



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:07 AM UTC

PDB ID : 9FMD / pdb\_00009fmd  
EMDB ID : EMD-4525  
Title : Integrative model of the human post-catalytic spliceosome (P-complex)  
Authors : Rothe, P.; Plaschka, C.; Vorlaender, M.K.  
Deposited on : 2024-06-05  
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](mailto: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>.

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

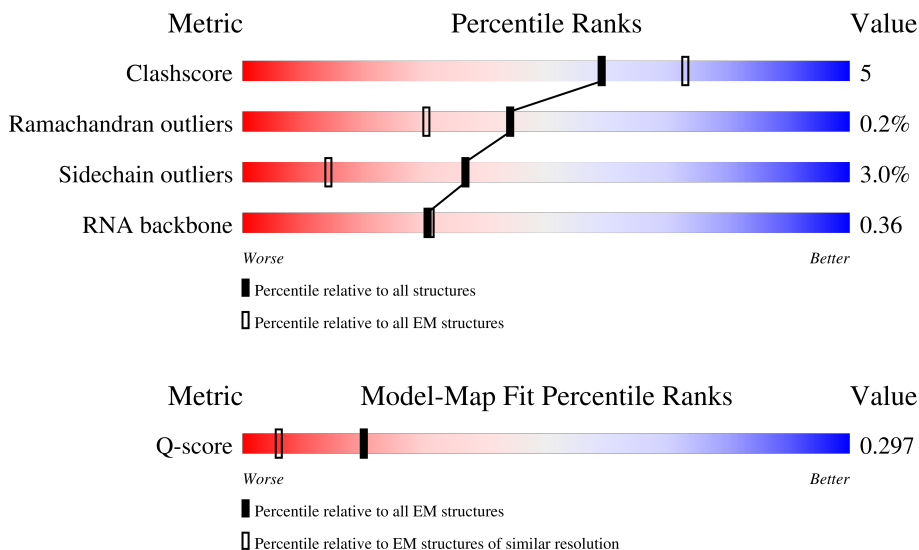
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 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.



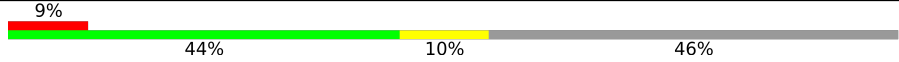
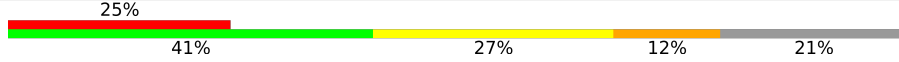


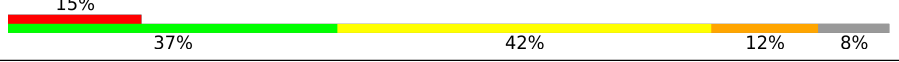
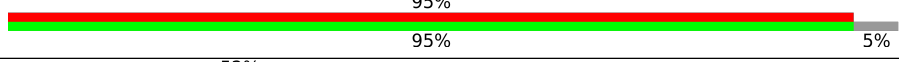

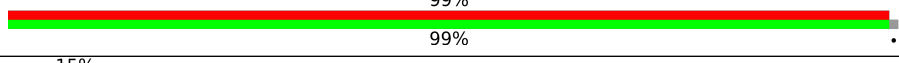
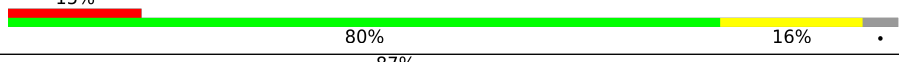




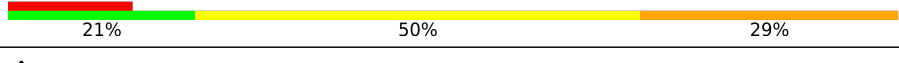






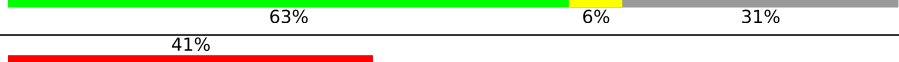
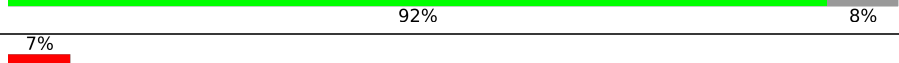

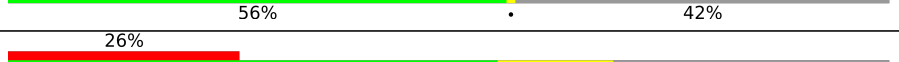
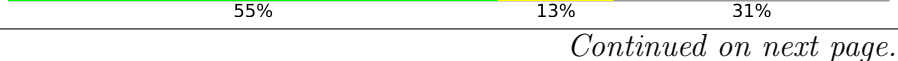
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 ( 2.80 - 3.80 )

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  $\geq 3$ , 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	1	184	
2	2	187	
3	3	476	

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Mol	Chain	Length	Quality of chain
4	32	112	
5	5	116	
6	50	339	
7	56	222	
8	6	106	
9	7	411	
10	8	174	
11	9	146	
12	A	2335	
13	B	2136	
14	C	972	
15	D	285	
16	E	357	
17	EX	14	
18	F	758	
19	H	908	
20	I	855	
21	IN	113	
22	J	848	
23	K	225	
24	L	802	
25	M	243	
26	N	144	
27	NO	301	
28	O	420	

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Mol	Chain	Length	Quality of chain
29	P	229	8% 41% 54%
30	Q	1485	89% 89% 11%
31	R	536	21% 51% 10% 39%
32	S	166	22% 83% 16%
33	SR	2752	97%
34	T	514	9% 56% 14% 29%
35	U	586	13% 41% 9% 50%
36	V	1220	57% 60% 40%
37	W	579	11% 67% 21% 11%
38	X	451	14% 14% 85%
39	Z	166	32% 31% 68%
40	a	126	32% 53% 13% 33%
40	h	126	30% 52% 14% 34%
41	b	240	23% 27% 9% 64%
41	i	240	29% 27% 7% 66%
42	c	119	61% 51% 16% 33%
42	j	119	62% 48% 19% 33%
43	d	118	75% 61% 14% 25%
43	k	118	78% 69% 12% 19%
44	e	92	86% 76% 10% 14%
44	l	92	73% 74% 14% 12%
45	f	86	81% 69% 15% 16%
45	m	86	76% 71% 13% 16%
46	g	76	76% 78% 18%
46	n	76	54% 68% 28%

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Mol	Chain	Length	Quality of chain
47	o	255	<p>63% 54% 10% 36%</p>
48	p	225	<p>40% 35% 6% 59%</p>
49	q	504	<p>20% 20% 80%</p>
49	r	504	<p>24% 24% 76%</p>
49	s	504	<p>26% 26% 74%</p>
49	t	504	<p>20% 20% 80%</p>
50	w	646	<p>82% 81% 18%</p>
51	x	289	<p>43% 43% 56%</p>
52	y	301	<p>26% 26% 74%</p>
53	z	415	<p>10% 15% 83%</p>

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 120489 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	123	1013	635	193	180	5	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	120	2535	1135	428	852	120	0	0

- Molecule 3 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	82	408	244	82	82	0	0

- Molecule 4 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	32	60	504	314	96	92	2	0	0

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	92	1936	867	322	655	92	0	0

- Molecule 6 is a protein called Protein FAM50A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
6	50	226	1124	671	226	227	0	0

- Molecule 7 is a protein called STING ER exit protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	56	101	Total	C	N	O	0	0
			498	296	101	101		

- Molecule 8 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 9 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	7	390	Total	C	N	O	0	0
			1928	1147	390	391		

- Molecule 10 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8	91	Total	C	N	O	0	0
			445	263	91	91		

- Molecule 11 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	9	144	Total	C	N	O	0	0
			712	423	144	145		

- Molecule 12 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	2250	Total	C	N	O	S	0	0
			17802	11405	3151	3176	70		

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	1864	Total	C	N	O	S	0	0
			15004	9583	2569	2775	77		

- Molecule 14 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	894	7069	4521	1178	1336	34	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	D	72	358	214	72	72	0	0

- Molecule 16 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	E	303	2370	1489	416	452	13	0	0

- Molecule 17 is a RNA chain called Exon.

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

- Molecule 18 is a protein called Splicing factor Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	122	1089	714	197	176	2	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	459	2932	1827	533	560	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	I	727	3610	2156	727	727	0	0

- Molecule 21 is a RNA chain called INTRON.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	IN	42	893	400	158	293	42	0	0

- Molecule 22 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	J	602	2998	1794	602	602	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	K	189	941	563	189	189	0	0

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	L	555	3642	2233	706	695	8	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	M	224	1115	666	224	225	0	0

- Molecule 26 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	N	144	1189	748	218	211	12	0	0

- Molecule 27 is a protein called Nitric oxide synthase-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	NO	174	864	516	174	174	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	289	Total	C	N	O	S	0	0
			2327	1459	416	432	20		

- Molecule 29 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	106	Total	C	N	O	S	0	0
			889	544	174	169	2		

- Molecule 30 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	1322	Total	C	N	O		0	0
			6554	3910	1322	1322			

- Molecule 31 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	R	328	Total	C	N	O	P	S	0	0
			2618	1634	479	489	2	14		

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	164	Total	C	N	O	S	0	0
			1271	810	220	234	7		

- Molecule 33 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SR	70	Total	C	N	O	S	0	0
			412	251	80	80	1		

- Molecule 34 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	363	Total	C	N	O	S	0	0
			2881	1820	525	526	10		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	295	Total	C	N	O	S	0	0
			2425	1525	431	461	8		

- Molecule 36 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	V	733	Total	C	N	O	0	0
			3629	2163	733	733		

- Molecule 37 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	513	Total	C	N	O	S	0	0
			4158	2643	719	772	24		

- Molecule 38 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	X	66	Total	C	N	O	0	0
			328	196	66	66		

- Molecule 39 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
40	h	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b	87	Total	C	N	O	S	0	0
			654	412	120	115	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	c	80	Total	C	N	O	S	0	0
			634	404	111	115	4		
42	j	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	89	Total	C	N	O	S	0	0
			723	454	133	131	5		
43	k	95	Total	C	N	O	S	0	0
			774	486	141	142	5		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein E.

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

- Molecule 45 is a protein called Small nuclear ribonucleoprotein F.

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

- Molecule 46 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 47 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 48 is a protein called U2 small nuclear ribonucleoprotein B'.

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

- Molecule 49 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	q	103	514	308	103	103	0	0
49	r	119	594	356	119	119	0	0
49	s	132	659	395	132	132	0	0
49	t	103	514	308	103	103	0	0

- Molecule 50 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	w	528	2605	1548	528	529	0	0

- Molecule 51 is a protein called Splicing factor C9orf78.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	x	128	636	379	128	129	0	0

- Molecule 52 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	y	79	318	160	79	79	0	0

- Molecule 53 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	z	70	430	259	83	86	2	0	0

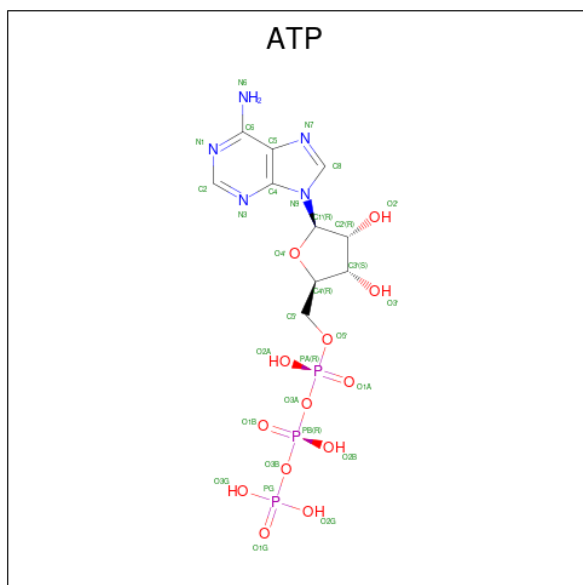
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	6	5	5	5	0
54	7	1	1	1	0

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
55	6	1	1	1	0

- Molecule 56 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

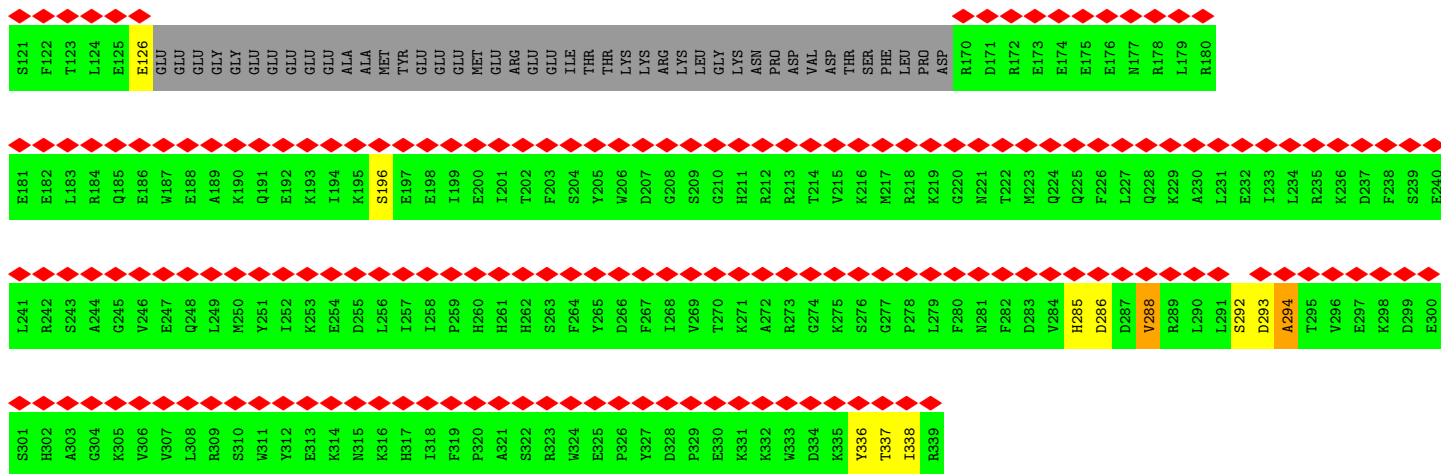




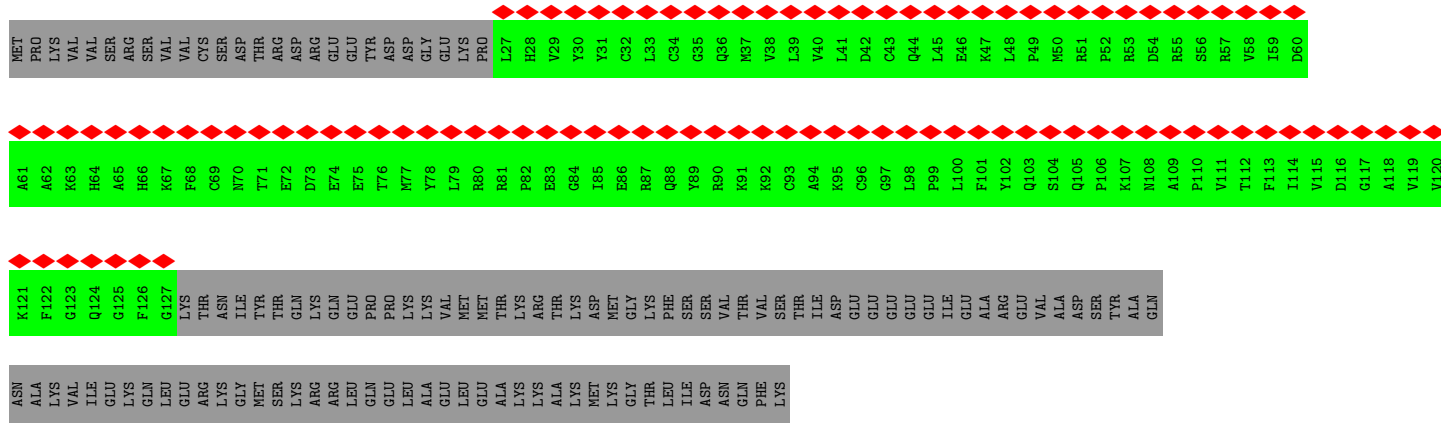
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
59	U	1	36	6	24	6	0



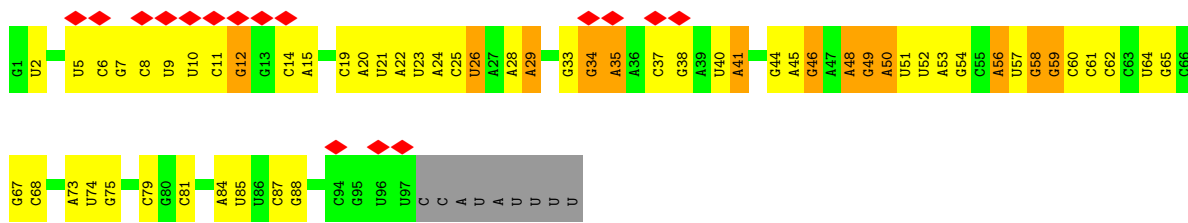




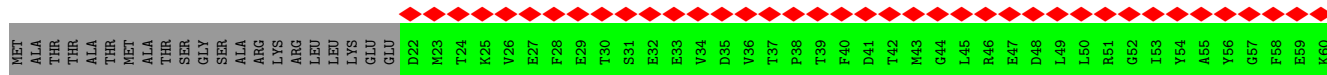
• Molecule 7: STING ER exit protein



• Molecule 8: U6 snRNA

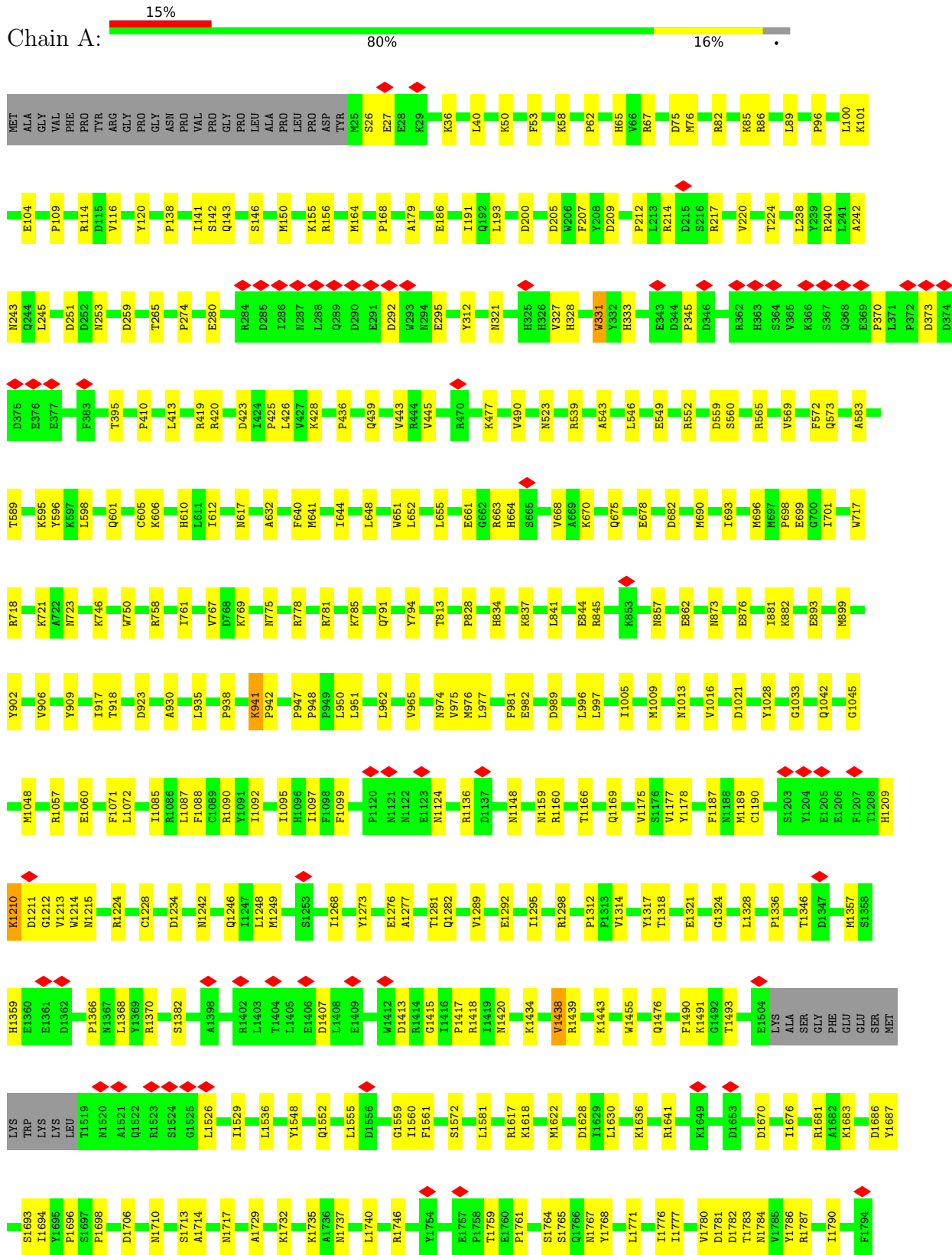


• Molecule 9: Eukaryotic initiation factor 4A-III





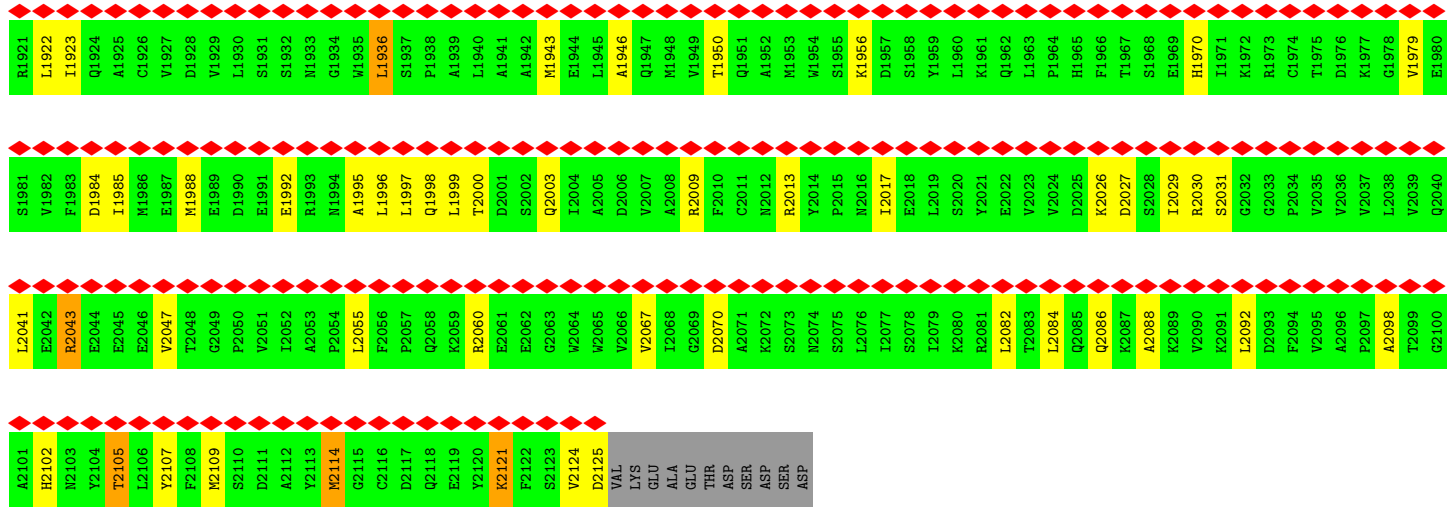
• Molecule 12: Pre-mRNA-processing-splicing factor 8



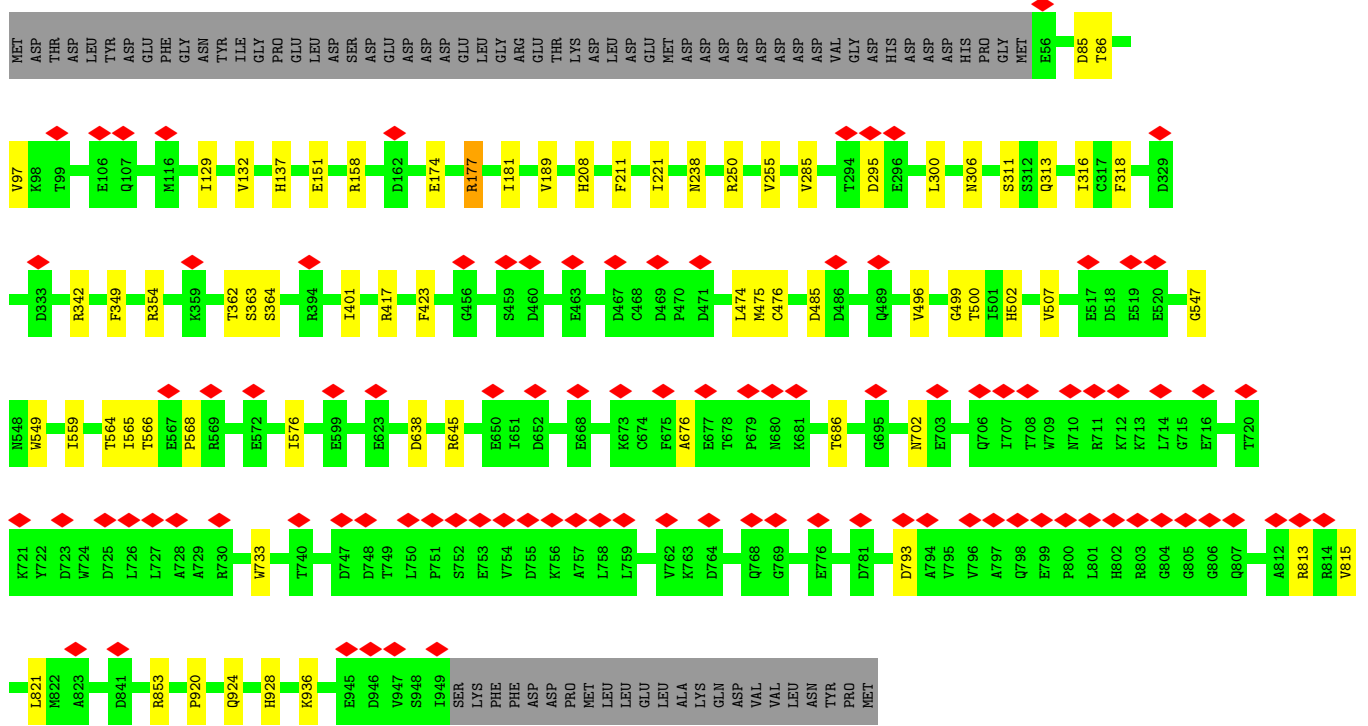
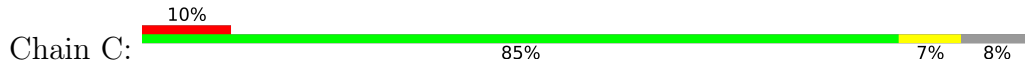


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TYR	GLN	LEU	HIS	GLU	THR	GLU	LYS	GLU	ASP	LEU	ILE	ARG	GLU	ARG	SER	ARG	ARG	GLU	VAL	ARG	GLN	SER	SER	ARG	MET	ASP	THR	LEU	LEU	GLN	GLY	ALA	ALA	LEU	A404	P405	R406	Q407	V408	L409	D410	L411	E412	D413	L414	V415	F416	T417	Q418	G419	S420								

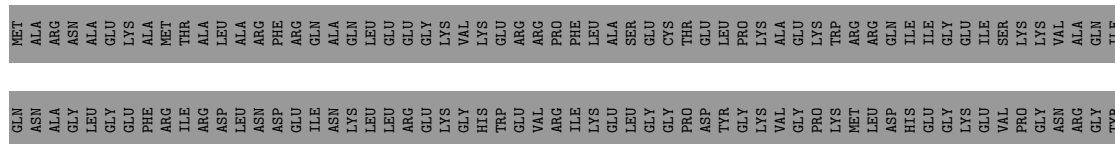
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E1201	L1202	T1203	I1204	T1205	P1206	D1207	F1208	Q1209	M1210	D1211	E1212	K1213	V1214	H1215	G1216	S1217	S1218	E1219	A1220	F1221	W1222	L1223	L1224	V1225	I1226	D1227	V1228	D1229	S1230	E1231	P1232	L1233	L1234	H1235	H1236	E1237	Y1238	F1239	L1240	L1241	K1242	A1243	K1244	Y1245	A1246	Q1247	D1248	E1249	H1250	L1251	I1252	T1253	F1254	F1255	V1256	P1257	F1259	E1260				
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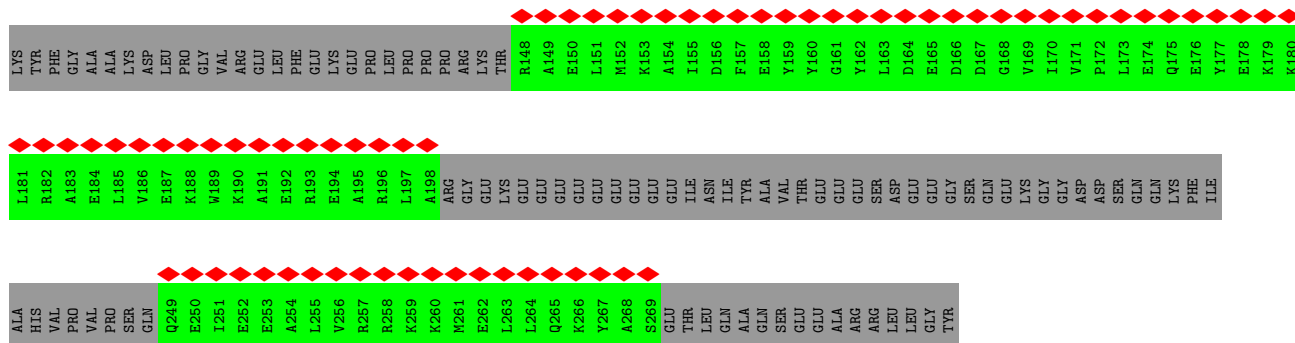


• Molecule 14: 116 kDa U5 small nuclear ribonucleoprotein component

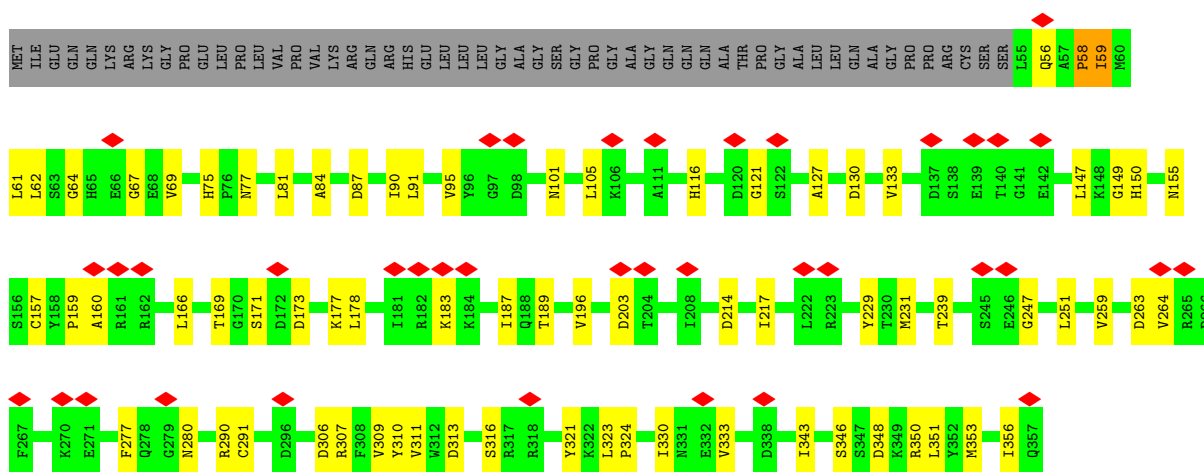


• Molecule 15: Pre-mRNA-splicing factor ISY1 homolog





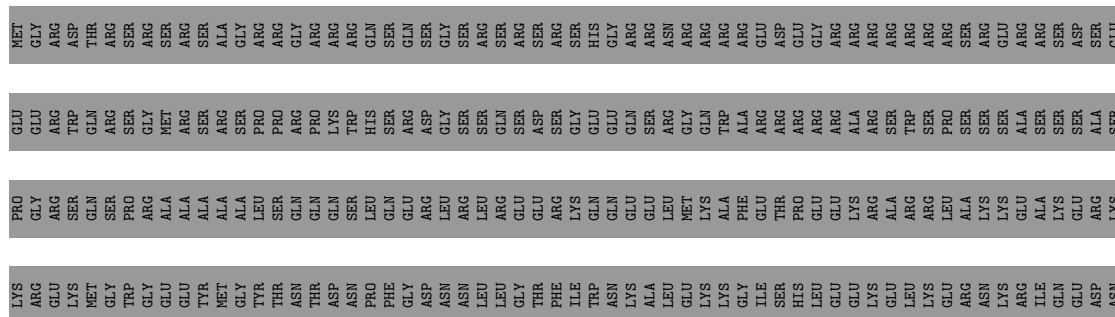
• Molecule 16: U5 small nuclear ribonucleoprotein 40 kDa protein



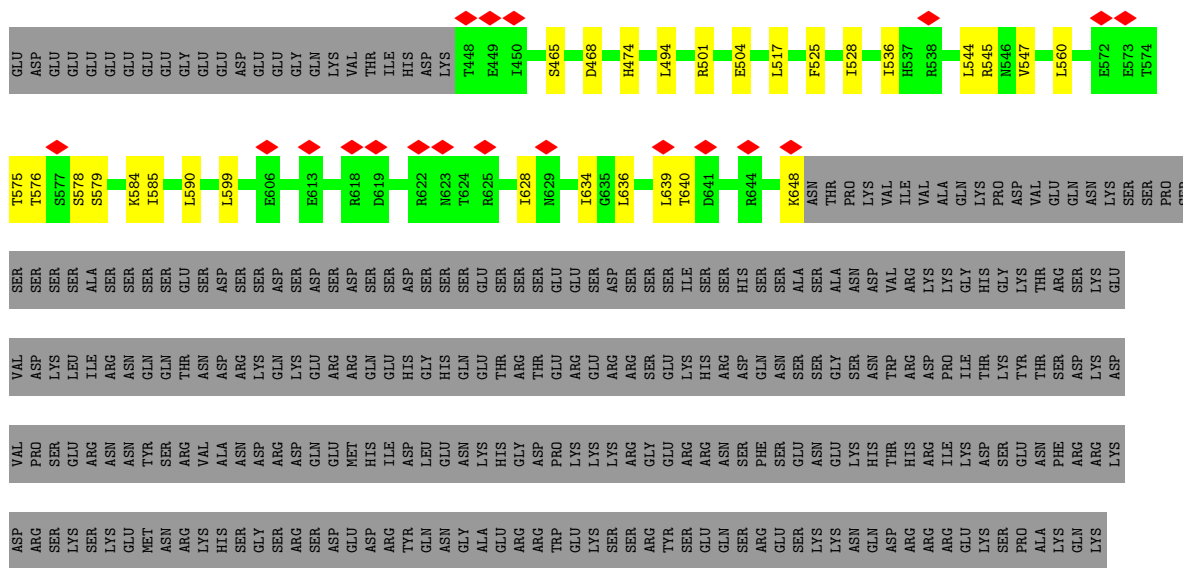
• Molecule 17: Exon



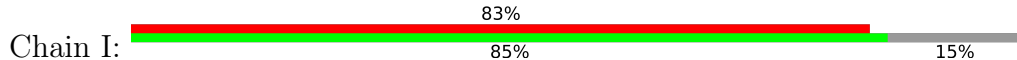
• Molecule 18: Splicing factor Cactin





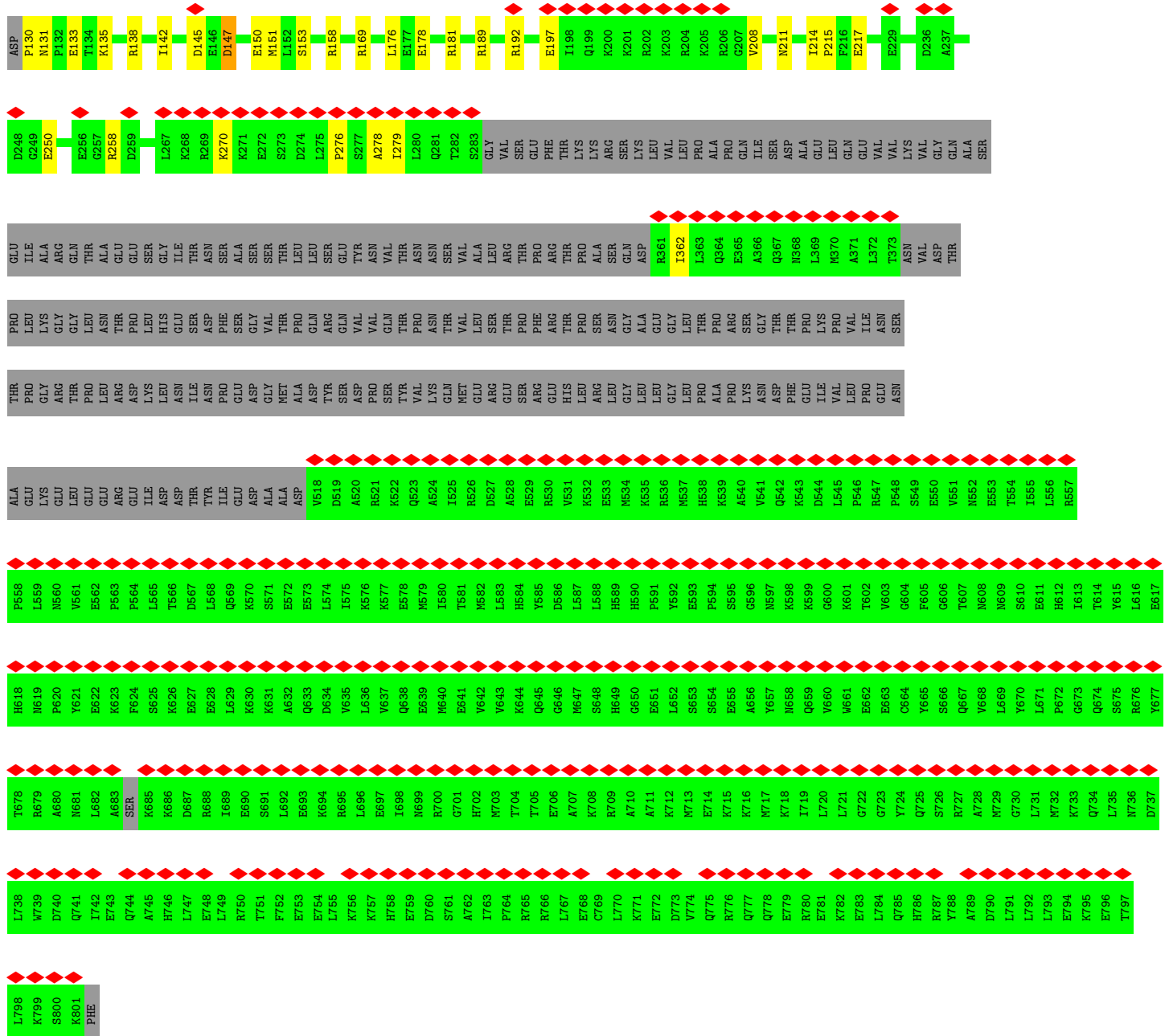


● Molecule 20: Pre-mRNA-splicing factor SYF1

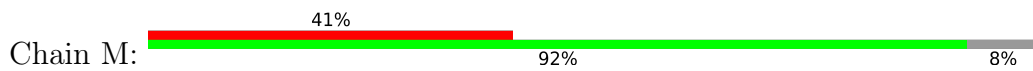








● Molecule 25: Pre-mRNA-splicing factor SYF2







T361	R362	E363	S364	L365	V366	K367	F368	F369	G370	P371	L372	S373	S374	N375	T376	L377	H378	Q379	V380	A381	S382	Y383	L384	C385	L386	L387	P388	L389	L390	P391	K392	N393	E394	D395	T396	F397	F398	D399	K400	E401	F402	L403	L404	E405	L406	L407	V408	S409	R410	H411	E412	R413	R414	I415	S416	Q417	I418	Q419	Q420					
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	K454	L455	N456	L457	L458	F459	L460	T461	L462	H463	D464	Y465	L466	L467	R468	N469	F470	N471	L472	F473	R474	L475	E476	S477	T478	Y479	E480					
I481	R482	Q483	D484	I485	E486	D487	S488	V489	S490	R491	M492	K493	P494	W495	Q496	GLU	T497	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	E527	G528	E529	N530	W531	P532	T533	R534	V535	R536	A537	D538	V539	T540						
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I721	E722	H723	L724	K725	A726	S727	F728	P729	G730	H731	N732	K733	R734	V735	T736	E737	F738	D739	P740	A741	R742	V743	I744	P745	F746	F747	R748	I749	T750	F751	F752	ARG	SER	GLY	LYS	LYS	LYS	ARG	ASP	ALA	VAL	GLU	ASP	GLU	THR	GLU	E773	A774	K775	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	G822	G823	P824	P825	L826	G826	T827	G828	K829	T830	D831	V832	A833	V834	Q835	I836	I837	S838	N839	I840				
H841	H842	N843	F844	P845	E846	R847	R848	T849	L850	I851	V852	T853	H854	L855	N856	Q857	A858	L859	N860	Q861	L862	F863	E864	K865	L866	M867	A868	L869	E869	D870	I871	D872	E873	R874	H875	L876	L877	R878	L879	G880	H881	GLU	E884	E885	K890	D891	F892	S893	K894	Y895	G896	R897	V898	N899	Y900									
V901	L902	A903	R904	R905	L906	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	R939	H1000	V940	M941	S942	R943	W944	F1005	E945	E946	E947	Y947	L1008	I948	S949	K950	V951	N951	K952	N953	LYS	GLY	SER	THR	LEU	P959	D960
V961	T962	E963	V964	S965	T966	F967	F968	P969	F970	H971	E972	K1033	Y973	F974	A975	N976	A977	GLN	PRO	I981	F982	K983	G984	R985	S986	Y987	E988	E989	D990	M991	E992	I993	A994	E995	G996	C997	F998	R999	H1000	I1001	K1002	K1003	K1004	F1005	T1006	Q1007	L1008	E1009	E1010	F1011	F1012	I1013	A1013	S1014	E1015	P1075	L1016	L1017	R1018	S1019	G1020			
L1021	D1022	R1023	S1024	K1025	Y1026	L1027	L1028	V1029	K1030	E1031	A1032	K1033	I1034	I1035	A1036	M1037	T1038	C1039	T1040	H1041	A1042	A1043	L1044	K1045	R1046	H1047	D1048	L1049	V1050	K1051	L1052	G1053	F1054	K1055	G996	C997	F998	R999	H1000	I1001	K1002	K1003	K1004	F1005	T1006	Q1007	L1008	E1009	E1010	F1011	F1012	I1013	A1013	S1014	E1015	P1075	L1016	L1017	R1018	S1019	G1020			
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	G1137	R1138	A1139	R1140					











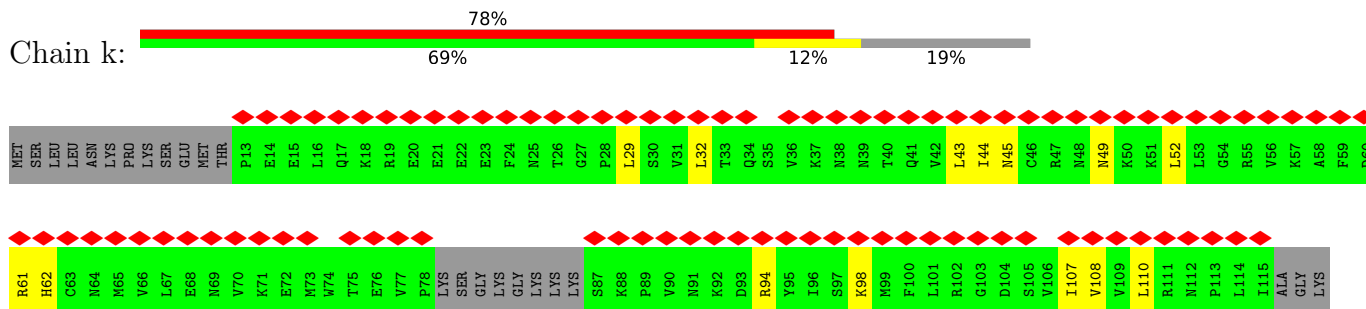




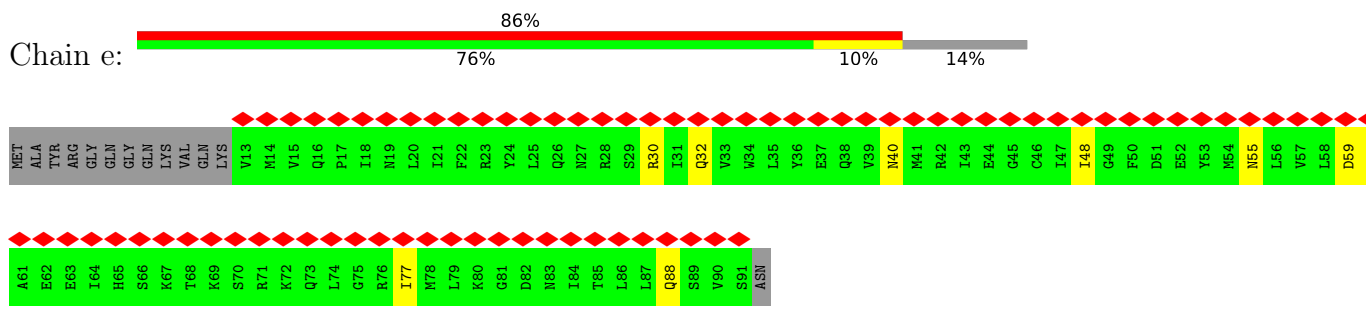




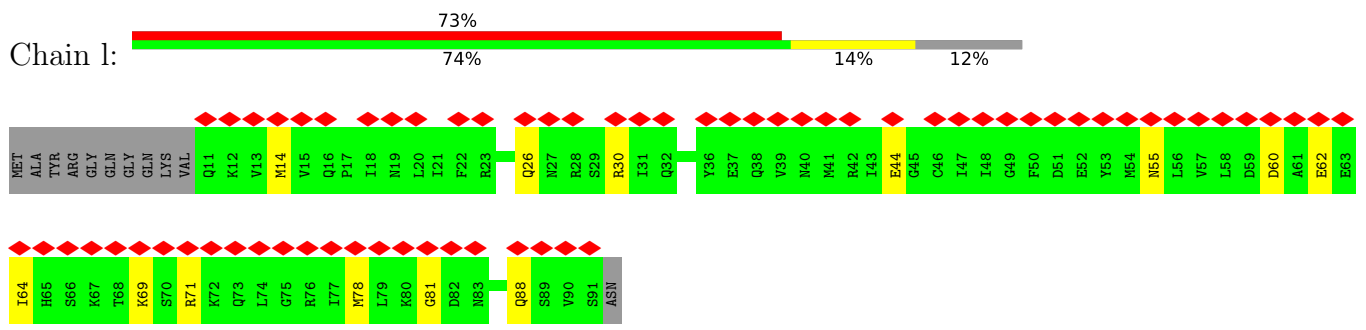
• Molecule 43: Small nuclear ribonucleoprotein Sm D2



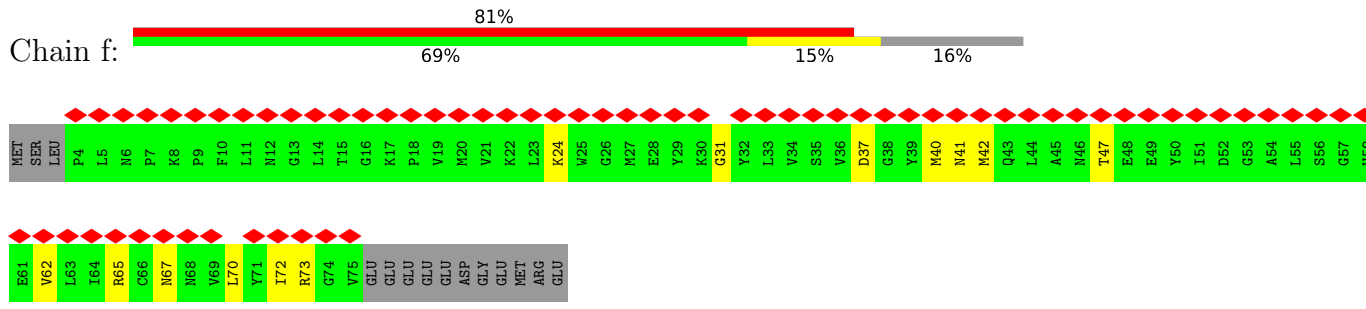
• Molecule 44: Small nuclear ribonucleoprotein E



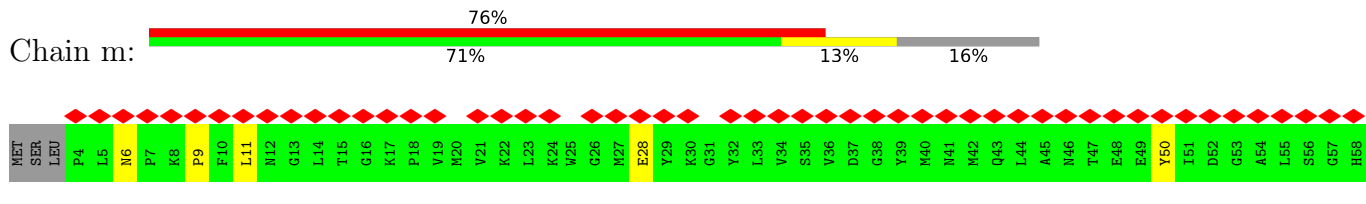
• Molecule 44: Small nuclear ribonucleoprotein E

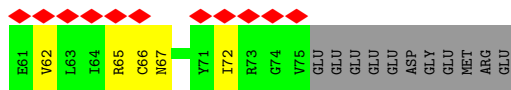


• Molecule 45: Small nuclear ribonucleoprotein F

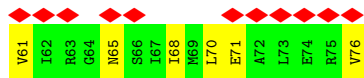
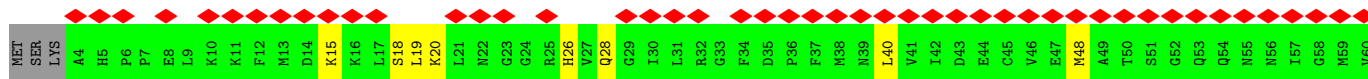
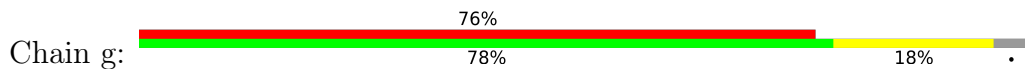


• Molecule 45: Small nuclear ribonucleoprotein F

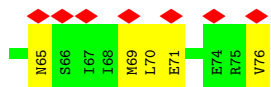
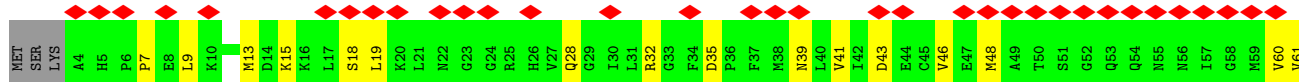




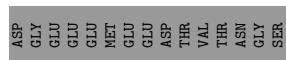
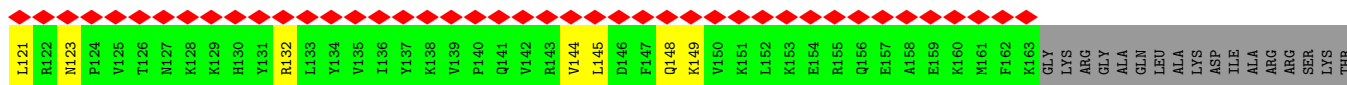
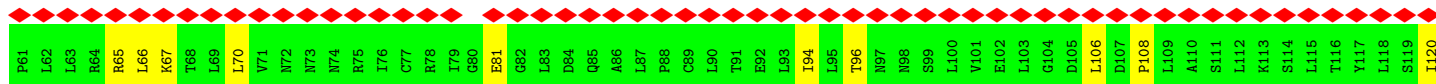
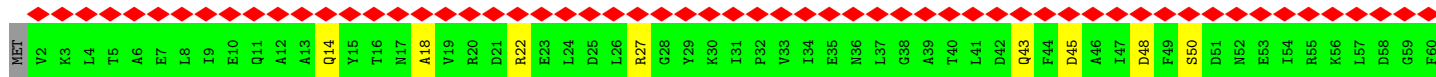
• Molecule 46: Small nuclear ribonucleoprotein G



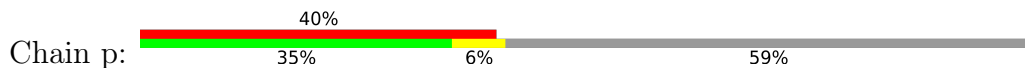
• Molecule 46: Small nuclear ribonucleoprotein G



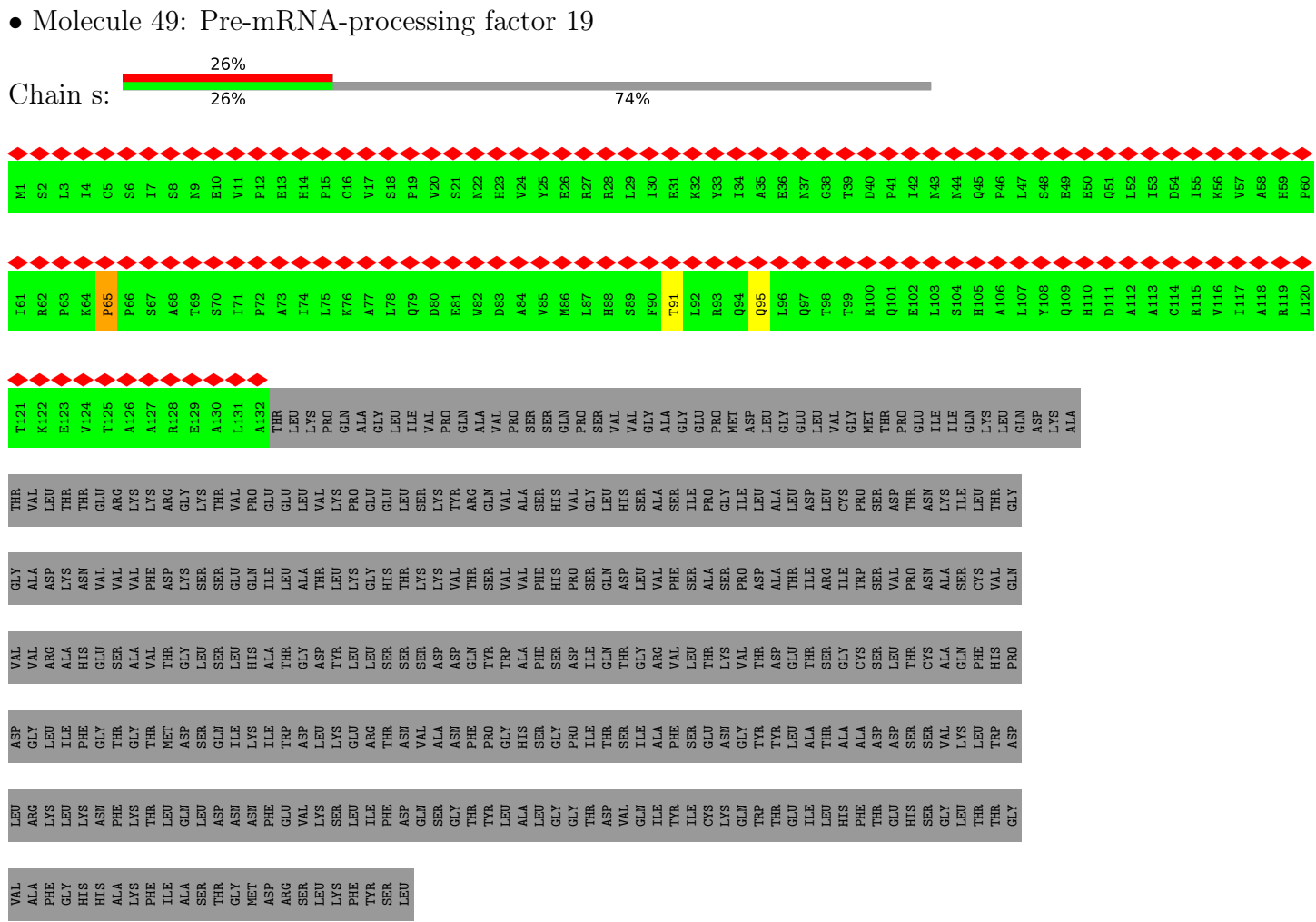
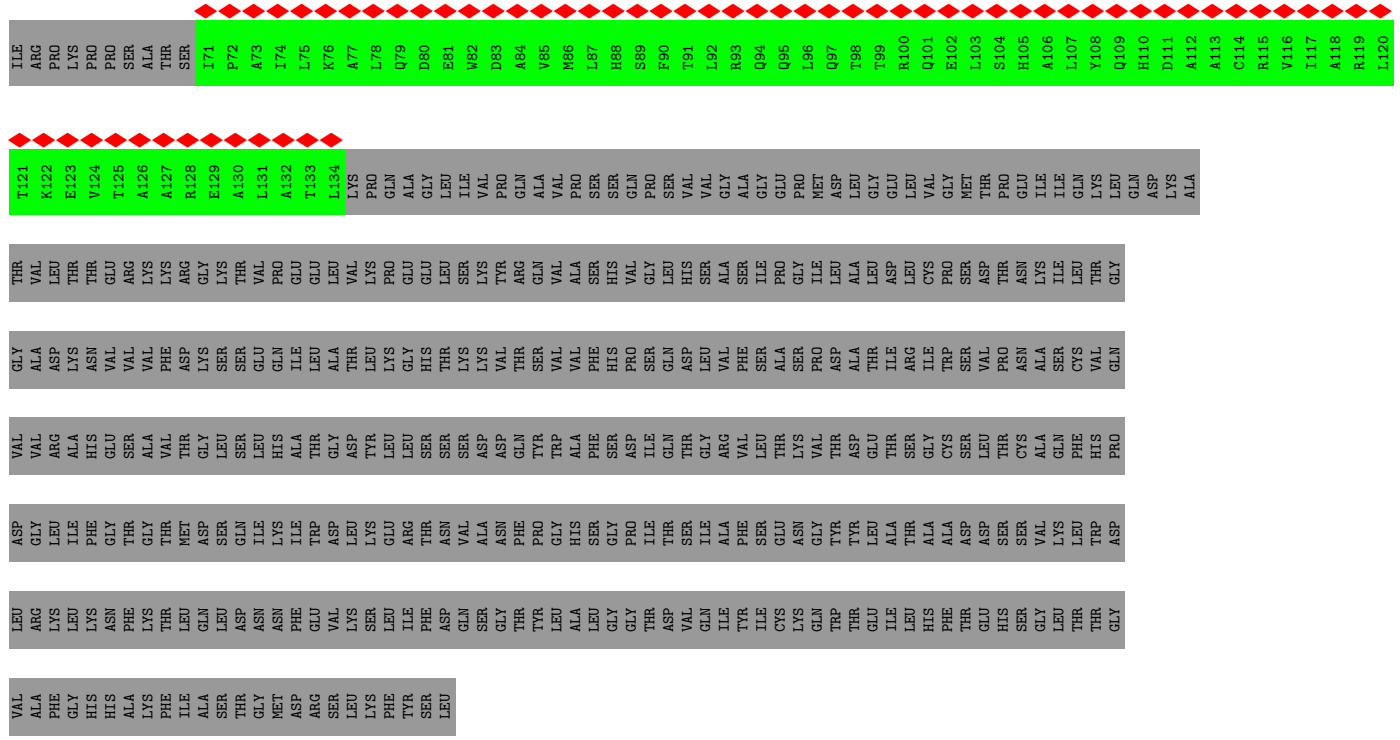
• Molecule 47: U2 small nuclear ribonucleoprotein A'



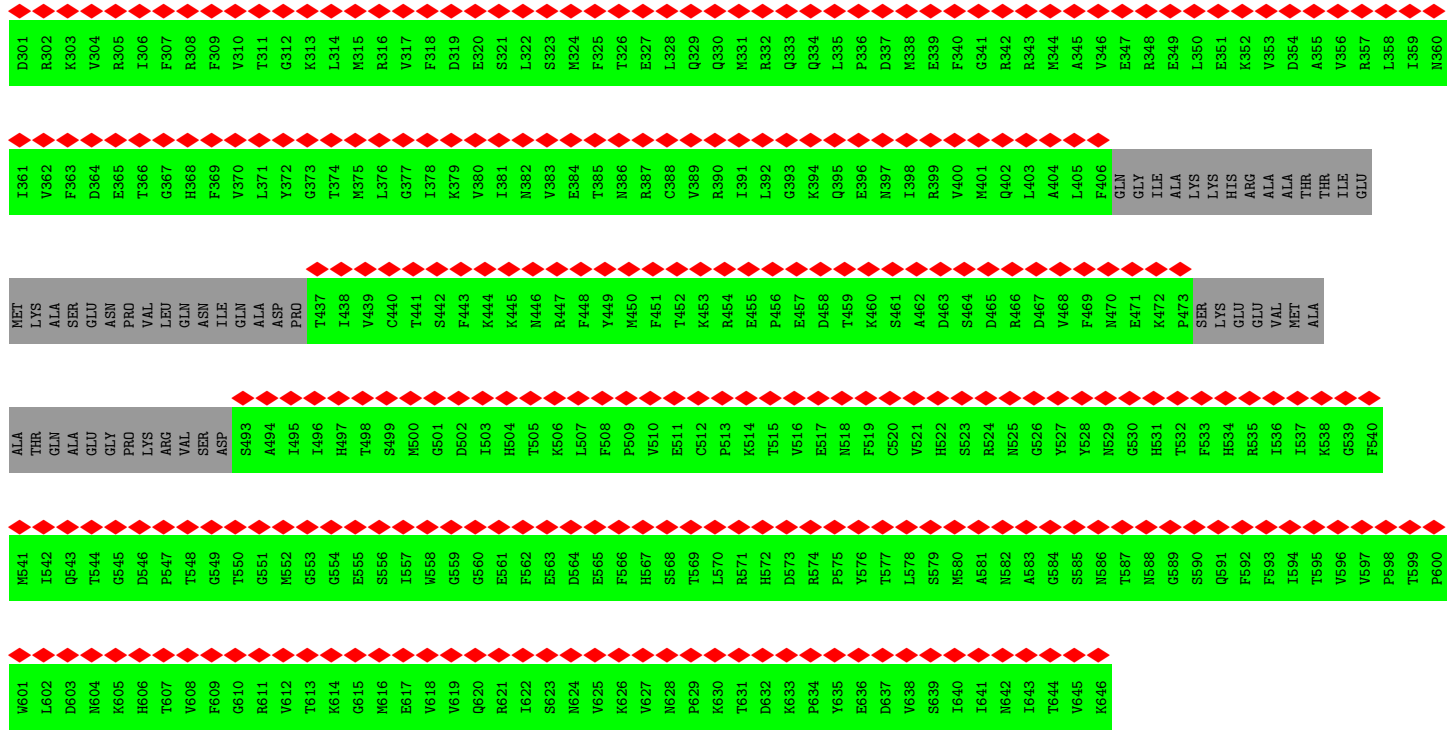
• Molecule 48: U2 small nuclear ribonucleoprotein B''



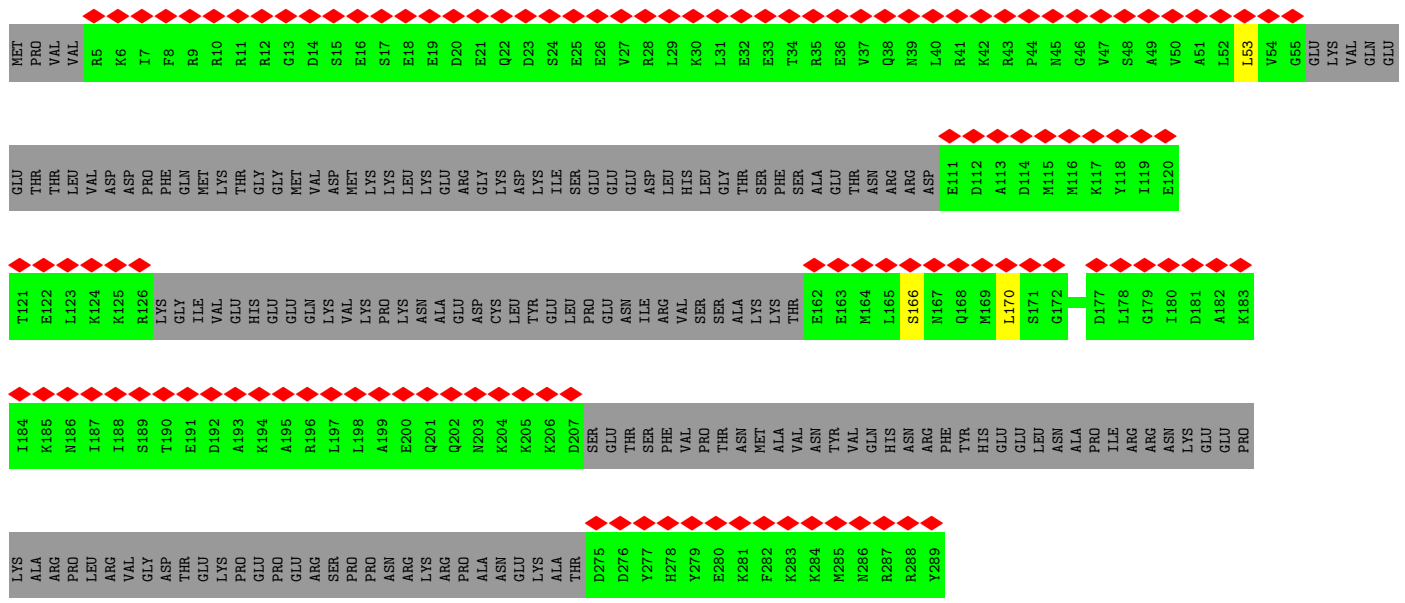




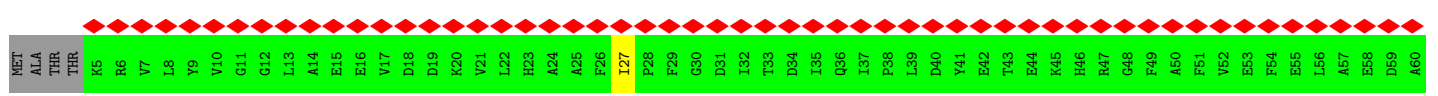




• Molecule 51: Splicing factor C9orf78



• Molecule 52: Peptidyl-prolyl cis-trans isomerase E





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
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	Not provided	
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: IHP, MG, GTP, K, ATP, ZN, SEP

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	1	0.33	0/1030	0.67	0/1371
2	2	0.38	0/2827	0.60	2/4393 (0.0%)
3	3	0.32	0/406	0.83	0/564
4	32	0.34	0/513	0.66	0/683
5	5	0.54	0/2157	0.79	6/3351 (0.2%)
6	50	0.63	0/1122	1.40	4/1562 (0.3%)
7	56	0.26	0/497	0.65	0/690
8	6	0.54	0/2323	0.66	1/3619 (0.0%)
9	7	0.35	0/1927	1.00	0/2681
10	8	0.34	0/444	0.91	0/614
11	9	0.38	0/711	0.94	0/987
12	A	0.58	0/18250	0.71	3/24798 (0.0%)
13	B	0.36	0/15311	0.92	13/20733 (0.1%)
14	C	0.53	0/7228	0.91	2/9822 (0.0%)
15	D	0.38	0/356	0.87	0/494
16	E	0.59	1/2424 (0.0%)	0.78	7/3285 (0.2%)
17	EX	0.91	0/329	1.68	8/510 (1.6%)
18	F	0.38	0/1134	0.65	0/1530
19	H	0.41	0/2965	0.83	1/4049 (0.0%)
20	I	0.37	0/3609	0.99	0/5036
21	IN	0.39	0/996	0.81	4/1544 (0.3%)
22	J	0.42	0/2997	1.03	0/4187
23	K	0.38	0/940	0.97	0/1312
24	L	0.42	0/3674	0.78	0/4988
25	M	0.34	0/1114	0.81	0/1553
26	N	0.49	0/1215	0.72	0/1627
27	NO	0.37	0/861	0.88	0/1197
28	O	0.43	0/2375	0.59	0/3204
29	P	0.41	0/903	0.64	0/1201
30	Q	0.36	0/6545	0.88	0/9115
31	R	0.43	0/2647	0.72	0/3554
32	S	0.31	0/1305	0.56	0/1767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	SR	0.48	0/414	0.73	0/568
34	T	0.66	0/2957	0.79	0/4023
35	U	0.43	0/2483	0.72	0/3341
36	V	0.34	0/3626	0.87	0/5050
37	W	0.47	0/4266	0.70	0/5761
38	X	0.29	0/326	0.87	0/452
39	Z	0.32	0/263	0.93	0/365
40	a	0.32	0/666	0.66	0/897
40	h	0.33	0/660	0.70	0/889
41	b	0.24	0/663	0.54	0/885
41	i	0.25	0/674	0.57	0/899
42	c	0.21	0/642	0.50	0/867
42	j	0.22	0/642	0.51	0/867
43	d	0.21	0/732	0.56	0/984
43	k	0.24	0/784	0.58	0/1053
44	e	0.24	0/659	0.63	0/885
44	l	0.26	0/677	0.63	0/908
45	f	0.32	0/574	0.71	0/775
45	m	0.29	0/574	0.65	0/775
46	g	0.29	0/575	0.63	0/768
46	n	0.27	0/575	0.60	0/768
47	o	0.25	0/1299	0.65	0/1761
48	p	0.22	0/759	0.50	0/1016
49	q	0.38	0/512	0.85	0/713
49	r	0.43	0/592	0.87	0/825
49	s	0.42	0/658	0.98	1/919 (0.1%)
49	t	0.40	0/512	0.96	0/713
50	w	0.33	0/2602	0.83	0/3615
51	x	0.33	0/632	0.90	0/874
52	y	0.25	0/317	0.77	1/396 (0.3%)
53	z	0.34	0/431	0.67	0/582
All	All	0.44	1/122881 (0.0%)	0.81	53/169215 (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
12	A	0	2
13	B	0	20
14	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	E	0	1
29	P	0	1
31	R	0	2
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	58	PRO	C-N	22.51	1.54	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	58	PRO	CA-C-N	13.57	138.10	122.36
16	E	58	PRO	C-N-CA	13.57	138.10	122.36
16	E	58	PRO	O-C-N	-13.42	104.26	122.24
6	50	196	SER	CA-C-N	13.16	139.56	120.87
6	50	196	SER	C-N-CA	13.16	139.56	120.87

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	1418	ARG	Sidechain
12	A	941	LYS	Peptide
13	B	129	ARG	Sidechain
13	B	728	ARG	Sidechain
13	B	739	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	1	1013	0	1058	10	0
2	2	2535	0	1281	29	0
3	3	408	0	181	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	32	504	0	509	11	0
5	5	1936	0	982	29	0
6	50	1124	0	485	31	0
7	56	498	0	220	0	0
8	6	2075	0	1048	29	0
9	7	1928	0	856	0	0
10	8	445	0	203	0	0
11	9	712	0	299	0	0
12	A	17802	0	17006	245	0
13	B	15004	0	15162	114	0
14	C	7069	0	7089	33	0
15	D	358	0	167	0	0
16	E	2370	0	2306	49	0
17	EX	296	0	153	2	0
18	F	1089	0	1023	25	0
19	H	2932	0	2204	17	0
20	I	3610	0	1639	0	0
21	IN	893	0	453	13	0
22	J	2998	0	1333	3	0
23	K	941	0	424	0	0
24	L	3642	0	2904	31	0
25	M	1115	0	513	0	0
26	N	1189	0	1192	17	0
27	NO	864	0	371	1	0
28	O	2327	0	2315	44	0
29	P	889	0	865	8	0
30	Q	6554	0	2828	1	0
31	R	2618	0	2664	36	0
32	S	1271	0	1244	17	0
33	SR	412	0	287	7	0
34	T	2881	0	2836	41	0
35	U	2425	0	2370	40	0
36	V	3629	0	1603	0	0
37	W	4158	0	4060	87	0
38	X	328	0	156	1	0
39	Z	265	0	114	1	0
40	a	658	0	675	17	0
40	h	652	0	670	15	0
41	b	654	0	667	18	0
41	i	664	0	690	14	0
42	c	634	0	680	14	0
42	j	634	0	680	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	d	723	0	750	12	0
43	k	774	0	802	13	0
44	e	651	0	671	7	0
44	l	669	0	692	11	0
45	f	562	0	574	9	0
45	m	562	0	574	11	0
46	g	568	0	590	9	0
46	n	568	0	590	13	0
47	o	1282	0	1305	15	0
48	p	745	0	767	9	0
49	q	514	0	236	0	0
49	r	594	0	270	0	0
49	s	659	0	299	1	0
49	t	514	0	236	0	0
50	w	2605	0	1124	3	0
51	x	636	0	276	10	0
52	y	318	0	88	0	0
53	z	430	0	321	3	0
54	6	5	0	0	0	0
54	7	1	0	0	0	0
55	6	1	0	0	0	0
56	7	31	0	12	0	0
57	C	32	0	12	0	0
58	N	3	0	0	0	0
58	O	3	0	0	0	0
59	U	36	0	6	1	0
All	All	120489	0	96660	985	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 5.

The worst 5 of 985 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)
6:50:336:TYR:O	18:F:667:ASN:HB2	1.14	1.30
6:50:288:VAL:CB	51:x:170:LEU:CB	2.12	1.27
28:O:144:SER:OG	28:O:147:LEU:HB2	1.42	1.17
6:50:288:VAL:CB	51:x:170:LEU:CA	2.28	1.10
6:50:336:TYR:O	18:F:667:ASN:CB	2.07	1.01

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	121/184 (66%)	114 (94%)	6 (5%)	1 (1%)	16	45
3	3	78/476 (16%)	78 (100%)	0	0	100	100
4	32	58/112 (52%)	56 (97%)	2 (3%)	0	100	100
6	50	222/339 (66%)	214 (96%)	6 (3%)	2 (1%)	14	43
7	56	99/222 (45%)	98 (99%)	1 (1%)	0	100	100
9	7	388/411 (94%)	377 (97%)	10 (3%)	1 (0%)	36	65
10	8	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	11	39
11	9	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
12	A	2244/2335 (96%)	2107 (94%)	134 (6%)	3 (0%)	48	75
13	B	1856/2136 (87%)	1785 (96%)	68 (4%)	3 (0%)	43	71
14	C	892/972 (92%)	816 (92%)	72 (8%)	4 (0%)	30	60
15	D	68/285 (24%)	67 (98%)	1 (2%)	0	100	100
16	E	301/357 (84%)	281 (93%)	20 (7%)	0	100	100
18	F	120/758 (16%)	109 (91%)	11 (9%)	0	100	100
19	H	455/908 (50%)	439 (96%)	15 (3%)	1 (0%)	43	71
20	I	725/855 (85%)	710 (98%)	15 (2%)	0	100	100
22	J	600/848 (71%)	572 (95%)	26 (4%)	2 (0%)	36	65
23	K	187/225 (83%)	174 (93%)	12 (6%)	1 (0%)	24	55
24	L	545/802 (68%)	524 (96%)	20 (4%)	1 (0%)	43	71
25	M	222/243 (91%)	215 (97%)	6 (3%)	1 (0%)	24	55
26	N	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	9	33
27	NO	168/301 (56%)	158 (94%)	8 (5%)	2 (1%)	10	37
28	O	287/420 (68%)	271 (94%)	16 (6%)	0	100	100
29	P	100/229 (44%)	94 (94%)	6 (6%)	0	100	100
30	Q	1304/1485 (88%)	1267 (97%)	34 (3%)	3 (0%)	43	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	R	322/536 (60%)	296 (92%)	25 (8%)	1 (0%)	36	65
32	S	162/166 (98%)	148 (91%)	14 (9%)	0	100	100
33	SR	66/2752 (2%)	59 (89%)	7 (11%)	0	100	100
34	T	359/514 (70%)	340 (95%)	16 (4%)	3 (1%)	16	45
35	U	291/586 (50%)	272 (94%)	18 (6%)	1 (0%)	36	65
36	V	727/1220 (60%)	708 (97%)	18 (2%)	1 (0%)	48	75
37	W	511/579 (88%)	462 (90%)	49 (10%)	0	100	100
38	X	62/451 (14%)	59 (95%)	3 (5%)	0	100	100
39	Z	49/166 (30%)	49 (100%)	0	0	100	100
40	a	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
40	h	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
41	b	81/240 (34%)	80 (99%)	1 (1%)	0	100	100
41	i	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
42	c	78/119 (66%)	73 (94%)	5 (6%)	0	100	100
42	j	78/119 (66%)	76 (97%)	2 (3%)	0	100	100
43	d	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
43	k	91/118 (77%)	88 (97%)	3 (3%)	0	100	100
44	e	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
44	l	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
45	f	70/86 (81%)	70 (100%)	0	0	100	100
45	m	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
46	g	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
46	n	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
47	o	160/255 (63%)	146 (91%)	14 (9%)	0	100	100
48	p	90/225 (40%)	88 (98%)	2 (2%)	0	100	100
49	q	99/504 (20%)	98 (99%)	1 (1%)	0	100	100
49	r	115/504 (23%)	111 (96%)	4 (4%)	0	100	100
49	s	130/504 (26%)	125 (96%)	4 (3%)	1 (1%)	16	45
49	t	99/504 (20%)	96 (97%)	2 (2%)	1 (1%)	12	40
50	w	522/646 (81%)	504 (97%)	18 (3%)	0	100	100
51	x	120/289 (42%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
53	z	66/415 (16%)	64 (97%)	1 (2%)	1 (2%)	8	32
All	All	16534/28198 (59%)	15754 (95%)	743 (4%)	37 (0%)	44	71

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	50	285	HIS
13	B	1584	ILE
30	Q	1078	LEU
49	s	65	PRO
9	7	340	GLY

### 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	
1	1	106/157 (68%)	106 (100%)	0	100	100
4	32	54/99 (54%)	54 (100%)	0	100	100
12	A	1732/2108 (82%)	1721 (99%)	11 (1%)	78	81
13	B	1662/1908 (87%)	1496 (90%)	166 (10%)	7	27
14	C	109/866 (13%)	106 (97%)	3 (3%)	38	62
16	E	87/300 (29%)	86 (99%)	1 (1%)	65	76
18	F	100/655 (15%)	100 (100%)	0	100	100
24	L	233/709 (33%)	228 (98%)	5 (2%)	47	67
26	N	130/130 (100%)	130 (100%)	0	100	100
28	O	258/361 (72%)	256 (99%)	2 (1%)	73	79
29	P	94/203 (46%)	92 (98%)	2 (2%)	47	67
31	R	275/457 (60%)	275 (100%)	0	100	100
32	S	133/134 (99%)	132 (99%)	1 (1%)	73	79
33	SR	21/2432 (1%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	T	316/441 (72%)	308 (98%)	8 (2%)	42	64
35	U	258/520 (50%)	251 (97%)	7 (3%)	39	63
37	W	451/502 (90%)	447 (99%)	4 (1%)	70	78
40	a	74/101 (73%)	74 (100%)	0	100	100
40	h	73/101 (72%)	73 (100%)	0	100	100
41	b	68/177 (38%)	67 (98%)	1 (2%)	57	72
41	i	75/177 (42%)	75 (100%)	0	100	100
42	c	75/101 (74%)	75 (100%)	0	100	100
42	j	75/101 (74%)	75 (100%)	0	100	100
43	d	85/110 (77%)	84 (99%)	1 (1%)	63	75
43	k	91/110 (83%)	91 (100%)	0	100	100
44	e	74/84 (88%)	74 (100%)	0	100	100
44	l	76/84 (90%)	76 (100%)	0	100	100
45	f	61/74 (82%)	60 (98%)	1 (2%)	55	72
45	m	61/74 (82%)	61 (100%)	0	100	100
46	g	63/66 (96%)	62 (98%)	1 (2%)	55	72
46	n	63/66 (96%)	61 (97%)	2 (3%)	34	60
47	o	139/218 (64%)	137 (99%)	2 (1%)	59	73
48	p	81/195 (42%)	81 (100%)	0	100	100
53	z	25/366 (7%)	25 (100%)	0	100	100
All	All	7278/14187 (51%)	7060 (97%)	218 (3%)	37	61

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	B	1368	LEU
13	B	1788	LEU
35	U	181	ILE
13	B	1419	LEU
13	B	1481	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
40	h	40	ASN
42	j	21	ASN
47	o	72	ASN
13	B	1528	GLN
13	B	1449	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	EX	14/14 (100%)	5 (35%)	1 (7%)
2	2	117/187 (62%)	30 (25%)	5 (4%)
21	IN	39/113 (34%)	19 (48%)	3 (7%)
5	5	90/116 (77%)	23 (25%)	2 (2%)
8	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	356/536 (66%)	114 (32%)	16 (4%)

5 of 114 RNA backbone outliers are listed below:

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

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	IN	95	U
21	IN	90	C
8	6	33	G
17	EX	-12	G
8	6	5	U

## 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
31	SEP	R	232	31	8,9,10	1.64	1 (12%)	7,12,14	1.06	0
31	SEP	R	224	31	8,9,10	1.52	1 (12%)	7,12,14	0.89	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
31	SEP	R	232	31	-	3/6/8/10	-
31	SEP	R	224	31	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	232	SEP	P-O1P	3.52	1.61	1.50
31	R	224	SEP	P-O1P	3.21	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	R	232	SEP	CB-OG-P-O1P
31	R	232	SEP	CB-OG-P-O2P
31	R	232	SEP	CB-OG-P-O3P
31	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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
59	IHP	U	601	-	36,36,36	1.38	6 (16%)	60,60,60	1.17	7 (11%)
56	ATP	7	501	54	32,33,33	0.53	1 (3%)	48,52,52	0.72	1 (2%)
57	GTP	C	1500	-	33,34,34	1.00	1 (3%)	50,54,54	1.72	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	IHP	U	601	-	-	6/30/54/54	0/1/1/1
56	ATP	7	501	54	-	0/22/38/38	0/3/3/3
57	GTP	C	1500	-	-	1/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	U	601	IHP	P3-O13	2.76	1.64	1.59
59	U	601	IHP	P6-O16	2.64	1.64	1.59
59	U	601	IHP	P2-O12	2.41	1.63	1.59
57	C	1500	GTP	C5-N7	-2.34	1.34	1.39
59	U	601	IHP	P5-O15	2.30	1.63	1.59

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	1500	GTP	C5-C4-N3	-5.09	120.29	128.39
57	C	1500	GTP	C2-N3-C4	4.37	119.83	112.30
57	C	1500	GTP	N9-C4-N3	3.58	133.11	125.95
57	C	1500	GTP	C2-N1-C6	-3.31	119.11	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	U	601	IHP	C6-C1-C2	-3.04	103.75	110.43

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

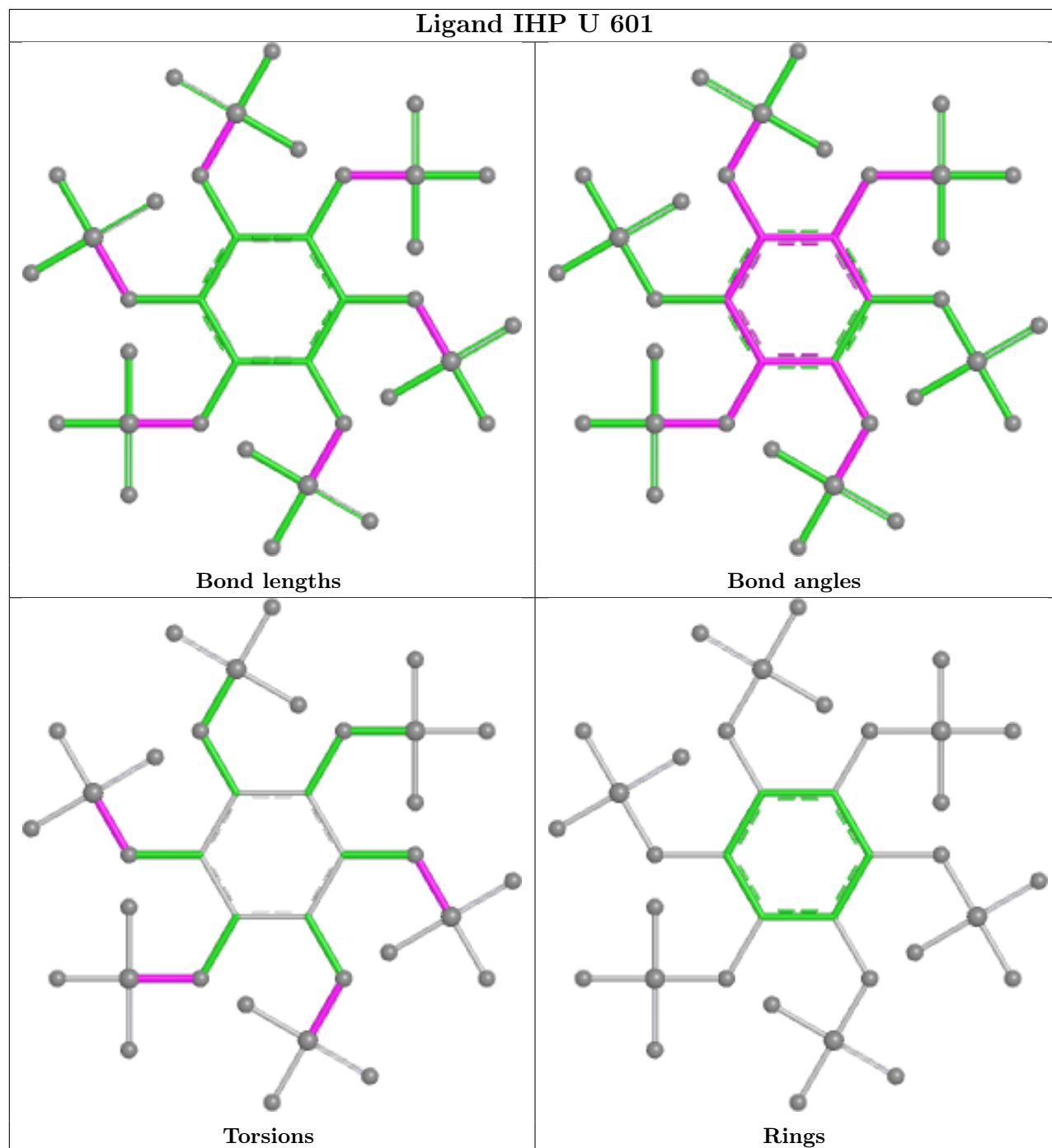
Mol	Chain	Res	Type	Atoms
59	U	601	IHP	C5-O15-P5-O25
59	U	601	IHP	C1-O11-P1-O31
59	U	601	IHP	C2-O12-P2-O42
59	U	601	IHP	C6-O16-P6-O46
59	U	601	IHP	C1-O11-P1-O41

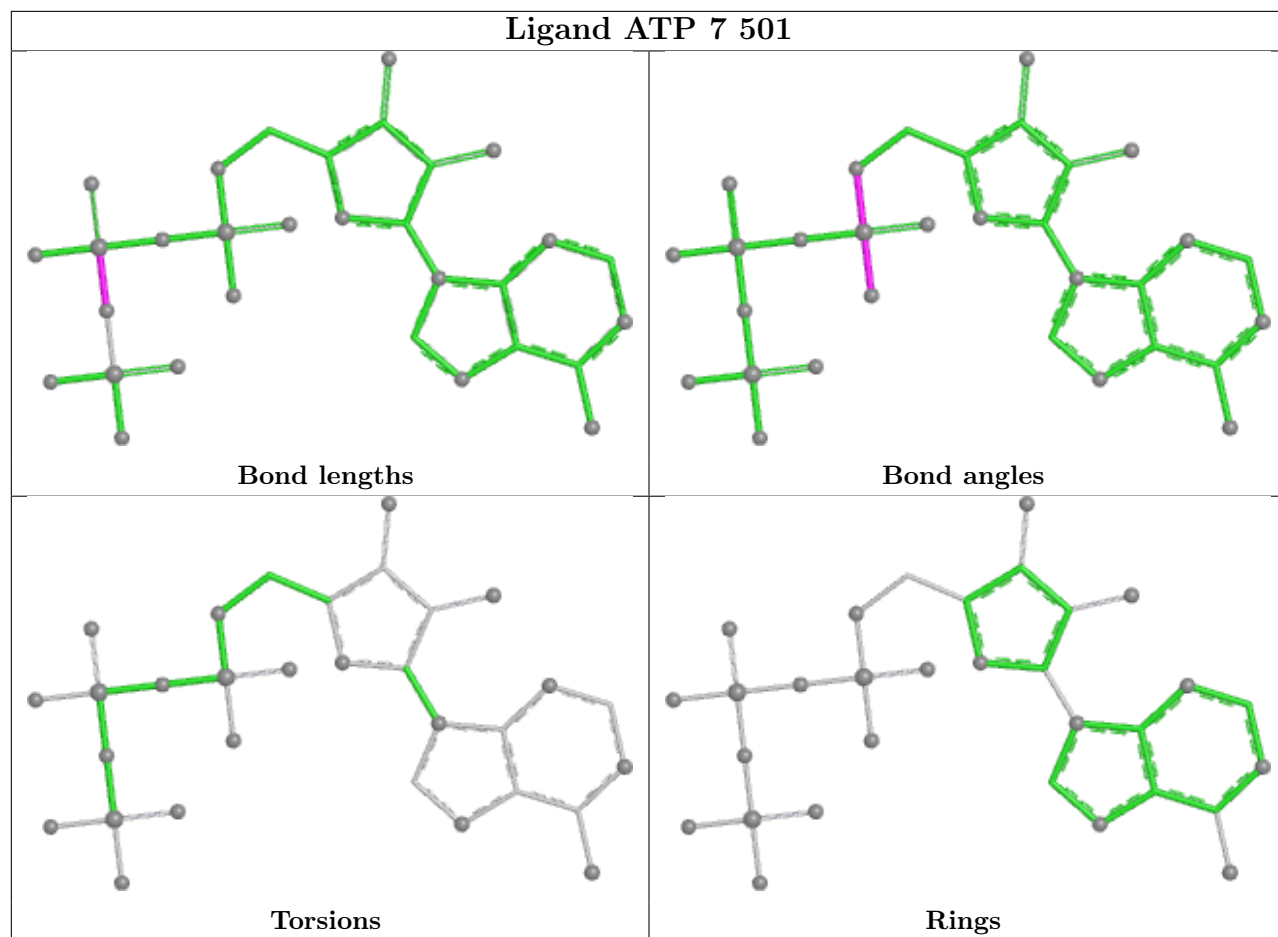
There are no ring outliers.

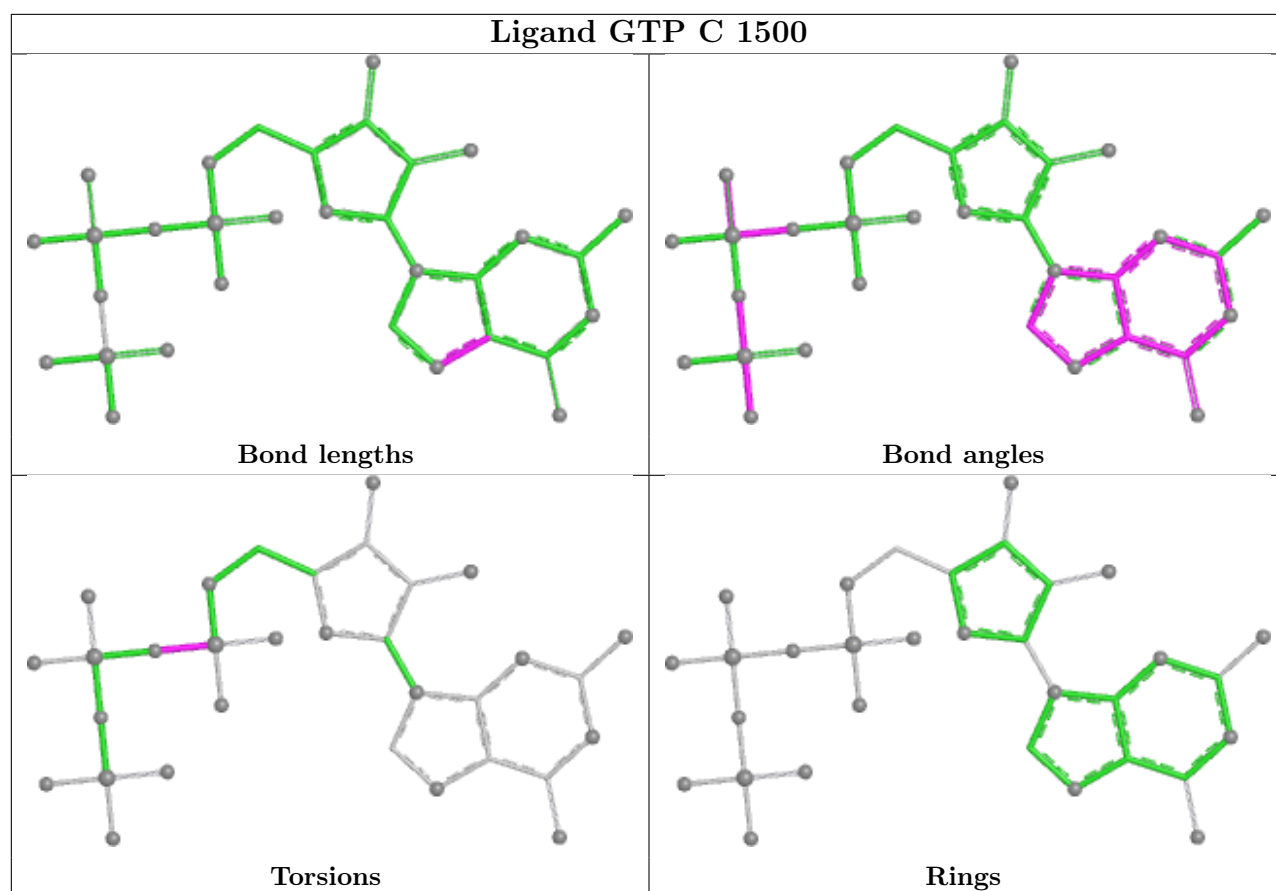
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	U	601	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.

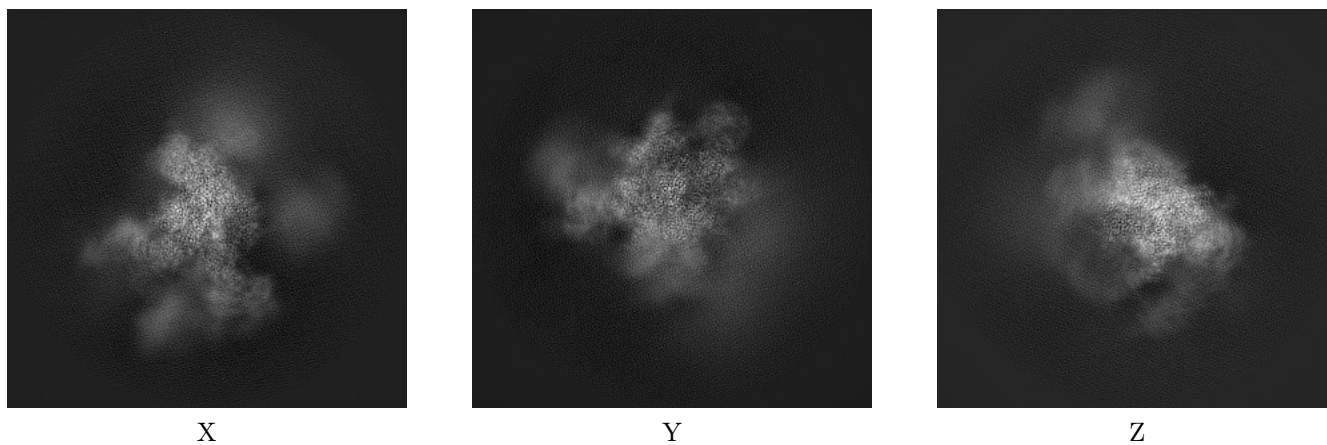
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-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](#)

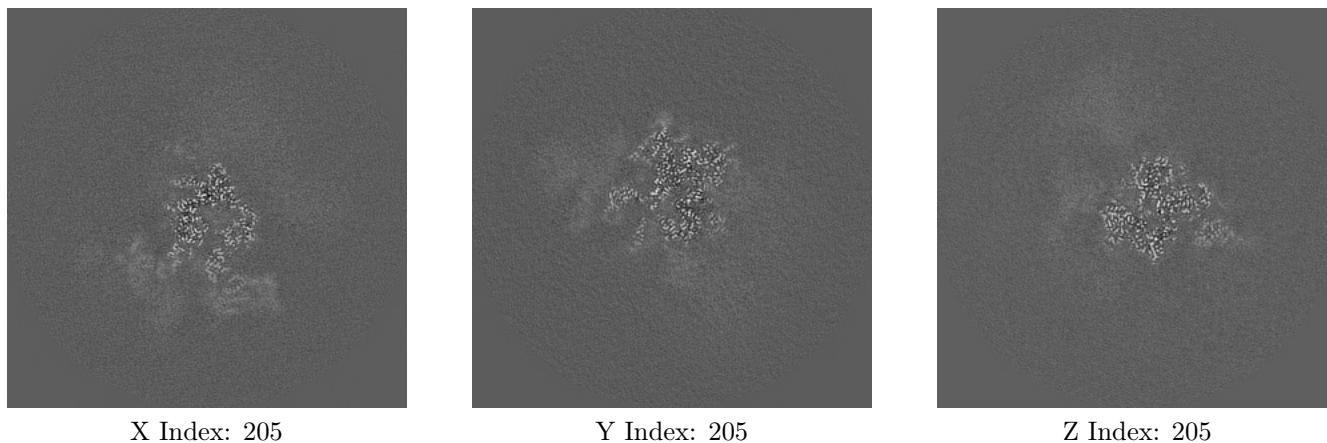
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

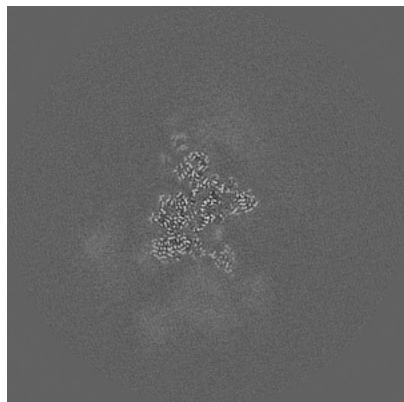
#### 6.2.1 Primary map



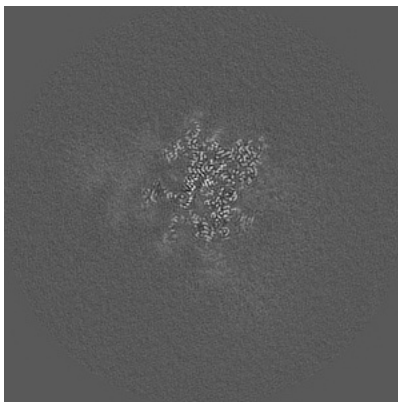
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

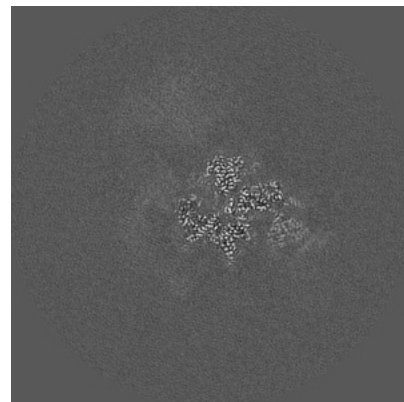
### 6.3.1 Primary map



X Index: 231



Y Index: 203

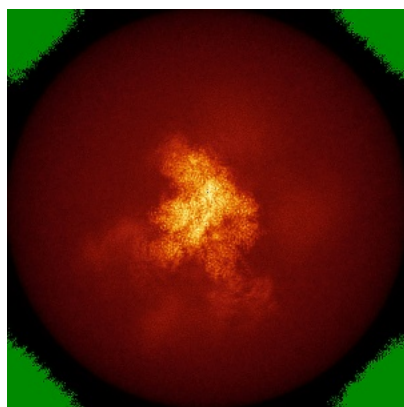


Z Index: 202

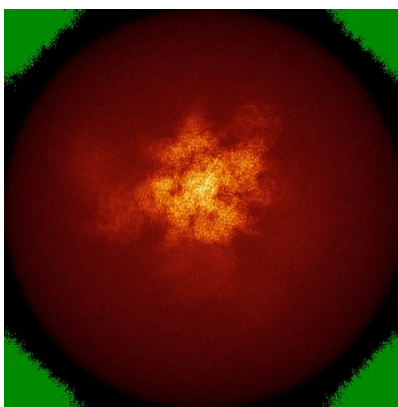
The images above show the largest variance slices of the map in three orthogonal directions.

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

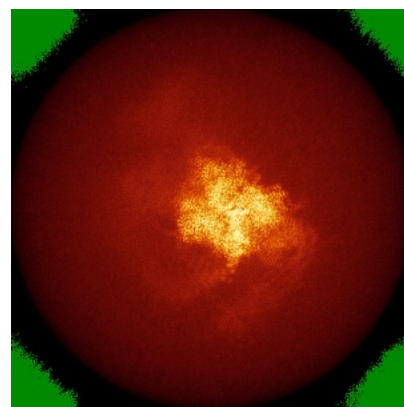
### 6.4.1 Primary map



X



Y



Z

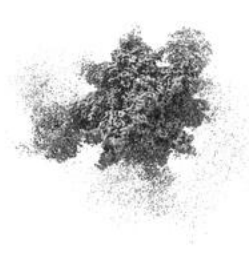
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

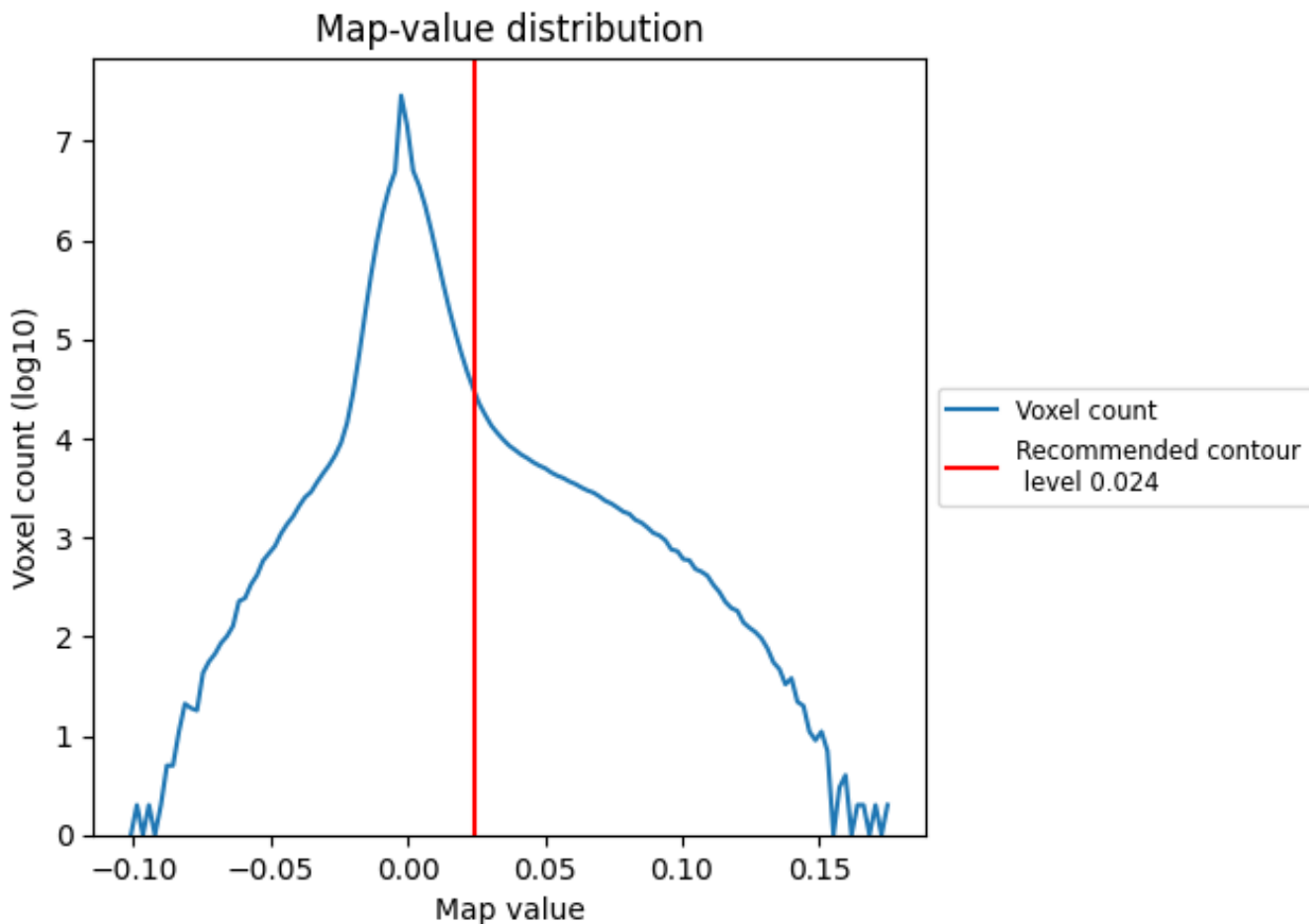
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

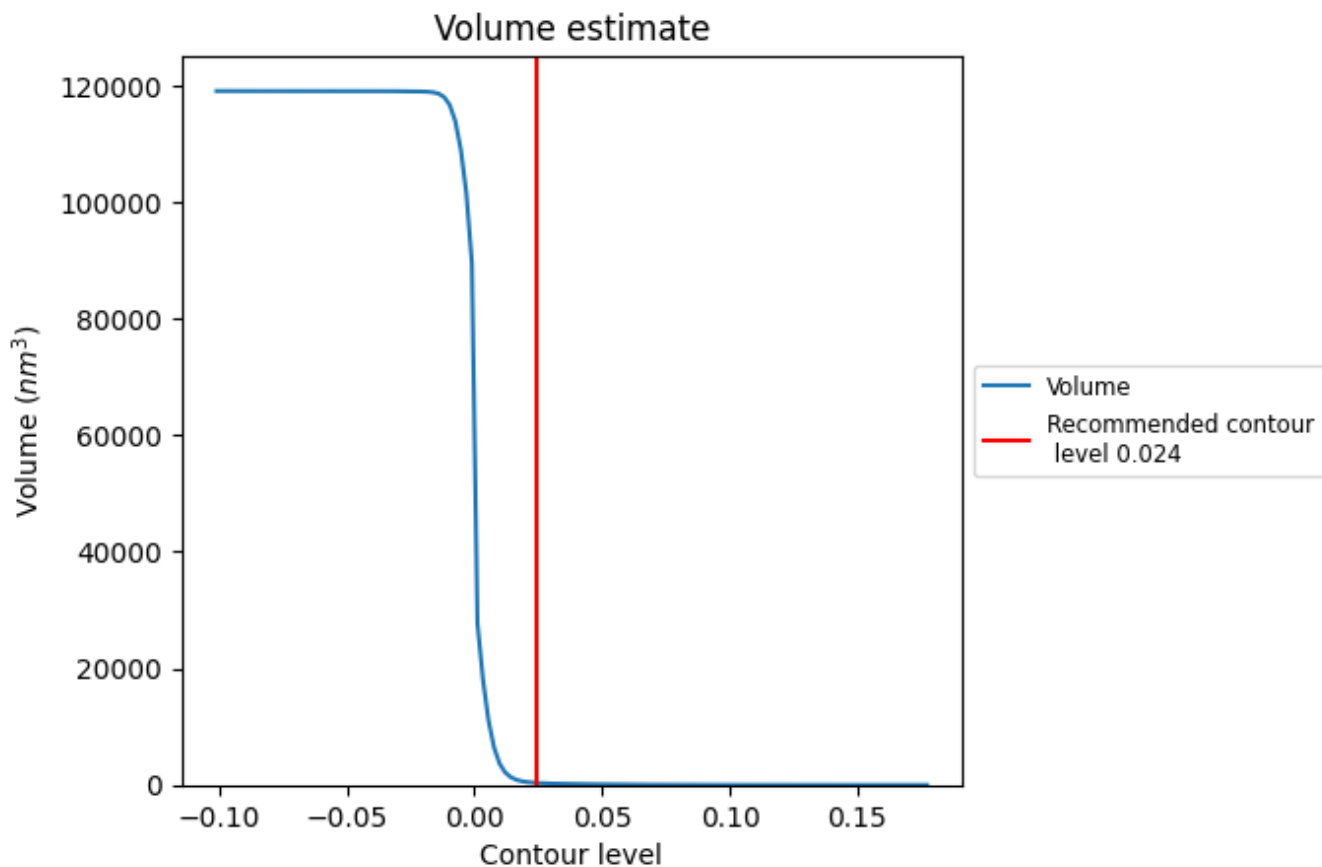
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

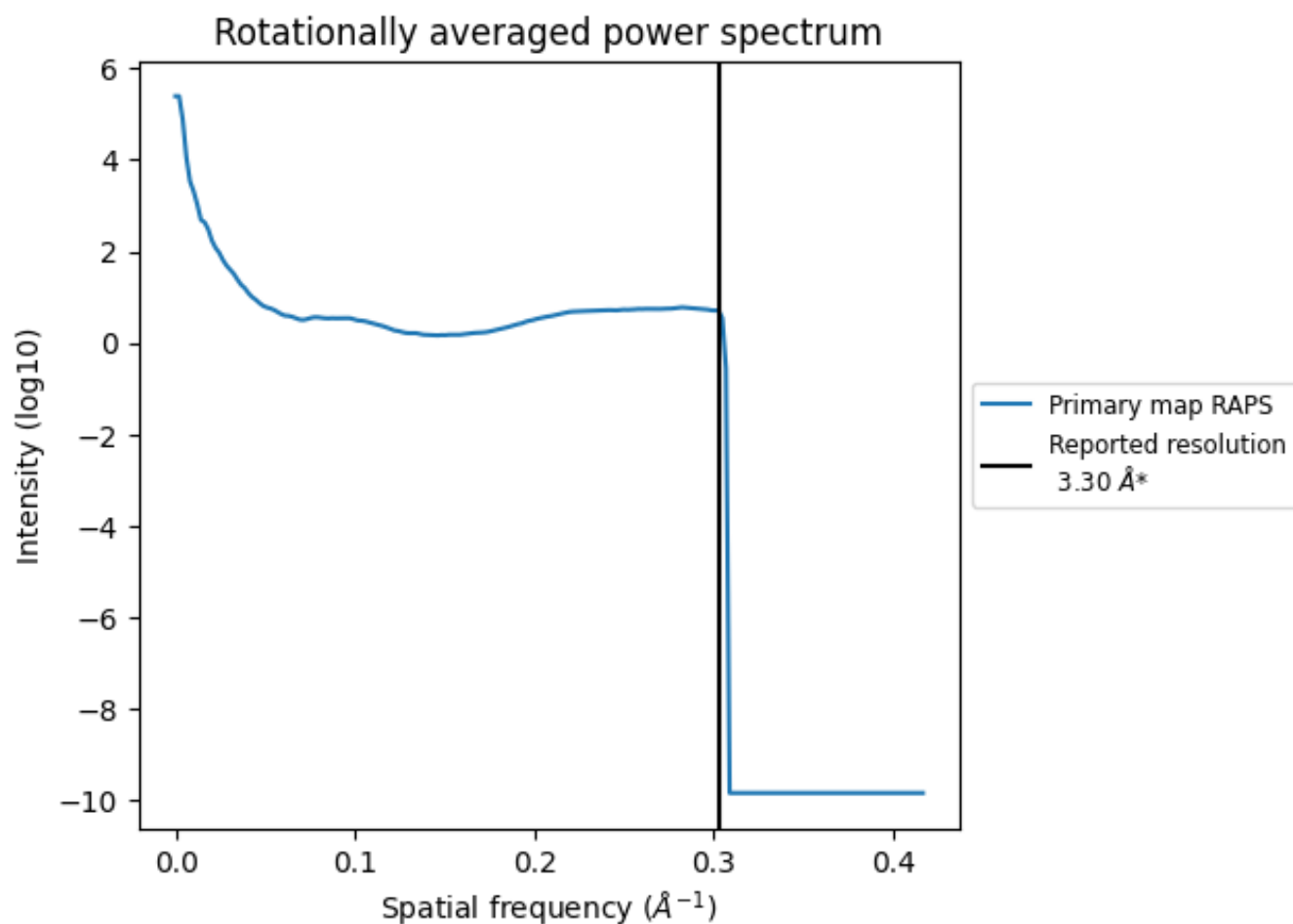
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm<sup>3</sup>; 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 [\(i\)](#)

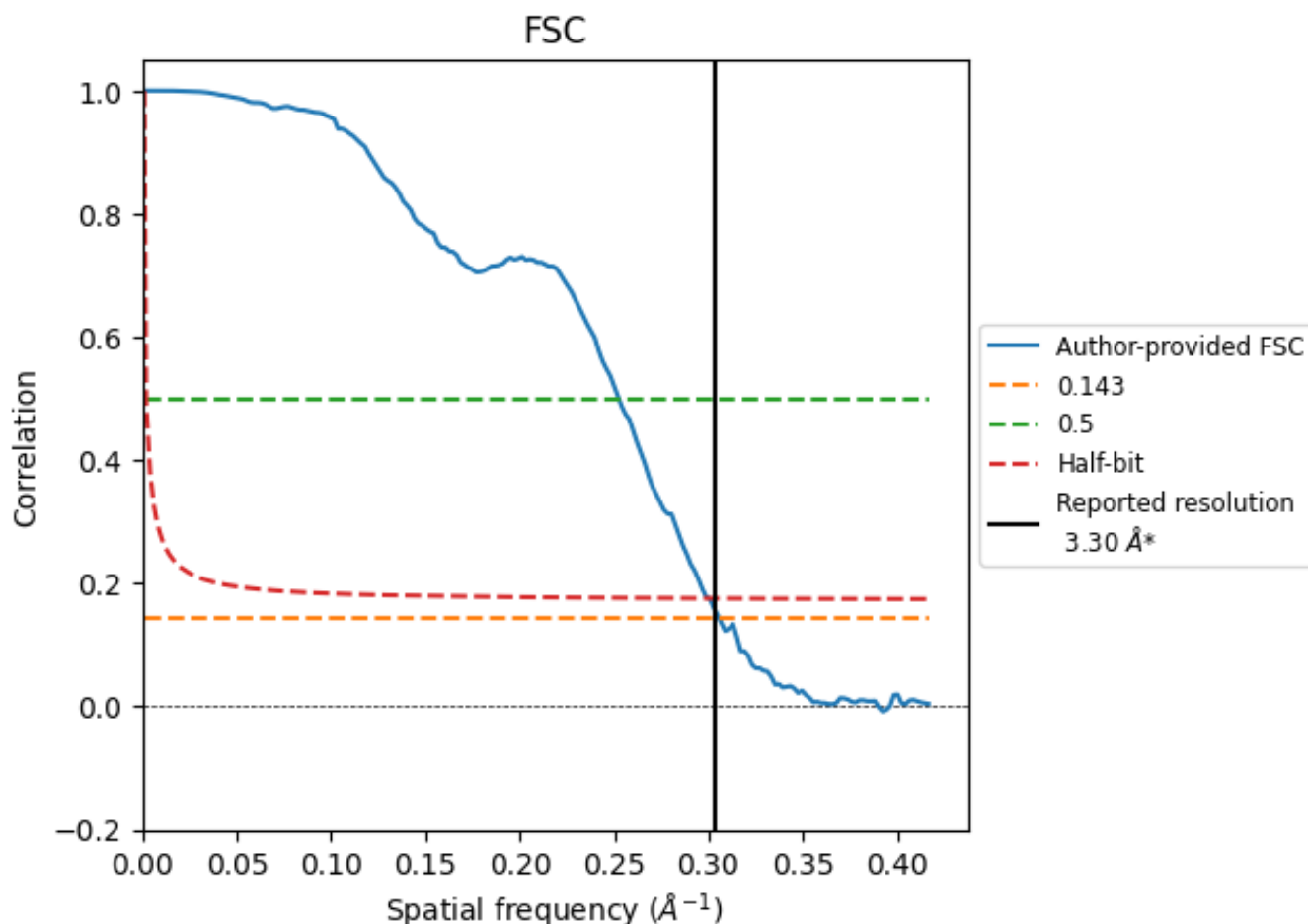


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

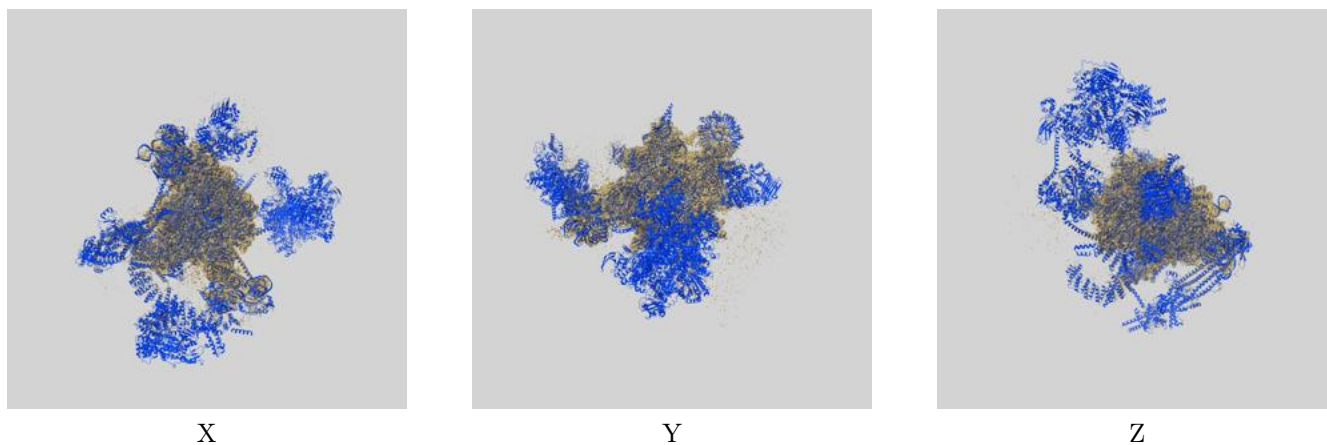
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

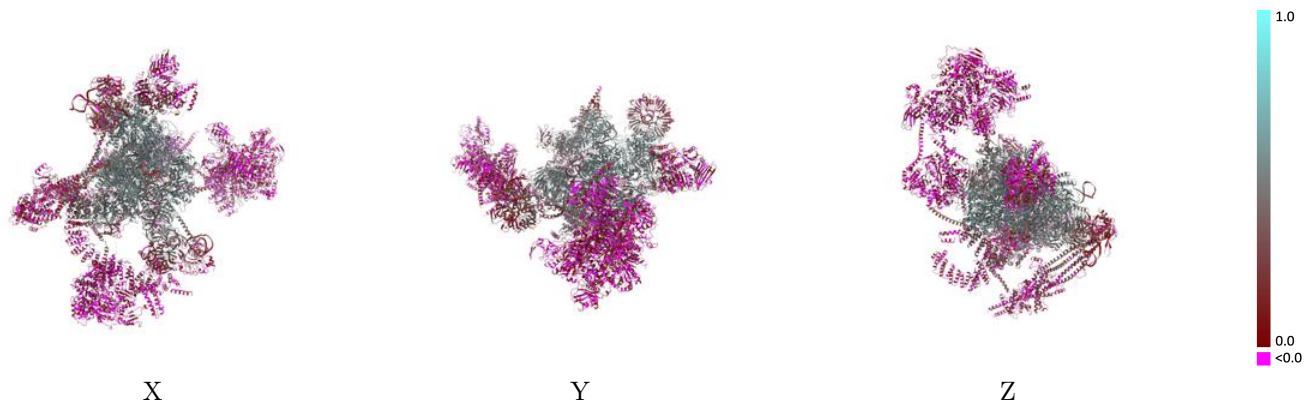
This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 9FMD. Per-residue inclusion information can be found in section [3](#) on page [17](#).

### 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](#)

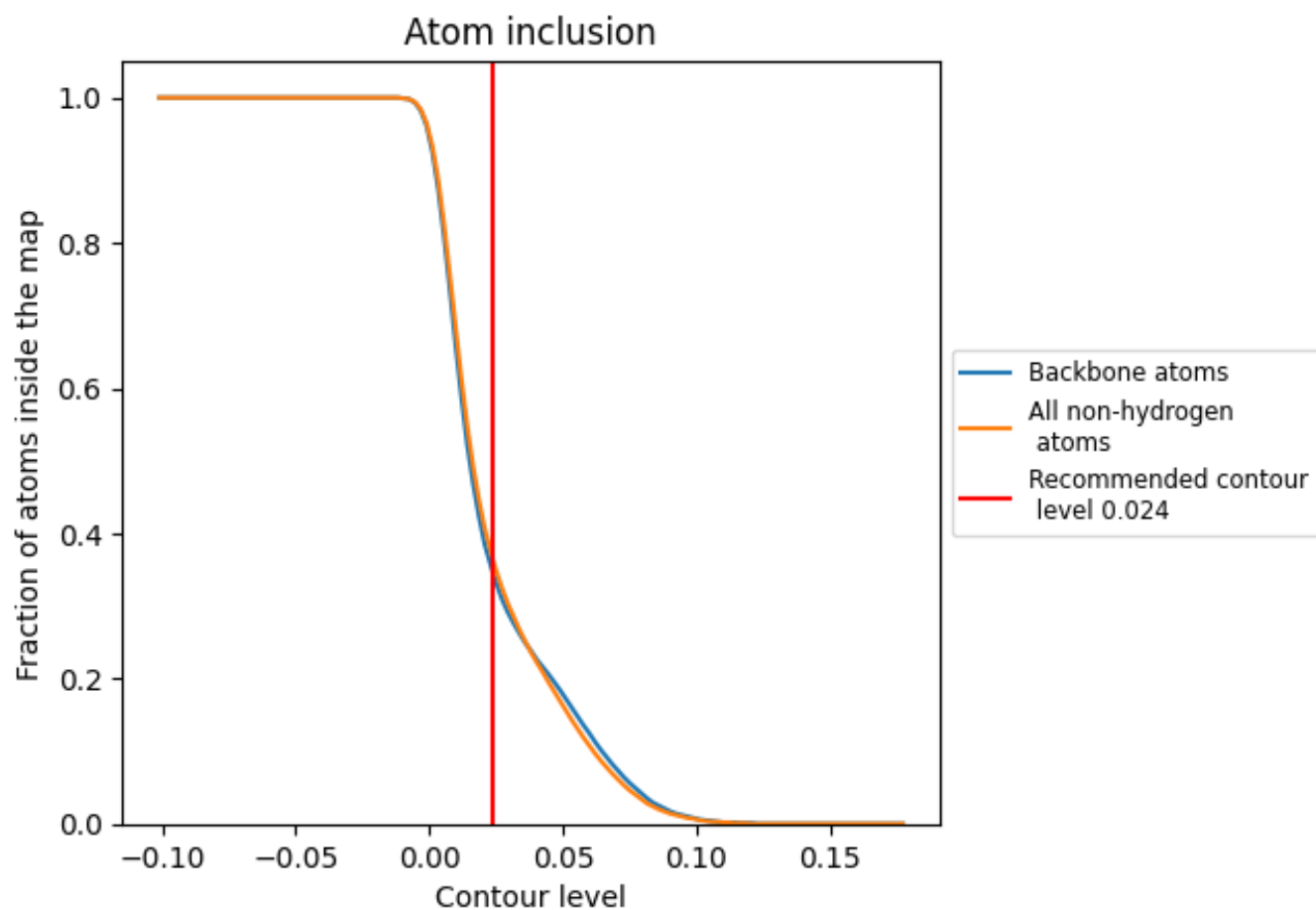


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 34% 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	 0.3610	 0.2970
1	 0.4060	 0.3790
2	 0.4230	 0.3010
3	 0.1450	 0.2540
32	 0.5850	 0.5090
5	 0.6140	 0.3800
50	 0.0160	 0.0940
56	 0.0000	 -0.0080
6	 0.7320	 0.4560
7	 0.0070	 0.1120
8	 0.0000	 0.0520
9	 0.0000	 0.0410
A	 0.7230	 0.5070
B	 0.0010	 0.0490
C	 0.6930	 0.4900
D	 0.0000	 0.0980
E	 0.6300	 0.4760
EX	 0.8110	 0.5290
F	 0.6270	 0.4680
H	 0.4160	 0.3540
I	 0.0520	 0.1010
IN	 0.5690	 0.3790
J	 0.3950	 0.2850
K	 0.1140	 0.1850
L	 0.4040	 0.3650
M	 0.4950	 0.3800
N	 0.7540	 0.5330
NO	 0.0010	 0.1280
O	 0.5190	 0.4460
P	 0.6500	 0.5200
Q	 0.0020	 0.0540
R	 0.5290	 0.4400
S	 0.5720	 0.4560
SR	 0.4090	 0.3340
T	 0.7370	 0.5080



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Chain	Atom inclusion	Q-score
U	 0.5840	 0.4550
V	 0.0500	 0.0800
W	 0.6700	 0.5010
X	 0.0150	 0.1510
Z	 0.0150	 0.0570
a	 0.4280	 0.4140
b	 0.3330	 0.3340
c	 0.1390	 0.2060
d	 0.0680	 0.1490
e	 0.0870	 0.1940
f	 0.0470	 0.1550
g	 0.2180	 0.3330
h	 0.3940	 0.3510
i	 0.2460	 0.2900
j	 0.1200	 0.2020
k	 0.0810	 0.1590
l	 0.2390	 0.2770
m	 0.1380	 0.1770
n	 0.3620	 0.3680
o	 0.0250	 0.1130
p	 0.0560	 0.1370
q	 0.0430	 0.1160
r	 0.0180	 0.0870
s	 0.0290	 0.1440
t	 0.0120	 0.0880
w	 0.0000	 0.0340
x	 0.0270	 0.1330
y	 0.0060	 0.1250
z	 0.3540	 0.2970