



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 12:43 am GMT

PDB ID : 6QX9  
EMDB ID : EMD-4665  
Title : Structure of a human fully-assembled precatalytic spliceosome (pre-B complex).  
Authors : Charenton, C.; Wilkinson, M.E.; Nagai, K.  
Deposited on : 2019-03-07  
Resolution : 3.28 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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:

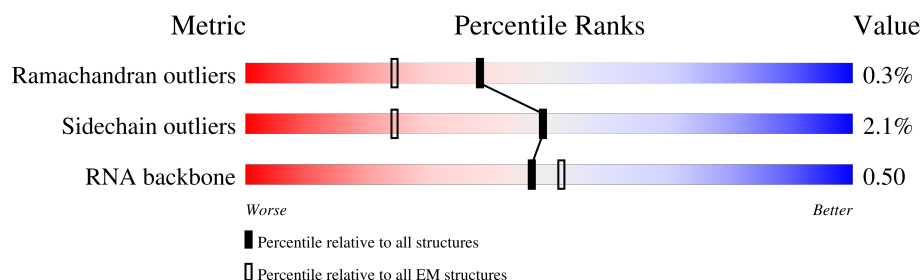
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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  $\geq 3$ , 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	164	<div> <div>100%</div> <div> <div>66%</div> <div>30%</div> <div>.</div> </div> </div>
2	6	106	<div> <div>17%</div> <div>36%</div> <div>12%</div> <div>.</div> <div>50%</div> </div>
3	5O	357	<div> <div>75%</div> <div>85%</div> <div>.</div> <div>14%</div> </div>
4	B4	424	<div> <div>18%</div> <div>18%</div> <div>82%</div> </div>
5	13	126	<div> <div>64%</div> <div>56%</div> <div>6%</div> <div>.</div> <div>36%</div> </div>
5	23	126	<div> <div>66%</div> <div>66%</div> <div>34%</div> </div>
5	43	126	<div> <div>53%</div> <div>65%</div> <div>.</div> <div>34%</div> </div>
5	53	126	<div> <div>.</div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
6	4B	522	
7	1e	92	
7	2e	92	
7	4e	92	
7	5e	92	
8	I	62	
9	1K	437	
10	4C	499	
11	11	119	
11	21	119	
11	41	119	
11	51	119	
12	R	480	
13	1f	86	
13	2f	86	
13	4f	86	
13	5f	86	
14	66	80	
15	X	155	
16	12	118	
16	22	118	
16	42	118	
16	52	118	
17	5	117	
18	67	103	


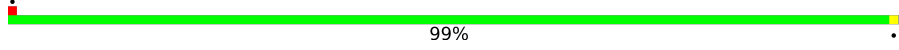
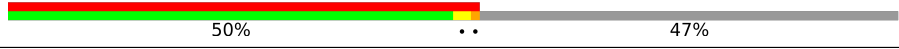
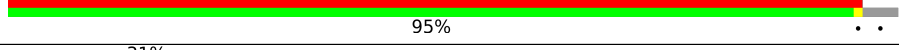


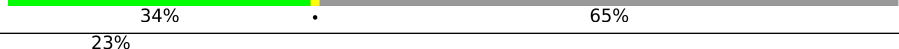

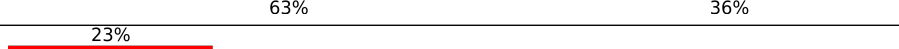


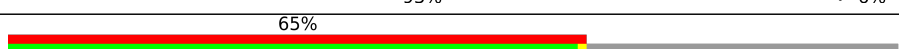
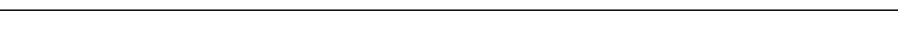
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Mol	Chain	Length	Quality of chain
19	62	95	
20	2B	225	
21	A2	209	
22	B2	895	
23	5C	854	
24	5X	820	
25	1b	240	
25	2b	240	
25	4b	240	
25	5b	240	
26	B5	86	
27	1A	282	
28	S	800	
29	5J	850	
30	4D	128	
31	63	102	
32	2	188	
33	B3	1217	
34	1g	76	
34	2g	76	
34	4g	76	
34	5g	76	
35	68	96	
36	5A	2311	
37	A3	501	

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Mol	Chain	Length	Quality of chain
38	U	555	
39	5D	142	
40	64	139	
41	BP	104	
42	1C	159	
43	K	1007	
44	4A	683	
45	4	146	
46	2A	255	
47	A1	647	
48	65	91	
49	5B	2136	
50	B1	1304	

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 137494 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 U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	164	Total	C	N	O	P	0	0
			3485	1555	607	1159	164		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	53	Total	C	N	O	P	0	0
			1133	506	203	371	53		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5O	306	Total	C	N	O	S	0	0
			2394	1501	422	457	14		

- Molecule 4 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B4	78	Total	C	N	O	S	0	0
			618	399	101	115	3		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	13	81	Total	C	N	O	S	0	0
			637	400	112	119	6		
5	53	84	Total	C	N	O	S	0	0
			657	412	116	123	6		
5	23	83	Total	C	N	O	S	0	0
			652	409	115	122	6		
5	43	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4B	359	Total	C	N	O	S	0	0
			2842	1793	509	521	19		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		
7	4e	76	Total	C	N	O	S	0	0
			631	400	112	114	5		
7	1e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		
7	2e	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 8 is a RNA chain called AdML pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	25	Total	C	N	O	P	0	0
			530	237	92	177	24		

- Molecule 9 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1K	201	Total	C	N	O	S	0	0
			1649	1036	317	291	5		

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4C	301	Total	C	N	O	S	0	0
			2375	1486	418	456	15		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	41	81	Total	C	N	O	S	0	0
			641	408	112	118	3		
11	11	81	Total	C	N	O	S	0	0
			641	408	112	118	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	51	81	Total	C	N	O	S	0	0
			641	408	112	118	3		
11	21	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

- Molecule 12 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	106	Total	C	N	O	S	0	0
			874	553	160	157	4		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
13	2f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
13	5f	73	Total	C	N	O	S	0	0
			567	367	94	101	5		
13	4f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	66	72	Total	C	N	O	S	0	0
			567	360	97	108	2		

- Molecule 15 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	49	Total	C	N	O	S	0	0
			394	247	74	69	4		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	22	95	Total	C	N	O	S	0	0
			774	486	141	142	5		
16	42	92	Total	C	N	O	S	0	0
			737	463	138	131	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	52	98	Total	C	N	O	S	0	0
			796	498	144	148	6		
16	12	95	Total	C	N	O	S	0	0
			777	486	141	144	6		

- Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	67	77	Total	C	N	O	S	0	0
			604	383	102	116	3		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	62	95	Total	C	N	O	S	0	0
			761	486	126	145	4		

- Molecule 20 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2B	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 21 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A2	144	Total	C	N	O	S	0	0
			1221	782	219	214	6		

- Molecule 22 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B2	208	Total	C	N	O	S	0	0
			1699	1093	302	295	9		

- Molecule 23 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5C	852	Total	C	N	O	S	0	0
			6727	4300	1127	1266	34		

- Molecule 24 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5X	583	Total	C	N	O	S	7	0
			4780	3014	855	893	18		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1b	86	Total	C	N	O	S	0	0
			692	435	126	124	7		
25	2b	82	Total	C	N	O	S	0	0
			664	419	121	117	7		
25	5b	73	Total	C	N	O	S	0	0
			594	376	108	103	7		
25	4b	82	Total	C	N	O	S	0	0
			669	423	122	117	7		

- Molecule 26 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B5	69	Total	C	N	O	S	0	0
			567	360	99	103	5		

- Molecule 27 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1A	98	Total	C	N	O	S	0	0
			787	506	134	143	4		

- Molecule 28 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	120	Total	C	N	O	S	0	0
			917	576	168	168	5		

- Molecule 29 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5J	803	Total	C	N	O	S	0	0
			6316	3963	1155	1170	28		

- Molecule 30 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4D	123	Total	C	N	O	S	0	0
			955	604	170	176	5		

- Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	63	85	Total	C	N	O	S	0	0
			699	440	120	136	3		

- Molecule 32 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2	94	Total	C	N	O	P	0	0
			1984	887	331	672	94		

- Molecule 33 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B3	1186	Total	C	N	O	S	0	0
			9296	5898	1580	1773	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
34	2g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
34	5g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
34	4g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		

- Molecule 35 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	68	95	Total	C	N	O	S	0	0
			722	446	124	151	1		

- Molecule 36 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5A	2212	Total	C	N	O	S	0	0
			18366	11840	3193	3253	80		

- Molecule 37 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A3	383	Total	C	N	O	S	0	0
			3227	2029	566	618	14		

- Molecule 38 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	U	456	Total	C	N	O	S	0	0
			3750	2427	635	674	14		

- Molecule 39 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5D	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 40 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	64	73	Total	C	N	O	S	0	0
			596	376	105	109	6		

- Molecule 41 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	100	Total	C	N	O	S	0	0
			766	473	135	145	13		

- Molecule 42 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1C	50	Total	C	N	O	S	0	0
			425	266	73	82	4		

- Molecule 43 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	322	Total	C	N	O	S	0	0
			2626	1682	462	467	15		

- Molecule 44 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	4A	239	Total	C	N	O	S	0	0
			1946	1237	360	342	7		

- Molecule 45 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4	126	Total	C	N	O	P	0	0
			2690	1202	474	888	126		

- Molecule 46 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2A	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 47 is a protein called Splicing factor 3A subunit 1,Splicing factor 3A subunit 1,Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	A1	168	Total	C	N	O	S	0	0
			1339	855	237	245	2		

- Molecule 48 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	65	76	Total	C	N	O	S	0	0
			587	373	96	114	4		

- Molecule 49 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5B	2001	Total	C	N	O	S	0	0
			16077	10235	2767	2991	84		

- Molecule 50 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B1	848	Total	C	N	O	S	0	0
			6749	4330	1160	1220	39		

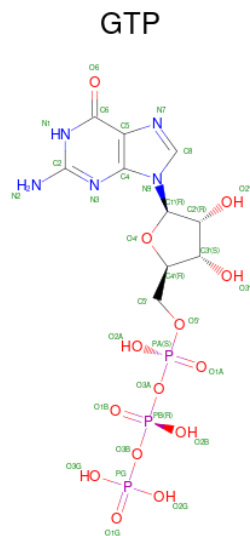
- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	A2	1	Total	Zn	0
			1	1	
51	U	1	Total	Zn	0
			1	1	
51	BP	3	Total	Zn	0
			3	3	
51	1C	1	Total	Zn	0
			1	1	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

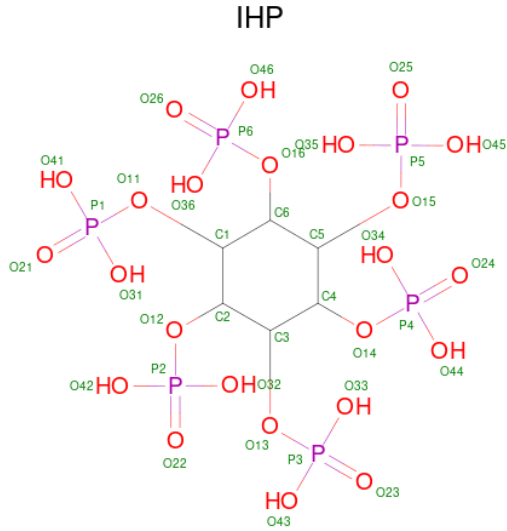
Mol	Chain	Residues	Atoms		AltConf
52	5C	1	Total	Mg	0
			1	1	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
53	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

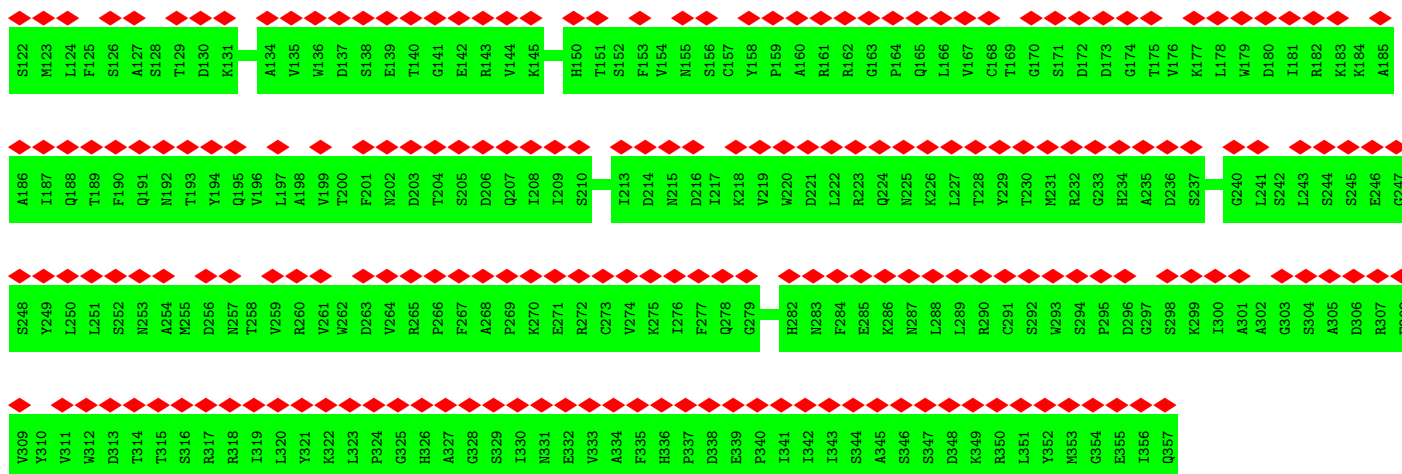
- Molecule 54 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$ ).



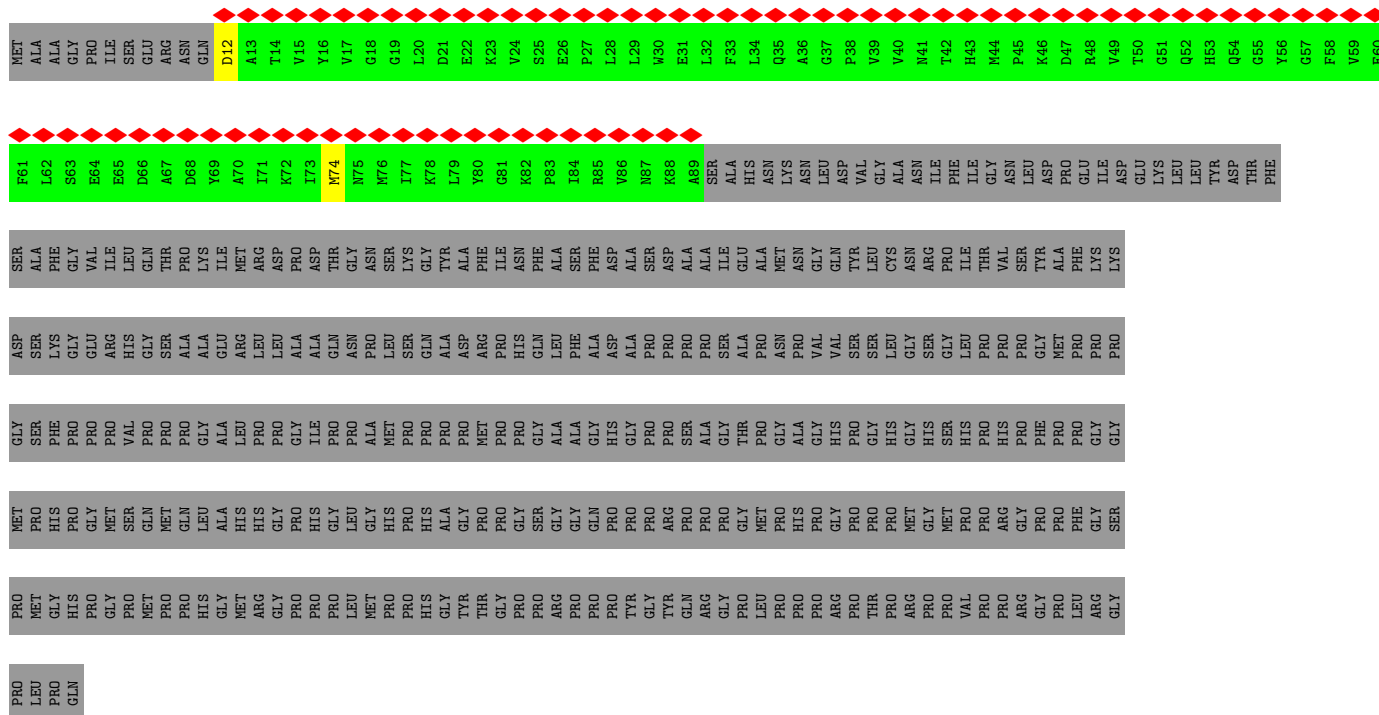
Mol	Chain	Residues	Atoms				AltConf
54	5A	1	Total	C	O	P	0
			36	6	24	6	



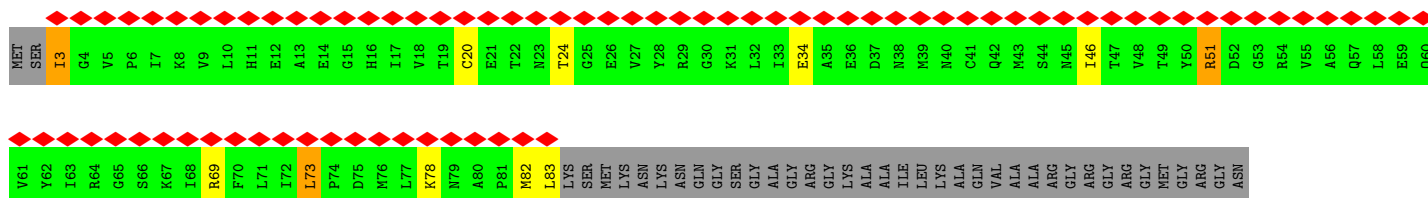




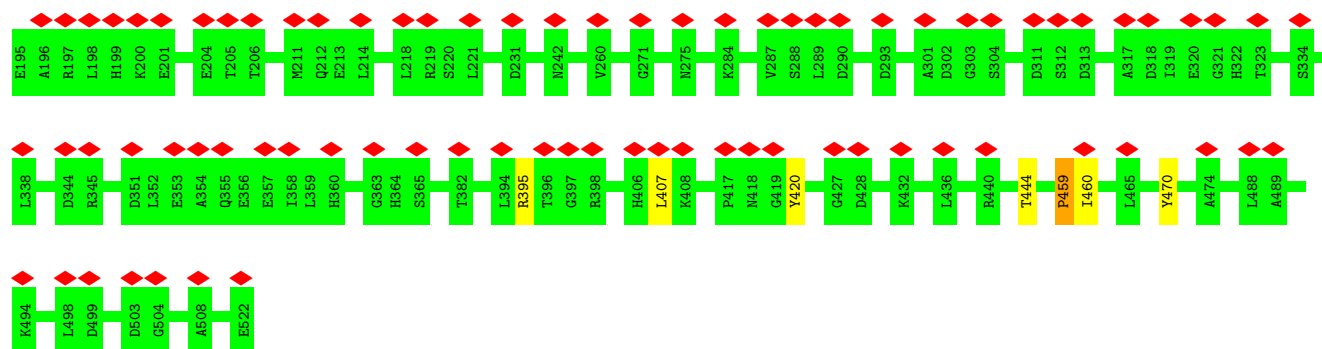
- Molecule 4: Splicing factor 3B subunit 4



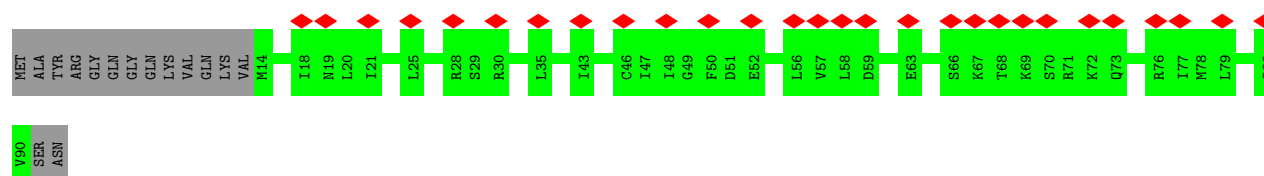
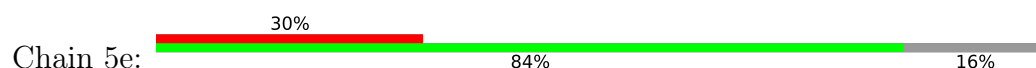
- Molecule 5: Small nuclear ribonucleoprotein Sm D3



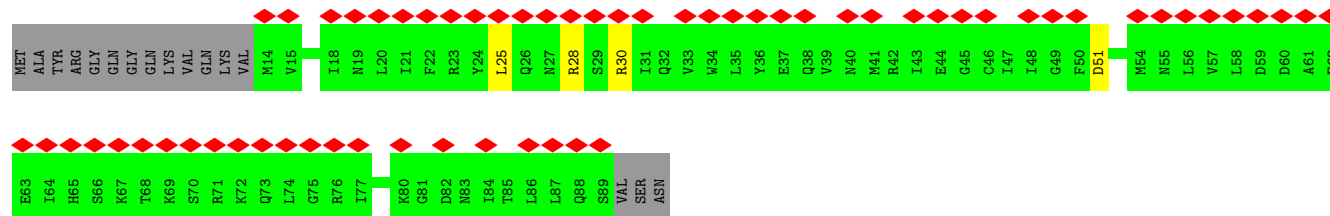
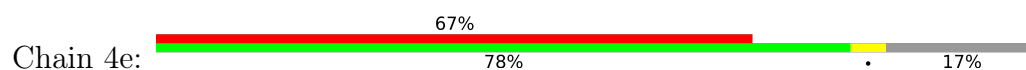
LEU PHE GLY GLU GLY PRO ALA GLU ARG ARG GLU ARG LEU ARG ASN ILE LEU SER SER VAL VAL GLY THR ASP ALA LEU LYS LYS THR LYS LYS ASP ASP GLU LYS SER LYS LYS TYR GLU TYR Q164 G170 P171 M172 S173 V176 A177 M183 M190 K191 R192 L193



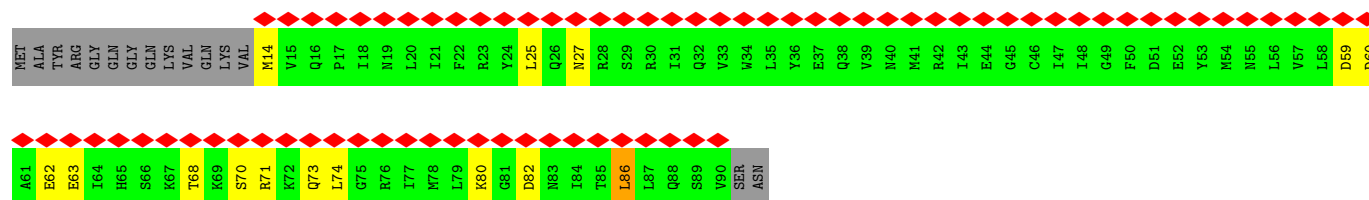
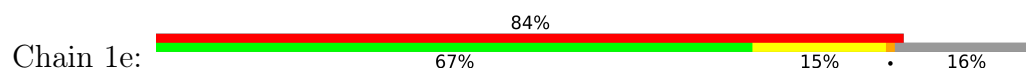
- Molecule 7: Small nuclear ribonucleoprotein E



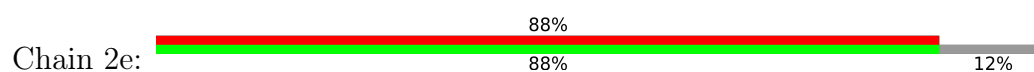
- Molecule 7: Small nuclear ribonucleoprotein E

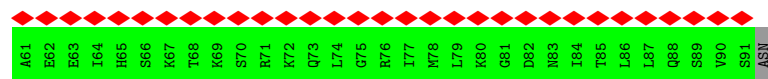


- Molecule 7: Small nuclear ribonucleoprotein E

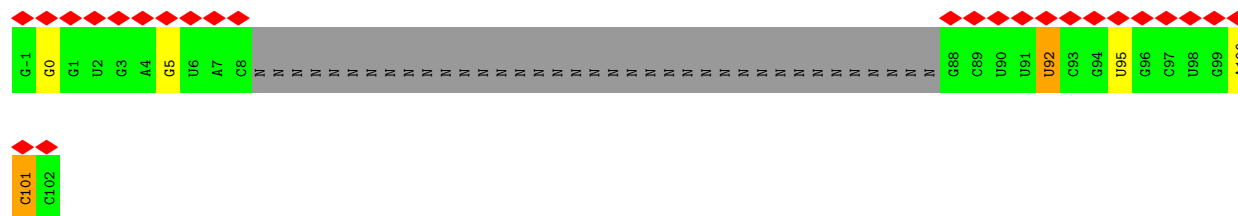


- Molecule 7: Small nuclear ribonucleoprotein E

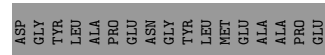
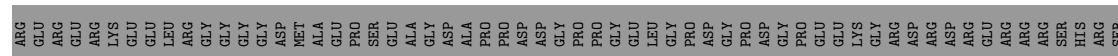
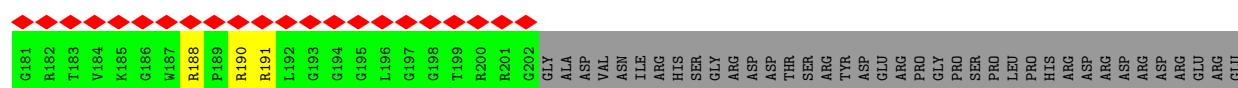
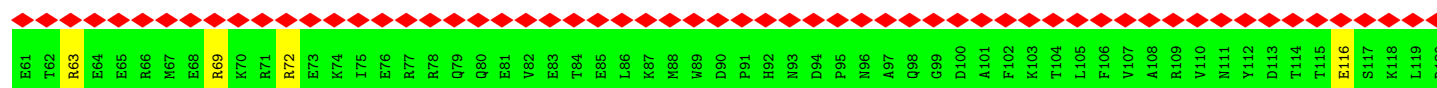
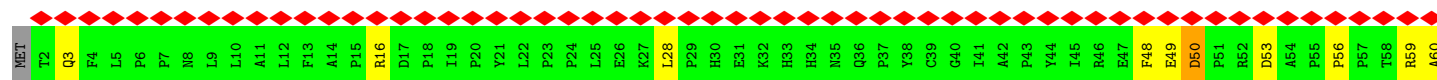
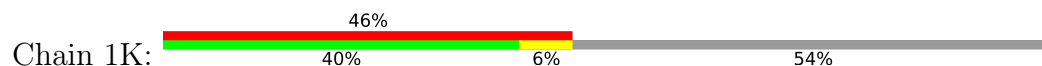




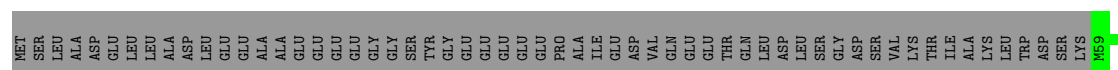
• Molecule 8: AdML pre-mRNA

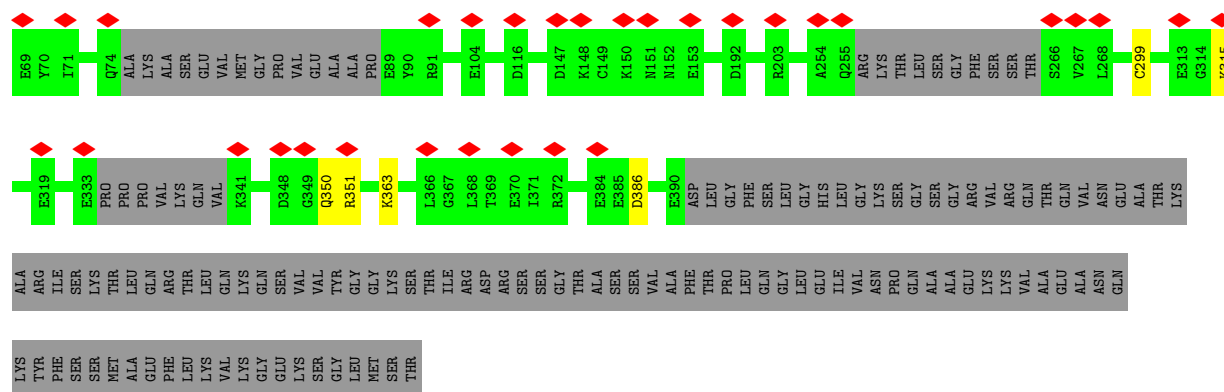


• Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

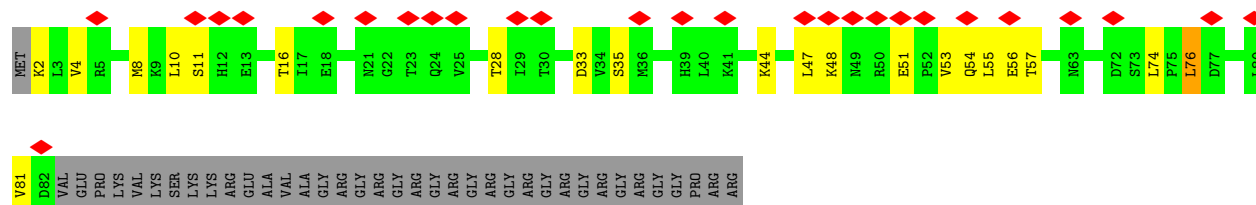


• Molecule 10: U4/U6 small nuclear ribonucleoprotein Prp31

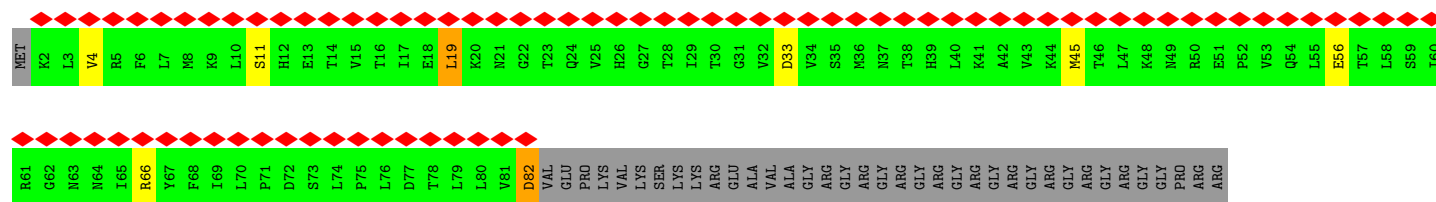




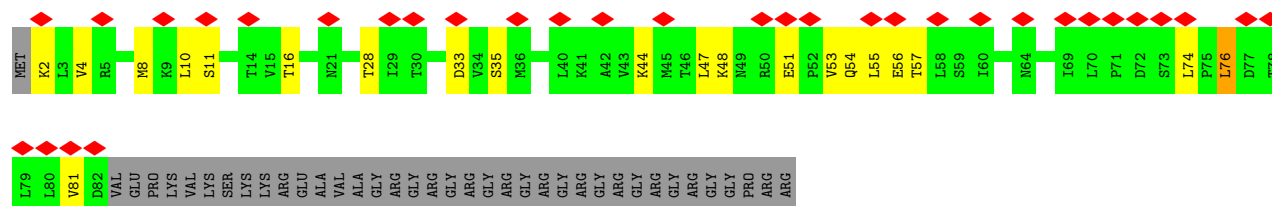
• Molecule 11: Small nuclear ribonucleoprotein Sm D1



• Molecule 11: Small nuclear ribonucleoprotein Sm D1



• Molecule 11: Small nuclear ribonucleoprotein Sm D1

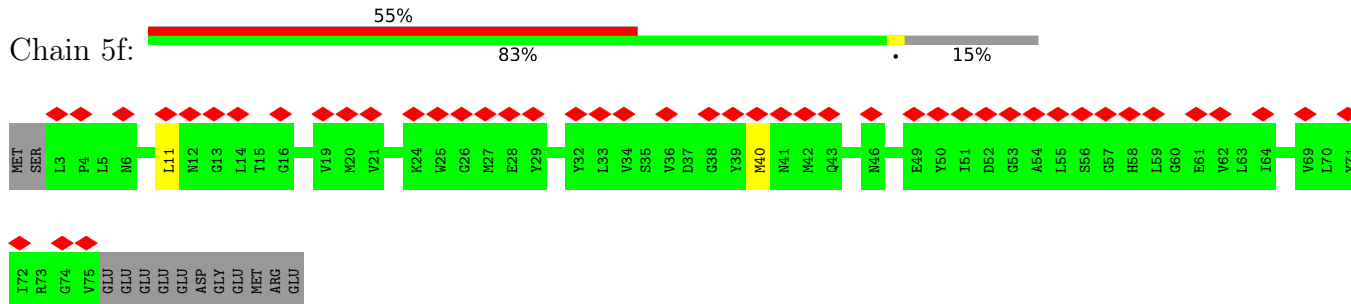


• Molecule 11: Small nuclear ribonucleoprotein Sm D1

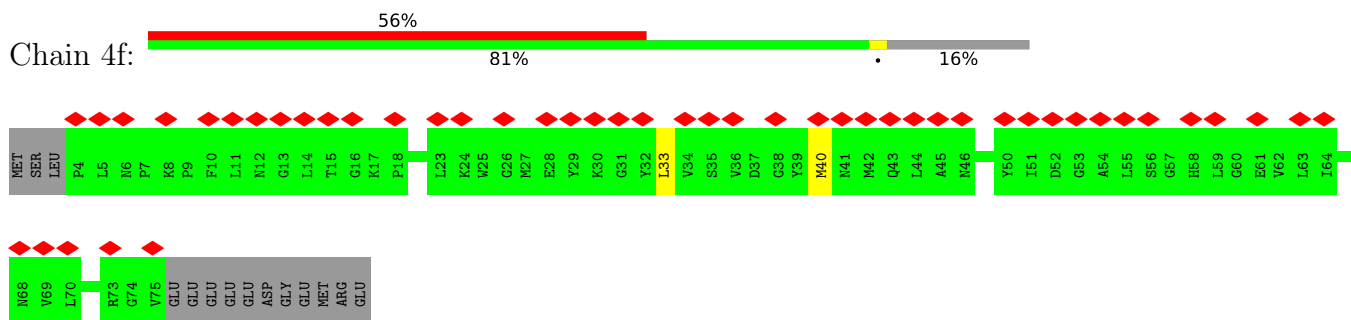




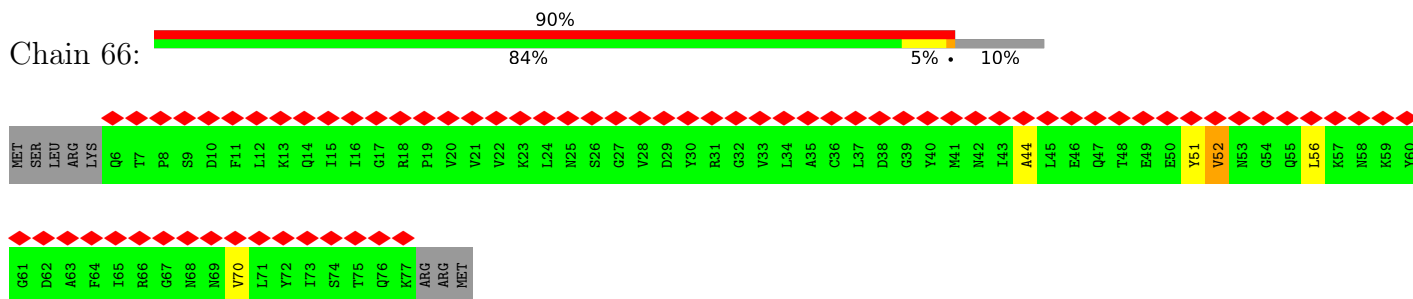
- Molecule 13: Small nuclear ribonucleoprotein F



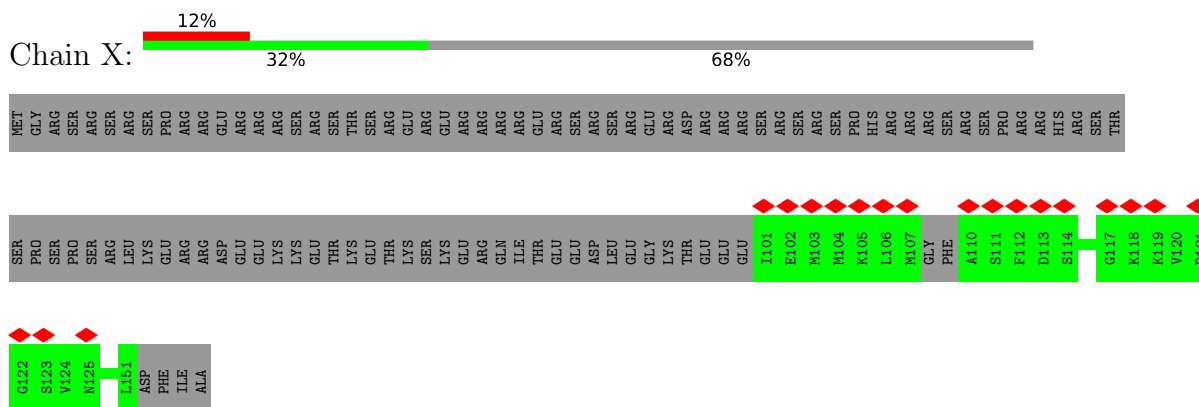
- Molecule 13: Small nuclear ribonucleoprotein F



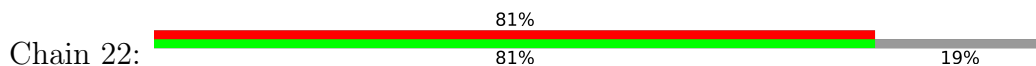
- Molecule 14: U6 snRNA-associated Sm-like protein LSm6



- Molecule 15: U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein

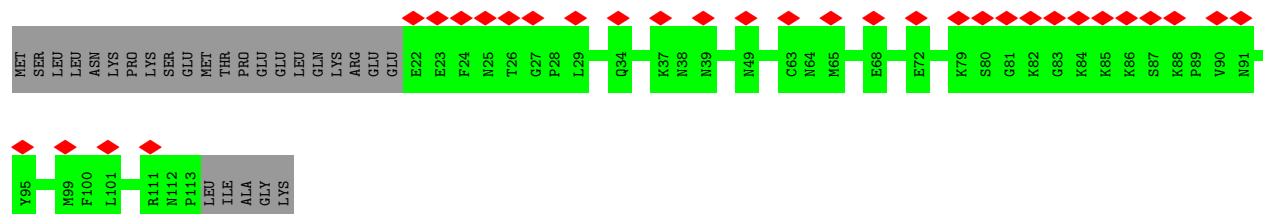
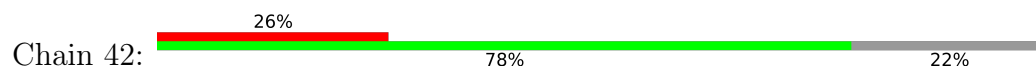


- Molecule 16: Small nuclear ribonucleoprotein Sm D2

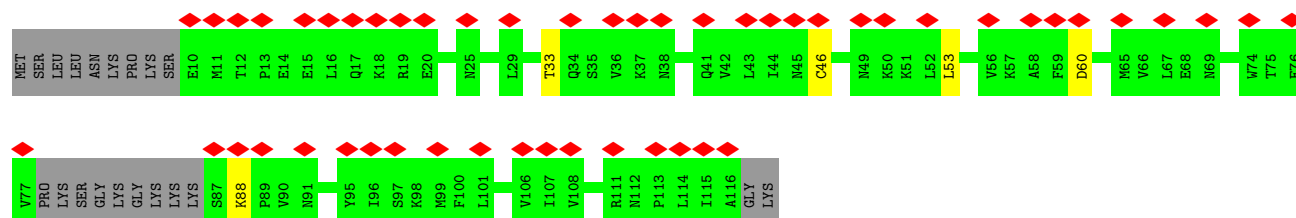
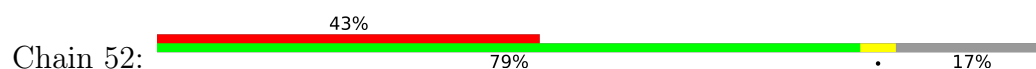




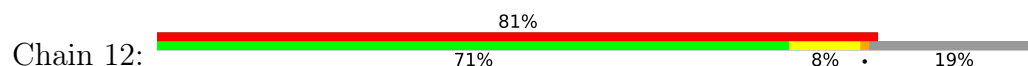
• Molecule 16: Small nuclear ribonucleoprotein Sm D2



• Molecule 16: Small nuclear ribonucleoprotein Sm D2



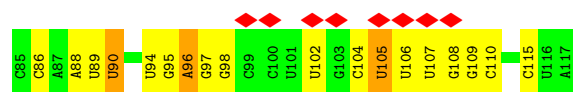
• Molecule 16: Small nuclear ribonucleoprotein Sm D2



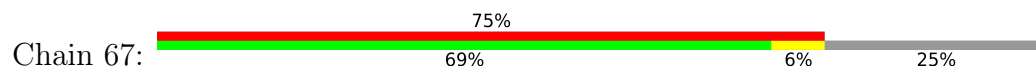
• Molecule 17: U5 snRNA







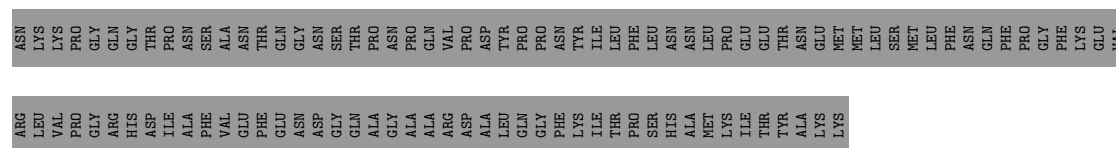
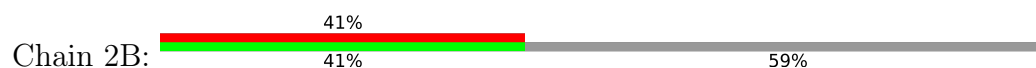
- Molecule 18: U6 snRNA-associated Sm-like protein LSm7



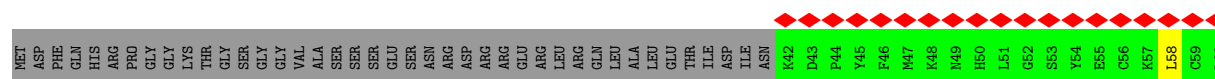
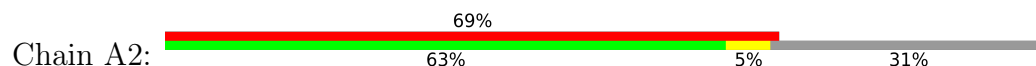
- Molecule 19: U6 snRNA-associated Sm-like protein LSm2



- Molecule 20: U2 small nuclear ribonucleoprotein B''

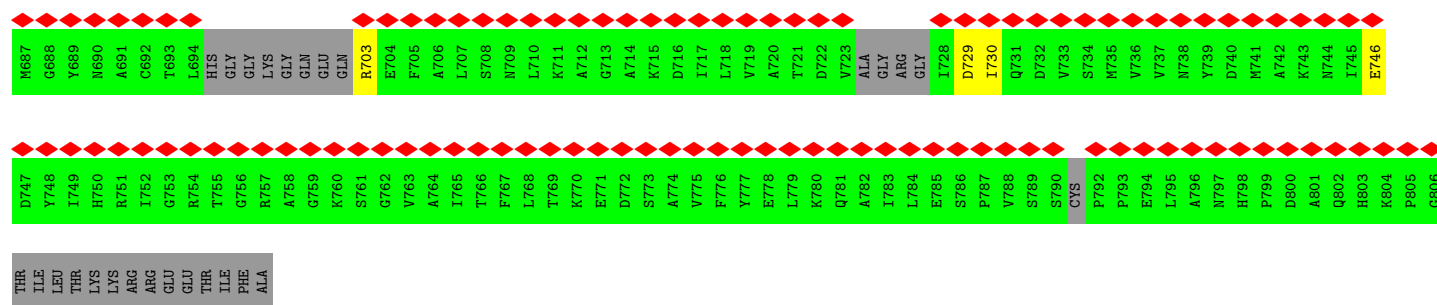


- Molecule 21: Splicing factor 3A subunit 2

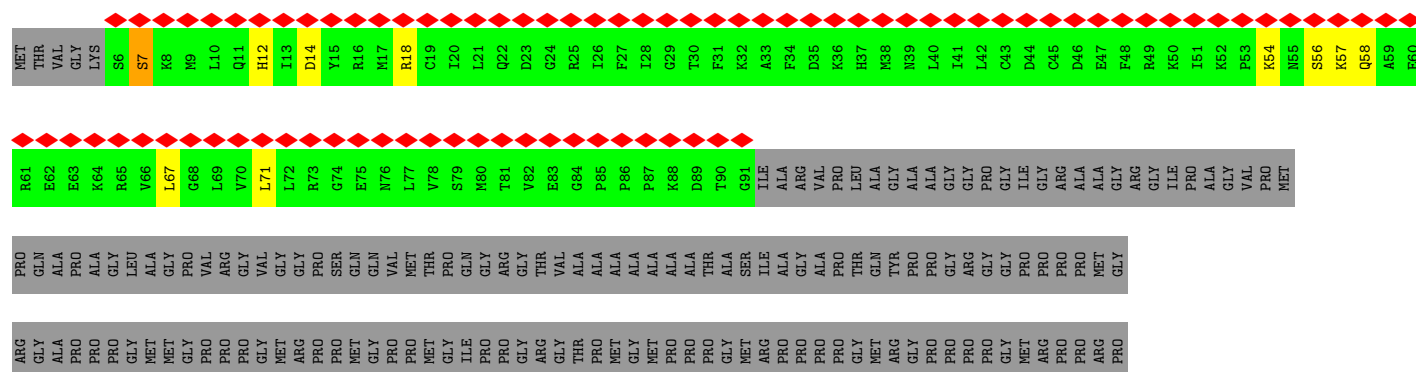




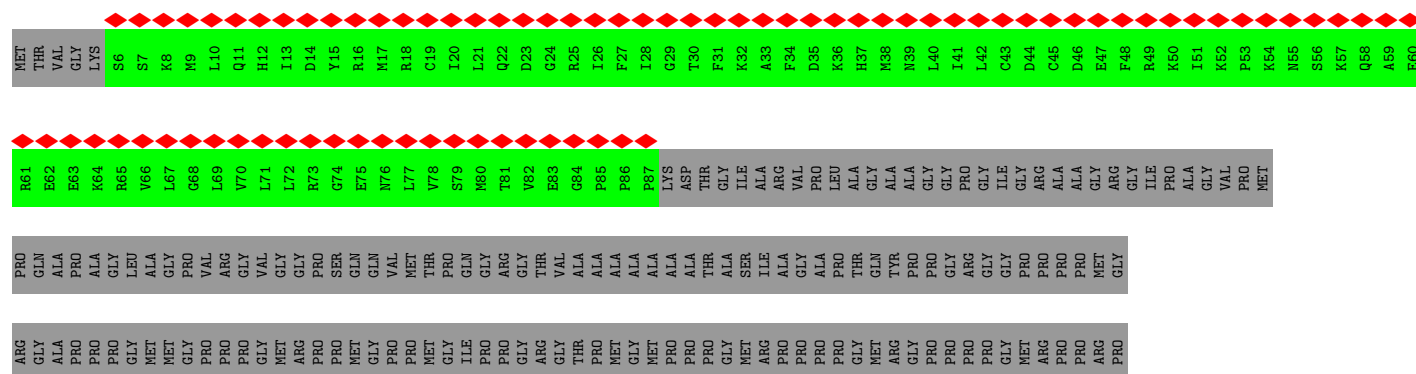
V627	V628	I629	G630	SR	A632	G633	K634	P635	H636	E637	R638	V639	E640	G641	K642	V643	F644	L645	M646	S647	E648	S649	E650	K651	R652	K653	K654	L655	L656	A657	E658	L659	E660	G661	G662	F663	D664	P665	P666	I667	I668	I669	F670	V671	M672	G673	K674	K675	G676	G677	D678	V679	L680	A681	K682	S683	L684	E685
------	------	------	------	----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



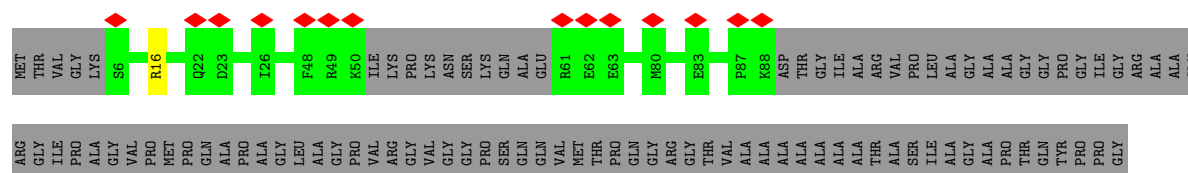
- Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

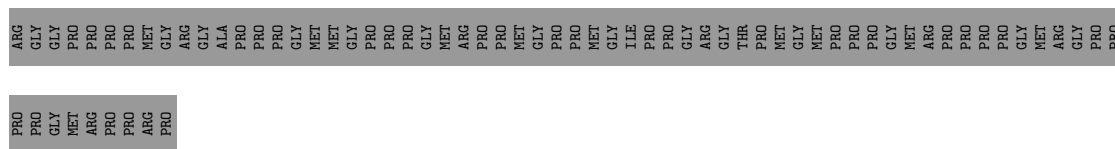


- Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

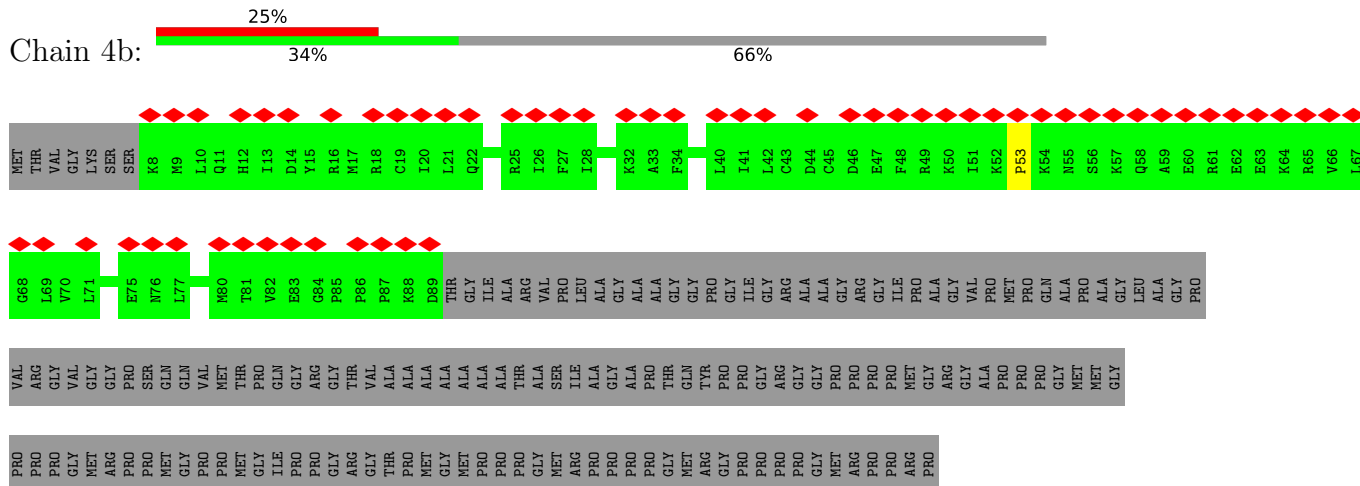


- Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

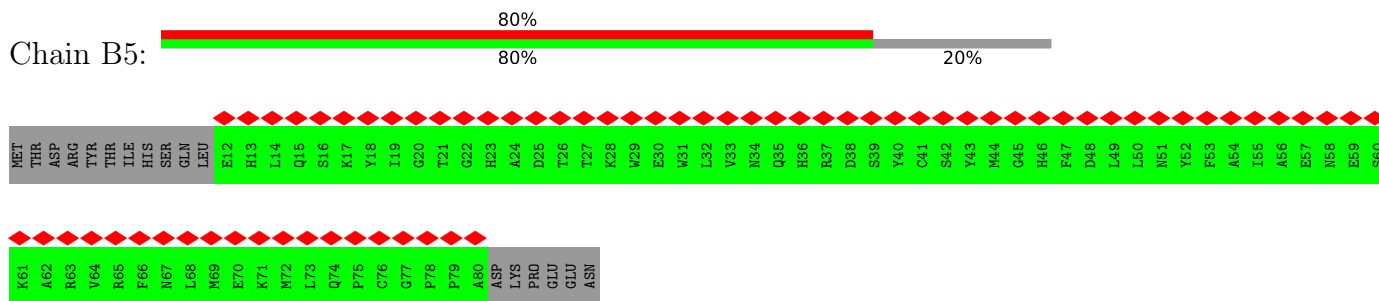




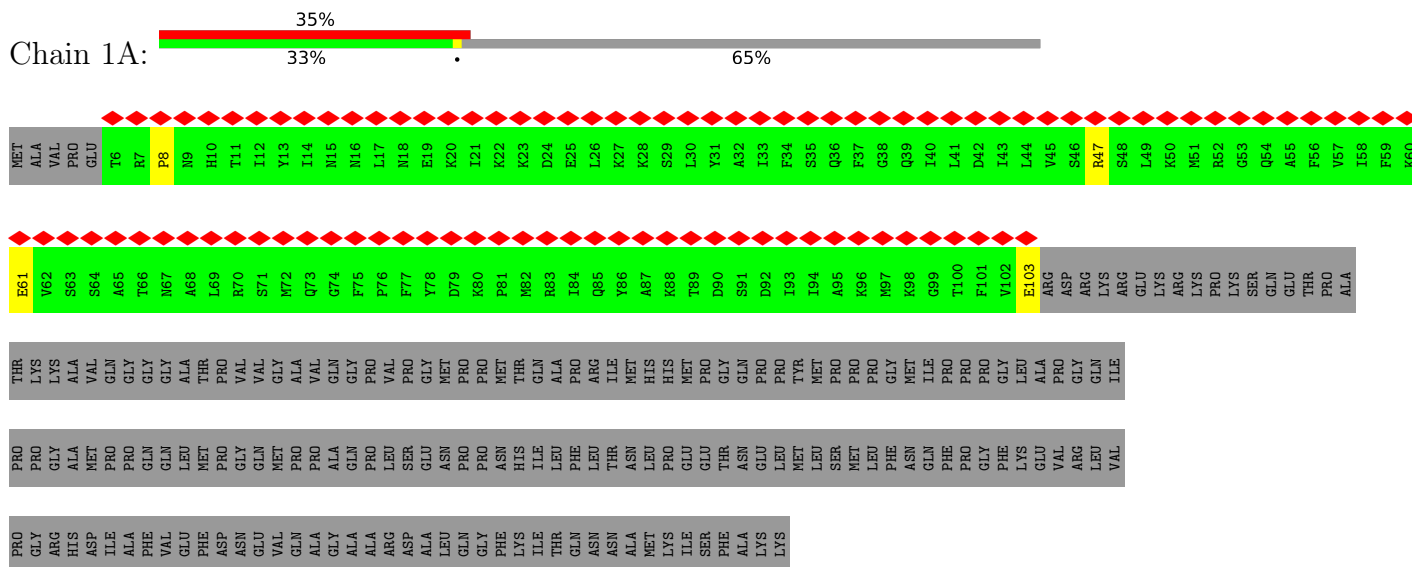
- Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'



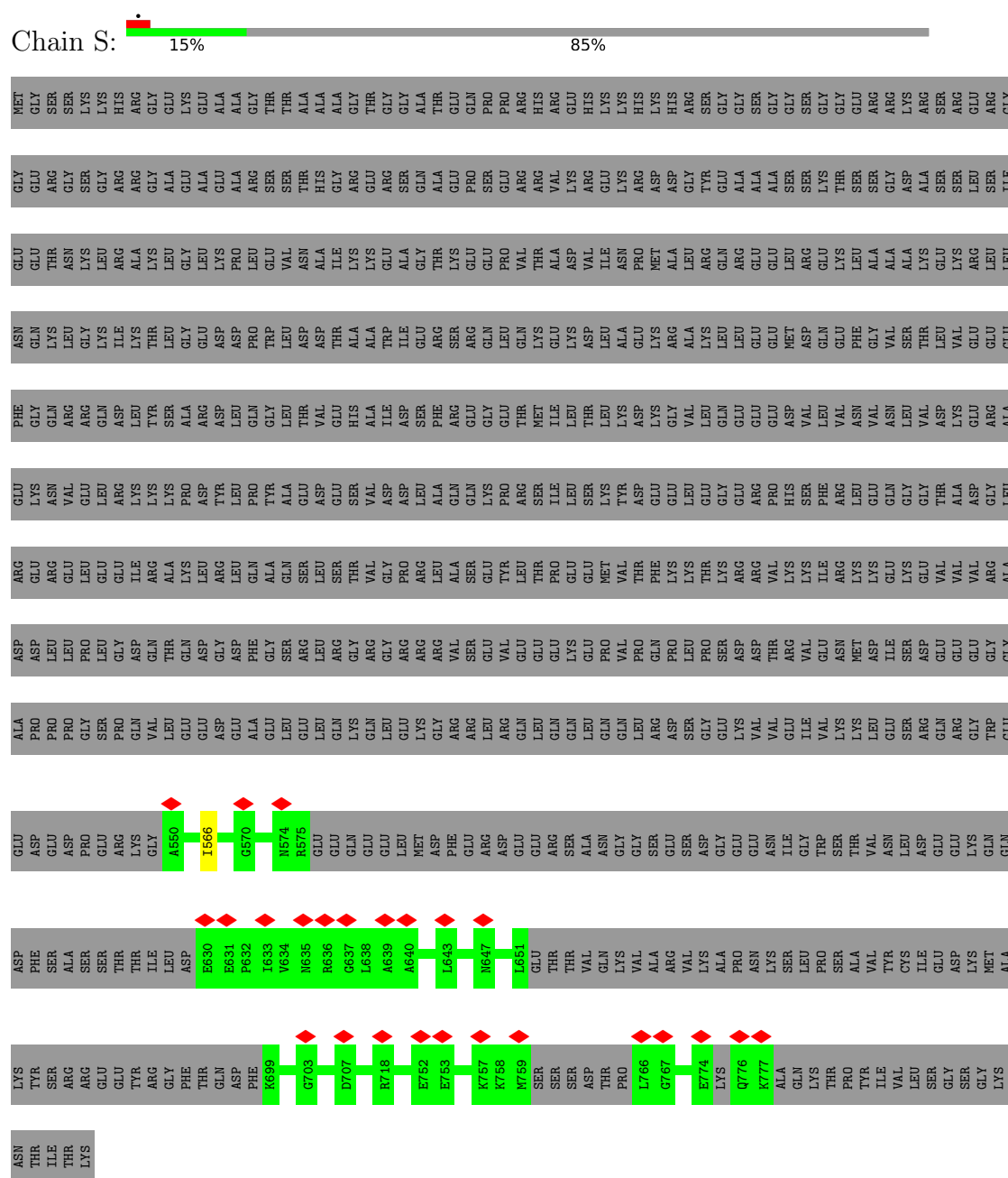
- Molecule 26: Splicing factor 3B subunit 5



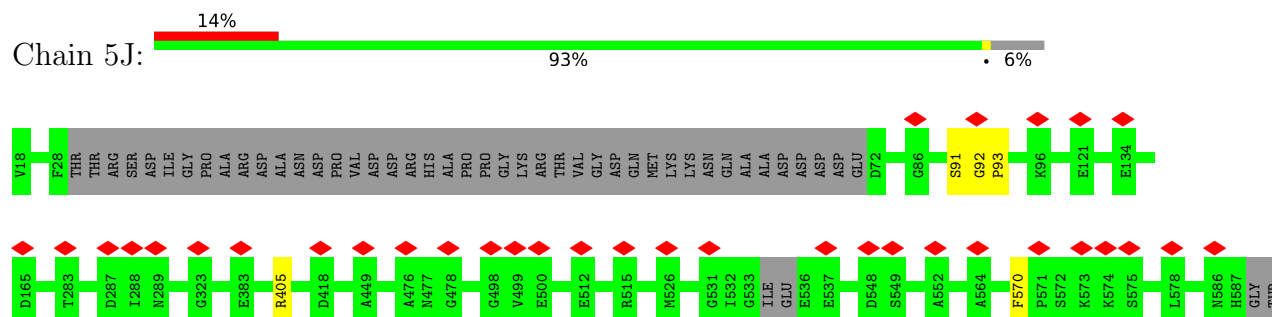
- Molecule 27: U1 small nuclear ribonucleoprotein A

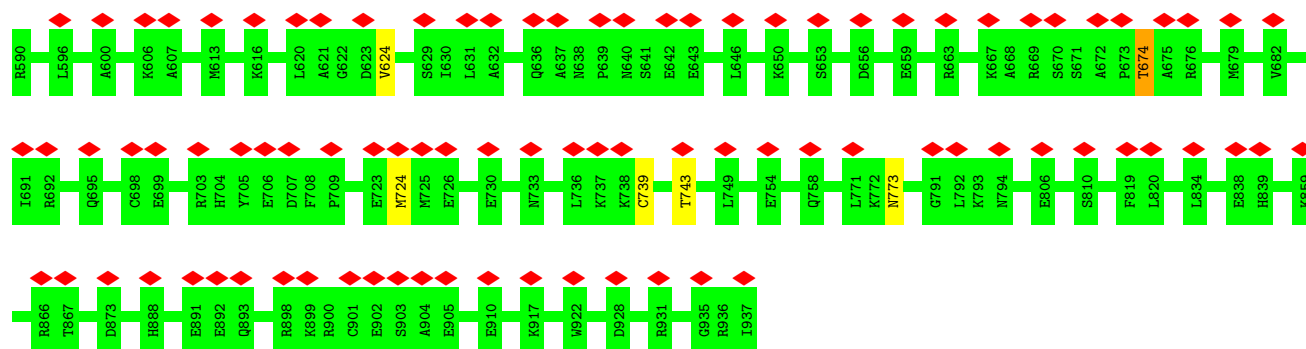


• Molecule 28: U4/U6.U5 tri-snRNP-associated protein 1

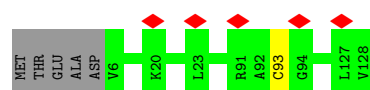


• Molecule 29: Pre-mRNA-processing factor 6

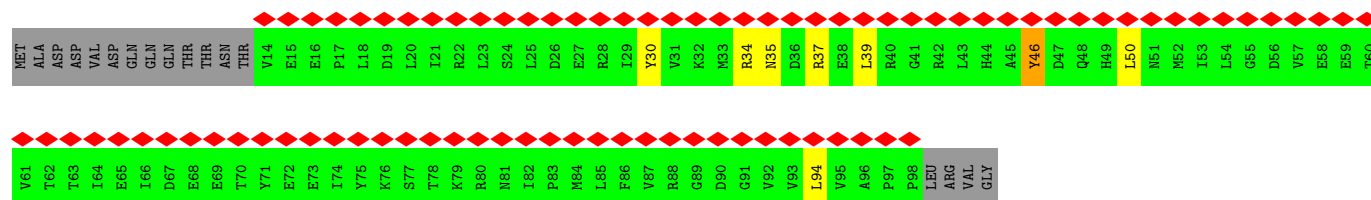
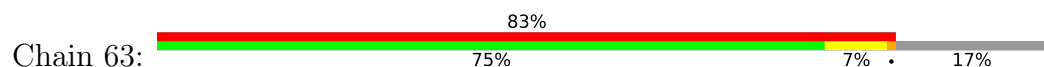




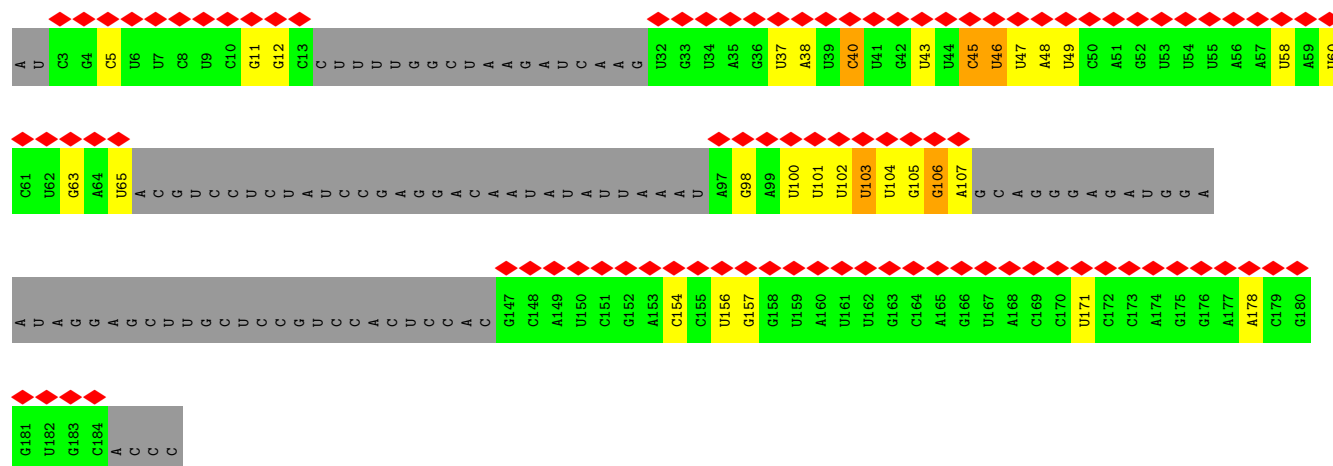
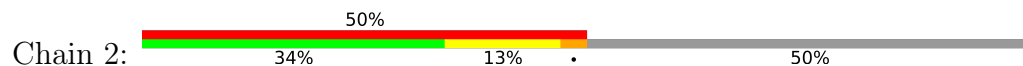
• Molecule 30: NHP2-like protein 1



• Molecule 31: U6 snRNA-associated Sm-like protein LSm3



• Molecule 32: U2 snRNA

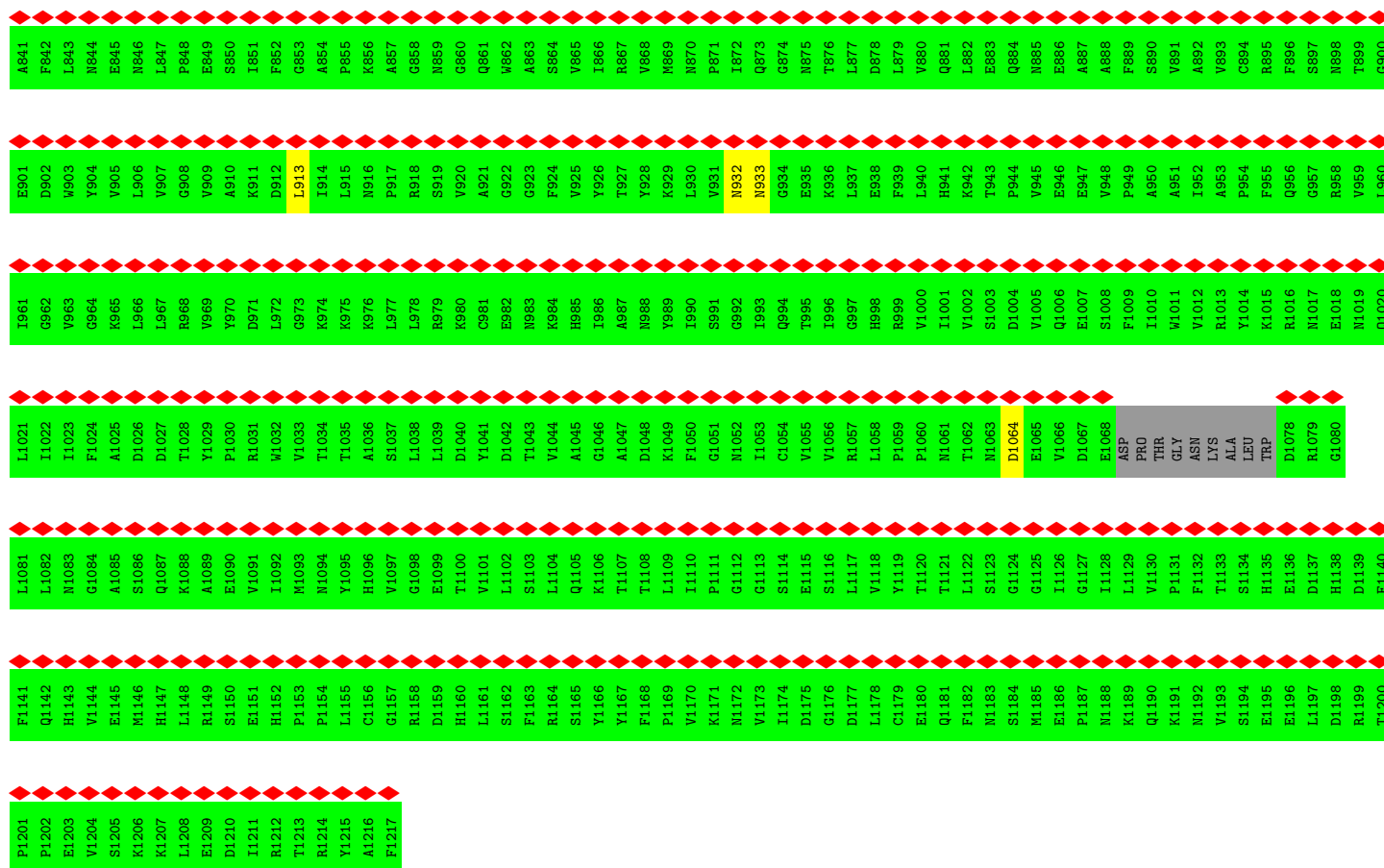


• Molecule 33: Splicing factor 3B subunit 3



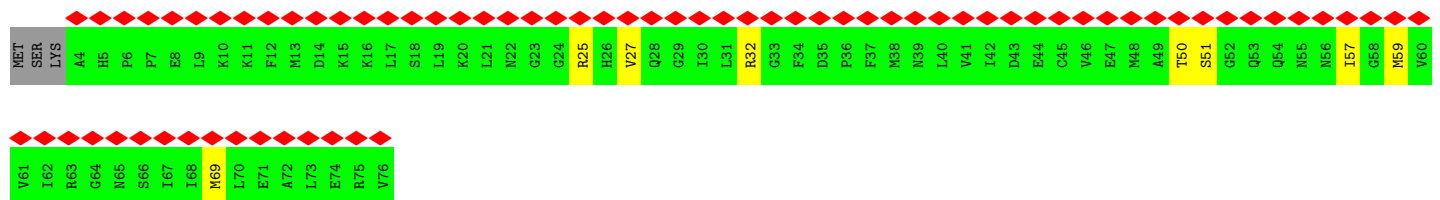






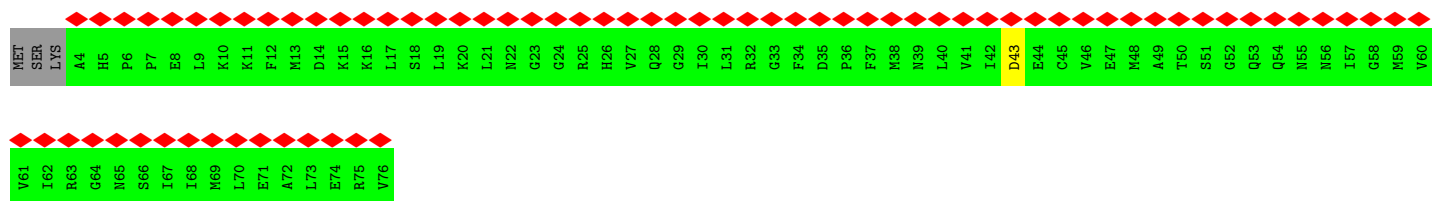
• Molecule 34: Small nuclear ribonucleoprotein G

Chain 1g:



• Molecule 34: Small nuclear ribonucleoprotein G

Chain 2g:



• Molecule 34: Small nuclear ribonucleoprotein G

Chain 5g:

- Molecule 34: Small nuclear ribonucleoprotein G

Chain 4g:

- Molecule 35: U6 snRNA-associated Sm-like protein LSm8

Chain 68:

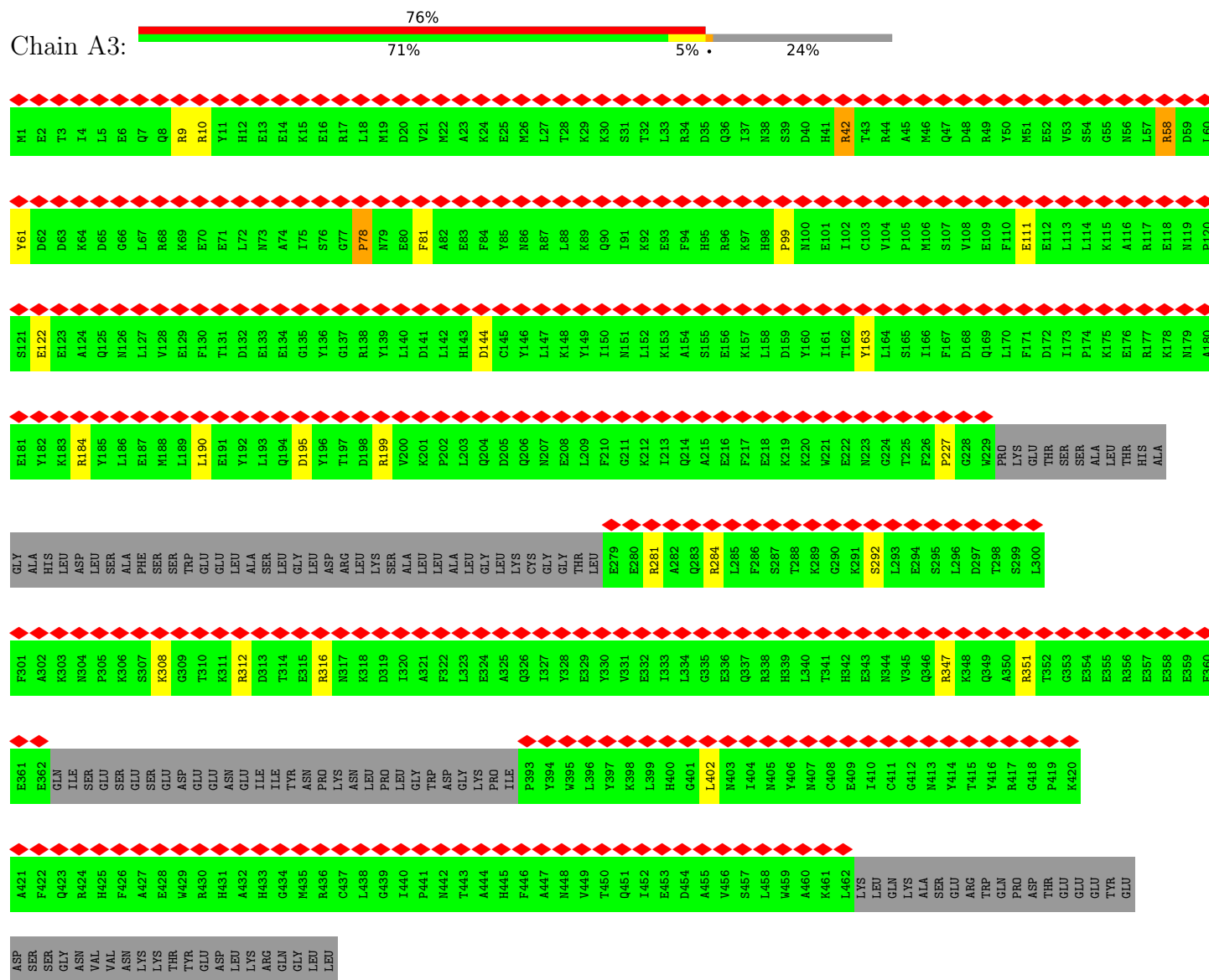
- Molecule 36: Pre-mRNA-processing-splicing factor 8

Chain 5A:

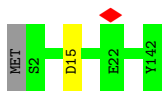


- Molecule 37: Splicing factor 3A subunit 3

Chain A3:

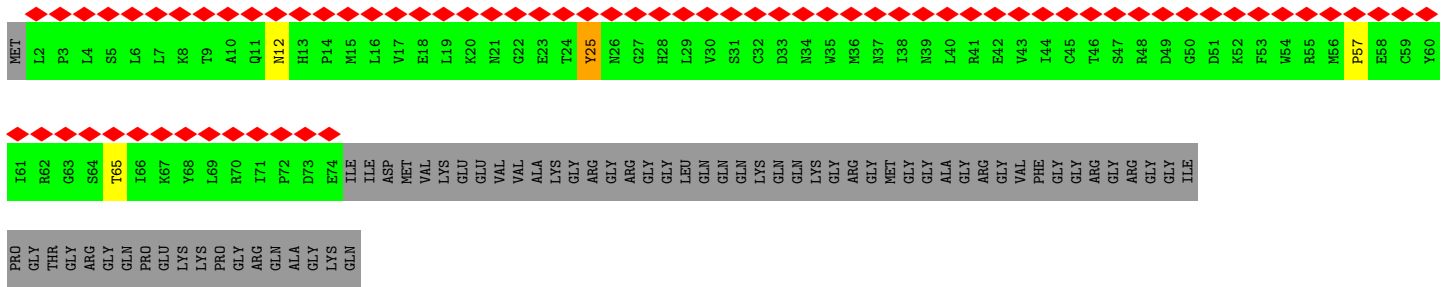


Chain 5D:  99%



- Molecule 40: U6 snRNA-associated Sm-like protein LSm4

Chain 64:  53% 50% 47%



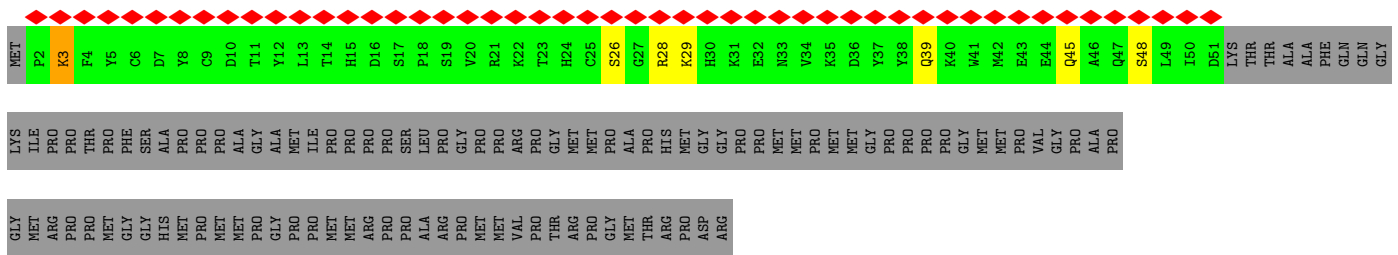
- Molecule 41: PHD finger-like domain-containing protein 5A

Chain BP: 



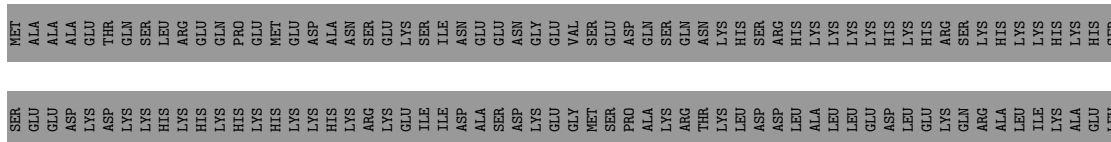
- Molecule 42: U1 small nuclear ribonucleoprotein C

Chain 1C: 



- Molecule 43: Serine/threonine-protein kinase PRP4 homolog

Chain K:  32% 29% 68%

















## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86146	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	429.24, 429.24, 429.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.022, 1.022, 1.022	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, IHP, GTP, MG, M7M

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	0.75	8/3891 (0.2%)	0.87	9/6061 (0.1%)
2	6	0.72	5/1264 (0.4%)	1.19	8/1961 (0.4%)
3	5O	0.31	0/2448	0.58	0/3316
4	B4	0.72	0/632	1.02	2/855 (0.2%)
5	13	0.53	0/645	1.19	6/870 (0.7%)
5	23	0.48	0/660	0.61	0/889
5	43	0.34	0/660	0.67	1/889 (0.1%)
5	53	0.44	0/665	0.56	0/896
6	4B	0.48	0/2921	0.65	0/3966
7	1e	0.62	0/646	1.27	5/867 (0.6%)
7	2e	0.48	0/677	0.60	0/908
7	4e	0.37	0/639	0.78	1/857 (0.1%)
7	5e	0.37	0/646	0.70	0/867
8	I	0.86	0/590	1.30	8/916 (0.9%)
9	1K	1.13	2/1695 (0.1%)	1.19	15/2288 (0.7%)
10	4C	0.34	0/2406	0.56	0/3232
11	11	0.68	0/649	1.24	7/878 (0.8%)
11	21	0.40	0/642	0.56	0/867
11	41	0.40	0/649	0.73	1/878 (0.1%)
11	51	0.40	0/649	0.73	1/878 (0.1%)
12	R	0.39	0/891	0.77	0/1188
13	1f	0.66	1/588 (0.2%)	1.18	4/795 (0.5%)
13	2f	0.49	0/574	0.59	0/775
13	4f	0.42	0/574	0.74	1/775 (0.1%)
13	5f	0.41	0/579	0.78	0/783
14	66	0.83	1/575 (0.2%)	1.25	3/776 (0.4%)
15	X	0.42	0/398	0.59	0/524
16	12	0.69	0/786	1.15	3/1055 (0.3%)
16	22	0.43	0/784	0.56	0/1053
16	42	0.43	0/747	0.66	0/1000
16	52	0.40	0/805	0.74	1/1081 (0.1%)
17	5	0.63	0/2444	1.47	59/3798 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	67	0.81	1/611 (0.2%)	1.29	3/824 (0.4%)
19	62	0.79	0/773	1.21	4/1043 (0.4%)
20	2B	0.38	0/759	0.50	0/1016
21	A2	0.65	0/1254	0.93	4/1682 (0.2%)
22	B2	0.67	3/1747 (0.2%)	0.88	7/2356 (0.3%)
23	5C	0.54	0/6879	0.61	3/9344 (0.0%)
24	5X	0.52	1/4859 (0.0%)	0.61	0/6522
25	1b	0.64	0/702	1.16	3/936 (0.3%)
25	2b	0.45	0/674	0.55	0/899
25	4b	0.33	0/679	0.62	0/905
25	5b	0.38	0/602	0.57	0/801
26	B5	0.60	0/584	0.59	0/789
27	1A	1.04	0/801	1.02	2/1074 (0.2%)
28	S	0.39	0/925	0.66	0/1229
29	5J	0.35	0/6430	0.62	6/8681 (0.1%)
30	4D	0.51	1/967 (0.1%)	0.56	0/1305
31	63	0.80	0/709	1.22	3/959 (0.3%)
32	2	0.72	3/2209 (0.1%)	1.15	14/3429 (0.4%)
33	B3	0.48	0/9485	0.61	0/12870
34	1g	0.58	0/575	1.17	4/768 (0.5%)
34	2g	0.48	0/575	0.62	0/768
34	4g	0.41	0/584	0.71	1/779 (0.1%)
34	5g	0.41	0/584	0.72	1/779 (0.1%)
35	68	0.80	0/728	1.30	7/987 (0.7%)
36	5A	0.48	1/18874 (0.0%)	0.59	10/25606 (0.0%)
37	A3	0.70	0/3294	1.07	12/4423 (0.3%)
38	U	0.54	0/3846	0.63	2/5208 (0.0%)
39	5D	0.39	0/1198	0.58	1/1620 (0.1%)
40	64	0.82	0/609	1.25	2/824 (0.2%)
41	BP	0.65	0/779	0.56	0/1047
42	1C	0.56	0/437	1.16	4/587 (0.7%)
43	K	0.37	0/2673	0.54	0/3593
44	4A	0.42	0/1983	0.59	2/2657 (0.1%)
45	4	0.59	2/2967 (0.1%)	1.00	7/4610 (0.2%)
46	2A	0.32	0/1299	0.62	0/1761
47	A1	0.71	0/1234	1.03	4/1657 (0.2%)
48	65	0.83	0/593	1.25	3/800 (0.4%)
49	5B	0.44	0/16393	0.59	3/22174 (0.0%)
50	B1	0.53	0/6878	0.65	3/9315 (0.0%)
All	All	0.54	29/141171 (0.0%)	0.77	250/193369 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	4B	0	3
7	4e	0	1
9	1K	0	1
10	4C	0	2
13	4f	0	1
13	5f	0	1
14	66	0	1
16	12	0	1
16	52	0	3
18	67	0	1
19	62	0	1
21	A2	0	4
23	5C	0	2
25	4b	0	1
29	5J	0	2
31	63	0	2
33	B3	0	1
35	68	0	3
36	5A	0	2
37	A3	0	6
38	U	0	3
40	64	0	1
44	4A	0	2
45	4	0	1
47	A1	0	4
49	5B	0	2
50	B1	0	4
All	All	0	56

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	78	U	O3'-P	-19.56	1.37	1.61
1	1	2	U	O3'-P	-18.25	1.39	1.61
45	4	87	C	O3'-P	11.52	1.75	1.61
1	1	35	A	O3'-P	-7.25	1.52	1.61
22	B2	629	PRO	N-CD	-7.23	1.37	1.47
24	5X	543	CYS	CB-SG	-6.93	1.70	1.82
22	B2	629	PRO	CA-C	-6.80	1.39	1.52
2	6	87	C	C1'-N1	6.66	1.58	1.48
2	6	95	G	C1'-N9	-6.46	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	11	G	C1'-N9	-6.46	1.37	1.46
30	4D	93	CYS	CB-SG	-6.33	1.71	1.82
2	6	93	G	C1'-N9	-6.29	1.38	1.46
18	67	61	GLN	C-O	-6.24	1.11	1.23
32	2	12	G	C1'-N9	-6.13	1.38	1.46
2	6	86	U	C1'-N1	5.96	1.57	1.48
1	1	25	C	O3'-P	-5.91	1.54	1.61
1	1	23	A	O3'-P	-5.83	1.54	1.61
1	1	33	C	O3'-P	-5.82	1.54	1.61
9	1K	124	GLU	CD-OE1	5.61	1.31	1.25
2	6	89	U	C1'-N1	5.60	1.57	1.48
45	4	91	A	O3'-P	-5.42	1.54	1.61
32	2	5	C	C1'-N1	5.41	1.56	1.48
9	1K	116	GLU	CD-OE1	-5.34	1.19	1.25
22	B2	629	PRO	C-N	-5.23	1.24	1.34
36	5A	492	VAL	CB-CG1	-5.11	1.42	1.52
1	1	20	G	O3'-P	-5.09	1.55	1.61
14	66	70	VAL	C-O	-5.09	1.13	1.23
13	1f	4	PRO	N-CD	5.07	1.54	1.47
1	1	22	U	O3'-P	-5.05	1.55	1.61

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5J	92	GLY	C-N-CD	-13.53	90.84	120.60
17	5	57	G	O4'-C1'-N9	12.51	118.20	108.20
1	1	78	U	P-O3'-C3'	12.36	134.54	119.70
42	1C	28	ARG	NE-CZ-NH1	12.33	126.47	120.30
17	5	58	U	O5'-P-OP2	-10.23	96.50	105.70
5	13	73	LEU	CB-CG-CD2	10.20	128.34	111.00
17	5	23	C	C2-N1-C1'	10.20	130.01	118.80
17	5	22	U	N1-C2-O2	10.18	129.93	122.80
29	5J	674	THR	N-CA-C	-10.17	83.54	111.00
13	1f	73	ARG	NE-CZ-NH1	-10.09	115.26	120.30
17	5	22	U	C2-N1-C1'	9.91	129.60	117.70
17	5	115	C	C2-N1-C1'	9.69	129.46	118.80
17	5	22	U	N3-C2-O2	-9.49	115.56	122.20
17	5	58	U	C5-C6-N1	9.46	127.43	122.70
7	1e	59	ASP	CB-CG-OD2	9.31	126.68	118.30
40	64	65	THR	CA-CB-CG2	-9.22	99.49	112.40
17	5	71	C	N1-C2-O2	9.02	124.31	118.90
47	A1	193	TYR	CB-CG-CD1	8.71	126.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	23	C	N1-C2-O2	8.59	124.06	118.90
13	1f	73	ARG	NE-CZ-NH2	8.57	124.58	120.30
17	5	90	U	N1-C2-O2	8.56	128.79	122.80
21	A2	115	PRO	CA-N-CD	-8.51	99.59	111.50
18	67	69	ARG	NE-CZ-NH1	8.46	124.53	120.30
31	63	37	ARG	NE-CZ-NH1	8.30	124.45	120.30
7	1e	71	ARG	NE-CZ-NH2	-8.24	116.18	120.30
19	62	68	ARG	NE-CZ-NH1	8.21	124.41	120.30
9	1K	121	ARG	NE-CZ-NH1	8.18	124.39	120.30
47	A1	246	ARG	NE-CZ-NH1	8.17	124.38	120.30
36	5A	1551	PHE	N-CA-C	-8.10	89.14	111.00
50	B1	557	ASP	CB-CG-OD1	8.09	125.58	118.30
17	5	58	U	C2-N1-C1'	8.09	127.40	117.70
45	4	87	C	O3'-P-O5'	8.07	119.33	104.00
35	68	8	TYR	CB-CG-CD1	8.04	125.82	121.00
47	A1	193	TYR	CB-CG-CD2	-8.04	116.18	121.00
18	67	55	MET	CG-SD-CE	-8.04	87.34	100.20
17	5	71	C	C2-N1-C1'	8.01	127.61	118.80
25	1b	18	ARG	NE-CZ-NH2	-8.01	116.30	120.30
5	13	51	ARG	NE-CZ-NH2	7.96	124.28	120.30
11	11	56	GLU	OE1-CD-OE2	-7.94	113.77	123.30
5	13	69	ARG	NE-CZ-NH1	7.82	124.21	120.30
17	5	71	C	N3-C2-O2	-7.75	116.48	121.90
17	5	90	U	N3-C2-O2	-7.73	116.79	122.20
9	1K	191	ARG	NE-CZ-NH2	-7.72	116.44	120.30
17	5	58	U	N1-C2-O2	7.69	128.18	122.80
17	5	110	C	C5-C6-N1	7.67	124.83	121.00
25	1b	14	ASP	CB-CG-OD2	-7.66	111.41	118.30
17	5	23	C	N3-C2-O2	-7.66	116.54	121.90
1	1	67	U	O5'-P-OP2	-7.63	98.83	105.70
29	5J	739	CYS	C-N-CD	-7.55	104.00	120.60
17	5	90	U	C2-N1-C1'	7.52	126.72	117.70
37	A3	284	ARG	NE-CZ-NH2	7.51	124.05	120.30
17	5	110	C	C6-N1-C2	-7.50	117.30	120.30
37	A3	351	ARG	NE-CZ-NH2	7.49	124.05	120.30
37	A3	10	ARG	NE-CZ-NH2	7.45	124.02	120.30
17	5	58	U	N3-C2-O2	-7.43	117.00	122.20
8	I	101	C	C6-N1-C2	-7.42	117.33	120.30
48	65	49	MET	CG-SD-CE	-7.42	88.33	100.20
7	1e	86	LEU	CA-CB-CG	7.39	132.29	115.30
17	5	58	U	C6-N1-C2	-7.37	116.58	121.00
17	5	71	C	C6-N1-C2	-7.33	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	128	U	O5'-P-OP1	-7.32	99.11	105.70
5	13	51	ARG	NE-CZ-NH1	-7.30	116.65	120.30
2	6	31	U	N1-C2-O2	7.28	127.89	122.80
45	4	87	C	P-O3'-C3'	-7.28	110.97	119.70
37	A3	184	ARG	NE-CZ-NH2	7.13	123.87	120.30
39	5D	15	ASP	CB-CG-OD1	7.11	124.70	118.30
9	1K	144	ARG	NE-CZ-NH1	7.04	123.82	120.30
17	5	115	C	N1-C2-O2	6.98	123.09	118.90
17	5	23	C	C6-N1-C1'	-6.97	112.44	120.80
32	2	103	U	OP2-P-O3'	6.93	120.45	105.20
11	11	66	ARG	NE-CZ-NH2	6.93	123.76	120.30
17	5	23	C	C6-N1-C2	-6.91	117.54	120.30
32	2	46	U	P-O3'-C3'	6.91	127.99	119.70
19	62	69	TYR	CB-CG-CD2	-6.89	116.86	121.00
11	11	45	MET	CG-SD-CE	-6.89	89.17	100.20
1	1	37	G	O5'-P-OP2	-6.88	99.51	105.70
17	5	115	C	C6-N1-C1'	-6.88	112.55	120.80
17	5	22	U	C6-N1-C1'	-6.87	111.58	121.20
37	A3	42	ARG	NE-CZ-NH2	6.87	123.73	120.30
2	6	31	U	N3-C2-O2	-6.86	117.40	122.20
13	4f	33	LEU	CA-CB-CG	6.86	131.07	115.30
22	B2	629	PRO	N-CA-CB	6.84	111.51	103.30
42	1C	28	ARG	NE-CZ-NH2	-6.77	116.91	120.30
36	5A	1557	LEU	CA-CB-CG	6.75	130.83	115.30
34	1g	32	ARG	NE-CZ-NH2	6.74	123.67	120.30
36	5A	853	LYS	N-CA-C	-6.69	92.94	111.00
45	4	87	C	OP2-P-O3'	-6.68	90.50	105.20
17	5	115	C	C5-C6-N1	6.67	124.34	121.00
17	5	55	C	C6-N1-C2	-6.64	117.64	120.30
32	2	103	U	P-O3'-C3'	6.60	127.62	119.70
38	U	378	ASP	CB-CG-OD2	6.60	124.24	118.30
17	5	105	U	N1-C2-O2	6.59	127.42	122.80
19	62	47	ASP	CB-CA-C	6.59	123.59	110.40
2	6	47	A	P-O3'-C3'	6.58	127.60	119.70
9	1K	165	ASP	CB-CG-OD1	6.54	124.19	118.30
9	1K	191	ARG	CG-CD-NE	-6.53	98.09	111.80
4	B4	74	MET	CG-SD-CE	-6.52	89.77	100.20
17	5	4	C	C2-N1-C1'	6.50	125.95	118.80
32	2	106	G	P-O3'-C3'	6.50	127.50	119.70
35	68	8	TYR	CB-CG-CD2	-6.50	117.10	121.00
36	5A	1833	LEU	CA-CB-CG	6.47	130.19	115.30
22	B2	629	PRO	CB-CA-C	-6.47	95.83	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	57	G	P-O3'-C3'	6.46	127.45	119.70
1	1	126	A	O5'-P-OP1	-6.44	99.90	105.70
8	I	101	C	C2-N1-C1'	6.42	125.86	118.80
17	5	105	U	N3-C2-O2	-6.42	117.71	122.20
36	5A	779	LEU	CB-CG-CD1	-6.41	100.11	111.00
16	12	99	MET	CG-SD-CE	-6.39	89.98	100.20
19	62	69	TYR	CB-CG-CD1	6.38	124.83	121.00
17	5	110	C	N1-C2-O2	6.36	122.72	118.90
49	5B	821	LEU	CA-CB-CG	6.35	129.90	115.30
34	1g	25	ARG	NE-CZ-NH2	-6.34	117.13	120.30
42	1C	3	LYS	CB-CG-CD	6.32	128.03	111.60
36	5A	1819	LEU	CA-CB-CG	6.28	129.75	115.30
17	5	72	U	N1-C2-O2	6.28	127.19	122.80
17	5	55	C	N1-C2-O2	6.28	122.67	118.90
35	68	63	ARG	NE-CZ-NH2	-6.27	117.16	120.30
8	I	101	C	C5-C6-N1	6.25	124.12	121.00
17	5	96	A	N7-C8-N9	6.20	116.90	113.80
37	A3	190	LEU	CB-CG-CD1	-6.13	100.58	111.00
17	5	55	C	N3-C2-O2	-6.11	117.62	121.90
4	B4	12	ASP	CB-CG-OD2	-6.09	112.82	118.30
13	1f	3	LEU	C-N-CD	6.08	141.16	128.40
9	1K	50	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	1	35	A	O5'-P-OP2	-6.07	100.24	105.70
35	68	79	SER	N-CA-CB	6.06	119.59	110.50
36	5A	851	SER	N-CA-C	-6.06	94.64	111.00
17	5	115	C	C6-N1-C2	-6.03	117.89	120.30
17	5	72	U	N3-C2-O2	-6.02	117.98	122.20
9	1K	190	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	6	105	U	C5-C4-O4	5.98	129.49	125.90
47	A1	237	ARG	NE-CZ-NH1	5.96	123.28	120.30
32	2	58	U	N3-C2-O2	-5.96	118.03	122.20
14	66	52	VAL	CA-CB-CG1	5.95	119.83	110.90
8	I	92	U	N3-C2-O2	-5.92	118.05	122.20
14	66	56	LEU	CB-CG-CD1	-5.92	100.93	111.00
11	11	19	LEU	CB-CG-CD2	5.92	121.06	111.00
32	2	58	U	N1-C2-O2	5.91	126.94	122.80
9	1K	180	ARG	NE-CZ-NH1	5.91	123.25	120.30
11	11	33	ASP	CB-CG-OD2	-5.89	113.00	118.30
8	I	92	U	N1-C2-O2	5.88	126.91	122.80
17	5	71	C	C5-C6-N1	5.88	123.94	121.00
9	1K	69	ARG	NE-CZ-NH1	5.87	123.23	120.30
29	5J	739	CYS	CA-CB-SG	5.87	124.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	63	46	TYR	CB-CG-CD1	-5.86	117.49	121.00
5	43	10	LEU	CA-CB-CG	5.85	128.75	115.30
8	I	92	U	C2-N1-C1'	5.84	124.70	117.70
45	4	8	C	C6-N1-C2	-5.83	117.97	120.30
7	4e	25	LEU	CA-CB-CG	5.79	128.61	115.30
36	5A	638	LEU	CB-CG-CD1	-5.78	101.17	111.00
34	1g	25	ARG	NE-CZ-NH1	5.78	123.19	120.30
34	5g	19	LEU	CB-CG-CD2	-5.75	101.23	111.00
37	A3	199	ARG	NE-CZ-NH2	5.73	123.17	120.30
17	5	105	U	C2-N1-C1'	5.72	124.57	117.70
22	B2	644	SER	N-CA-CB	-5.72	101.91	110.50
34	4g	19	LEU	CB-CG-CD2	-5.72	101.27	111.00
37	A3	58	ARG	NE-CZ-NH1	5.72	123.16	120.30
23	5C	298	LEU	CA-CB-CG	5.71	128.43	115.30
11	11	66	ARG	CG-CD-NE	5.71	123.78	111.80
27	1A	47	ARG	NE-CZ-NH1	5.69	123.14	120.30
36	5A	1550	GLY	N-CA-C	5.68	127.29	113.10
37	A3	9	ARG	NE-CZ-NH1	5.67	123.14	120.30
14	66	44	ALA	N-CA-CB	5.66	118.02	110.10
9	1K	69	ARG	NE-CZ-NH2	-5.66	117.47	120.30
7	1e	74	LEU	CB-CG-CD1	5.64	120.59	111.00
50	B1	811	LEU	CA-CB-CG	5.64	128.27	115.30
17	5	96	A	C4-N9-C1'	5.62	136.42	126.30
1	1	2	U	OP1-P-O3'	5.61	117.55	105.20
17	5	32	C	C6-N1-C2	-5.60	118.06	120.30
29	5J	773	ASN	C-N-CD	-5.59	108.30	120.60
22	B2	565	ASP	CB-CG-OD1	5.58	123.33	118.30
45	4	130	U	N3-C2-O2	-5.56	118.31	122.20
45	4	3	C	C6-N1-C2	-5.54	118.08	120.30
42	1C	28	ARG	CD-NE-CZ	5.53	131.34	123.60
32	2	156	U	N1-C2-O2	5.52	126.67	122.80
31	63	50	LEU	CB-CG-CD2	-5.52	101.61	111.00
49	5B	2084	LEU	CA-CB-CG	5.52	128.00	115.30
40	64	25	TYR	CB-CG-CD2	-5.50	117.70	121.00
27	1A	47	ARG	NE-CZ-NH2	-5.50	117.55	120.30
17	5	7	U	N1-C2-O2	5.47	126.63	122.80
25	1b	7	SER	CA-CB-OG	5.46	125.94	111.20
8	I	95	U	C5-C6-N1	5.46	125.43	122.70
38	U	145	GLY	N-CA-C	5.45	126.73	113.10
17	5	4	C	C5-C6-N1	5.45	123.72	121.00
2	6	31	U	C2-N1-C1'	5.44	124.23	117.70
17	5	18	C	C5-C6-N1	5.44	123.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	60	U	N1-C2-O2	5.42	126.59	122.80
1	1	126	A	O5'-P-OP2	5.42	117.20	110.70
1	1	65	A	O5'-P-OP2	5.41	117.19	110.70
17	5	22	U	O4'-C1'-N1	-5.39	103.89	108.20
22	B2	619	MET	CG-SD-CE	-5.38	91.59	100.20
35	68	96	HIS	CB-CA-C	-5.35	99.70	110.40
2	6	66	C	C6-N1-C2	-5.34	118.17	120.30
8	I	101	C	N1-C2-O2	5.33	122.10	118.90
11	11	82	ASP	CB-CG-OD1	5.33	123.10	118.30
9	1K	179	GLU	OE1-CD-OE2	-5.32	116.91	123.30
17	5	56	C	N1-C2-O2	5.31	122.09	118.90
9	1K	16	ARG	NE-CZ-NH1	5.31	122.95	120.30
9	1K	49	GLU	OE1-CD-OE2	-5.31	116.93	123.30
22	B2	633	LEU	CB-CG-CD2	5.31	120.02	111.00
17	5	9	G	C4-N9-C1'	5.30	133.39	126.50
32	2	154	C	N3-C2-O2	-5.30	118.19	121.90
5	13	3	ILE	CA-CB-CG2	5.29	121.48	110.90
17	5	110	C	N3-C2-O2	-5.29	118.20	121.90
36	5A	422	LEU	CA-CB-CG	5.29	127.46	115.30
11	51	76	LEU	CA-CB-CG	5.29	127.46	115.30
17	5	96	A	C8-N9-C4	-5.28	103.69	105.80
23	5C	440	SER	C-N-CD	-5.27	109.00	120.60
34	1g	32	ARG	NE-CZ-NH1	-5.26	117.67	120.30
48	65	70	ASP	CA-CB-CG	5.25	124.95	113.40
37	A3	347	ARG	NE-CZ-NH2	5.25	122.92	120.30
11	41	76	LEU	CA-CB-CG	5.24	127.35	115.30
32	2	156	U	N3-C2-O2	-5.23	118.54	122.20
17	5	7	U	C2-N1-C1'	5.23	123.97	117.70
22	B2	629	PRO	N-CD-CG	5.21	111.01	103.20
21	A2	124	ASP	CB-CG-OD2	5.21	122.99	118.30
17	5	38	C	N1-C2-O2	5.21	122.02	118.90
16	52	53	LEU	CA-CB-CG	5.18	127.22	115.30
23	5C	828	MET	C-N-CA	5.18	134.65	121.70
37	A3	144	ASP	CB-CG-OD1	5.17	122.95	118.30
2	6	77	C	N1-C2-O2	5.15	121.99	118.90
32	2	156	U	C2-N1-C1'	5.15	123.88	117.70
48	65	65	ARG	NE-CZ-NH2	5.14	122.87	120.30
16	12	102	ARG	NE-CZ-NH1	-5.13	117.73	120.30
50	B1	974	LEU	CA-CB-CG	5.13	127.11	115.30
5	13	73	LEU	CB-CG-CD1	-5.13	102.28	111.00
13	1f	73	ARG	CG-CD-NE	5.12	122.56	111.80
32	2	40	C	N1-C2-O2	5.12	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	68	88	ALA	C-N-CA	5.12	134.51	121.70
2	6	105	U	C6-N1-C1'	5.12	128.37	121.20
44	4A	426	PRO	C-N-CD	5.11	139.12	128.40
44	4A	551	LEU	CA-CB-CG	5.11	127.04	115.30
16	12	61	ARG	NE-CZ-NH1	-5.09	117.75	120.30
17	5	7	U	N3-C2-O2	-5.08	118.64	122.20
9	1K	72	ARG	NE-CZ-NH1	5.08	122.84	120.30
29	5J	739	CYS	C-N-CA	5.07	143.31	122.00
45	4	3	C	C5-C6-N1	5.07	123.53	121.00
37	A3	316	ARG	NE-CZ-NH2	5.07	122.83	120.30
9	1K	53	ASP	CB-CG-OD2	5.06	122.86	118.30
32	2	45	C	C5-C6-N1	5.06	123.53	121.00
21	A2	148	ARG	NE-CZ-NH2	5.04	122.82	120.30
21	A2	58	LEU	CA-CB-CG	5.04	126.89	115.30
7	1e	73	GLN	CA-CB-CG	5.04	124.48	113.40
49	5B	299	ASP	CB-CG-OD1	5.03	122.83	118.30
18	67	69	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
17	5	110	C	C2-N1-C1'	5.02	124.33	118.80
17	5	23	C	C5-C6-N1	5.02	123.51	121.00
32	2	46	U	OP2-P-O3'	5.02	116.24	105.20
35	68	63	ARG	NE-CZ-NH1	5.01	122.80	120.30
17	5	4	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	12	17	GLN	Peptide
9	1K	56	PRO	Peptide
45	4	90	G	Sidechain
44	4A	421	PRO	Peptide
44	4A	538	SER	Peptide
6	4B	420	TYR	Peptide
6	4B	459	PRO	Peptide
6	4B	470	TYR	Peptide
10	4C	350	GLN	Peptide
10	4C	386	ASP	Peptide
25	4b	53	PRO	Peptide
7	4e	51	ASP	Peptide
13	4f	40	MET	Peptide
16	52	46	CYS	Peptide
16	52	60	ASP	Peptide

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Mol	Chain	Res	Type	Group
16	52	88	LYS	Peptide
36	5A	1416	ILE	Peptide
36	5A	1792	LYS	Peptide
49	5B	1265	GLN	Peptide
49	5B	526	ASN	Peptide
23	5C	167	TYR	Peptide
23	5C	439	PRO	Peptide
29	5J	624	VAL	Peptide
29	5J	724	MET	Peptide
13	5f	40	MET	Peptide
19	62	69	TYR	Sidechain
31	63	30	TYR	Sidechain
31	63	46	TYR	Sidechain
40	64	25	TYR	Sidechain
14	66	51	TYR	Sidechain
18	67	62	TYR	Sidechain
35	68	60	TYR	Sidechain
35	68	8	TYR	Sidechain
35	68	89	GLU	Peptide
47	A1	191	ARG	Sidechain
47	A1	193	TYR	Sidechain
47	A1	199	ARG	Sidechain
47	A1	255	ARG	Sidechain
21	A2	138	TYR	Sidechain
21	A2	175	PRO	Peptide
21	A2	176	TYR	Sidechain
21	A2	201	ARG	Sidechain
37	A3	163	TYR	Sidechain
37	A3	281	ARG	Sidechain
37	A3	312	ARG	Sidechain
37	A3	42	ARG	Sidechain
37	A3	58	ARG	Sidechain
37	A3	61	TYR	Sidechain
50	B1	1050	VAL	Peptide
50	B1	460	PRO	Peptide
50	B1	483	ASP	Peptide
50	B1	488	SER	Peptide
33	B3	913	LEU	Peptide
38	U	244	LEU	Peptide
38	U	423	PHE	Peptide
38	U	531	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

## 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	
3	5O	304/357 (85%)	283 (93%)	19 (6%)	2 (1%)	19	49
4	B4	76/424 (18%)	76 (100%)	0	0	100	100
5	13	79/126 (63%)	75 (95%)	4 (5%)	0	100	100
5	23	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
5	43	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
5	53	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
6	4B	357/522 (68%)	330 (92%)	25 (7%)	2 (1%)	22	52
7	1e	75/92 (82%)	70 (93%)	5 (7%)	0	100	100
7	2e	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
7	4e	74/92 (80%)	71 (96%)	3 (4%)	0	100	100
7	5e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
9	1K	199/437 (46%)	184 (92%)	12 (6%)	3 (2%)	8	33
10	4C	293/499 (59%)	275 (94%)	18 (6%)	0	100	100
11	11	79/119 (66%)	77 (98%)	2 (2%)	0	100	100
11	21	78/119 (66%)	75 (96%)	3 (4%)	0	100	100
11	41	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
11	51	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
12	R	104/480 (22%)	91 (88%)	13 (12%)	0	100	100
13	1f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
13	2f	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
13	4f	70/86 (81%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	5f	71/86 (83%)	64 (90%)	7 (10%)	0	100	100
14	66	70/80 (88%)	69 (99%)	0	1 (1%)	9	34
15	X	45/155 (29%)	39 (87%)	6 (13%)	0	100	100
16	12	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
16	22	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
16	42	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
16	52	94/118 (80%)	87 (93%)	7 (7%)	0	100	100
18	67	75/103 (73%)	72 (96%)	2 (3%)	1 (1%)	10	36
19	62	93/95 (98%)	84 (90%)	6 (6%)	3 (3%)	3	19
20	2B	90/225 (40%)	88 (98%)	2 (2%)	0	100	100
21	A2	138/209 (66%)	123 (89%)	11 (8%)	4 (3%)	3	21
22	B2	204/895 (23%)	181 (89%)	22 (11%)	1 (0%)	25	56
23	5C	850/854 (100%)	817 (96%)	31 (4%)	2 (0%)	44	72
24	5X	574/820 (70%)	561 (98%)	13 (2%)	0	100	100
25	1b	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
25	2b	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
25	4b	80/240 (33%)	71 (89%)	9 (11%)	0	100	100
25	5b	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
26	B5	67/86 (78%)	61 (91%)	6 (9%)	0	100	100
27	1A	96/282 (34%)	94 (98%)	2 (2%)	0	100	100
28	S	110/800 (14%)	101 (92%)	8 (7%)	1 (1%)	14	44
29	5J	793/850 (93%)	748 (94%)	44 (6%)	1 (0%)	48	77
30	4D	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
31	63	83/102 (81%)	79 (95%)	3 (4%)	1 (1%)	11	38
33	B3	1176/1217 (97%)	1082 (92%)	92 (8%)	2 (0%)	44	72
34	1g	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
34	2g	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
34	4g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
34	5g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
35	68	93/96 (97%)	81 (87%)	6 (6%)	6 (6%)	1	7
36	5A	2198/2311 (95%)	2094 (95%)	102 (5%)	2 (0%)	48	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	A3	377/501 (75%)	346 (92%)	26 (7%)	5 (1%)	10	36
38	U	454/555 (82%)	424 (93%)	27 (6%)	3 (1%)	19	49
39	5D	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
40	64	71/139 (51%)	66 (93%)	3 (4%)	2 (3%)	4	22
41	BP	98/104 (94%)	92 (94%)	6 (6%)	0	100	100
42	1C	48/159 (30%)	47 (98%)	1 (2%)	0	100	100
43	K	316/1007 (31%)	294 (93%)	18 (6%)	4 (1%)	10	36
44	4A	229/683 (34%)	210 (92%)	18 (8%)	1 (0%)	30	61
46	2A	160/255 (63%)	147 (92%)	13 (8%)	0	100	100
47	A1	138/647 (21%)	129 (94%)	7 (5%)	2 (1%)	9	34
48	65	74/91 (81%)	70 (95%)	2 (3%)	2 (3%)	4	22
49	5B	1989/2136 (93%)	1885 (95%)	103 (5%)	1 (0%)	48	77
50	B1	846/1304 (65%)	792 (94%)	53 (6%)	1 (0%)	48	77
All	All	15337/23178 (66%)	14438 (94%)	846 (6%)	53 (0%)	38	67

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	5O	59	ILE
9	1K	59	ARG
9	1K	63	ARG
19	62	47	ASP
19	62	53	HIS
21	A2	165	ARG
28	S	566	ILE
29	5J	93	PRO
35	68	89	GLU
37	A3	78	PRO
38	U	408	GLN
43	K	697	VAL
47	A1	192	ASN
6	4B	460	ILE
9	1K	60	ALA
14	66	52	VAL
35	68	86	ILE
35	68	90	PRO
37	A3	227	PRO

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Mol	Chain	Res	Type
37	A3	292	SER
43	K	851	VAL
48	65	87	GLU
33	B3	932	ASN
33	B3	933	ASN
35	68	79	SER
36	5A	189	GLU
37	A3	308	LYS
47	A1	218	ILE
3	5O	58	PRO
19	62	55	LEU
23	5C	943	LEU
31	63	35	ASN
35	68	43	GLU
40	64	12	ASN
43	K	699	SER
21	A2	115	PRO
21	A2	208	LEU
23	5C	107	GLN
35	68	59	LEU
36	5A	60	ASP
37	A3	99	PRO
38	U	146	ARG
40	64	57	PRO
43	K	722	ASN
44	4A	539	GLN
18	67	19	ILE
49	5B	756	SER
6	4B	459	PRO
21	A2	188	ILE
50	B1	489	PRO
22	B2	521	PRO
38	U	362	PRO
48	65	47	VAL

### 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	
3	5O	263/300 (88%)	263 (100%)	0	100	100
4	B4	66/336 (20%)	66 (100%)	0	100	100
5	13	71/101 (70%)	61 (86%)	10 (14%)	3	13
5	23	73/101 (72%)	73 (100%)	0	100	100
5	43	73/101 (72%)	73 (100%)	0	100	100
5	53	73/101 (72%)	73 (100%)	0	100	100
6	4B	306/442 (69%)	303 (99%)	3 (1%)	73	84
7	1e	72/84 (86%)	61 (85%)	11 (15%)	2	10
7	2e	76/84 (90%)	76 (100%)	0	100	100
7	4e	71/84 (84%)	69 (97%)	2 (3%)	38	63
7	5e	72/84 (86%)	72 (100%)	0	100	100
9	1K	170/373 (46%)	161 (95%)	9 (5%)	19	46
10	4C	255/424 (60%)	251 (98%)	4 (2%)	58	75
11	11	76/101 (75%)	72 (95%)	4 (5%)	19	46
11	21	75/101 (74%)	75 (100%)	0	100	100
11	41	76/101 (75%)	55 (72%)	21 (28%)	0	1
11	51	76/101 (75%)	55 (72%)	21 (28%)	0	1
12	R	94/369 (26%)	91 (97%)	3 (3%)	34	60
13	1f	63/74 (85%)	56 (89%)	7 (11%)	5	20
13	2f	61/74 (82%)	61 (100%)	0	100	100
13	4f	61/74 (82%)	61 (100%)	0	100	100
13	5f	61/74 (82%)	60 (98%)	1 (2%)	58	75
14	66	62/70 (89%)	62 (100%)	0	100	100
15	X	42/144 (29%)	42 (100%)	0	100	100
16	12	91/110 (83%)	83 (91%)	8 (9%)	8	28
16	22	91/110 (83%)	91 (100%)	0	100	100
16	42	86/110 (78%)	86 (100%)	0	100	100
16	52	93/110 (84%)	92 (99%)	1 (1%)	70	82
18	67	69/91 (76%)	68 (99%)	1 (1%)	62	78
19	62	88/88 (100%)	86 (98%)	2 (2%)	45	68
20	2B	81/195 (42%)	81 (100%)	0	100	100
21	A2	129/180 (72%)	128 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	B2	187/776 (24%)	185 (99%)	2 (1%)	70	82
23	5C	754/756 (100%)	751 (100%)	3 (0%)	89	93
24	5X	517/721 (72%)	501 (97%)	16 (3%)	35	61
25	1b	78/177 (44%)	70 (90%)	8 (10%)	6	22
25	2b	75/177 (42%)	75 (100%)	0	100	100
25	4b	75/177 (42%)	75 (100%)	0	100	100
25	5b	67/177 (38%)	66 (98%)	1 (2%)	60	77
26	B5	60/77 (78%)	60 (100%)	0	100	100
27	1A	85/240 (35%)	82 (96%)	3 (4%)	31	57
28	S	91/681 (13%)	91 (100%)	0	100	100
29	5J	636/715 (89%)	631 (99%)	5 (1%)	79	87
30	4D	107/111 (96%)	107 (100%)	0	100	100
31	63	79/94 (84%)	76 (96%)	3 (4%)	28	55
33	B3	1027/1051 (98%)	1021 (99%)	6 (1%)	84	90
34	1g	63/66 (96%)	57 (90%)	6 (10%)	7	25
34	2g	63/66 (96%)	62 (98%)	1 (2%)	58	75
34	4g	64/66 (97%)	46 (72%)	18 (28%)	0	1
34	5g	64/66 (97%)	46 (72%)	18 (28%)	0	1
35	68	81/82 (99%)	77 (95%)	4 (5%)	21	49
36	5A	2002/2090 (96%)	1990 (99%)	12 (1%)	84	90
37	A3	345/446 (77%)	339 (98%)	6 (2%)	56	74
38	U	418/503 (83%)	414 (99%)	4 (1%)	73	84
39	5D	129/130 (99%)	129 (100%)	0	100	100
40	64	68/111 (61%)	68 (100%)	0	100	100
41	BP	86/90 (96%)	85 (99%)	1 (1%)	67	81
42	1C	48/135 (36%)	42 (88%)	6 (12%)	3	16
43	K	291/919 (32%)	259 (89%)	32 (11%)	5	20
44	4A	210/599 (35%)	208 (99%)	2 (1%)	73	84
46	2A	139/218 (64%)	138 (99%)	1 (1%)	81	88
47	A1	130/550 (24%)	127 (98%)	3 (2%)	45	68
48	65	68/80 (85%)	67 (98%)	1 (2%)	60	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	5B	1779/1908 (93%)	1766 (99%)	13 (1%)	81	88
50	B1	733/1104 (66%)	729 (100%)	4 (0%)	86	91
All	All	13735/20051 (68%)	13447 (98%)	288 (2%)	49	70

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	13	3	ILE
5	13	20	CYS
5	13	24	THR
5	13	34	GLU
5	13	46	ILE
5	13	51	ARG
5	13	73	LEU
5	13	78	LYS
5	13	82	MET
5	13	83	LEU
6	4B	395	ARG
6	4B	407	LEU
6	4B	444	THR
9	1K	3	GLN
9	1K	28	LEU
9	1K	48	PHE
9	1K	50	ASP
9	1K	140	SER
9	1K	167	LYS
9	1K	168	LYS
9	1K	172	ARG
9	1K	188	ARG
10	4C	299	CYS
10	4C	315	LYS
10	4C	351	ARG
10	4C	363	LYS
11	41	2	LYS
11	41	4	VAL
11	41	8	MET
11	41	10	LEU
11	41	11	SER
11	41	16	THR
11	41	28	THR
11	41	33	ASP

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Mol	Chain	Res	Type
11	41	35	SER
11	41	44	LYS
11	41	47	LEU
11	41	48	LYS
11	41	51	GLU
11	41	53	VAL
11	41	54	GLN
11	41	55	LEU
11	41	56	GLU
11	41	57	THR
11	41	74	LEU
11	41	76	LEU
11	41	81	VAL
12	R	377	ASP
12	R	379	ASP
12	R	431	ASP
13	1f	3	LEU
13	1f	8	LYS
13	1f	14	LEU
13	1f	23	LEU
13	1f	27	MET
13	1f	51	ILE
13	1f	65	ARG
7	4e	28	ARG
7	4e	30	ARG
18	67	17	LYS
19	62	44	SER
19	62	72	LEU
21	A2	189	ASP
22	B2	600	ARG
22	B2	604	LYS
23	5C	507	VAL
23	5C	735	PHE
23	5C	919	ARG
24	5X	270	ARG
24	5X	389	PRO
24	5X	395	ASP
24	5X	472	ILE
24	5X	491	PHE
24	5X	516	ARG
24	5X	532	VAL
24	5X	664	ASP

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Mol	Chain	Res	Type
24	5X	674	LYS
24	5X	675	LYS
24	5X	679	VAL
24	5X	685	GLU
24	5X	703	ARG
24	5X	729	ASP
24	5X	730	ILE
24	5X	746	GLU
11	11	4	VAL
11	11	11	SER
11	11	19	LEU
11	11	82	ASP
25	1b	7	SER
25	1b	12	HIS
25	1b	54	LYS
25	1b	56	SER
25	1b	57	LYS
25	1b	58	GLN
25	1b	67	LEU
25	1b	71	LEU
27	1A	8	PRO
27	1A	61	GLU
27	1A	103	GLU
13	5f	11	LEU
29	5J	91	SER
29	5J	405	ARG
29	5J	570	PHE
29	5J	674	THR
29	5J	743	THR
11	51	2	LYS
11	51	4	VAL
11	51	8	MET
11	51	10	LEU
11	51	11	SER
11	51	16	THR
11	51	28	THR
11	51	33	ASP
11	51	35	SER
11	51	44	LYS
11	51	47	LEU
11	51	48	LYS
11	51	51	GLU

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Mol	Chain	Res	Type
11	51	53	VAL
11	51	54	GLN
11	51	55	LEU
11	51	56	GLU
11	51	57	THR
11	51	74	LEU
11	51	76	LEU
11	51	81	VAL
31	63	34	ARG
31	63	39	LEU
31	63	94	LEU
33	B3	175	VAL
33	B3	248	VAL
33	B3	278	LEU
33	B3	532	ARG
33	B3	703	ARG
33	B3	1064	ASP
34	1g	27	VAL
34	1g	50	THR
34	1g	51	SER
34	1g	57	ILE
34	1g	59	MET
34	1g	69	MET
25	5b	16	ARG
35	68	13	VAL
35	68	19	ASP
35	68	90	PRO
35	68	91	LEU
7	1e	14	MET
7	1e	25	LEU
7	1e	27	ASN
7	1e	60	ASP
7	1e	62	GLU
7	1e	63	GLU
7	1e	68	THR
7	1e	70	SER
7	1e	80	LYS
7	1e	82	ASP
7	1e	86	LEU
36	5A	86	ARG
36	5A	165	ARG
36	5A	284	ARG

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Mol	Chain	Res	Type
36	5A	342	THR
36	5A	563	GLN
36	5A	579	GLN
36	5A	741	ARG
36	5A	1126	VAL
36	5A	1298	ARG
36	5A	1925	LYS
36	5A	1958	LYS
36	5A	2249	LYS
37	A3	78	PRO
37	A3	81	PHE
37	A3	111	GLU
37	A3	122	GLU
37	A3	195	ASP
37	A3	402	LEU
38	U	100	ARG
38	U	101	ARG
38	U	235	ASP
38	U	289	ARG
34	2g	43	ASP
16	52	33	THR
16	12	20	GLU
16	12	37	LYS
16	12	42	VAL
16	12	51	LYS
16	12	61	ARG
16	12	75	THR
16	12	94	ARG
16	12	114	LEU
41	BP	30	CYS
42	1C	3	LYS
42	1C	26	SER
42	1C	29	LYS
42	1C	39	GLN
42	1C	45	GLN
42	1C	48	SER
34	5g	3	LYS
34	5g	10	LYS
34	5g	11	LYS
34	5g	15	LYS
34	5g	27	VAL
34	5g	35	ASP

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Mol	Chain	Res	Type
34	5g	43	ASP
34	5g	44	GLU
34	5g	46	VAL
34	5g	47	GLU
34	5g	50	THR
34	5g	51	SER
34	5g	59	MET
34	5g	62	ILE
34	5g	66	SER
34	5g	70	LEU
34	5g	71	GLU
34	5g	73	LEU
43	K	676	ARG
43	K	688	ASN
43	K	697	VAL
43	K	698	PHE
43	K	700	ASN
43	K	721	ASN
43	K	724	LEU
43	K	726	GLN
43	K	731	LYS
43	K	733	LEU
43	K	763	LEU
43	K	777	VAL
43	K	778	LEU
43	K	793	ARG
43	K	805	LEU
43	K	812	LEU
43	K	825	GLU
43	K	830	LEU
43	K	831	LYS
43	K	843	ASP
43	K	850	LEU
43	K	878	THR
43	K	882	LEU
43	K	886	LYS
43	K	892	LYS
43	K	920	ASP
43	K	946	MET
43	K	950	ASN
43	K	955	LEU
43	K	956	LEU

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Mol	Chain	Res	Type
43	K	1004	GLN
43	K	1005	GLU
44	4A	597	LEU
44	4A	646	MET
34	4g	3	LYS
34	4g	10	LYS
34	4g	11	LYS
34	4g	15	LYS
34	4g	27	VAL
34	4g	35	ASP
34	4g	43	ASP
34	4g	44	GLU
34	4g	46	VAL
34	4g	47	GLU
34	4g	50	THR
34	4g	51	SER
34	4g	59	MET
34	4g	62	ILE
34	4g	66	SER
34	4g	70	LEU
34	4g	71	GLU
34	4g	73	LEU
46	2A	120	ILE
47	A1	163	ASP
47	A1	223	LYS
47	A1	237	ARG
48	65	16	GLU
49	5B	287	ASP
49	5B	300	ARG
49	5B	406	ARG
49	5B	681	ARG
49	5B	753	ARG
49	5B	992	TYR
49	5B	998	VAL
49	5B	1030	ARG
49	5B	1152	ARG
49	5B	1228	VAL
49	5B	1518	VAL
49	5B	1521	VAL
49	5B	1843	ARG
50	B1	614	ARG
50	B1	632	PHE

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Mol	Chain	Res	Type
50	B1	695	VAL
50	B1	970	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
3	5O	101	ASN
3	5O	165	GLN
3	5O	225	ASN
6	4B	282	HIS
6	4B	414	ASN
7	5e	32	GLN
7	5e	38	GLN
7	5e	88	GLN
9	1K	36	GLN
9	1K	133	HIS
9	1K	158	HIS
10	4C	389	GLN
11	4I	24	GLN
12	R	393	ASN
12	R	471	GLN
14	66	69	ASN
19	62	53	HIS
19	62	71	GLN
20	2B	15	ASN
5	53	42	GLN
21	A2	79	GLN
21	A2	149	HIS
22	B2	496	ASN
13	2f	68	ASN
23	5C	137	HIS
23	5C	154	HIS
23	5C	571	ASN
23	5C	583	ASN
23	5C	702	ASN
23	5C	719	GLN
23	5C	743	ASN
23	5C	771	GLN
23	5C	903	HIS
23	5C	905	GLN
24	5X	297	GLN
24	5X	359	GLN

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Mol	Chain	Res	Type
24	5X	420	GLN
24	5X	428	ASN
24	5X	535	ASN
24	5X	597	HIS
24	5X	731	GLN
16	42	49	ASN
16	42	69	ASN
16	42	112	ASN
26	B5	34	ASN
26	B5	51	ASN
26	B5	58	ASN
28	S	728	GLN
13	5f	6	ASN
13	5f	68	ASN
29	5J	140	GLN
29	5J	308	HIS
29	5J	353	GLN
29	5J	587	HIS
29	5J	733	ASN
29	5J	741	HIS
29	5J	839	HIS
29	5J	865	HIS
11	51	63	ASN
11	51	64	ASN
30	4D	111	GLN
25	2b	76	ASN
33	B3	138	GLN
33	B3	260	ASN
33	B3	264	GLN
33	B3	760	ASN
33	B3	796	ASN
33	B3	885	ASN
33	B3	988	ASN
33	B3	1172	ASN
5	23	40	ASN
5	23	45	ASN
25	5b	22	GLN
36	5A	221	ASN
36	5A	325	HIS
36	5A	434	HIS
36	5A	448	GLN
36	5A	579	GLN

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Mol	Chain	Res	Type
36	5A	654	ASN
36	5A	711	GLN
36	5A	775	ASN
36	5A	875	HIS
36	5A	1003	HIS
36	5A	1014	ASN
36	5A	1159	ASN
36	5A	1172	ASN
36	5A	1332	HIS
36	5A	1345	GLN
36	5A	1487	HIS
36	5A	1543	ASN
36	5A	1737	ASN
36	5A	1752	GLN
36	5A	1830	GLN
36	5A	1875	HIS
36	5A	2166	HIS
36	5A	2203	ASN
36	5A	2260	GLN
36	5A	2276	GLN
36	5A	2306	HIS
37	A3	143	HIS
38	U	144	GLN
38	U	158	GLN
38	U	205	ASN
38	U	234	ASN
38	U	242	GLN
38	U	298	HIS
38	U	413	GLN
38	U	531	GLN
38	U	541	GLN
34	2g	26	HIS
39	5D	7	HIS
39	5D	32	HIS
16	52	41	GLN
7	2e	19	ASN
7	2e	88	GLN
34	5g	26	HIS
34	5g	55	ASN
43	K	695	GLN
43	K	707	ASN
43	K	722	ASN

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Mol	Chain	Res	Type
43	K	740	ASN
43	K	840	HIS
43	K	895	ASN
43	K	896	HIS
43	K	921	GLN
43	K	926	ASN
43	K	928	ASN
43	K	950	ASN
43	K	995	ASN
44	4A	425	ASN
44	4A	524	GLN
11	2I	64	ASN
34	4g	26	HIS
34	4g	55	ASN
46	2A	72	ASN
49	5B	259	HIS
49	5B	304	ASN
49	5B	313	ASN
49	5B	485	GLN
49	5B	498	ASN
49	5B	524	HIS
49	5B	638	ASN
49	5B	702	GLN
49	5B	785	HIS
49	5B	884	ASN
49	5B	885	GLN
49	5B	968	ASN
49	5B	999	GLN
49	5B	1003	GLN
49	5B	1086	GLN
49	5B	1209	GLN
49	5B	1247	GLN
49	5B	1265	GLN
49	5B	1423	ASN
49	5B	1441	GLN
49	5B	1659	HIS
49	5B	1674	HIS
49	5B	1769	ASN
49	5B	1885	ASN
49	5B	1994	ASN
50	B1	457	ASN
50	B1	533	ASN

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Mol	Chain	Res	Type
50	B1	698	GLN
50	B1	832	GLN
50	B1	1002	ASN
50	B1	1107	GLN
50	B1	1252	GLN
50	B1	1256	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	163/164 (99%)	49 (30%)	6 (3%)
17	5	101/117 (86%)	42 (41%)	4 (3%)
2	6	50/106 (47%)	5 (10%)	2 (4%)
32	2	90/188 (47%)	23 (25%)	4 (4%)
45	4	120/146 (82%)	25 (20%)	3 (2%)
8	I	23/62 (37%)	5 (21%)	0
All	All	547/783 (69%)	149 (27%)	19 (3%)

All (149) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	U
1	1	12	G
1	1	15	G
1	1	16	G
1	1	17	G
1	1	20	G
1	1	21	A
1	1	22	U
1	1	23	A
1	1	28	G
1	1	29	A
1	1	35	A
1	1	41	G
1	1	47	C
1	1	48	C
1	1	50	G
1	1	51	G
1	1	55	A
1	1	62	U
1	1	72	U

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Mol	Chain	Res	Type
1	1	73	C
1	1	75	G
1	1	88	C
1	1	90	U
1	1	91	G
1	1	92	C
1	1	93	G
1	1	94	A
1	1	103	A
1	1	105	U
1	1	108	G
1	1	112	A
1	1	114	C
1	1	115	U
1	1	117	G
1	1	118	A
1	1	119	C
1	1	123	A
1	1	124	U
1	1	126	A
1	1	128	U
1	1	130	G
1	1	132	G
1	1	133	G
1	1	135	A
1	1	136	G
1	1	137	U
1	1	138	G
1	1	158	U
2	6	48	A
2	6	49	G
2	6	74	U
2	6	77	C
2	6	106	U
8	I	0	G
8	I	5	G
8	I	92	U
8	I	100	A
8	I	101	C
17	5	4	C
17	5	5	U
17	5	6	C

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Mol	Chain	Res	Type
17	5	7	U
17	5	9	G
17	5	20	G
17	5	21	A
17	5	22	U
17	5	23	C
17	5	24	G
17	5	25	C
17	5	26	A
17	5	28	A
17	5	36	C
17	5	37	G
17	5	38	C
17	5	47	A
17	5	48	A
17	5	57	G
17	5	58	U
17	5	59	G
17	5	63	A
17	5	66	A
17	5	67	A
17	5	71	C
17	5	75	G
17	5	78	U
17	5	86	C
17	5	88	A
17	5	89	U
17	5	90	U
17	5	94	U
17	5	95	G
17	5	97	G
17	5	98	G
17	5	102	U
17	5	104	C
17	5	105	U
17	5	106	U
17	5	107	U
17	5	108	G
17	5	109	G
32	2	37	U
32	2	38	A
32	2	40	C

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Mol	Chain	Res	Type
32	2	43	U
32	2	45	C
32	2	46	U
32	2	47	U
32	2	48	A
32	2	49	U
32	2	63	G
32	2	65	U
32	2	98	G
32	2	100	U
32	2	101	U
32	2	102	U
32	2	103	U
32	2	104	U
32	2	105	G
32	2	106	G
32	2	107	A
32	2	157	G
32	2	171	U
32	2	178	A
45	4	2	G
45	4	19	U
45	4	20	A
45	4	25	A
45	4	26	G
45	4	30	A
45	4	36	U
45	4	37	U
45	4	38	U
45	4	40	U
45	4	44	A
45	4	45	G
45	4	51	A
45	4	52	U
45	4	67	A
45	4	68	A
45	4	69	C
45	4	114	U
45	4	115	G
45	4	121	U
45	4	122	U
45	4	123	U

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Mol	Chain	Res	Type
45	4	125	G
45	4	126	A
45	4	140	G

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	15	G
1	1	90	U
1	1	92	C
1	1	123	A
1	1	126	A
1	1	128	U
2	6	47	A
2	6	104	U
17	5	57	G
17	5	58	U
17	5	96	A
17	5	105	U
32	2	37	U
32	2	46	U
32	2	103	U
32	2	106	G
45	4	1	A
45	4	68	A
45	4	114	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	IHP	5A	2401	-	36,36,36	0.71	0	54,60,60	0.58	0
53	GTP	5C	1002	52	26,34,34	1.36	3 (11%)	32,54,54	1.61	7 (21%)

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
54	IHP	5A	2401	-	-	8/30/54/54	0/1/1/1
53	GTP	5C	1002	52	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	5C	1002	GTP	C5-C6	-4.45	1.38	1.47
53	5C	1002	GTP	C5-C4	-2.15	1.37	1.43
53	5C	1002	GTP	O4'-C4'	-2.11	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	5C	1002	GTP	PB-O3B-PG	-3.54	120.68	132.83
53	5C	1002	GTP	C5-C6-N1	3.51	120.14	113.95
53	5C	1002	GTP	C8-N7-C5	3.05	108.80	102.99
53	5C	1002	GTP	C2-N1-C6	-3.00	119.58	125.10
53	5C	1002	GTP	PA-O3A-PB	-2.50	124.26	132.83
53	5C	1002	GTP	O6-C6-C5	-2.35	119.79	124.37
53	5C	1002	GTP	C3'-C2'-C1'	2.22	104.32	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	5A	2401	IHP	C1-O11-P1-O41

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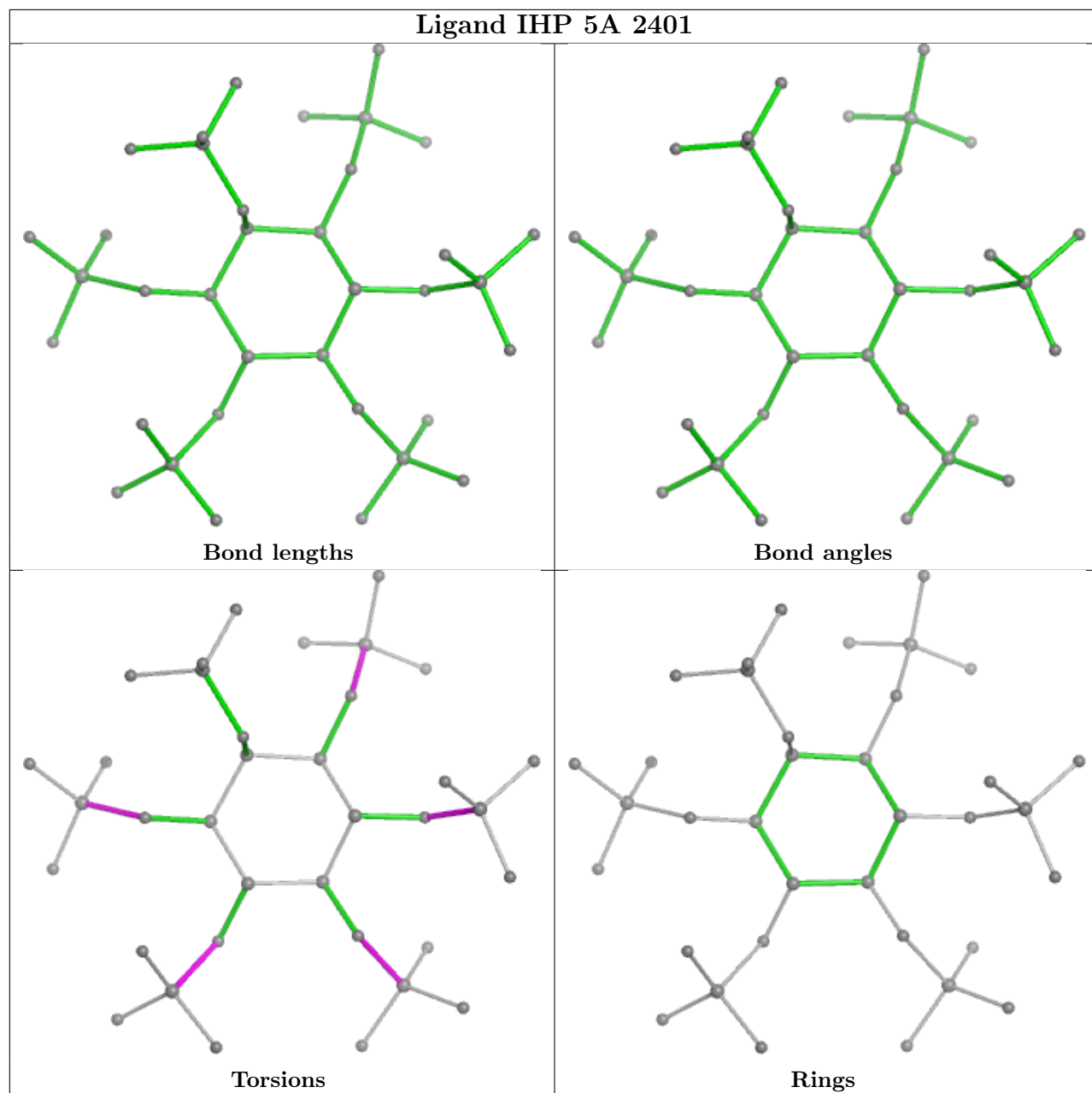
Mol	Chain	Res	Type	Atoms
54	5A	2401	IHP	C3-O13-P3-O23
53	5C	1002	GTP	O4'-C4'-C5'-O5'
53	5C	1002	GTP	PB-O3A-PA-O2A
53	5C	1002	GTP	C3'-C4'-C5'-O5'
54	5A	2401	IHP	C5-O15-P5-O25
54	5A	2401	IHP	C6-O16-P6-O26
54	5A	2401	IHP	C4-O14-P4-O34
54	5A	2401	IHP	C5-O15-P5-O35
54	5A	2401	IHP	C5-O15-P5-O45
54	5A	2401	IHP	C6-O16-P6-O46
53	5C	1002	GTP	C5'-O5'-PA-O1A

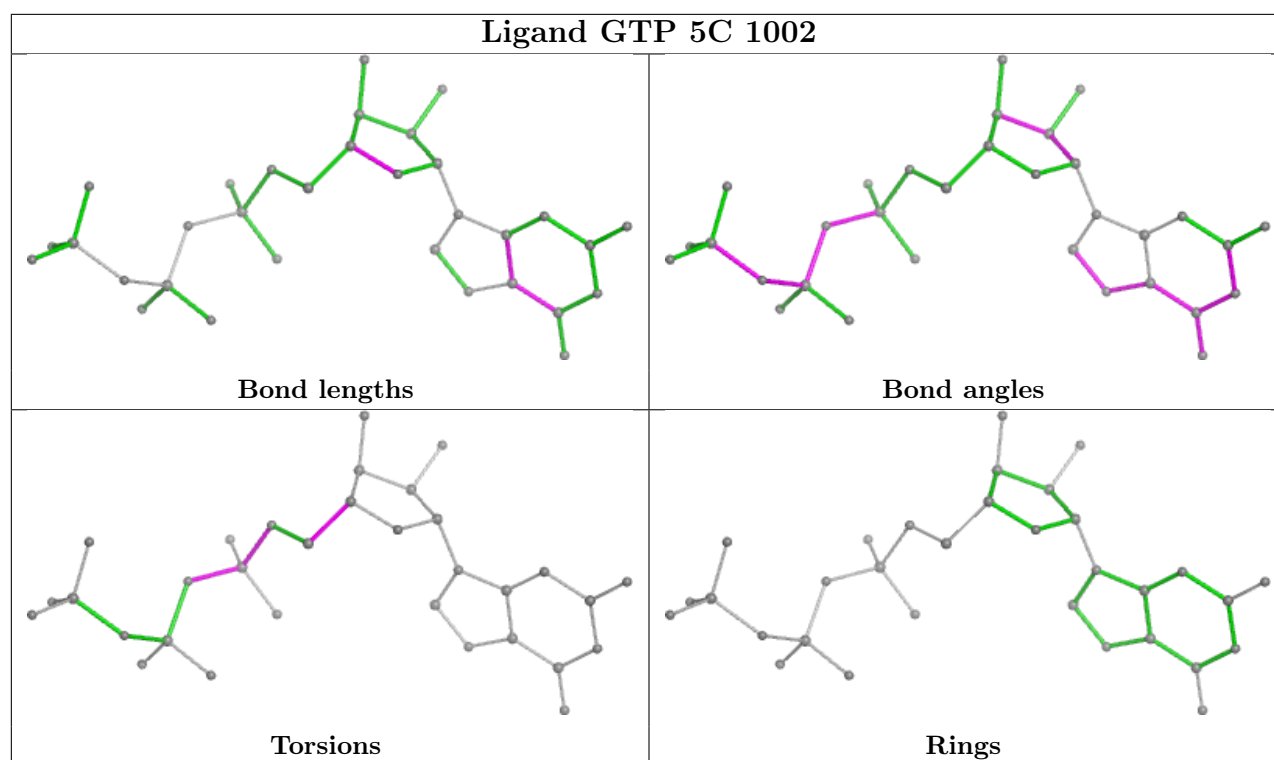
There are no ring outliers.

No monomer is involved in short contacts.

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

## Ligand IHP 5A 2401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	A1	2
1	1	2
29	5J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	282:VAL	C	422:UNK	N	108.26
1	5J	165:ASP	C	236:GLY	N	34.19
1	A1	447:UNK	C	455:VAL	N	4.52
1	1	2:U	O3'	3:A	P	1.39
1	1	78:U	O3'	79:G	P	1.37



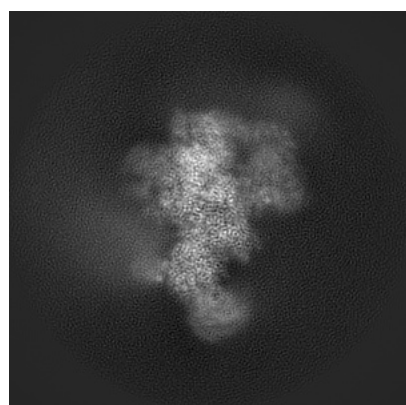
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4665. These allow visual inspection of the internal detail of the map and identification of artifacts.

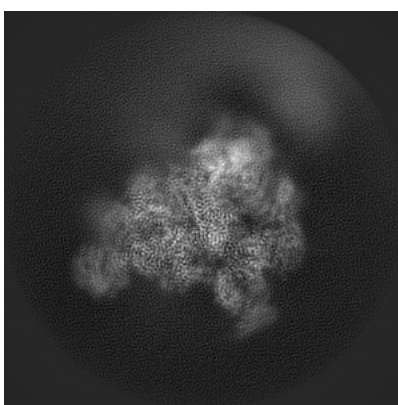
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

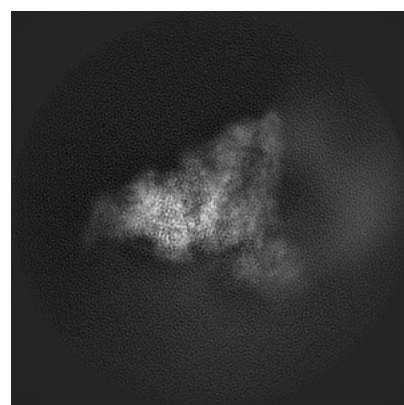
#### 6.1.1 Primary map



X



Y

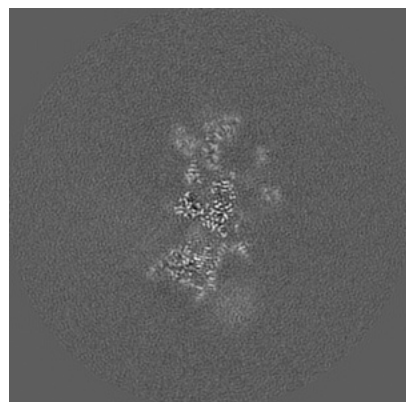


Z

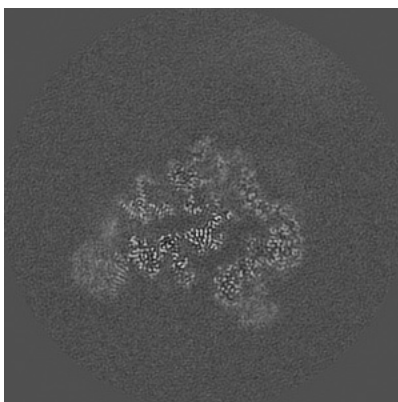
The images above show the map projected in three orthogonal directions.

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

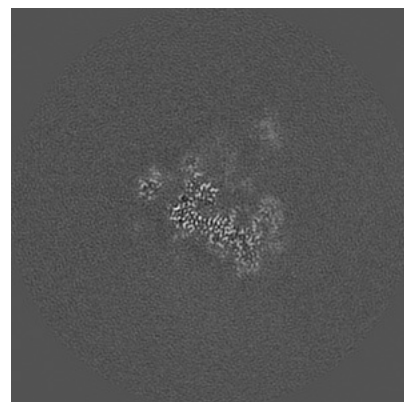
#### 6.2.1 Primary map



X Index: 210



Y Index: 210

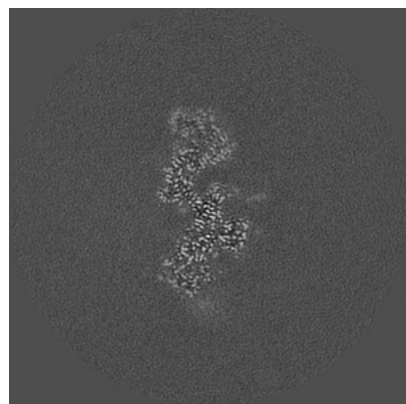


Z Index: 210

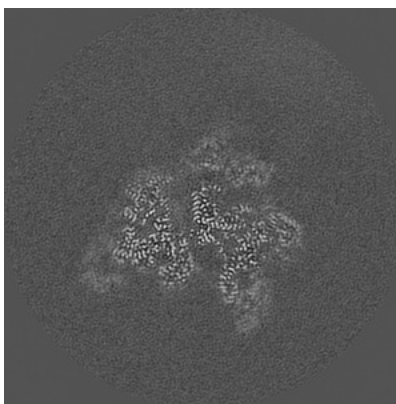
The images above show central slices of the map in three orthogonal directions.

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

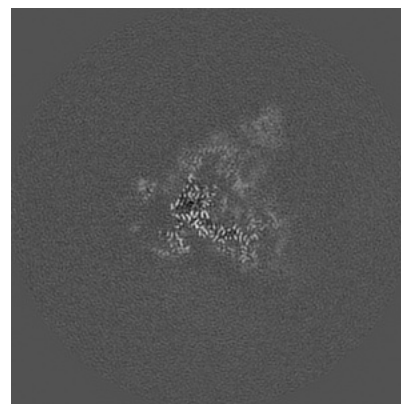
### 6.3.1 Primary map



X Index: 177



Y Index: 193

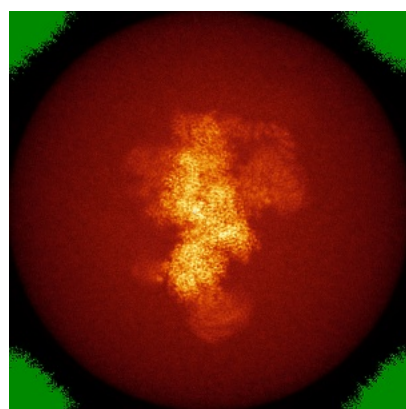


Z Index: 218

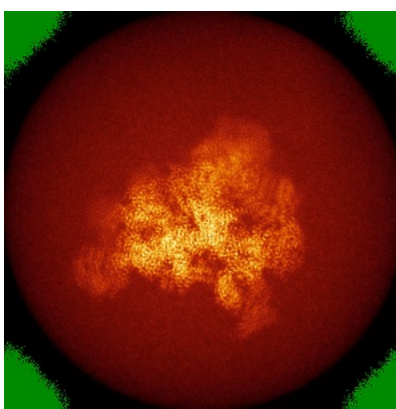
The images above show the largest variance slices of the map in three orthogonal directions.

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

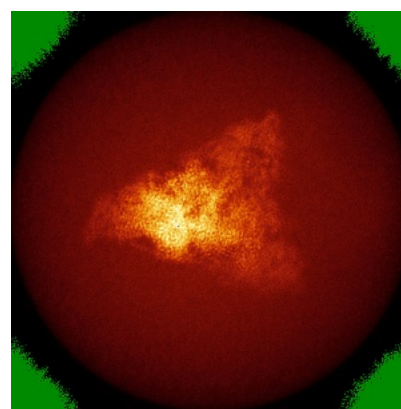
### 6.4.1 Primary map



X



Y

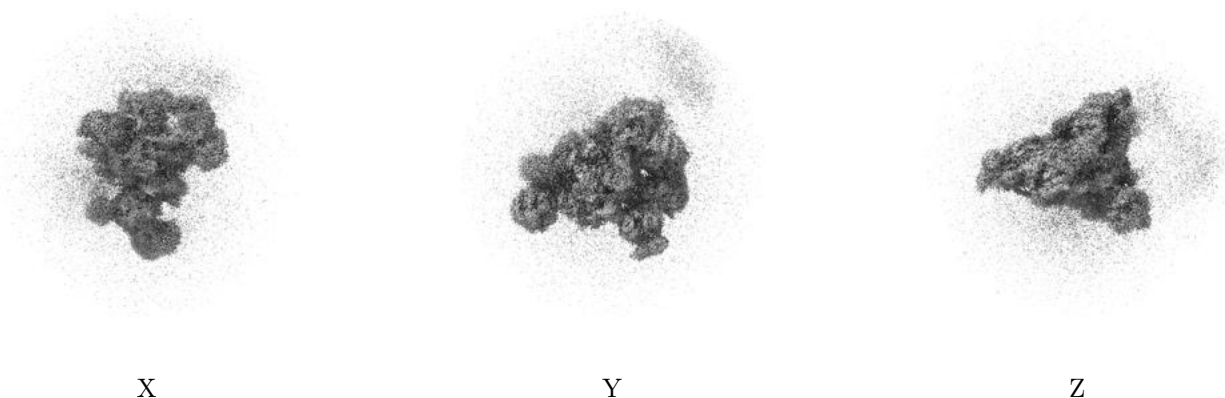


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

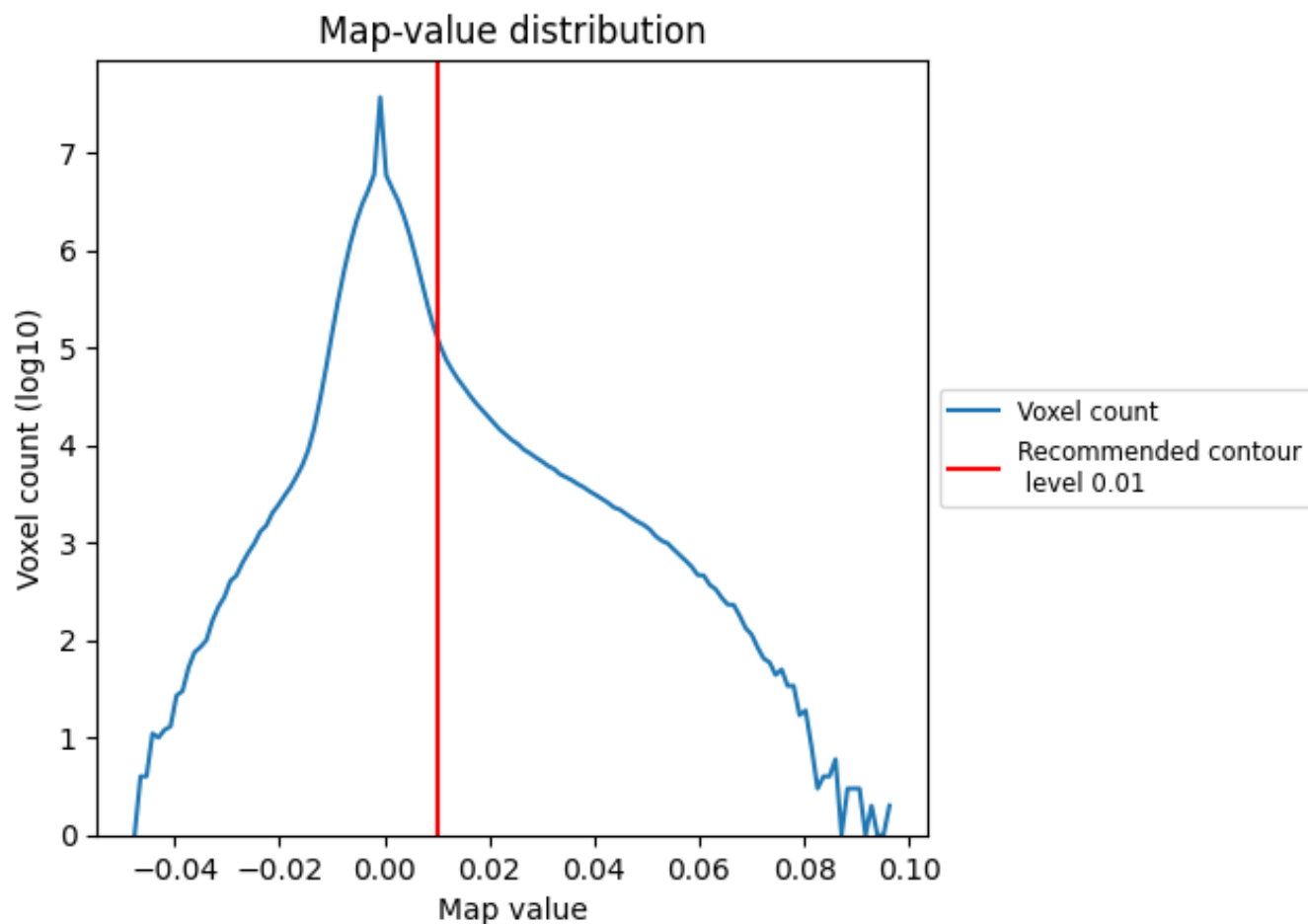
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

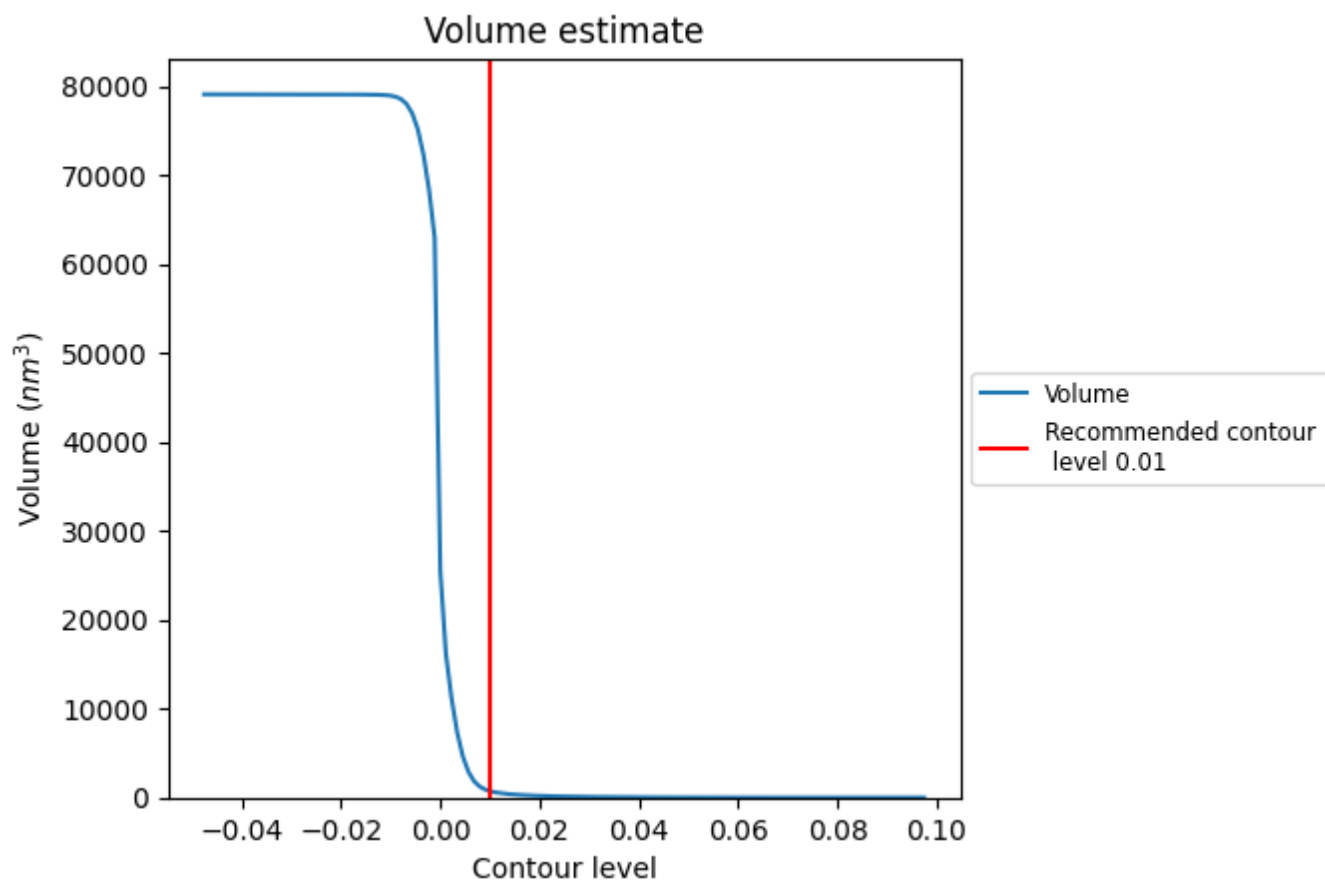
This section contains the results of statistical analysis of the map.

### 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.

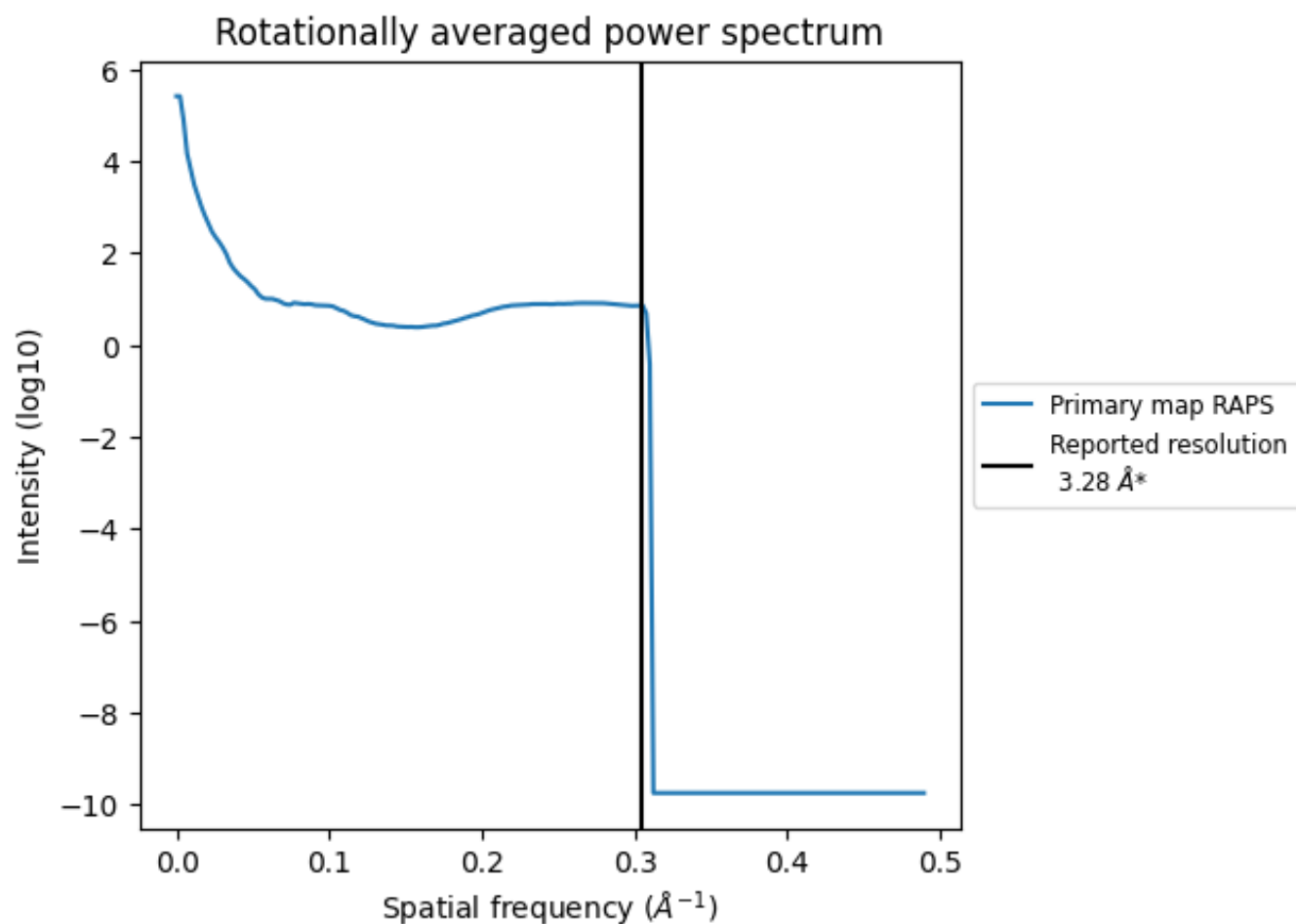
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 726  $\text{nm}^3$ ; this corresponds to an approximate mass of 656 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

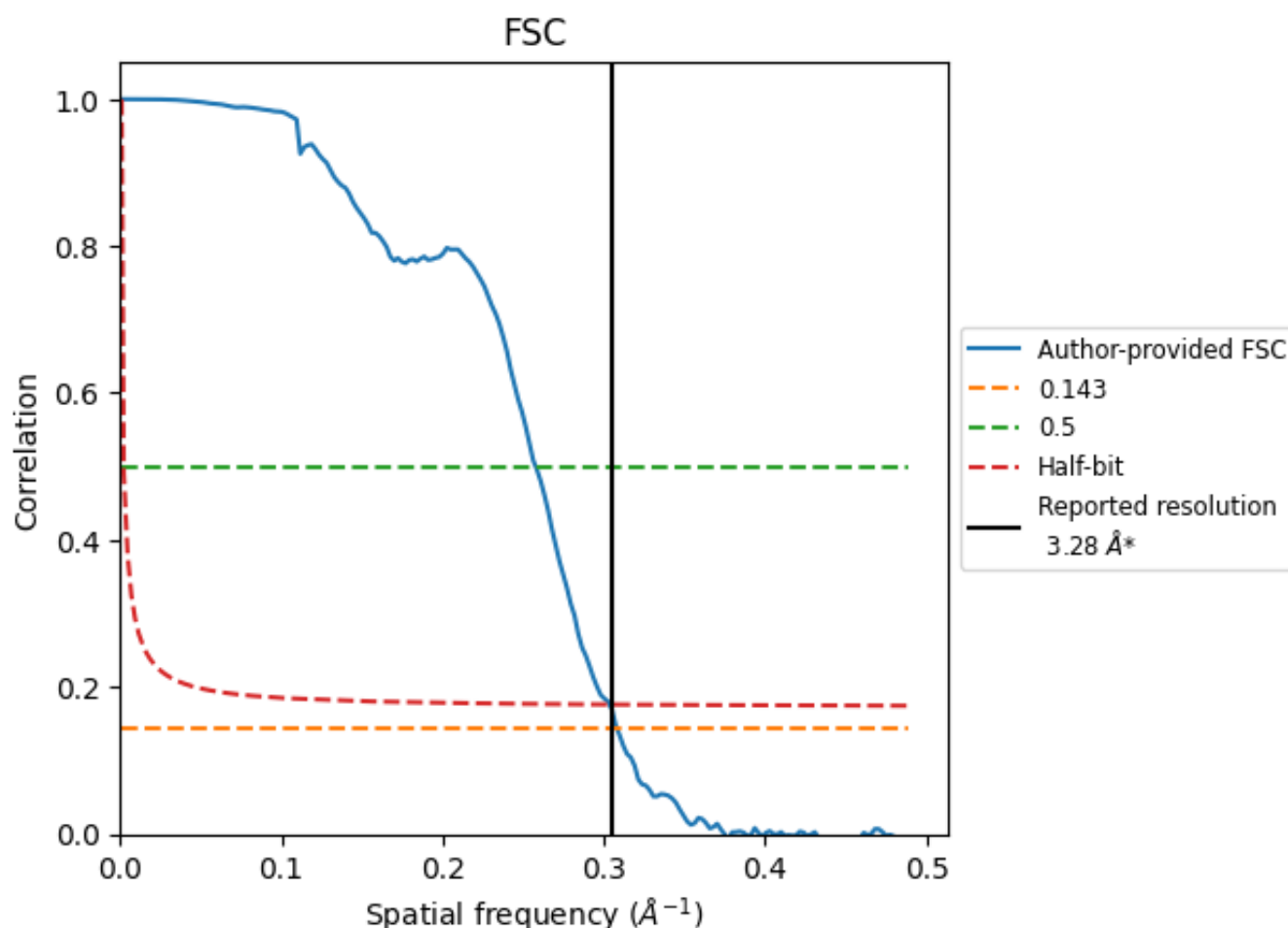


\*Reported resolution corresponds to spatial frequency of 0.305 Å<sup>-1</sup>

## 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 0.305 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	3.28	-	-
Author-provided FSC curve	3.24	3.88	3.29
Unmasked-calculated*	-	-	-

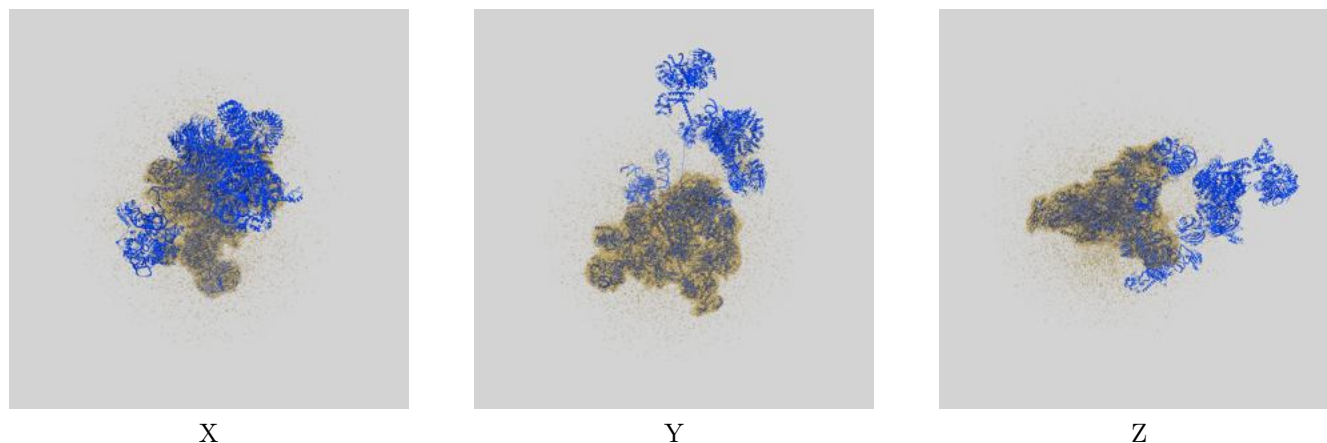
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



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

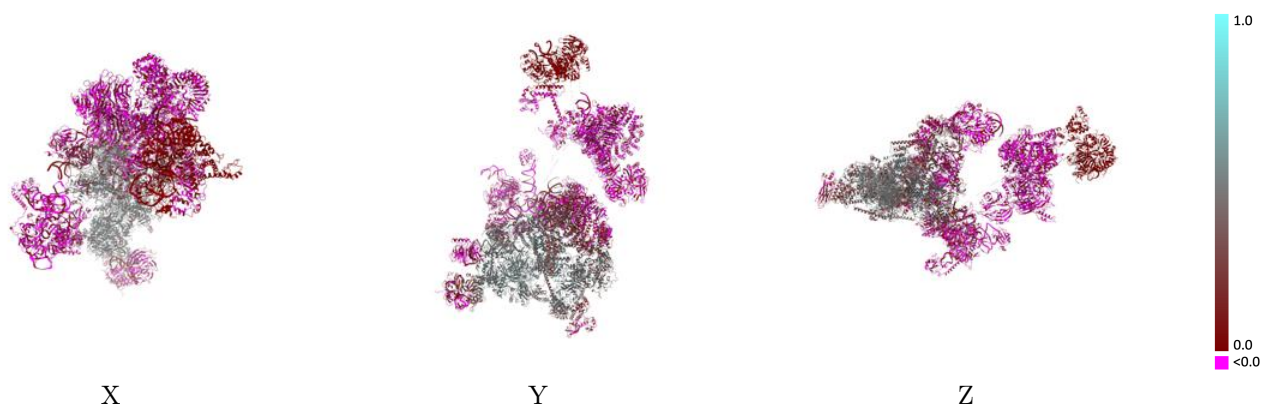
This section contains information regarding the fit between EMDB map EMD-4665 and PDB model 6QX9. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

### 9.1 Map-model overlay [i](#)



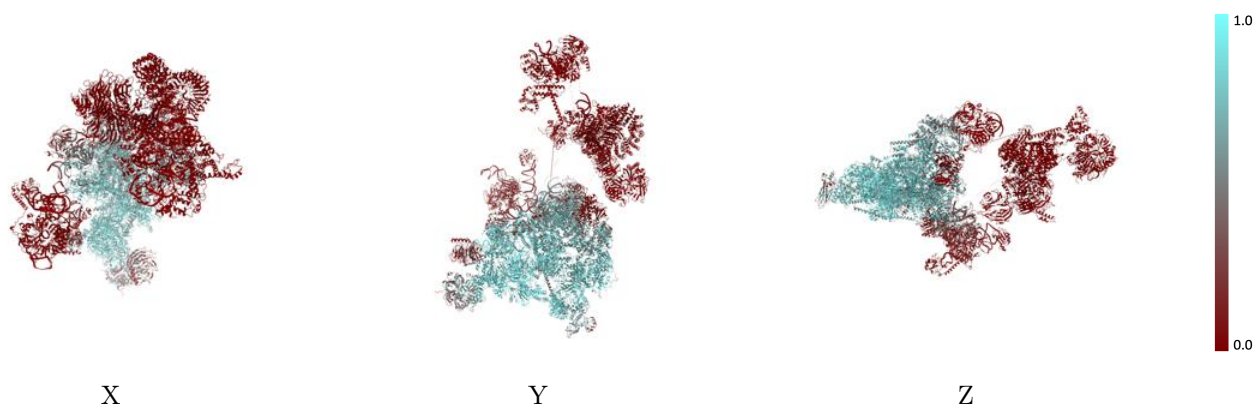
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



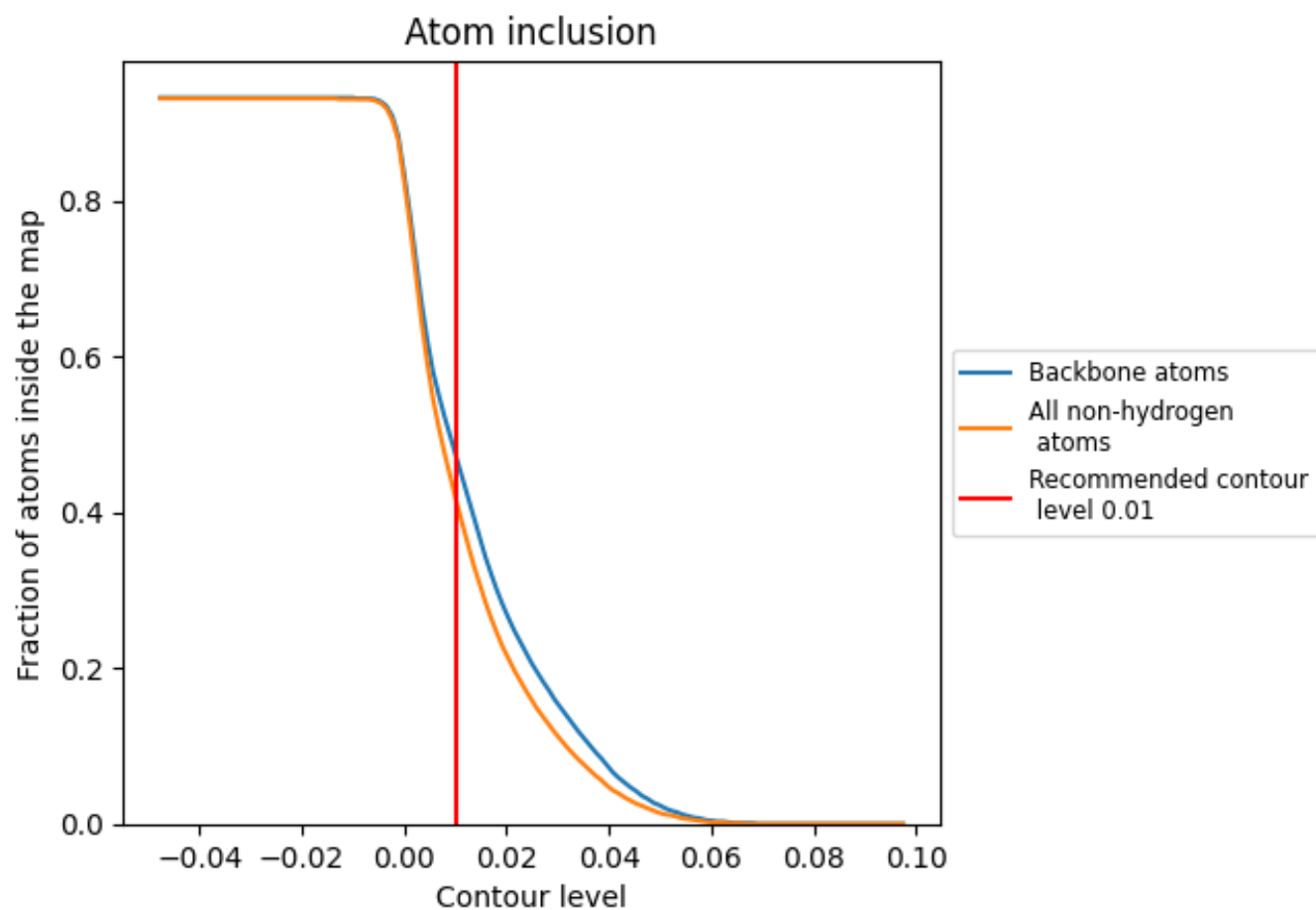
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 42% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4190	 0.2070
1	 0.0020	 0.0030
11	 0.0000	 -0.0020
12	 0.0000	 0.0170
13	 0.0000	 -0.0140
1A	 0.0000	 0.0280
1C	 0.0000	 0.0100
1K	 0.0010	 -0.0000
1b	 0.0030	 0.0140
1e	 0.0000	 0.0140
1f	 0.0020	 0.0020
1g	 0.0000	 0.0360
2	 0.0010	 0.0120
21	 0.0000	 0.0000
22	 0.0000	 0.0000
23	 0.0000	 0.0000
2A	 0.0000	 0.0000
2B	 0.0000	 0.0000
2b	 0.0000	 0.0000
2e	 0.0000	 0.0000
2f	 0.0000	 0.0000
2g	 0.0000	 0.0000
4	 0.6370	 0.2230
41	 0.4710	 0.2010
42	 0.4720	 0.2320
43	 0.2390	 0.0480
4A	 0.4880	 0.1430
4B	 0.5560	 0.1550
4C	 0.6880	 0.3260
4D	 0.6860	 0.3020
4b	 0.2840	 0.0870
4e	 0.2410	 0.0760
4f	 0.3330	 0.1270
4g	 0.2040	 0.0230
5	 0.7530	 0.2980



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Chain	Atom inclusion	Q-score
51	 0.4680	 0.1340
52	 0.4130	 0.1040
53	 0.7280	 0.3830
5A	 0.8230	 0.4690
5B	 0.7650	 0.3870
5C	 0.8730	 0.5100
5D	 0.8170	 0.4650
5J	 0.6500	 0.2450
5O	 0.1710	 0.0160
5X	 0.3060	 0.1470
5b	 0.5770	 0.2660
5e	 0.4730	 0.1160
5f	 0.3570	 0.0930
5g	 0.5680	 0.2690
6	 0.5610	 0.1990
62	 0.0050	 0.0140
63	 0.0100	 -0.0020
64	 0.0000	 -0.0470
65	 0.0020	 0.0290
66	 0.0000	 -0.0070
67	 0.0020	 -0.0100
68	 0.0010	 0.0250
A1	 0.1030	 0.0580
A2	 0.0000	 -0.0020
A3	 0.0000	 0.0040
B1	 0.0010	 0.0020
B2	 0.0020	 0.0090
B3	 0.0010	 -0.0030
B4	 0.0000	 -0.0010
B5	 0.0040	 -0.0090
BP	 0.0010	 -0.0110
I	 0.0040	 -0.0000
K	 0.0120	 0.0130
R	 0.6000	 0.2310
S	 0.6350	 0.3130
U	 0.8800	 0.5060
X	 0.5430	 0.2760