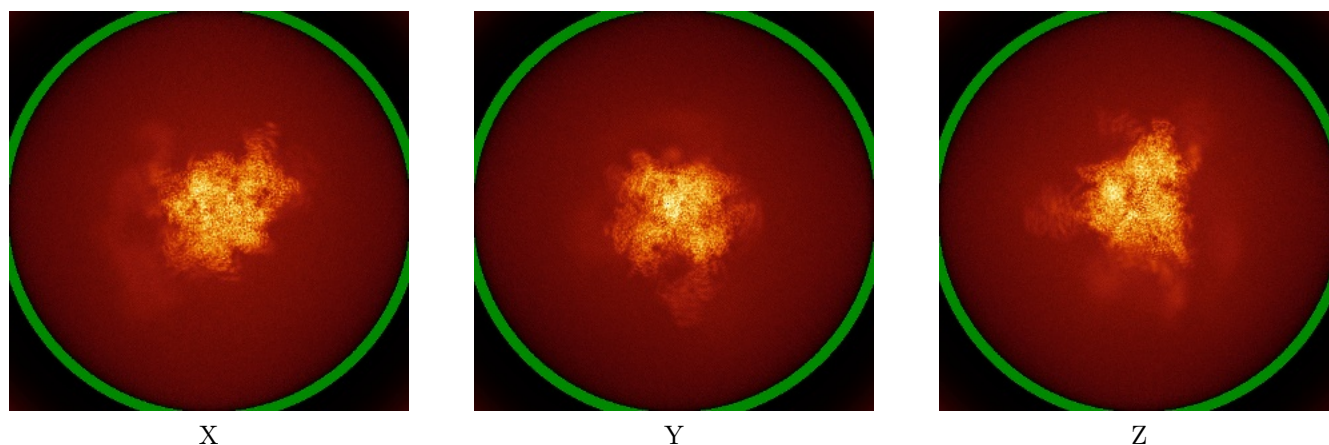
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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



X



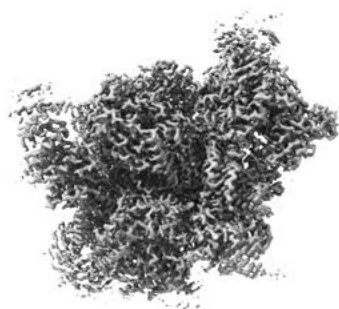
Y



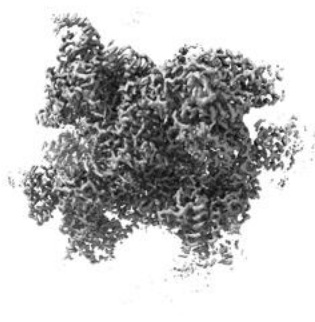
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

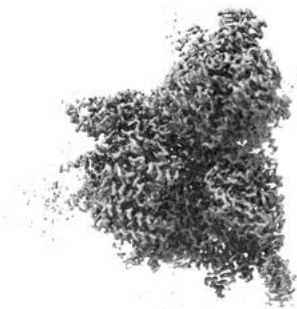
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

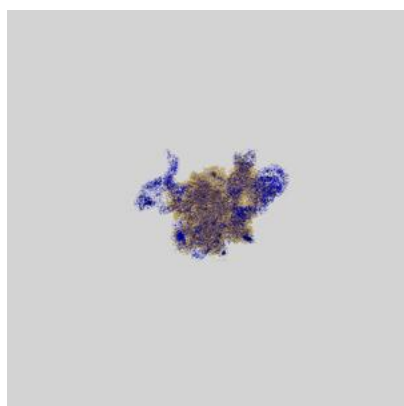
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

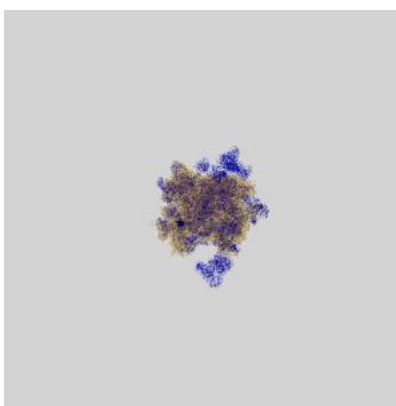
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

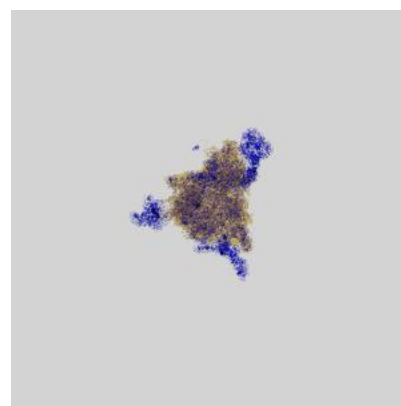
6.6.1 emd_47157_msk_1.map [i](#)



X



Y

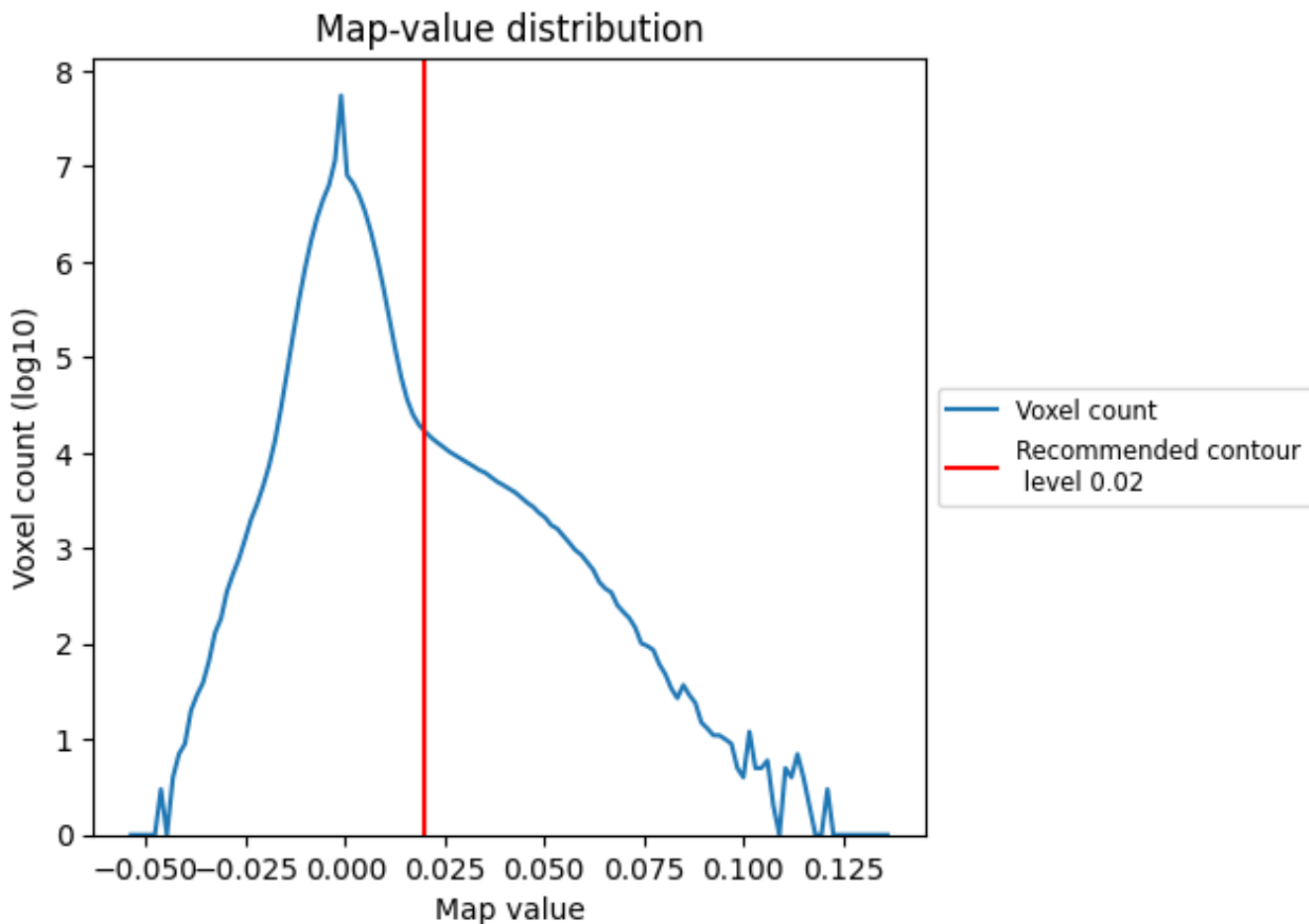


Z

7 Map analysis [i](#)

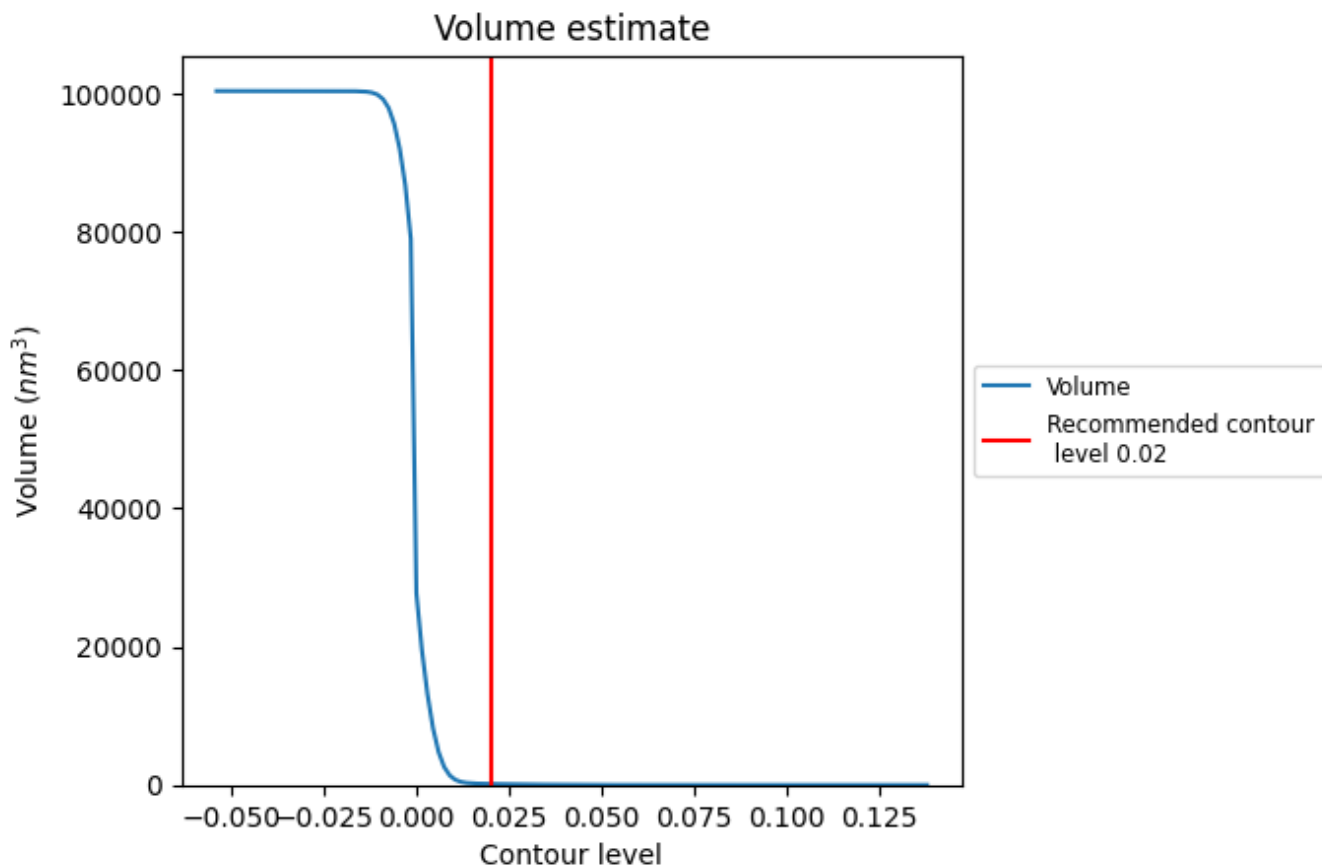
This section contains the results of statistical analysis of the map.

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.

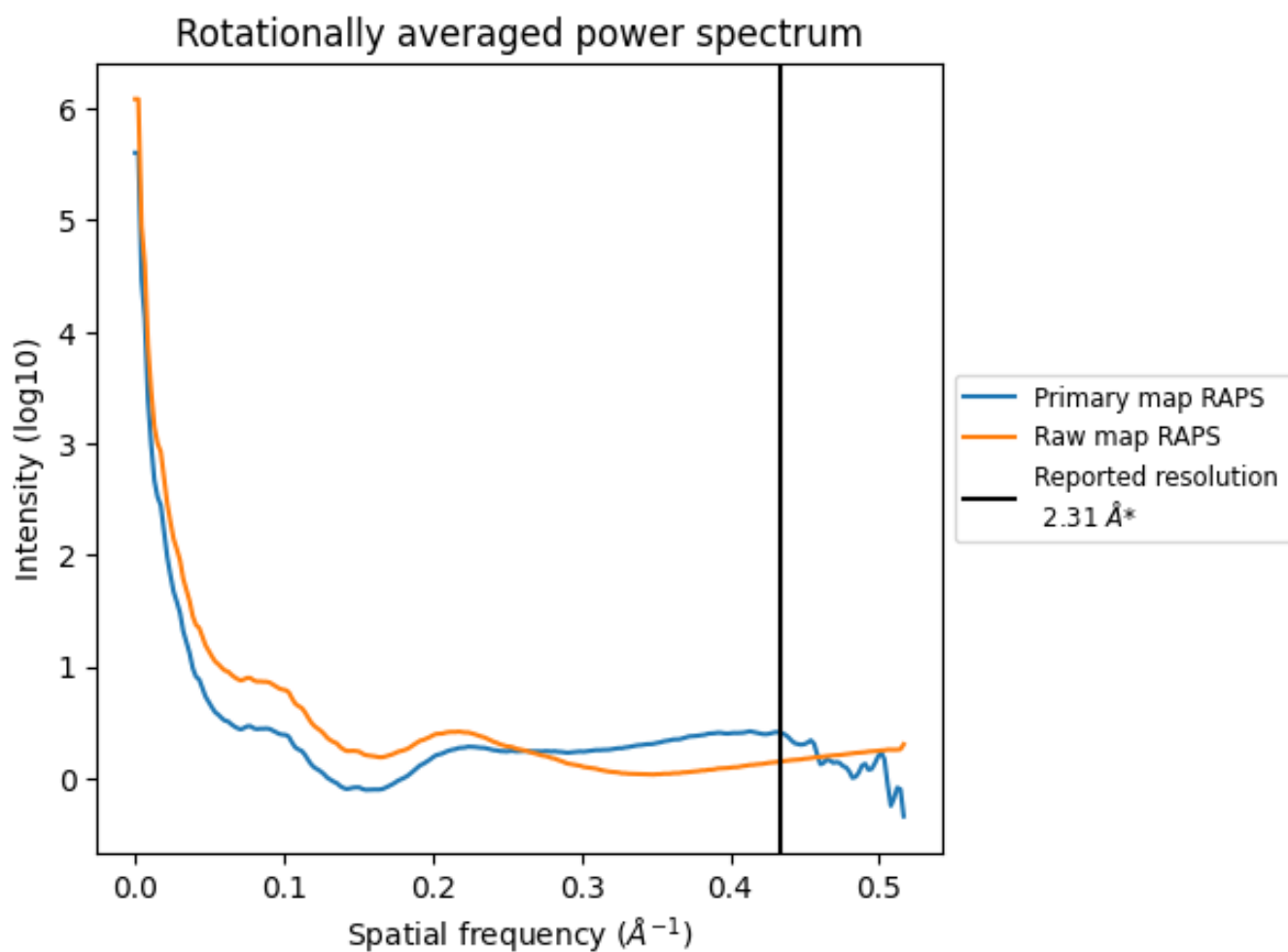
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 146 nm^3 ; this corresponds to an approximate mass of 132 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

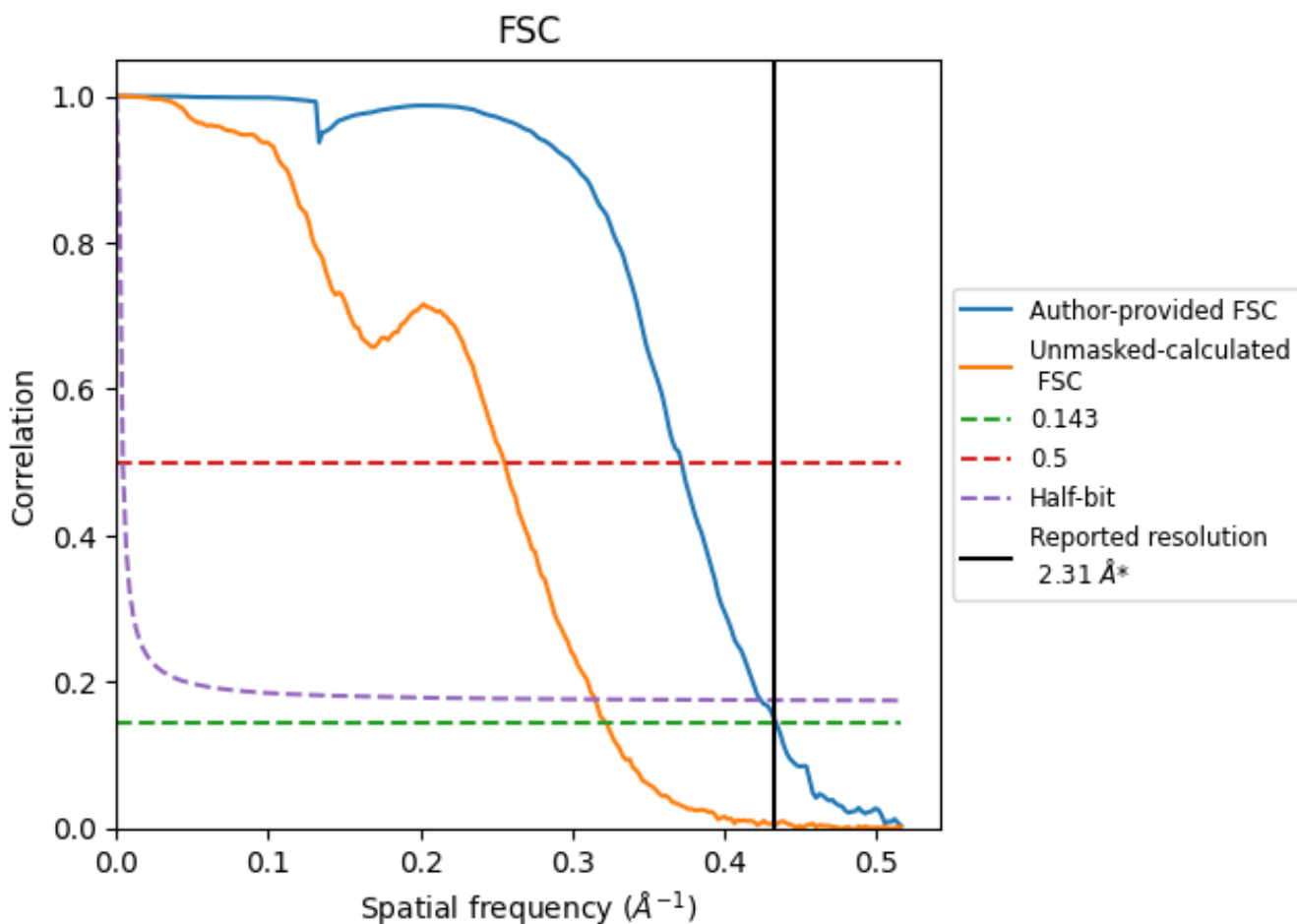


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

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 0.433 Å⁻¹

8.2 Resolution estimates [i](#)

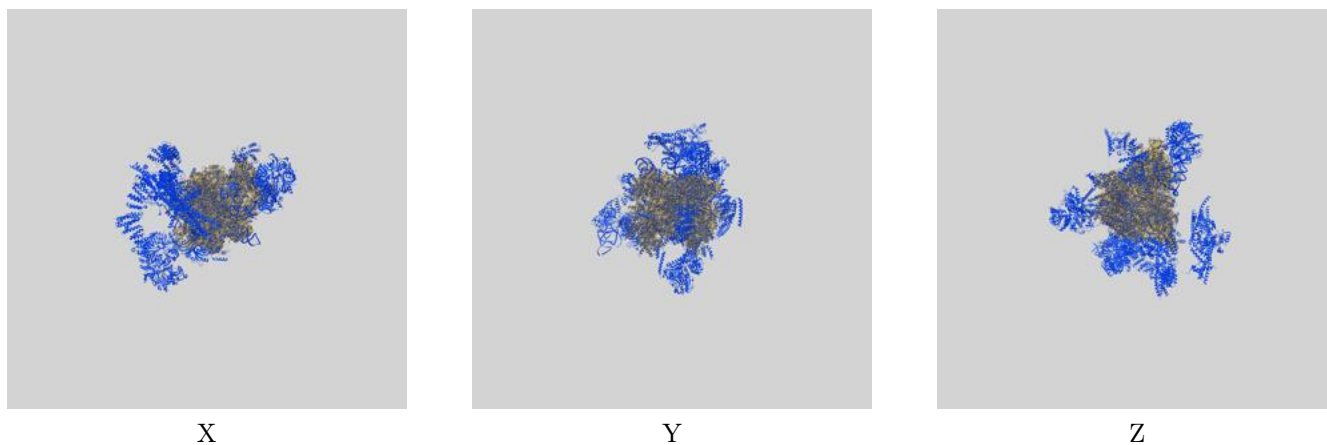
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.69	2.36
Unmasked-calculated*	3.10	3.92	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.31 by more than 10 %

9 Map-model fit [i](#)

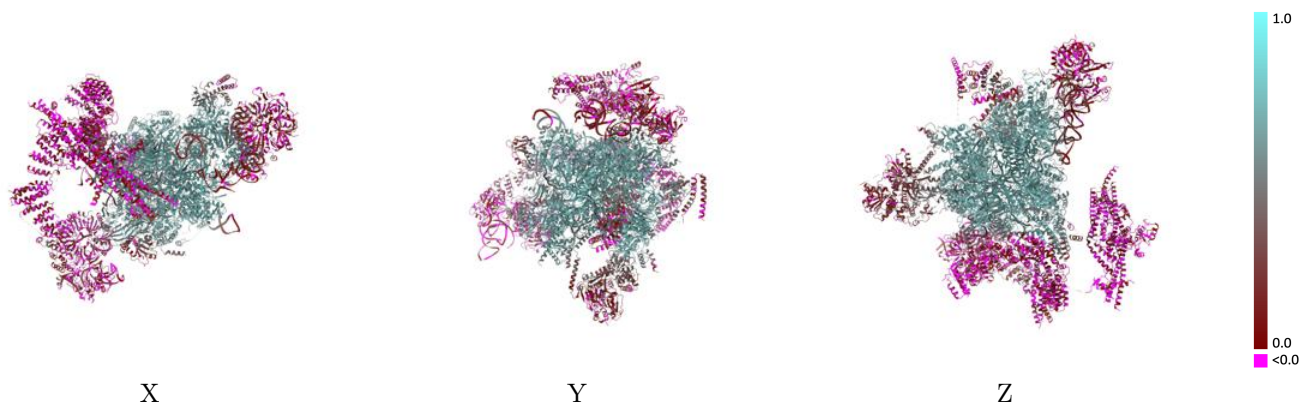
This section contains information regarding the fit between EMDB map EMD-47157 and PDB model 9DTR. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



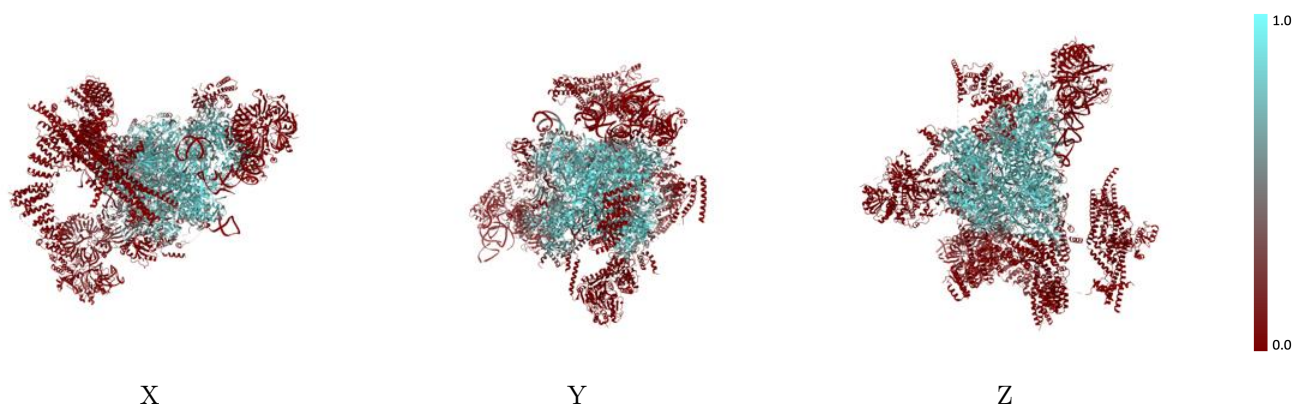
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



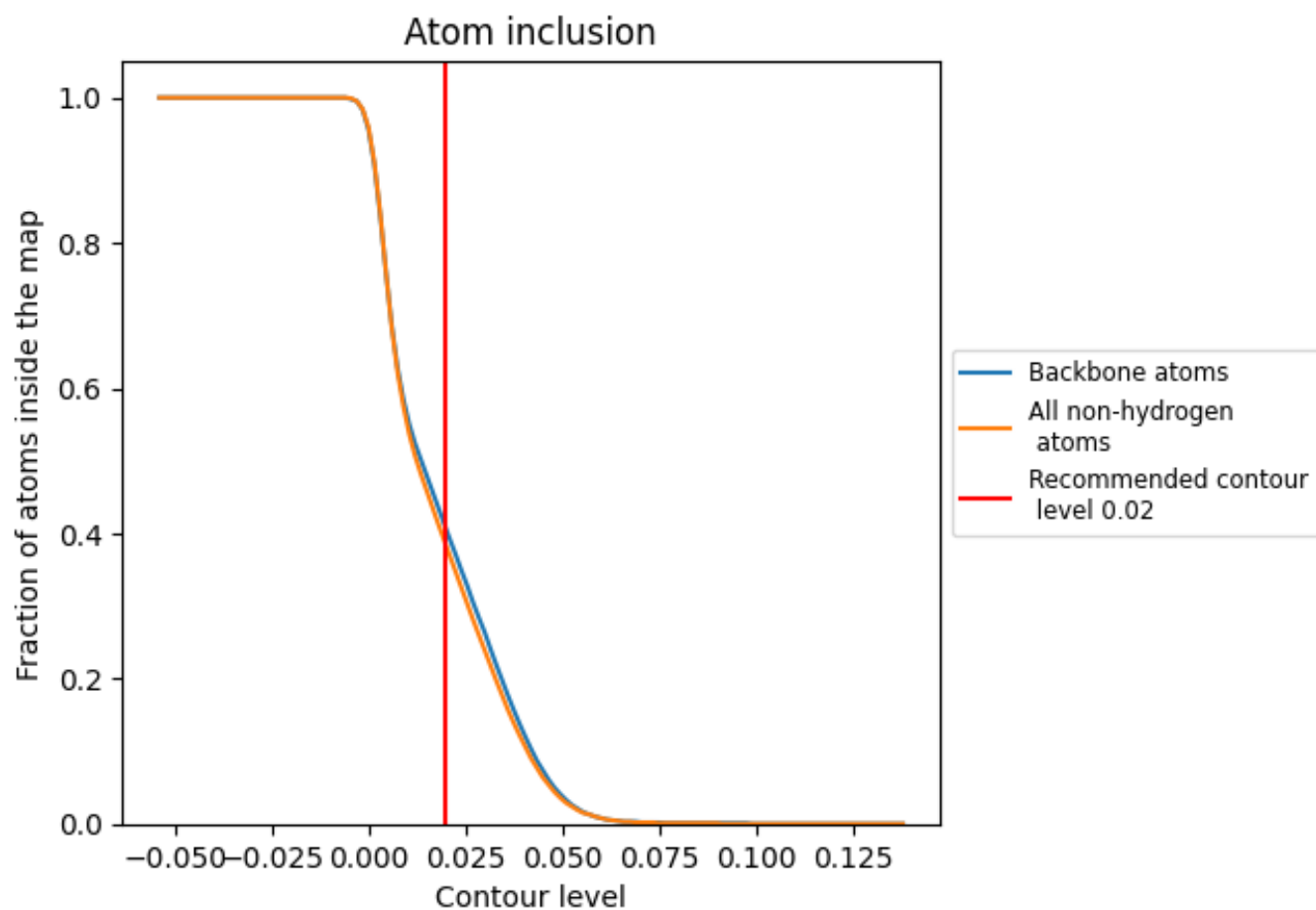
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 38% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3830	 0.4190
2	 0.1890	 0.1990
5	 0.4020	 0.3860
6	 0.6940	 0.6010
A	 0.8090	 0.6900
C	 0.6380	 0.6380
D	 0.1020	 0.3640
E	 0.3640	 0.4890
G	 0.0000	 0.2440
H	 0.2550	 0.3880
I	 0.4820	 0.5290
J	 0.7740	 0.6530
K	 0.6140	 0.6310
L	 0.7560	 0.6820
M	 0.5670	 0.6180
N	 0.3400	 0.4580
O	 0.4200	 0.4350
P	 0.6700	 0.6760
R	 0.3160	 0.3600
S	 0.3100	 0.3250
T	 0.0000	 0.0850
V	 0.0330	 0.2770
W	 0.0000	 0.0680
Y	 0.0000	 0.0490
Z	 0.0000	 0.0240
a	 0.4950	 0.5960
b	 0.0000	 0.1840
c	 0.3990	 0.5810
d	 0.0000	 0.2890
e	 0.0000	 0.0740
f	 0.0000	 0.0680
g	 0.0000	 0.1370
h	 0.0000	 0.1120
j	 0.0000	 0.0920
k	 0.0000	 0.0590



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Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.0000	 0.0350
m	 0.0000	 0.0140
n	 0.0000	 0.0770
o	 0.3940	 0.5910
p	 0.0000	 0.0230
q	 0.0000	 0.0210
r	 0.0000	 0.0590
s	 0.0000	 0.0340
t	 0.0000	 0.0360
u	 0.0000	 0.0180
v	 0.0000	 0.0450
w	 0.0000	 0.0390
y	 0.4080	 0.4650