



## Full wwPDB EM Validation Report ⓘ

May 2, 2024 – 05:27 PM JST

PDB ID : 8H6K  
EMDB ID : EMD-34507  
Title : Cryo-EM structure of human exon-defined spliceosome in the mature B state.  
Authors : Zhang, W.; Zhan, X.; Zhang, X.; Bai, R.; Lei, J.; Yan, C.; Shi, Y.  
Deposited on : 2022-10-18  
Resolution : 2.70 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:

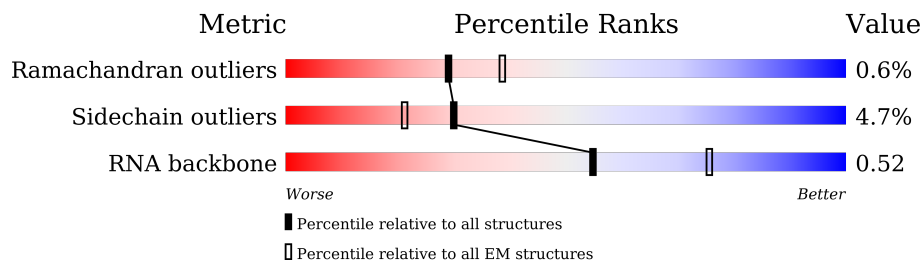
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	144	
2	5A	117	
3	5B	2335	
4	5C	972	
5	5D	2136	
6	5E	357	
7	2a	231	
7	4a	231	

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Mol	Chain	Length	Quality of chain
7	5a	231	32% 36% 64%
8	2b	119	69% 69% 31%
8	4b	119	68% 69% 31%
8	5b	119	65% 69% 31%
9	2c	118	72% 71% 28%
9	4c	118	63% 63% 37%
9	5c	118	75% 81% 18%
10	2d	86	86% 86% 14%
10	4d	86	81% 83% 17%
10	5d	86	80% 86% 14%
11	2e	92	86% 86% 14%
11	4e	92	85% 85% 15%
11	5e	92	85% 86% 14%
12	2f	76	89% 89% 11%
12	4f	76	95% 96% .
12	5f	76	84% 95% 5%
13	2g	126	63% 63% 37%
13	4g	126	56% 56% 44%
13	5g	126	49% 61% 39%
14	6A	107	16% 47% 9% 44%
15	6a	95	95% 91% . 5%
16	6b	102	73% 70% . 27%
17	6c	139	53% 53% . 47%
18	6d	91	79% 78% . 21%
19	6e	80	88% 85% . 12%

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Mol	Chain	Length	Quality of chain
20	6f	103	63% 63% 37%
21	6g	96	64% 63% 36%
22	4A	145	43% 64% 25% 11%
23	4B	683	36% 63%
24	4C	522	76% 5% 18%
25	4D	499	71% 25%
26	4E	128	93%
27	4F	142	94% 6%
28	4G	941	15% 82% 15%
29	4H	177	7% 95% 5%
30	4I	376	19% 80%
31	4J	800	18% 81%
32	4K	439	15% 41% 57%
33	4L	312	51% 5% 44%
34	4M	73	92% 8%
35	4N	199	35% 6% 60%
36	4Z	513	82% 82% 18%
37	2A	188	58% 33% 21% 42%
38	2B	255	64% 63% 36%
39	2C	225	42% 42% 58%
40	2D	793	16% 25% 74%
41	2E	464	20% 18% 80%
42	2F	501	84% 83% 16%
43	2G	1304	80% 78% 20%
44	2H	895	20% 23% 76%

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Mol	Chain	Length	Quality of chain
45	2I	1217	<p>96%</p> <p>94%</p>
46	2J	424	<p>18%</p> <p>82%</p>
47	2K	125	<p>86%</p> <p>83%</p> <p>14%</p>
48	2L	110	<p>81%</p> <p>19%</p>
49	2M	86	<p>77%</p> <p>73%</p> <p>23%</p>

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 98459 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 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	64	1334	597	209	464	64	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	115	2420	1084	403	818	115	0	0

- Molecule 3 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5B	2253	18639	11991	3249	3318	81	0	0

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5C	818	6430	4108	1085	1205	32	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5D	1696	13633	8715	2329	2519	70	0	0

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	5E	299	1196	598	299	299	0	0

- Molecule 7 is a protein called Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5a	84	Total	C	N	O	0	0
			336	168	84	84		
7	4a	64	Total	C	N	O	0	0
			256	128	64	64		
7	2a	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	5b	82	Total	C	N	O	0	0
			328	164	82	82		
8	4b	82	Total	C	N	O	0	0
			334	170	82	82		
8	2b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	5c	97	Total	C	N	O	0	0
			388	194	97	97		
9	4c	74	Total	C	N	O	0	0
			300	152	74	74		
9	2c	85	Total	C	N	O	0	0
			340	170	85	85		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	5d	74	Total	C	N	O	0	0
			296	148	74	74		
10	4d	71	Total	C	N	O	0	0
			292	150	71	71		
10	2d	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	5e	79	Total	C	N	O	0	0
			316	158	79	79		
11	4e	78	Total	C	N	O	0	0
			314	158	78	78		
11	2e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	5f	72	Total	C	N	O	0	0
			288	144	72	72		
12	4f	73	Total	C	N	O	0	0
			298	152	73	73		
12	2f	68	Total	C	N	O	0	0
			272	136	68	68		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	5g	77	Total	C	N	O	0	0
			308	154	77	77		
13	4g	71	Total	C	N	O	0	0
			288	146	71	71		
13	2g	80	Total	C	N	O	0	0
			320	160	80	80		

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6A	60	Total	C	N	O	P	0	0
			1273	568	235	410	60		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	6a	90	Total	C	N	O	0	0
			360	180	90	90		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm3.



Mol	Chain	Residues	Atoms				AltConf	Trace
16	6b	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6c	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	6d	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	6e	70	Total	C	N	O	0	0
			280	140	70	70		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	6f	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	6g	61	Total	C	N	O	0	0
			244	122	61	61		

- Molecule 22 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4A	129	Total	C	N	O	P	0	0
			2744	1225	472	917	130		

- Molecule 23 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4B	256	Total	C	N	O	S	0	0
			2076	1316	385	367	8		

- Molecule 24 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4C	426	Total	C	N	O	S	0	0
			3370	2118	612	620	20		

- Molecule 25 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4D	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

- Molecule 26 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4E	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 27 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4F	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 28 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4G	801	Total	C	N	O	S	0	0
			5504	3419	1043	1026	16		

- Molecule 29 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4H	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 30 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4I	75	Total	C	N	O	S	0	0
			494	304	96	91	3		

- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4J	152	Total	C	N	O	S	0	0
			1144	709	204	229	2		

- Molecule 32 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4K	188	Total	C	N	O	S	0	0
			1192	741	219	230	2		

- Molecule 33 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4L	175	Total	C	N	O	S	0	0
			1452	934	244	265	9		

- Molecule 34 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4M	73	Total	C	N	O	S	0	0
			599	383	103	109	4		

- Molecule 35 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4N	80	Total	C	N	O	S	0	0
			640	397	116	120	7		

- Molecule 36 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	4Z	420	Total	C	N	O	0	0
			2092	1252	420	420		

- Molecule 37 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	2A	109	2311	1032	396	774	109	0	0

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	2B	162	648	324	162	162	0	0

- Molecule 39 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	2C	94	376	188	94	94	0	0

- Molecule 40 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	2D	204	1134	644	238	250	2	0	0

- Molecule 41 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	2E	94	376	188	94	94	0	0

- Molecule 42 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	2F	423	1693	847	423	423	0	0

- Molecule 43 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	2G	1048	4192	2096	1048	1048	0	0

- Molecule 44 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2H	213	Total	C	N	O	S	0	0
			959	510	220	226	3		

- Molecule 45 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	2I	1168	Total	C	N	O	0	0
			4672	2336	1168	1168		

- Molecule 46 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	2J	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 47 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	2K	108	Total	C	N	O	0	0
			432	216	108	108		

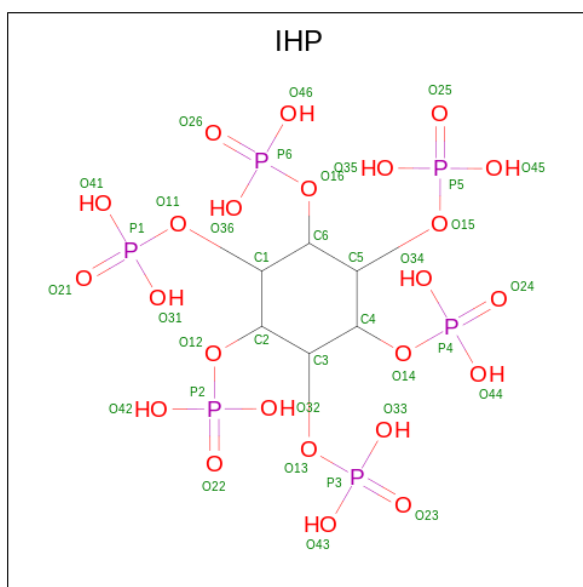
- Molecule 48 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	2L	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 49 is a protein called Splicing factor 3B subunit 5.

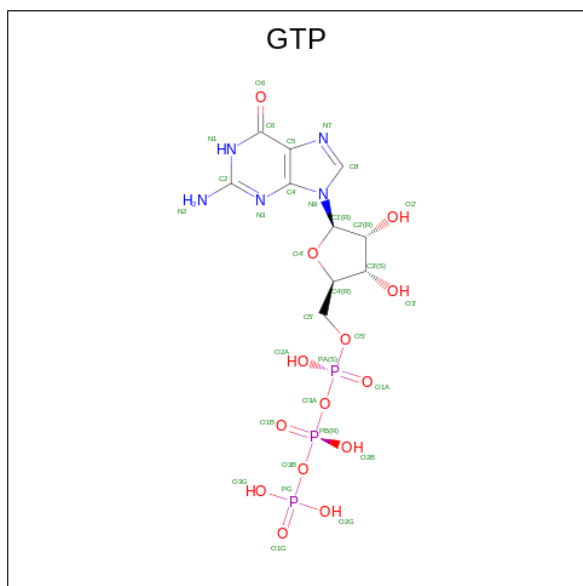
Mol	Chain	Residues	Atoms				AltConf	Trace
49	2M	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
50	5B	1	36	6	24	6	0

- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	5C	1	32	10	5	14	3	0

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

Mol	Chain	Residues	Atoms		AltConf
53	4I	1	Total	Zn	0
			1	1	
53	4N	1	Total	Zn	0
			1	1	

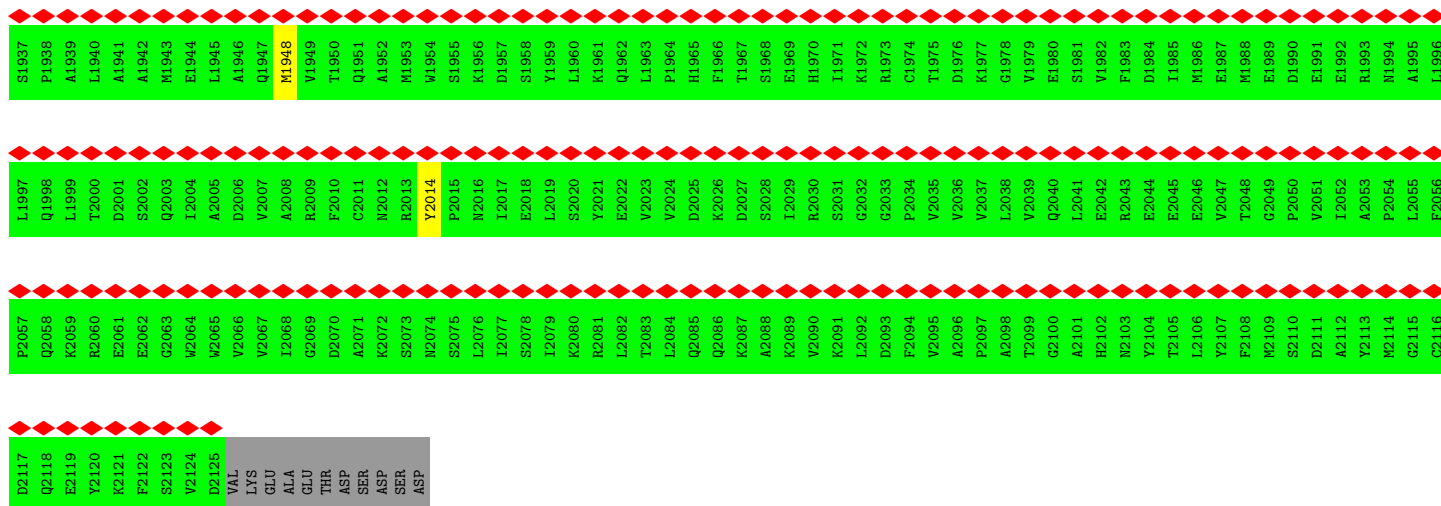




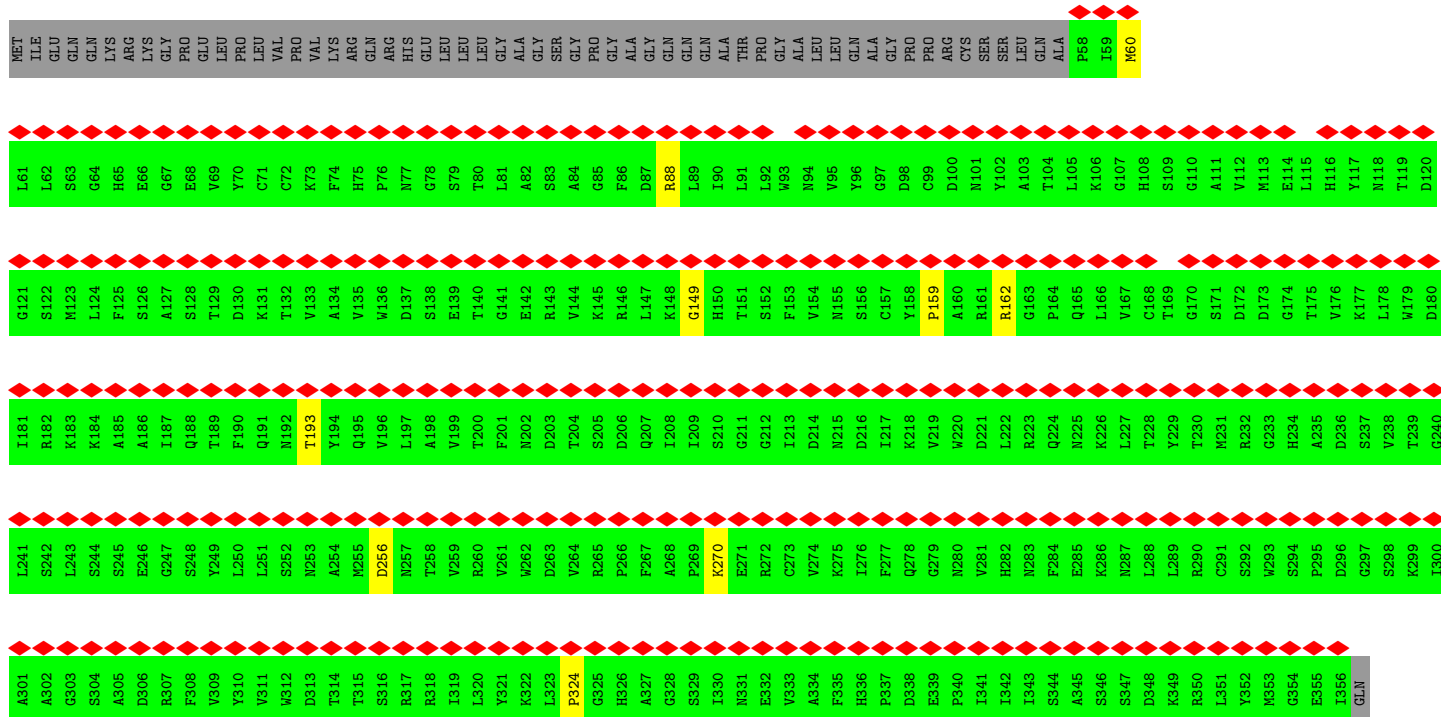
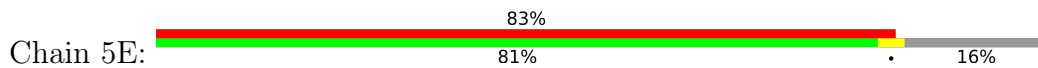




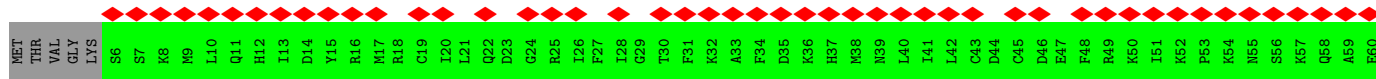
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L1276	S1277	C1278	E1279	L1282	P1283	V1284	S1285	F1286	M1287	H1288	L1289	I1290	L1291	P1292	E1293	K1294	L1295	P1296	P1297	P1298	L1299	E1300	L1301	L1302	L1303	L1304	Q1305	P1306	L1307	P1308	V1309	S1310	A1311	L1312	R1313	M1314	S1315	A1316	F1317	E1318	L1319	L1320	Y1321	Q1322	D1323	K1324	F1325	P1326	F1327	F1328	M1329	P1330	I1331	Q1332	T1333	Q1334	V1335	F1336		
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F1397	Q1398	D1399	R1400	L1401	M1402	K1403	K1404	V1405	V1406	L1407	L1408	T1409	G1410	E1411	T1412	S1413	T1414	D1415	L1416	K1417	L1418	C1419	G1420	K1421	G1422	M1423	I1424	L1425	I1426	S1427	T1428	P1429	E1430	K1431	W1432	D1433	I1434	L1435	S1436	R1437	R1438	W1439	K1440	Q1441	M1442	K1443	M1444	V1445	Q1446	M1447	I1448	M1449	L1450	F1451	V1452	V1453	D1454	E1455	V1456	
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● Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

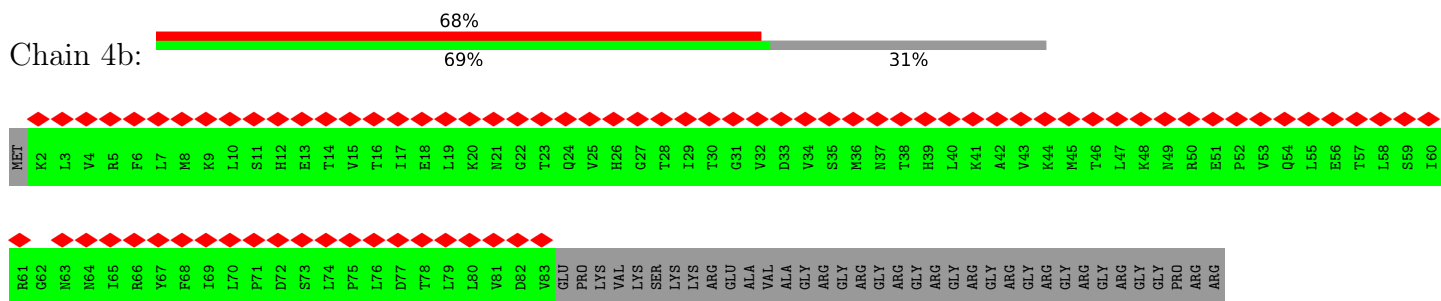


● Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

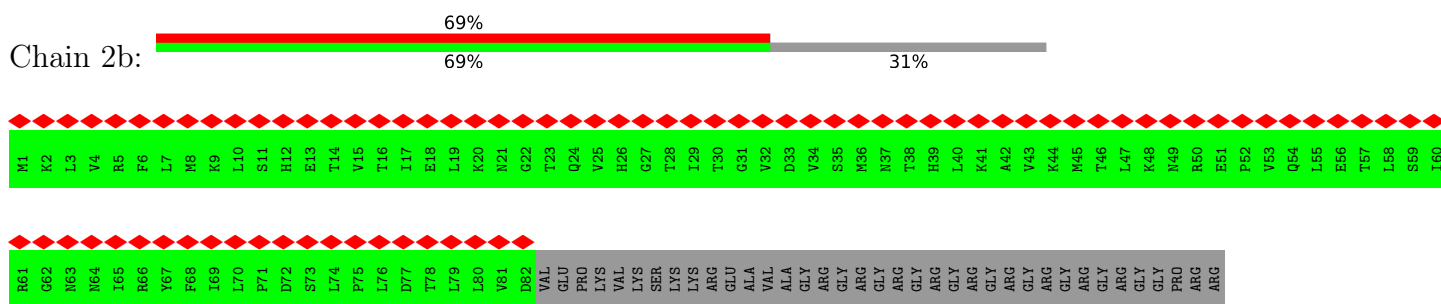




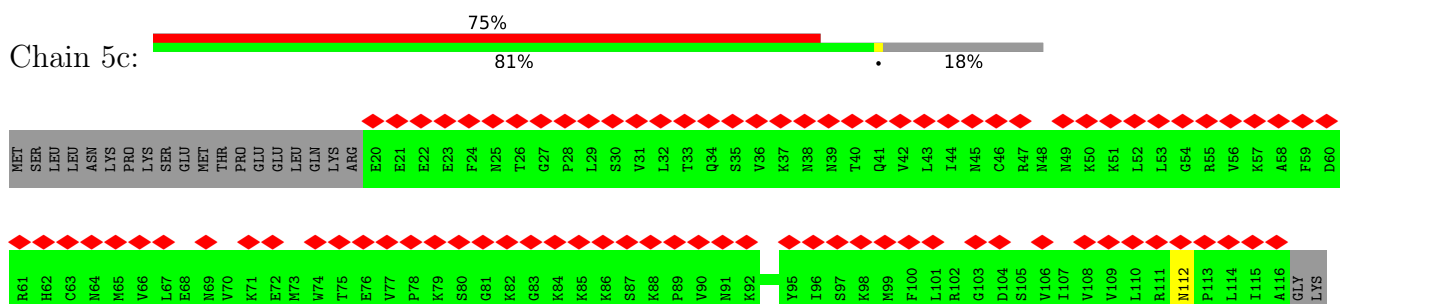
Molecule 8: Small nuclear ribonucleoprotein Sm D1



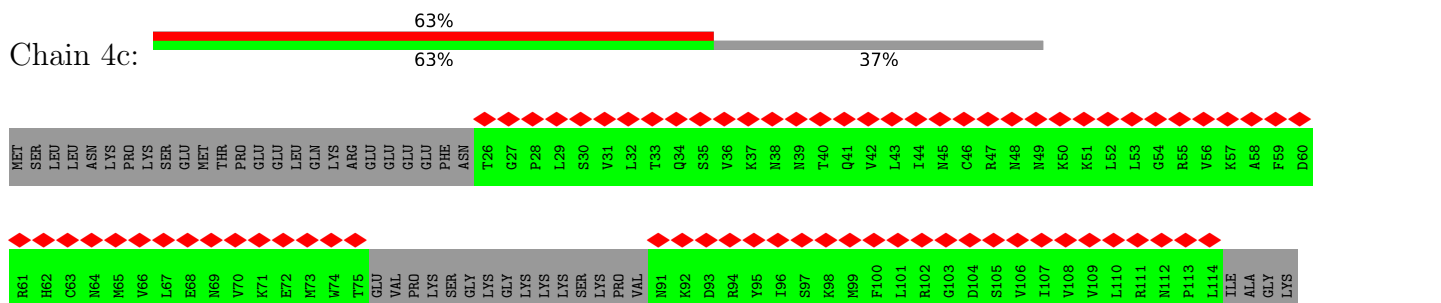
Molecule 8: Small nuclear ribonucleoprotein Sm D1



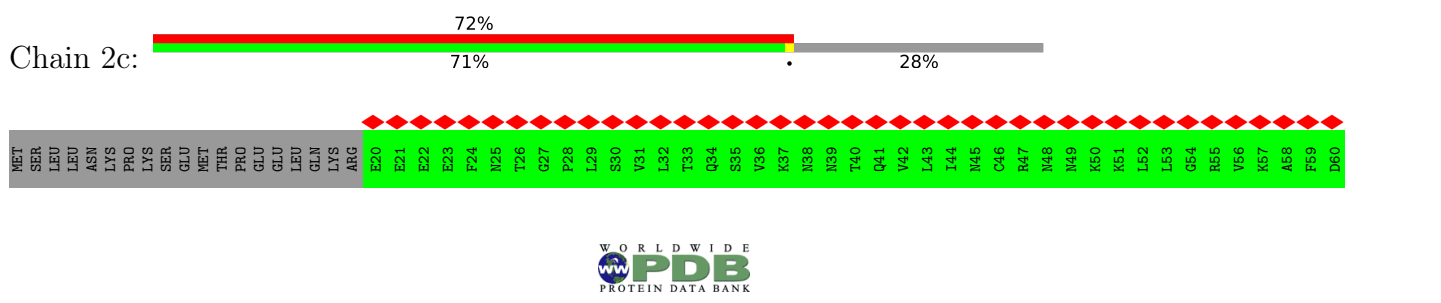
Molecule 9: Small nuclear ribonucleoprotein Sm D2

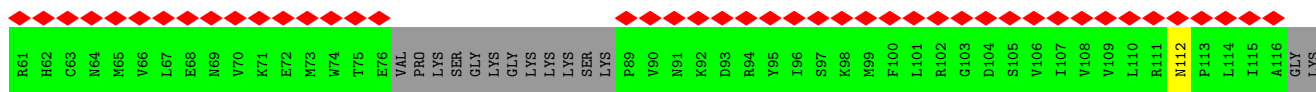


Molecule 9: Small nuclear ribonucleoprotein Sm D2

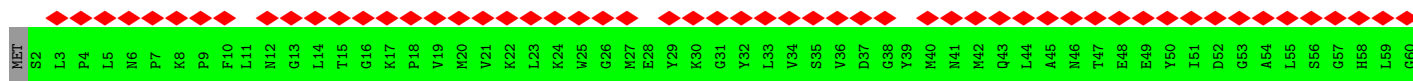
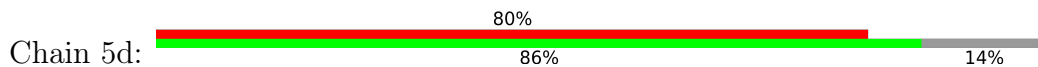


Molecule 9: Small nuclear ribonucleoprotein Sm D2

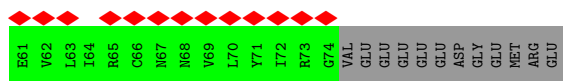
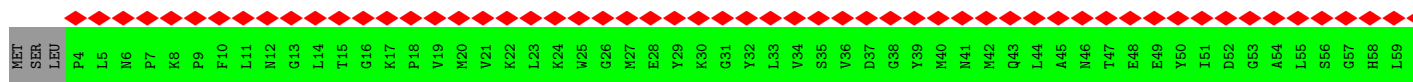
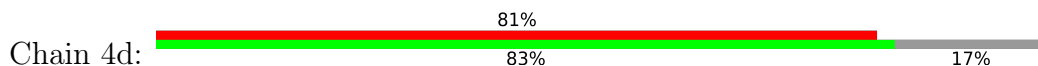




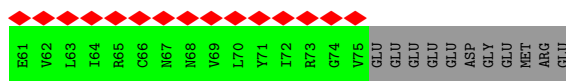
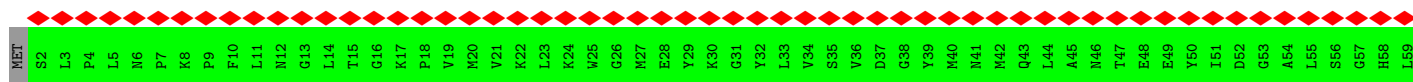
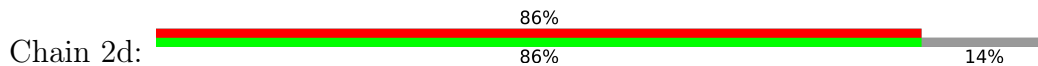
• Molecule 10: Small nuclear ribonucleoprotein F



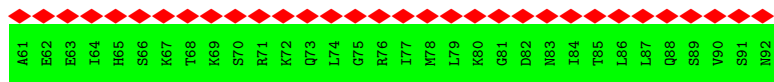
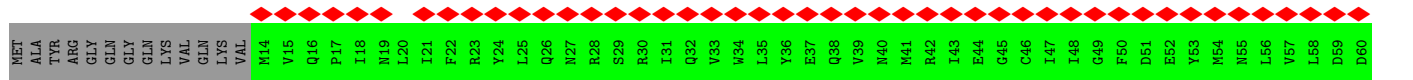
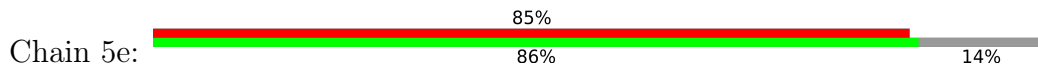
• Molecule 10: Small nuclear ribonucleoprotein F



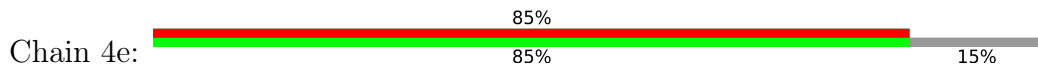
• Molecule 10: Small nuclear ribonucleoprotein F



• Molecule 11: Small nuclear ribonucleoprotein E

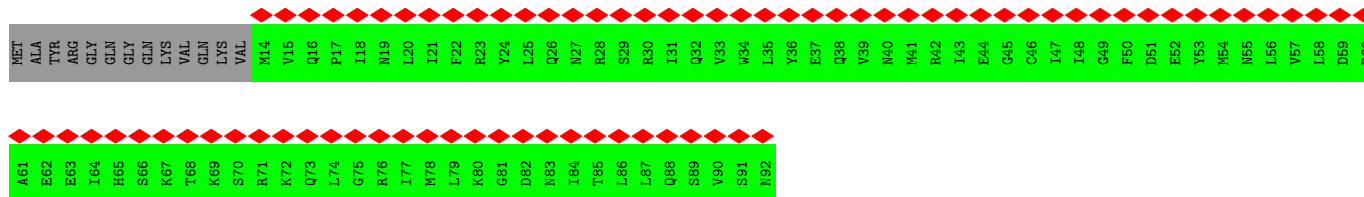
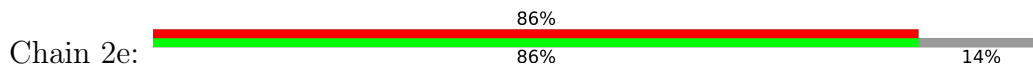


• Molecule 11: Small nuclear ribonucleoprotein E

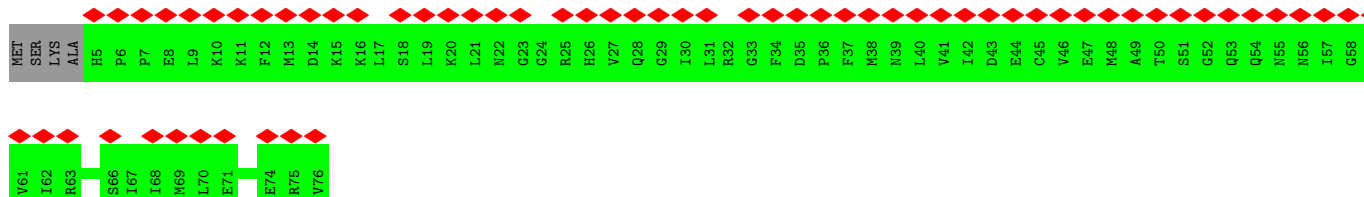
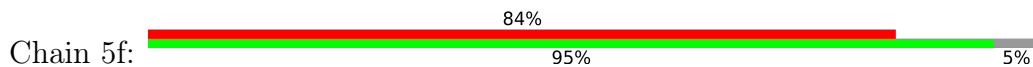




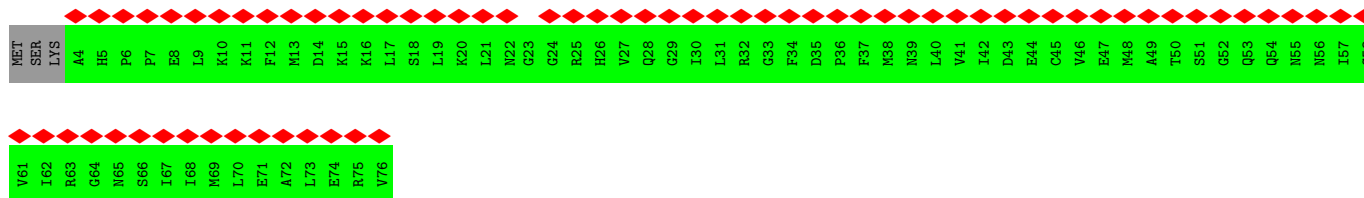
• Molecule 11: Small nuclear ribonucleoprotein E



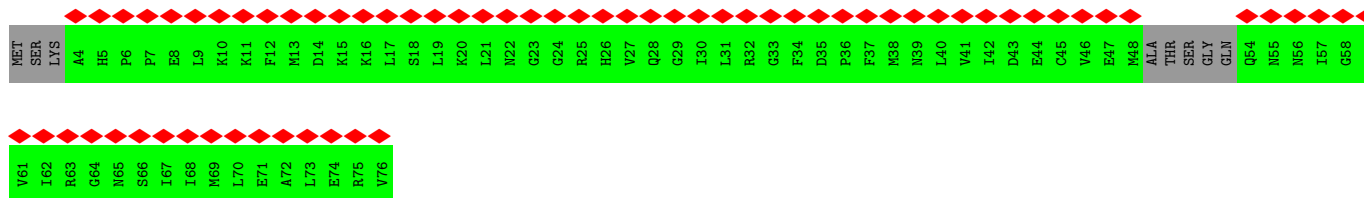
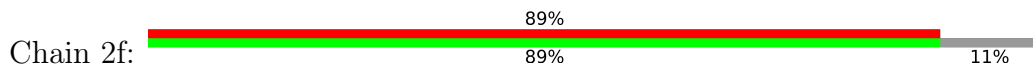
• Molecule 12: Small nuclear ribonucleoprotein G



• Molecule 12: Small nuclear ribonucleoprotein G

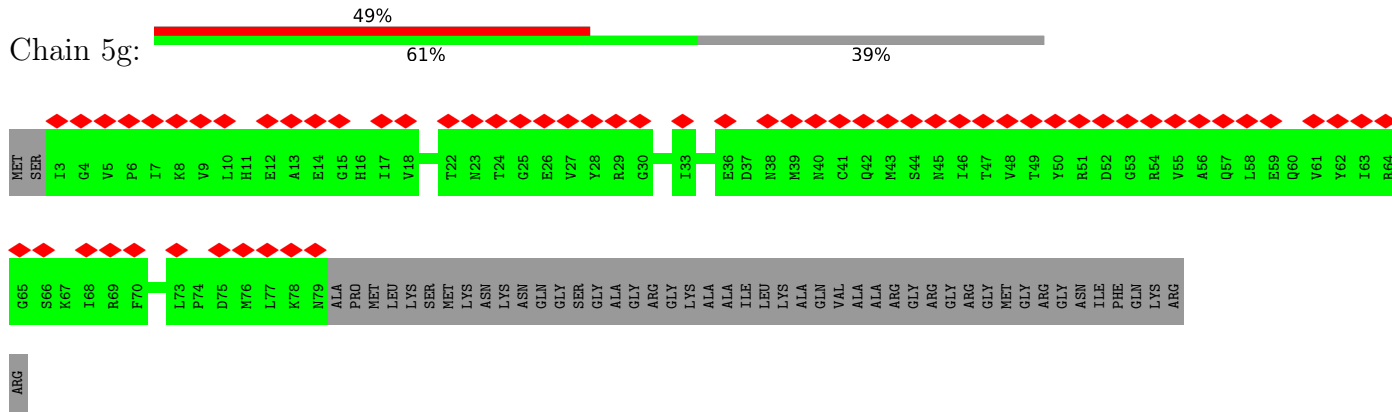


• Molecule 12: Small nuclear ribonucleoprotein G

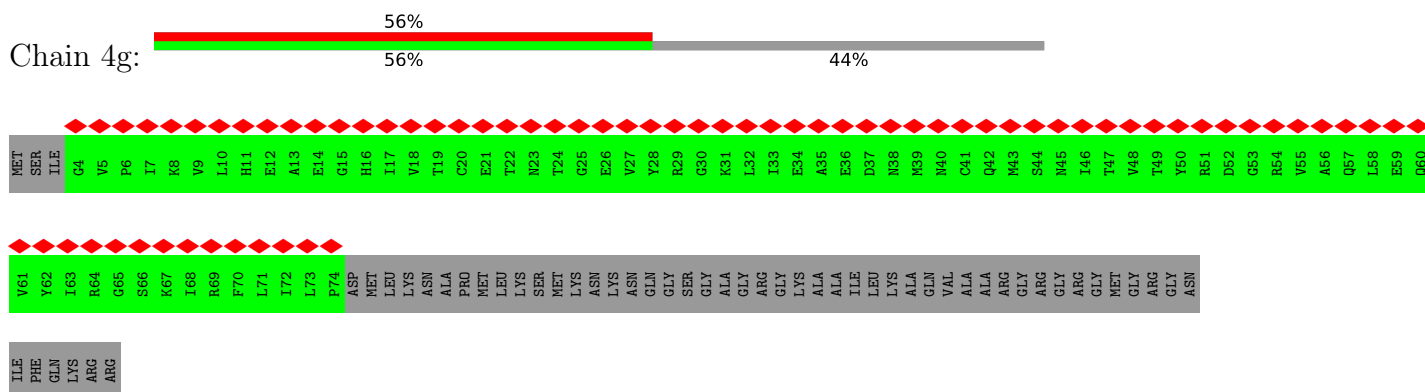




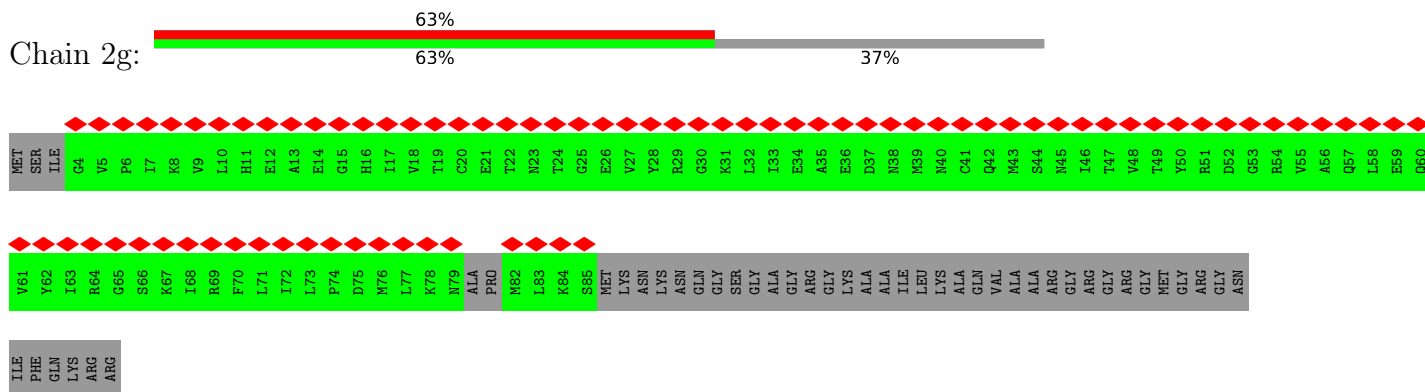
• Molecule 13: Small nuclear ribonucleoprotein Sm D3



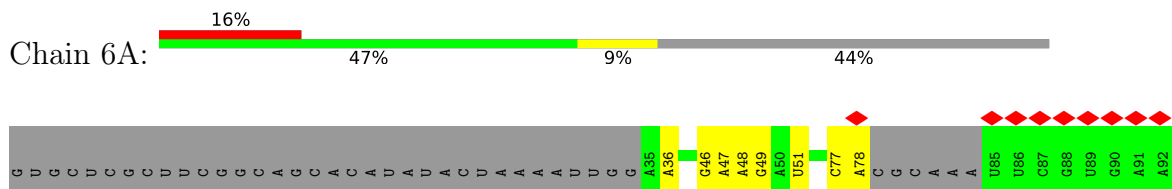
• Molecule 13: Small nuclear ribonucleoprotein Sm D3

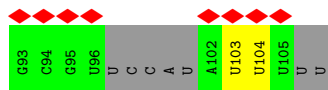


• Molecule 13: Small nuclear ribonucleoprotein Sm D3

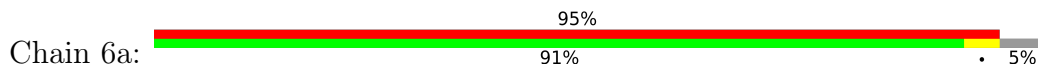


• Molecule 14: U6 snRNA

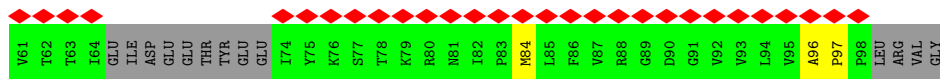
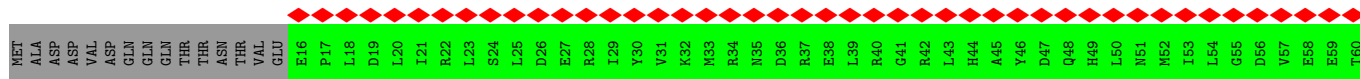
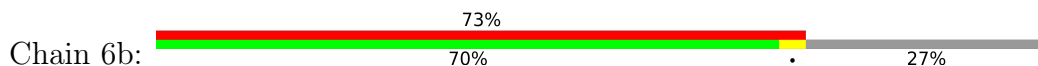




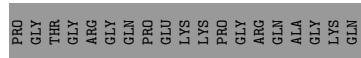
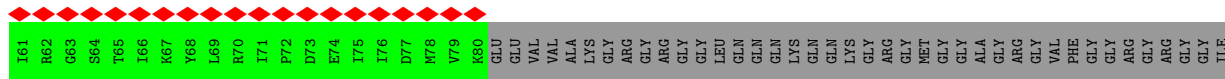
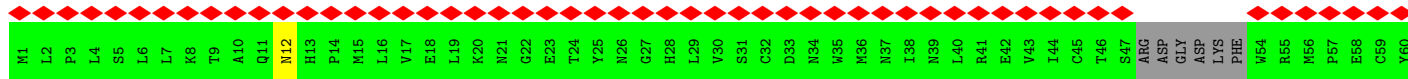
• Molecule 15: U6 snRNA-associated Sm-like protein LSm2



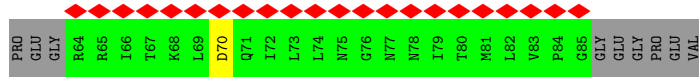
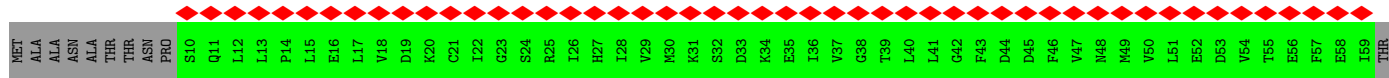
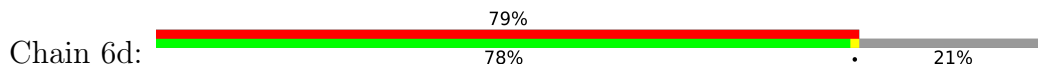
• Molecule 16: U6 snRNA-associated Sm-like protein LSm3



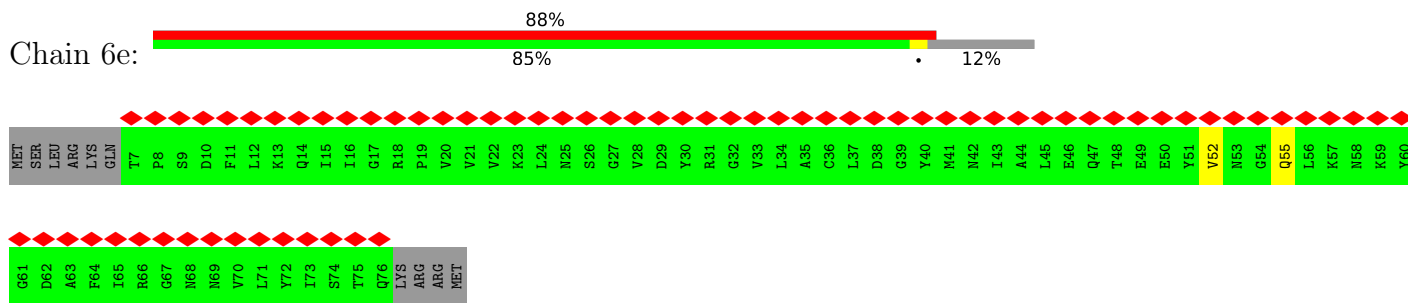
• Molecule 17: U6 snRNA-associated Sm-like protein LSm4



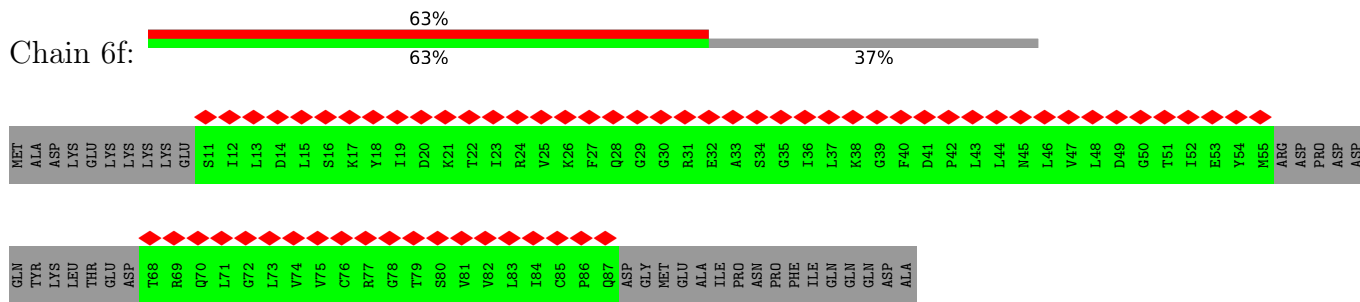
• Molecule 18: U6 snRNA-associated Sm-like protein LSm5



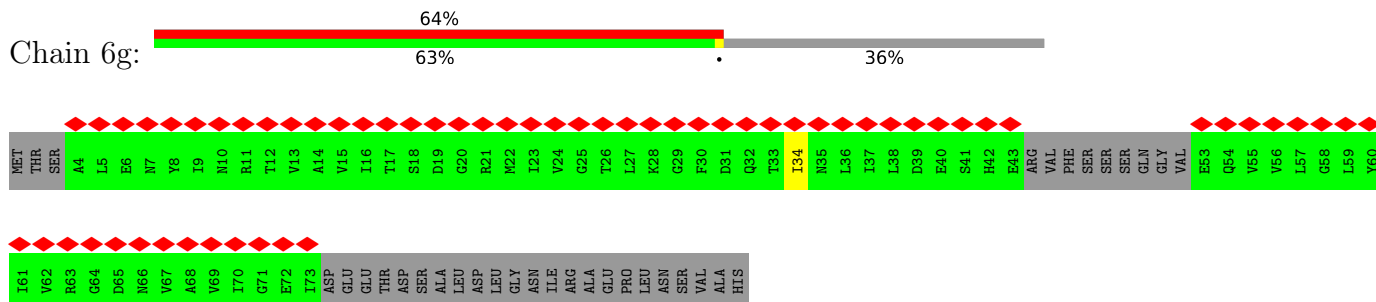
• Molecule 19: U6 snRNA-associated Sm-like protein LSm6



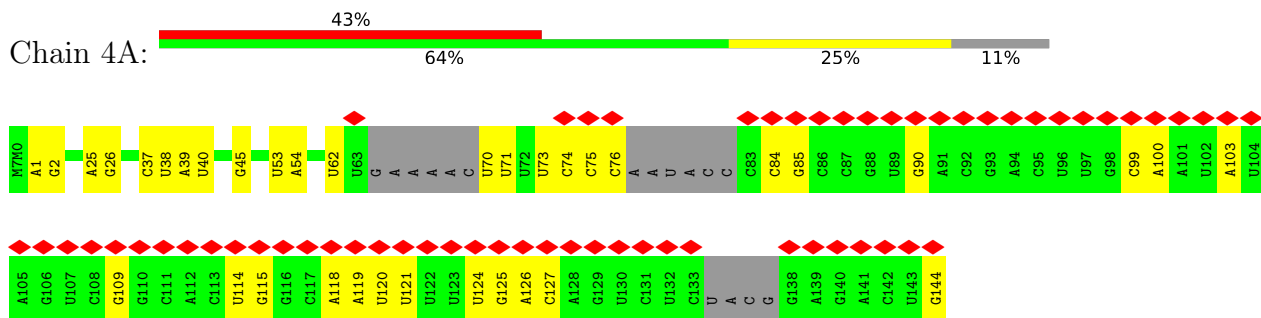
• Molecule 20: U6 snRNA-associated Sm-like protein LSm7



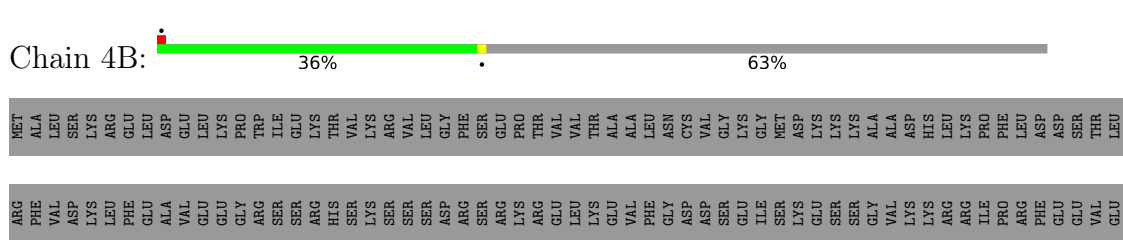
• Molecule 21: U6 snRNA-associated Sm-like protein LSm8

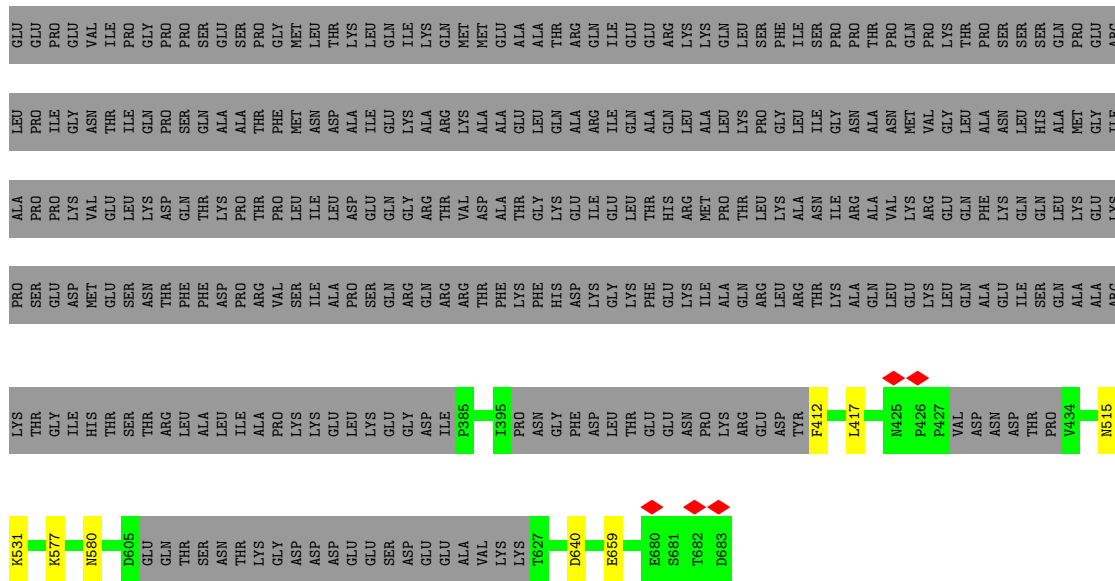


• Molecule 22: U4 snRNA

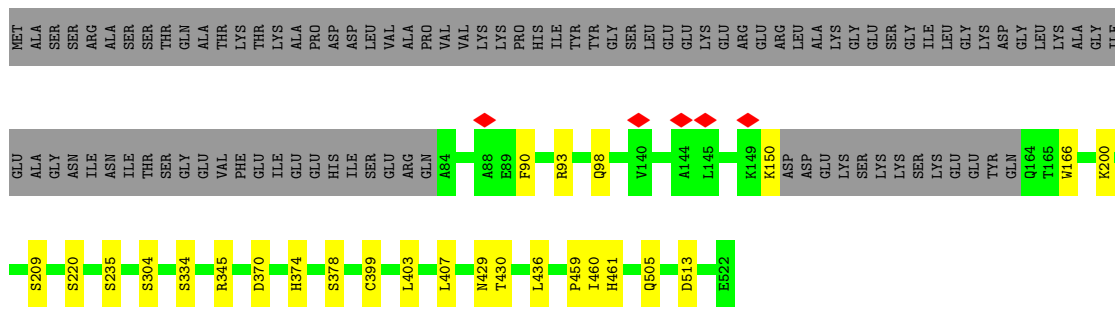
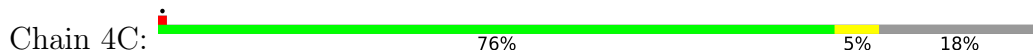


• Molecule 23: U4/U6 small nuclear ribonucleoprotein Prp3

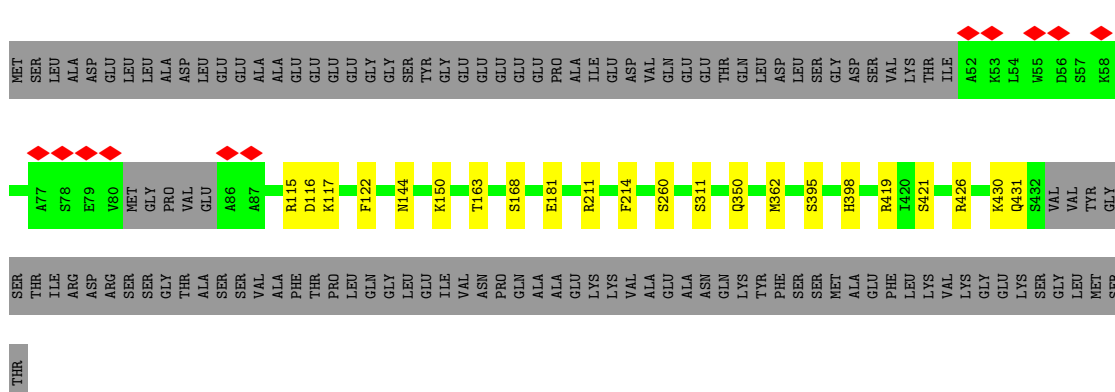




• Molecule 24: U4/U6 small nuclear ribonucleoprotein Prp4



• Molecule 25: U4/U6 small nuclear ribonucleoprotein Prp31



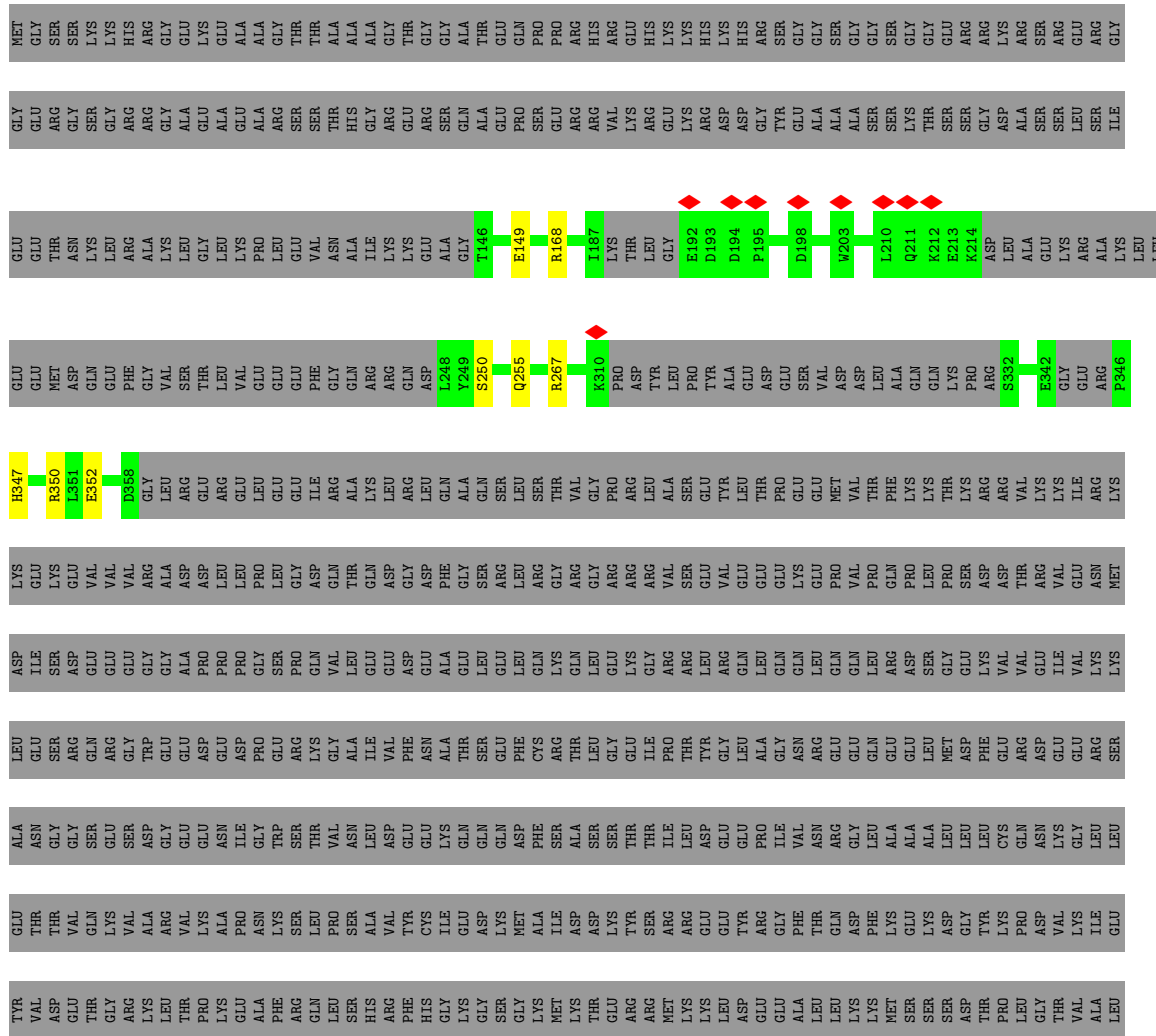
• Molecule 26: NHP2-like protein 1







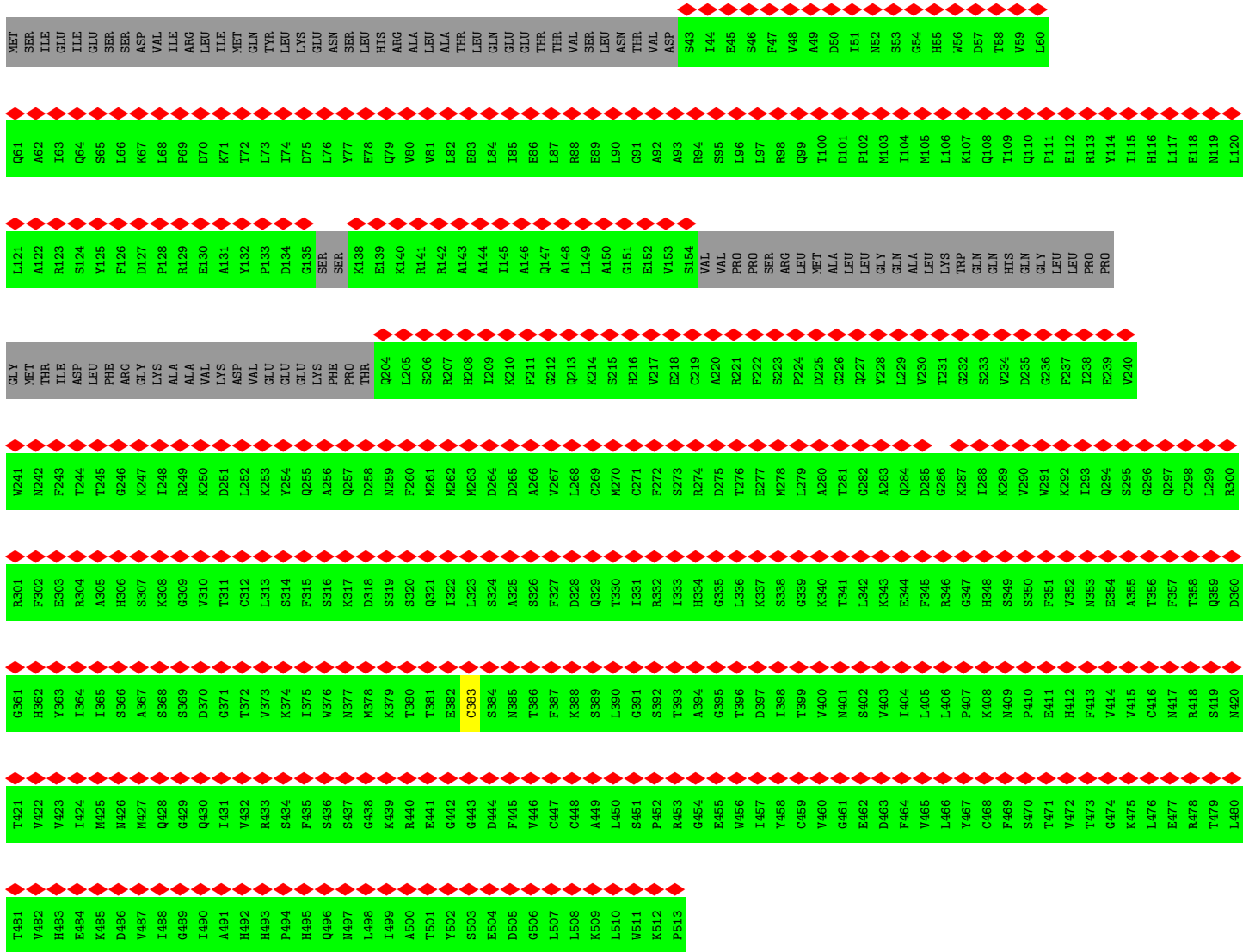
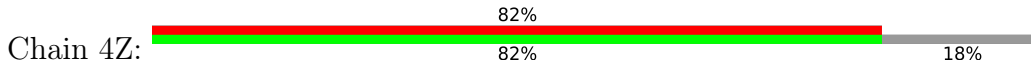
● Molecule 31: U4/U6.U5 tri-snRNP-associated protein 1



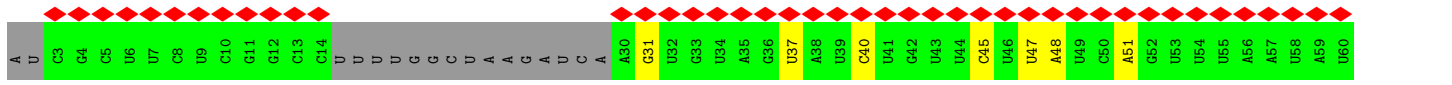
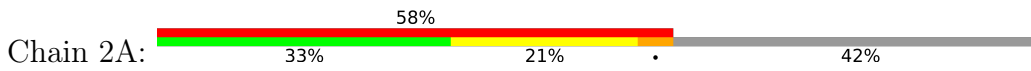




• Molecule 36: WD40 repeat-containing protein SMU1



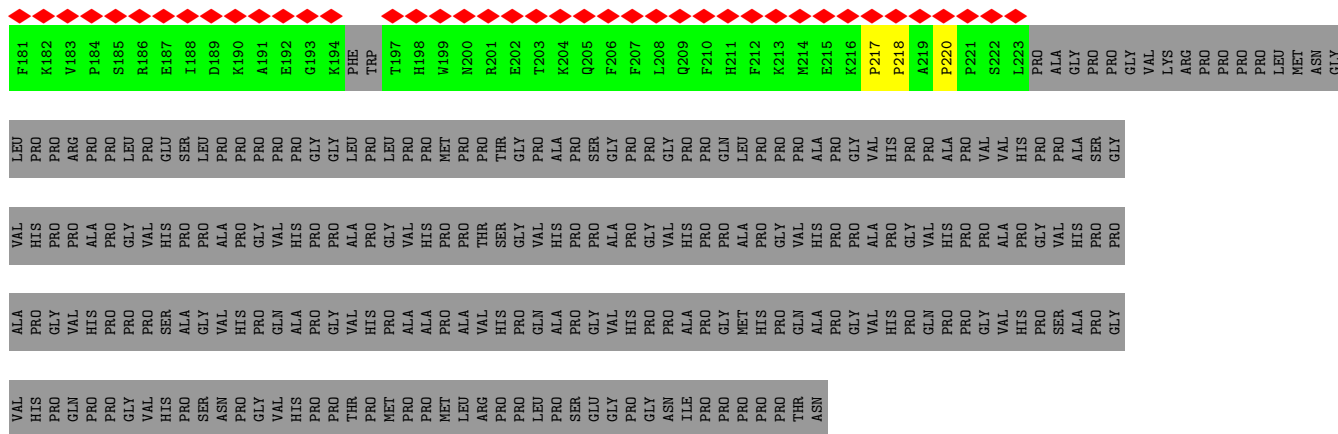
• Molecule 37: U2 snRNA



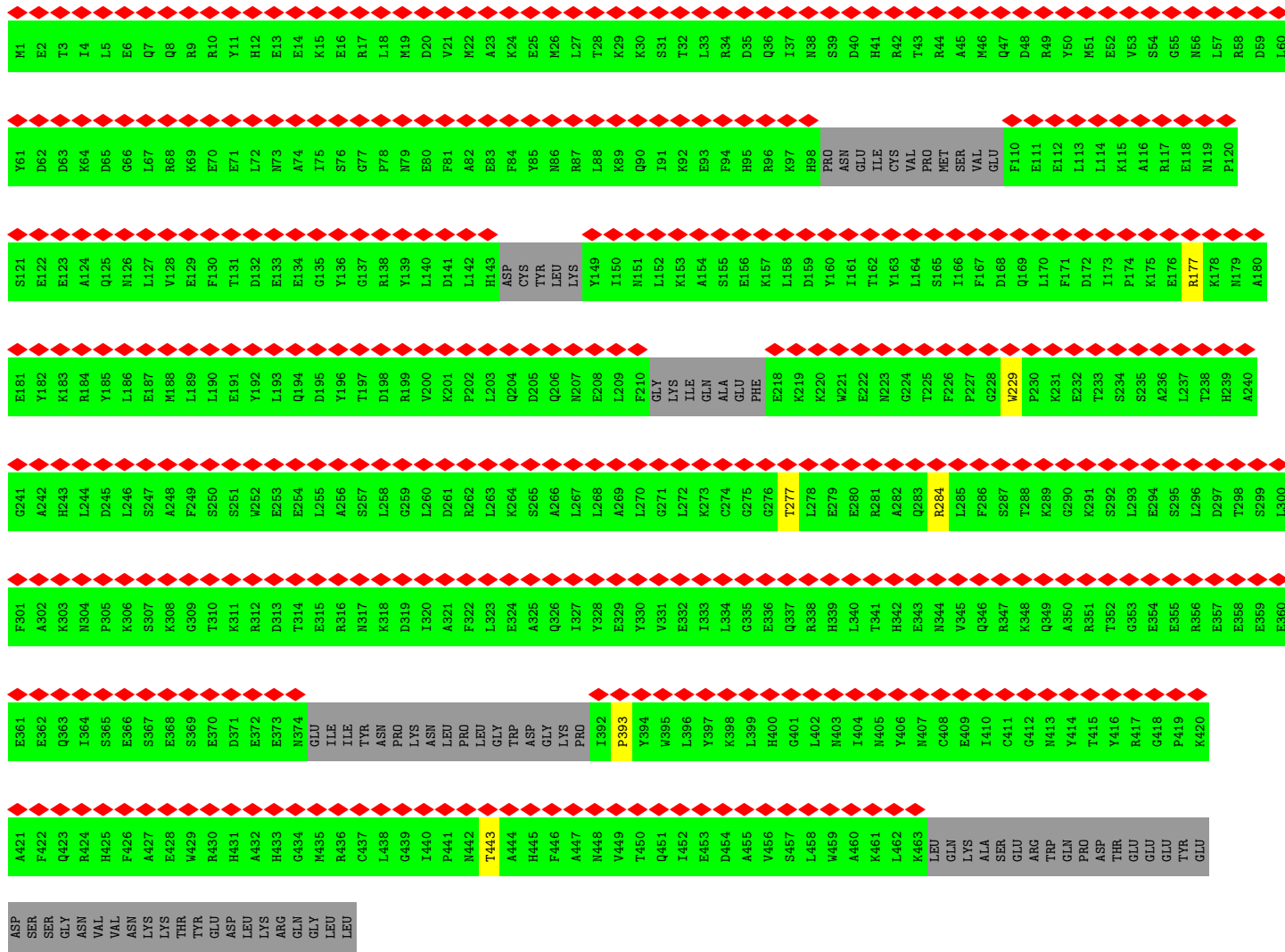
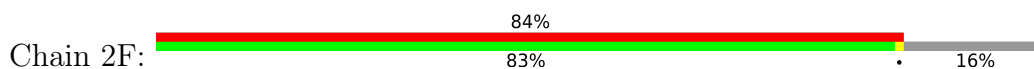








● Molecule 42: Splicing factor 3A subunit 3



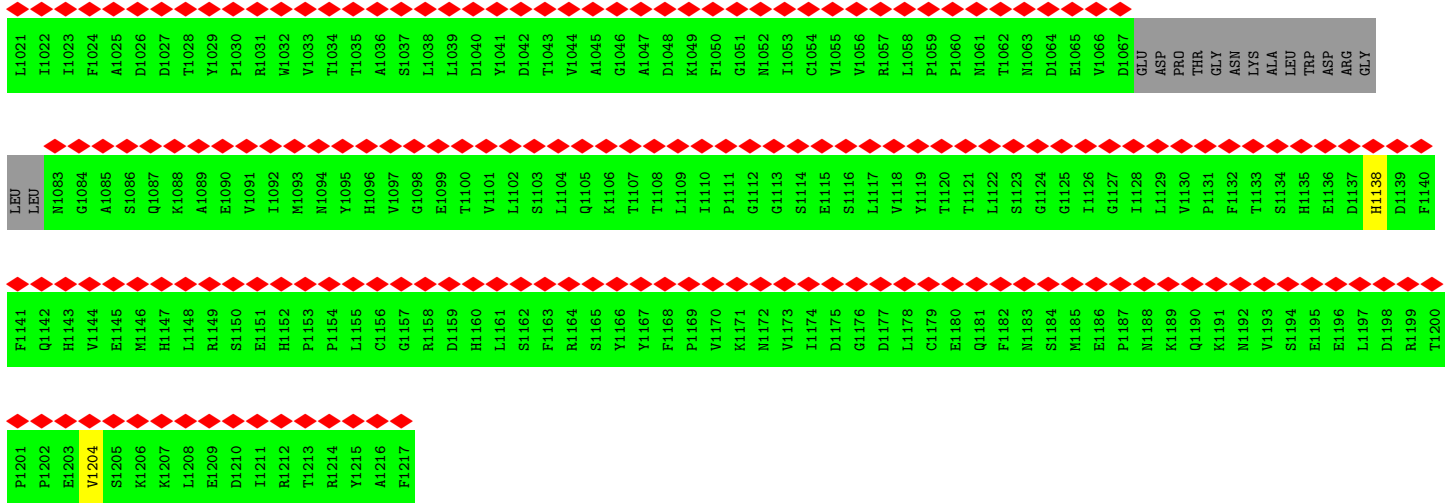
● Molecule 43: Splicing factor 3B subunit 1



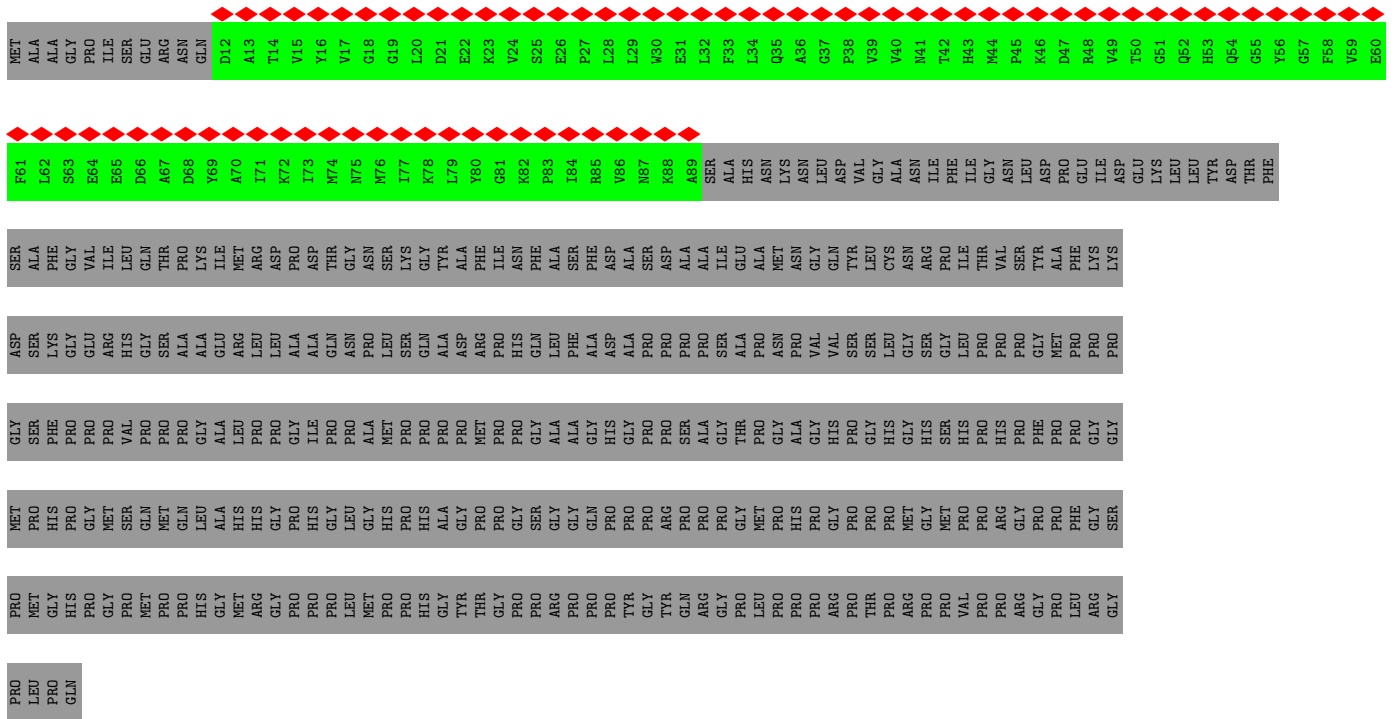




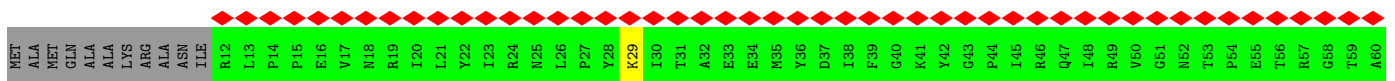
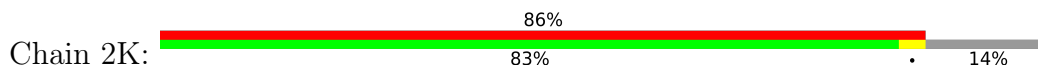
G241	S242	D243	G244	P245	S246	G247	V248	L249	I250	C251	S252	E253	N254	Y255	I256	T257	Y258	K259	N260	F261	G262	D263	Q264	P265	D266	I267	R268	C269	P270	I271	P272	R273	R274	R275	N276	D277	L278	D279	D280	P281	E282	R283	G284	M285	I286	F287	V288	C289	S290	A291	T292	H293	K294	T295	K296	S297	M298	F299	F300
F301	L302	A303	Q304	T305	E306	Q307	G308	D309	I310	F311	K312	I313	T314	L315	E316	T317	D318	E319	D320	M321	G322	T323	E324	I325	R326	L327	K328	S329	F330	D331	T332	V333	P334	V335	A336	A337	A338	M339	C340	V341	L342	K343	T344	M345	F346	L347	F348	V349	A350	S351	E352	F353	H354	N355	K356	Y357	L358	Y359	Q360
I361	A362	H363	L364	G365	D366	D367	D368	E369	E370	P371	E372	F373	S374	S375	A376	P377	PR0	LEU	GLU	GLU	GLY	ASP	T384	F385	F386	F387	Q388	P389	R390	P391	L392	K393	N394	L395	V396	L397	V398	D399	E400	L401	D402	S403	L404	S405	P406	I407	L408	F409	C410	Q411	I412	A413	D414	L415	A416	M417	E418	D419	T420
P421	Q422	L423	Y424	V425	A426	C427	G428	R429	G430	P431	R432	S433	S434	L435	R436	L438	R439	HIS	G441	L442	E443	V444	S445	E446	M447	A448	V449	S450	E451	L452	P453	G454	M455	P456	M457	A458	V459	W460	T461	V462	R463	R464	H465	I466	E467	D468	E469	F470	A471	I472	A473	I474	I475	V476	S477	F478	V479	M480	
A481	T482	L483	V484	L485	S486	I487	G488	E489	T490	V491	E492	E493	V494	T495	D496	G498	F499	L500	G501	T502	T503	P504	T505	L506	S507	C508	S509	L510	L511	G512	D513	D514	A515	L516	Q517	Q518	V519	Y520	P521	D522	G523	I524	H525	H526	I527	R528	A529	D530	K531	R532	V533	N534	E535	N536	K537	T538	P539	G540	
K541	K542	T543	I544	V545	K546	C547	A548	V549	N550	Q551	R552	Q553	V554	V555	I556	A557	L558	T559	G560	G561	E562	L563	V564	Y565	F566	E567	M568	D569	P570	S571	G572	Q573	D574	M575	E576	Y577	T578	E579	R580	K581	E582	M583	S584	A585	D586	V587	V588	C589	N590	S591	L592	A593	N594	V595	P596	P597	G598	E599	Q600
R601	S602	R603	F604	L605	A606	V607	G608	L609	V610	D611	N612	T613	V614	R615	L616	I617	S618	L619	D620	P621	S622	D623	G624	L625	Q626	P627	L628	S629	M630	Q631	A632	L633	P634	A635	Q636	P637	E638	S639	L640	C641	D642	V643	E644	M645	GLY	THR	GLU	LYS	GLN	ASP	GLU	LEU	ARG	GLY	GLU	ARG	ILE		
GLY	F662	L663	Y664	L665	N666	I667	L668	Q670	M671	G672	V673	L674	L675	R676	T677	V678	L679	D680	P681	V682	T683	G684	D685	L686	S687	D688	R689	R690	T691	ARG	TYR	LEU	G695	S696	R697	P698	V699	K700	L701	F702	R703	V704	R705	M706	Q707	G708	Q709	E710	A711	V712	L713	A714	F714	M715	S716	S717	R718	S719	M720
L721	S722	Y723	S724	Y725	Q726	T727	R728	F729	H730	L731	T732	P733	L734	S735	Y736	E737	T738	L739	E740	F741	A742	S743	G744	F745	A746	S747	E748	Q749	C750	P751	E752	G753	L754	V755	M756	A756	I757	S758	T759	N760	T761	L762	R763	L764	L765	L766	L767	E768	K769	L770	G771	ALA	V773	F774	M775	Q776	V777	F779	P780
L781	Q782	Y783	T784	P785	R786	K787	F788	V789	H790	H791	P792	E793	S794	M795	N796	L797	T798	I799	E800	E801	T802	D803	H804	N805	A806	Y807	T808	E809	A810	T811	K812	A813	O814	R815	K816	Q817	O818	R819	A820	E821	E822	H823	H824	E825	A826	A827	GLY	GLU	ASP	GLU	ARG	GLU	LEU	A835	A836	E837	M838	A839	A840
A841	F842	L843	N844	E845	N846	L847	P848	E849	S850	I851	F852	G853	A854	P855	K856	A857	G858	N859	G860	Q861	H862	A863	S864	Y865	I866	R867	V868	N869	H870	P871	L872	Q873	G874	N875	T876	L877	D878	L879	H880	Q881	L882	E883	O884	N885	E886	A887	A888	F889	S890	V891	A892	V893	C894	R895	F896	G897	N898	T899	G900
E901	D902	H903	Y904	V905	L906	Y907	G908	V909	A910	K911	D912	G913	I914	L915	N916	P917	R918	S919	V920	A921	G922	G923	F924	Y925	Y926	T927	Y928	R929	I930	Y931	N932	N933	O934	E935	K936	L937	E938	F939	L940	H941	L942	E883	O884	N885	E886	A887	V948	P949	A950	A951	I952	A953	P954	F955	Q956	G957	R958	V959	L960
I961	G962	V963	G964	K965	L966	L967	R968	V969	Y970	D971	L972	G973	K974	K975	K976	L977	L978	R979	K980	C981	N982	N983	K984	H985	I986	A987	N988	Y989	I990	S991	G992	I993	Q994	T995	I996	G997	H998	R999	I1000	I1001	I1002	S1003	D1004	V1005	Q1006	E1007	S1008	F1009	I1010	W1011	I1012	R1013	Y1014	X1015	R1016	N1017	I1018	N1019	Q1020



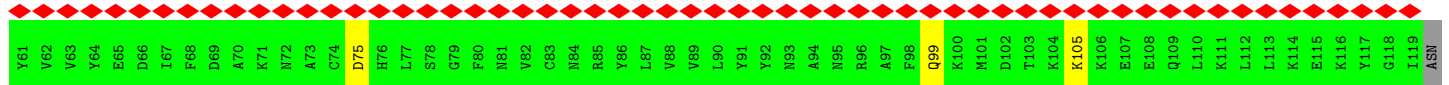
● Molecule 46: Splicing factor 3B subunit 4



● Molecule 47: Splicing factor 3B subunit 6

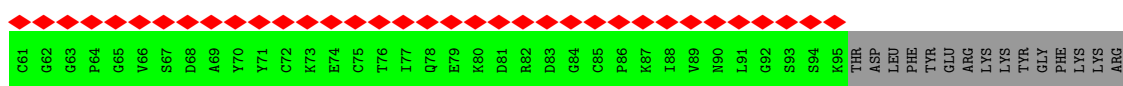
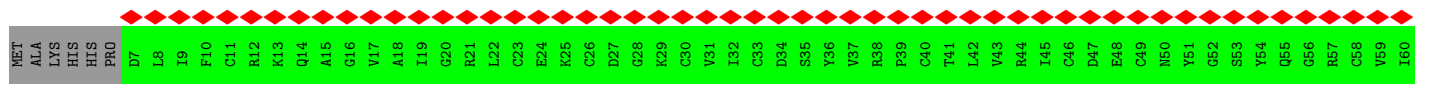
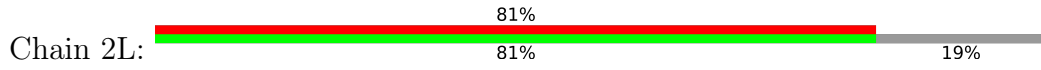




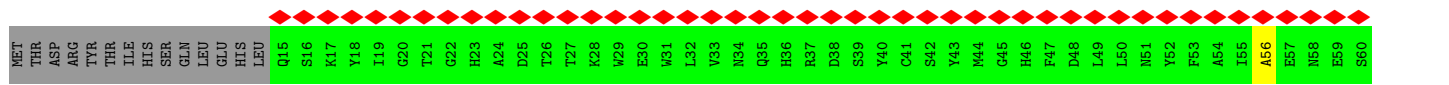
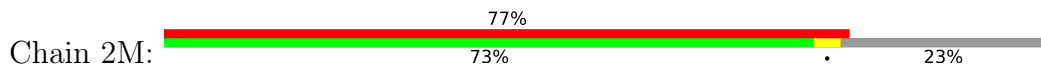


THR  
ASP  
PRO  
LYS

• Molecule 48: PHD finger-like domain-containing protein 5A



• Molecule 49: Splicing factor 3B subunit 5



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	414060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.110	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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: GTP, MG, M7M, IHP, ZN

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	A	0.65	3/1481 (0.2%)	0.92	0/2297
2	5A	0.29	0/2698	0.86	3/4195 (0.1%)
3	5B	0.26	0/19154	0.51	1/26000 (0.0%)
4	5C	0.26	0/6573	0.52	1/8929 (0.0%)
5	5D	0.26	0/13923	0.49	1/18868 (0.0%)
6	5E	0.67	0/1195	0.71	0/1492
7	2a	0.50	0/343	0.69	0/427
7	4a	0.22	0/254	0.48	0/314
7	5a	0.50	0/335	0.68	0/417
8	2b	0.56	0/327	0.68	0/407
8	4b	0.22	0/333	0.48	0/416
8	5b	0.57	0/327	0.67	0/407
9	2c	0.70	0/338	0.73	0/419
9	4c	0.23	0/298	0.48	0/370
9	5c	0.69	0/387	0.72	0/482
10	2d	0.77	0/295	0.76	0/367
10	4d	0.24	0/291	0.49	0/363
10	5d	0.77	0/295	0.76	0/367
11	2e	0.64	0/315	0.75	0/392
11	4e	0.22	0/313	0.49	0/390
11	5e	0.65	0/315	0.74	0/392
12	2f	0.55	0/270	0.63	0/334
12	4f	0.24	0/297	0.51	0/371
12	5f	0.54	0/287	0.61	0/357
13	2g	0.47	0/318	0.56	0/394
13	4g	0.23	0/287	0.49	0/358
13	5g	0.46	0/307	0.55	0/382
14	6A	0.24	0/1423	0.77	0/2211
15	6a	0.43	0/359	0.67	0/447
16	6b	0.46	0/294	0.75	0/364
17	6c	0.34	0/294	0.61	0/364
18	6d	0.43	0/286	0.59	0/354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	6e	0.43	0/279	0.72	0/347
20	6f	0.38	0/258	0.61	0/319
21	6g	0.41	0/242	0.64	0/299
22	4A	0.24	0/3025	0.76	2/4702 (0.0%)
23	4B	0.25	0/2114	0.50	0/2836
24	4C	0.25	0/3452	0.52	0/4675
25	4D	0.24	0/2912	0.50	0/3924
26	4E	0.24	0/974	0.47	0/1316
27	4F	0.29	0/1198	0.54	1/1620 (0.1%)
28	4G	0.24	0/5592	0.49	1/7615 (0.0%)
29	4H	0.26	0/853	0.46	0/1188
30	4I	0.25	0/502	0.44	0/683
31	4J	0.25	0/1149	0.52	0/1542
32	4K	0.24	0/1209	0.43	0/1655
33	4L	0.25	0/1481	0.52	0/1995
34	4M	0.23	0/609	0.49	0/819
35	4N	0.27	0/646	0.52	0/859
36	4Z	0.24	0/2100	0.45	0/2926
37	2A	0.86	11/2576 (0.4%)	1.43	55/4003 (1.4%)
38	2B	0.63	0/647	1.42	0/807
39	2C	0.61	0/375	1.20	0/467
40	2D	0.23	0/1139	0.49	0/1477
41	2E	0.22	0/373	0.58	1/461 (0.2%)
42	2F	0.25	0/1688	0.47	0/2102
43	2G	1.04	4/4184 (0.1%)	0.83	2/5216 (0.0%)
44	2H	0.65	0/957	0.67	0/1209
45	2I	0.85	0/4664	0.76	0/5816
46	2J	0.62	0/311	0.64	0/387
47	2K	0.79	0/431	0.79	0/537
48	2L	0.74	0/355	0.68	0/442
49	2M	1.01	0/263	0.77	0/327
All	All	0.44	18/100770 (0.0%)	0.64	68/136218 (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
3	5B	0	1
9	2c	0	1
9	5c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	2F	0	1
43	2G	0	11
44	2H	0	3
45	2I	0	11
47	2K	0	1
49	2M	0	1
All	All	0	31

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2G	407	MET	N-CA	12.36	1.71	1.46
43	2G	406	ALA	C-N	7.94	1.52	1.34
37	2A	142	C	C1'-N1	7.32	1.59	1.48
43	2G	1243	PRO	N-CA	-7.11	1.35	1.47
37	2A	182	U	C1'-N1	6.94	1.59	1.48
37	2A	150	U	C1'-N1	6.74	1.58	1.48
37	2A	151	C	C1'-N1	6.53	1.58	1.48
37	2A	97	G	C1'-N9	-6.41	1.37	1.46
37	2A	141	C	C1'-N1	6.38	1.58	1.48
37	2A	184	C	C1'-N1	6.35	1.58	1.48
37	2A	148	C	C1'-N1	6.33	1.58	1.48
43	2G	944	SER	N-CA	-5.72	1.34	1.46
37	2A	65	U	C1'-N1	5.54	1.57	1.48
37	2A	48	A	C1'-N9	-5.48	1.39	1.46
1	A	9	U	C1'-N1	5.14	1.56	1.48
1	A	8	U	C1'-N1	5.13	1.56	1.48
1	A	7	U	C1'-N1	5.13	1.56	1.48
37	2A	110	A	C1'-N9	-5.08	1.39	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2A	167	U	C5-C4-O4	11.61	132.87	125.90
43	2G	406	ALA	C-N-CA	10.28	147.39	121.70
37	2A	164	C	N1-C2-O2	-10.12	112.83	118.90
3	5B	1194	CYS	CA-CB-SG	9.09	130.36	114.00
37	2A	162	U	N3-C2-O2	-8.97	115.92	122.20
37	2A	164	C	C5'-C4'-O4'	-8.21	99.25	109.10
37	2A	169	C	P-O3'-C3'	8.20	129.54	119.70
37	2A	166	G	O4'-C1'-N9	8.03	114.62	108.20
37	2A	167	U	N3-C4-O4	-7.89	113.88	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2A	164	C	P-O3'-C3'	7.54	128.75	119.70
37	2A	167	U	N1-C2-O2	7.41	127.98	122.80
37	2A	164	C	N3-C2-O2	7.38	127.07	121.90
37	2A	113	G	OP2-P-O3'	7.26	121.17	105.20
37	2A	149	A	OP2-P-O3'	7.26	121.16	105.20
37	2A	141	C	OP2-P-O3'	7.24	121.13	105.20
37	2A	114	A	OP2-P-O3'	7.24	121.12	105.20
37	2A	183	G	OP2-P-O3'	7.22	121.08	105.20
37	2A	181	G	OP2-P-O3'	7.21	121.07	105.20
37	2A	182	U	OP2-P-O3'	7.21	121.07	105.20
37	2A	180	G	OP2-P-O3'	7.21	121.06	105.20
37	2A	150	U	OP2-P-O3'	7.20	121.05	105.20
37	2A	148	C	OP2-P-O3'	7.18	121.00	105.20
37	2A	168	A	P-O5'-C5'	-7.14	109.47	120.90
2	5A	77	G	P-O3'-C3'	-7.04	111.26	119.70
37	2A	167	U	N3-C2-O2	-6.96	117.33	122.20
37	2A	180	G	O3'-P-O5'	-6.83	91.02	104.00
37	2A	149	A	O3'-P-O5'	-6.83	91.03	104.00
43	2G	406	ALA	CA-C-O	-6.82	105.77	120.10
37	2A	155	C	P-O3'-C3'	6.82	127.88	119.70
37	2A	182	U	O3'-P-O5'	-6.81	91.06	104.00
37	2A	183	G	O3'-P-O5'	-6.79	91.11	104.00
37	2A	148	C	O3'-P-O5'	-6.78	91.12	104.00
37	2A	141	C	O3'-P-O5'	-6.77	91.14	104.00
37	2A	150	U	O3'-P-O5'	-6.75	91.17	104.00
37	2A	113	G	O3'-P-O5'	-6.75	91.19	104.00
37	2A	181	G	O3'-P-O5'	-6.74	91.19	104.00
37	2A	114	A	O3'-P-O5'	-6.73	91.21	104.00
4	5C	308	CYS	CA-CB-SG	6.22	125.20	114.00
37	2A	165	A	O4'-C1'-N9	-6.19	103.25	108.20
37	2A	166	G	N9-C4-C5	6.14	107.86	105.40
37	2A	166	G	C8-N9-C4	-6.11	103.96	106.40
37	2A	162	U	N1-C2-O2	6.07	127.05	122.80
37	2A	166	G	N3-C4-C5	-6.01	125.60	128.60
37	2A	168	A	C5'-C4'-C3'	-5.93	106.51	116.00
28	4G	707	ASP	C-N-CA	5.89	136.43	121.70
37	2A	172	C	P-O3'-C3'	5.80	126.66	119.70
2	5A	76	A	P-O3'-C3'	-5.78	112.77	119.70
37	2A	156	U	P-O3'-C3'	-5.77	112.78	119.70
41	2E	146	MET	C-N-CA	5.75	146.17	122.00
5	5D	583	THR	C-N-CA	5.75	136.07	121.70
37	2A	167	U	O3'-P-O5'	-5.74	93.09	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2A	164	C	C5-C4-N4	-5.72	116.20	120.20
27	4F	78	PRO	N-CD-CG	-5.55	94.88	103.20
37	2A	157	G	O4'-C1'-N9	-5.50	103.80	108.20
37	2A	166	G	C6-N1-C2	-5.46	121.83	125.10
37	2A	106	G	O5'-P-OP1	5.41	117.19	110.70
22	4A	1	A	OP1-P-OP2	5.36	127.64	119.60
37	2A	156	U	OP2-P-O3'	5.28	116.82	105.20
37	2A	160	A	P-O5'-C5'	-5.27	112.46	120.90
37	2A	170	C	O4'-C1'-C2'	-5.23	100.57	105.80
22	4A	70	U	C2-N1-C1'	5.20	123.94	117.70
37	2A	164	C	C6-N1-C2	5.17	122.37	120.30
37	2A	157	G	P-O5'-C5'	-5.15	112.66	120.90
37	2A	170	C	N3-C4-C5	-5.14	119.84	121.90
37	2A	156	U	C4'-C3'-C2'	5.08	107.69	102.60
2	5A	23	C	C2-N1-C1'	5.07	124.38	118.80
37	2A	162	U	C2-N3-C4	-5.03	123.98	127.00
37	2A	176	G	N9-C4-C5	5.01	107.41	105.40

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	2F	443	THR	Peptide
43	2G	1025	LYS	Peptide
43	2G	1122	THR	Peptide
43	2G	1127	THR	Peptide
43	2G	1179	ASP	Peptide
43	2G	1199	VAL	Peptide
43	2G	220	GLN	Peptide
43	2G	415	LEU	Peptide,Mainchain
43	2G	689	ILE	Peptide
43	2G	941	ASN	Peptide
43	2G	944	SER	Peptide
44	2H	553	MET	Peptide
44	2H	558	ARG	Peptide
44	2H	571	LEU	Peptide
45	2I	261	PHE	Peptide
45	2I	366	ASP	Peptide
45	2I	468	ASP	Peptide
45	2I	530	ASP	Peptide
45	2I	534	ASN	Peptide
45	2I	552	ARG	Peptide

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Mol	Chain	Res	Type	Group
45	2I	670	GLN	Peptide
45	2I	678	VAL	Peptide
45	2I	74	THR	Peptide
45	2I	980	LYS	Peptide
45	2I	986	ILE	Peptide
47	2K	29	LYS	Peptide
49	2M	74	GLN	Peptide
9	2c	112	ASN	Peptide
3	5B	941	LYS	Peptide
9	5c	112	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	5B	2249/2335 (96%)	2156 (96%)	93 (4%)	0	100	100
4	5C	814/972 (84%)	755 (93%)	58 (7%)	1 (0%)	51	78
5	5D	1694/2136 (79%)	1618 (96%)	75 (4%)	1 (0%)	51	78
6	5E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	4	10
7	2a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
7	4a	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
7	5a	82/231 (36%)	80 (98%)	2 (2%)	0	100	100
8	2b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
8	4b	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
8	5b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
9	2c	81/118 (69%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	4c	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
9	5c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
10	2d	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
10	4d	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
10	5d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
11	2e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	4e	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
11	5e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	2f	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
12	4f	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
12	5f	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
13	2g	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
13	4g	69/126 (55%)	69 (100%)	0	0	100	100
13	5g	75/126 (60%)	73 (97%)	2 (3%)	0	100	100
15	6a	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	5
16	6b	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	5
17	6c	70/139 (50%)	63 (90%)	6 (9%)	1 (1%)	11	28
18	6d	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	10	26
19	6e	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	4	10
20	6f	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
21	6g	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	8	21
23	4B	248/683 (36%)	235 (95%)	13 (5%)	0	100	100
24	4C	422/522 (81%)	393 (93%)	28 (7%)	1 (0%)	47	73
25	4D	372/499 (74%)	353 (95%)	19 (5%)	0	100	100
26	4E	122/128 (95%)	115 (94%)	7 (6%)	0	100	100
27	4F	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
28	4G	795/941 (84%)	747 (94%)	48 (6%)	0	100	100
29	4H	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
30	4I	73/376 (19%)	73 (100%)	0	0	100	100
31	4J	142/800 (18%)	136 (96%)	6 (4%)	0	100	100
32	4K	184/439 (42%)	174 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	4L	173/312 (55%)	165 (95%)	6 (4%)	2 (1%)	13	32
34	4M	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
35	4N	78/199 (39%)	77 (99%)	0	1 (1%)	12	30
36	4Z	414/513 (81%)	401 (97%)	12 (3%)	1 (0%)	47	73
38	2B	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	30
39	2C	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
40	2D	196/793 (25%)	180 (92%)	10 (5%)	6 (3%)	4	9
41	2E	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	0
42	2F	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	13	32
43	2G	1032/1304 (79%)	844 (82%)	166 (16%)	22 (2%)	7	18
44	2H	199/895 (22%)	179 (90%)	16 (8%)	4 (2%)	7	19
45	2I	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	17	40
46	2J	76/424 (18%)	75 (99%)	1 (1%)	0	100	100
47	2K	106/125 (85%)	85 (80%)	18 (17%)	3 (3%)	5	11
48	2L	87/110 (79%)	74 (85%)	13 (15%)	0	100	100
49	2M	64/86 (74%)	55 (86%)	7 (11%)	2 (3%)	4	9
All	All	14181/21253 (67%)	13204 (93%)	886 (6%)	91 (1%)	29	50

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	5D	1086	GLN
6	5E	193	THR
15	6a	55	LEU
16	6b	84	MET
18	6d	70	ASP
19	6e	52	VAL
19	6e	55	GLN
24	4C	459	PRO
36	4Z	383	CYS
40	2D	301	PRO
41	2E	139	PRO
41	2E	141	ILE
41	2E	146	MET
41	2E	162	PRO
41	2E	165	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	2E	218	PRO
42	2F	284	ARG
43	2G	208	PRO
43	2G	416	PRO
43	2G	418	PRO
43	2G	456	VAL
43	2G	717	THR
43	2G	941	ASN
43	2G	1107	GLN
45	2I	405	SER
45	2I	919	SER
47	2K	99	GLN
47	2K	105	LYS
15	6a	74	ALA
16	6b	97	PRO
17	6c	12	ASN
38	2B	160	LYS
40	2D	223	LYS
40	2D	280	VAL
42	2F	277	THR
43	2G	113	ALA
43	2G	1110	VAL
44	2H	597	PHE
45	2I	917	PRO
6	5E	60	MET
6	5E	88	ARG
6	5E	256	ASP
33	4L	39	CYS
42	2F	177	ARG
42	2F	393	PRO
44	2H	510	TYR
6	5E	162	ARG
16	6b	96	ALA
38	2B	32	PRO
40	2D	300	THR
43	2G	112	ILE
43	2G	437	PRO
43	2G	523	ALA
43	2G	909	VAL
43	2G	1006	MET
44	2H	463	ALA
44	2H	574	ALA

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Mol	Chain	Res	Type
45	2I	529	ALA
45	2I	578	THR
47	2K	75	ASP
6	5E	159	PRO
15	6a	73	PRO
35	4N	85	CYS
41	2E	147	PRO
41	2E	217	PRO
43	2G	1047	ALA
43	2G	1075	ARG
43	2G	1186	GLN
45	2I	95	SER
45	2I	229	GLU
6	5E	270	LYS
21	6g	34	ILE
33	4L	65	ILE
41	2E	220	PRO
43	2G	326	THR
43	2G	932	ILE
45	2I	918	ARG
45	2I	1138	HIS
49	2M	56	ALA
6	5E	149	GLY
43	2G	417	PRO
40	2D	221	PRO
43	2G	223	THR
42	2F	229	TRP
45	2I	1204	VAL
4	5C	439	PRO
6	5E	324	PRO
40	2D	298	PRO
43	2G	1031	VAL
49	2M	64	VAL
15	6a	52	PRO

### 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	5B	2033/2108 (96%)	1938 (95%)	95 (5%)	26	54
4	5C	717/866 (83%)	678 (95%)	39 (5%)	22	47
5	5D	1517/1908 (80%)	1492 (98%)	25 (2%)	62	85
23	4B	225/599 (38%)	217 (96%)	8 (4%)	35	64
24	4C	362/442 (82%)	336 (93%)	26 (7%)	14	34
25	4D	299/424 (70%)	277 (93%)	22 (7%)	13	32
26	4E	108/111 (97%)	103 (95%)	5 (5%)	27	54
27	4F	129/130 (99%)	122 (95%)	7 (5%)	22	47
28	4G	417/792 (53%)	389 (93%)	28 (7%)	16	37
29	4H	10/148 (7%)	10 (100%)	0	100	100
30	4I	32/333 (10%)	27 (84%)	5 (16%)	2	7
31	4J	112/681 (16%)	104 (93%)	8 (7%)	14	34
32	4K	66/395 (17%)	60 (91%)	6 (9%)	9	21
33	4L	159/293 (54%)	146 (92%)	13 (8%)	11	26
34	4M	66/66 (100%)	60 (91%)	6 (9%)	9	21
35	4N	75/181 (41%)	65 (87%)	10 (13%)	4	9
36	4Z	11/450 (2%)	11 (100%)	0	100	100
40	2D	70/709 (10%)	69 (99%)	1 (1%)	67	86
44	2H	26/776 (3%)	25 (96%)	1 (4%)	33	62
All	All	6434/11412 (56%)	6129 (95%)	305 (5%)	30	54

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5B	68	LYS
3	5B	81	PHE
3	5B	87	VAL
3	5B	104	GLU
3	5B	142	SER
3	5B	150	MET
3	5B	181	ASN
3	5B	183	LEU
3	5B	195	LEU
3	5B	200	ASP
3	5B	223	SER
3	5B	227	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	5B	236	SER
3	5B	248	ASP
3	5B	282	LEU
3	5B	305	ARG
3	5B	322	ASN
3	5B	330	THR
3	5B	339	PHE
3	5B	341	LYS
3	5B	351	TYR
3	5B	352	PHE
3	5B	353	ASP
3	5B	361	HIS
3	5B	379	GLU
3	5B	387	PHE
3	5B	417	ARG
3	5B	468	LYS
3	5B	484	SER
3	5B	506	LEU
3	5B	510	ARG
3	5B	513	LEU
3	5B	519	ASP
3	5B	528	LYS
3	5B	615	ARG
3	5B	650	ARG
3	5B	679	SER
3	5B	741	ARG
3	5B	748	ASP
3	5B	774	LYS
3	5B	819	SER
3	5B	821	ARG
3	5B	845	ARG
3	5B	855	ARG
3	5B	859	SER
3	5B	866	LEU
3	5B	934	ARG
3	5B	945	THR
3	5B	989	ASP
3	5B	991	THR
3	5B	994	ASN
3	5B	1032	ARG
3	5B	1089	CYS
3	5B	1091	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	5B	1104	ASP
3	5B	1122	ASN
3	5B	1129	ASN
3	5B	1137	ASP
3	5B	1140	MET
3	5B	1173	SER
3	5B	1176	SER
3	5B	1199	LYS
3	5B	1223	GLU
3	5B	1239	ARG
3	5B	1303	LEU
3	5B	1310	ARG
3	5B	1341	ARG
3	5B	1359	HIS
3	5B	1361	GLU
3	5B	1370	ARG
3	5B	1377	SER
3	5B	1402	ARG
3	5B	1413	ASP
3	5B	1420	ASN
3	5B	1438	VAL
3	5B	1536	LEU
3	5B	1544	ARG
3	5B	1634	SER
3	5B	1678	ARG
3	5B	1697	SER
3	5B	1753	LEU
3	5B	1765	SER
3	5B	1831	LYS
3	5B	1866	LYS
3	5B	1872	LEU
3	5B	1894	GLN
3	5B	1904	ASP
3	5B	1908	LYS
3	5B	2031	LYS
3	5B	2046	THR
3	5B	2056	THR
3	5B	2073	TRP
3	5B	2094	SER
3	5B	2231	THR
3	5B	2265	ASP
4	5C	121	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	5C	134	LEU
4	5C	198	TYR
4	5C	261	ASP
4	5C	273	ASP
4	5C	301	SER
4	5C	327	TYR
4	5C	352	LYS
4	5C	359	LYS
4	5C	394	ARG
4	5C	423	PHE
4	5C	458	ASP
4	5C	476	CYS
4	5C	507	VAL
4	5C	512	GLU
4	5C	514	TYR
4	5C	533	SER
4	5C	534	VAL
4	5C	543	ARG
4	5C	562	THR
4	5C	589	LYS
4	5C	592	VAL
4	5C	623	GLU
4	5C	649	SER
4	5C	713	LYS
4	5C	718	PHE
4	5C	721	LYS
4	5C	724	TRP
4	5C	727	LEU
4	5C	740	THR
4	5C	749	THR
4	5C	770	PHE
4	5C	780	CYS
4	5C	803	ARG
4	5C	826	ARG
4	5C	880	SER
4	5C	912	LEU
4	5C	919	ARG
4	5C	928	HIS
5	5D	685	LEU
5	5D	726	HIS
5	5D	780	TYR
5	5D	801	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	5D	844	LEU
5	5D	891	SER
5	5D	984	LEU
5	5D	990	HIS
5	5D	992	TYR
5	5D	1039	LYS
5	5D	1092	MET
5	5D	1148	PHE
5	5D	1159	ASN
5	5D	1320	LEU
5	5D	1325	PHE
5	5D	1376	CYS
5	5D	1417	LYS
5	5D	1478	SER
5	5D	1507	SER
5	5D	1580	CYS
5	5D	1607	SER
5	5D	1732	MET
5	5D	1841	LYS
5	5D	1948	MET
5	5D	2014	TYR
23	4B	412	PHE
23	4B	417	LEU
23	4B	515	ASN
23	4B	531	LYS
23	4B	577	LYS
23	4B	580	ASN
23	4B	640	ASP
23	4B	659	GLU
24	4C	90	PHE
24	4C	93	ARG
24	4C	98	GLN
24	4C	150	LYS
24	4C	166	TRP
24	4C	200	LYS
24	4C	206	THR
24	4C	209	SER
24	4C	220	SER
24	4C	235	SER
24	4C	304	SER
24	4C	334	SER
24	4C	345	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	4C	370	ASP
24	4C	374	HIS
24	4C	378	SER
24	4C	399	CYS
24	4C	403	LEU
24	4C	407	LEU
24	4C	429	ASN
24	4C	430	THR
24	4C	436	LEU
24	4C	460	ILE
24	4C	461	HIS
24	4C	505	GLN
24	4C	513	ASP
25	4D	115	ARG
25	4D	116	ASP
25	4D	117	LYS
25	4D	122	PHE
25	4D	144	ASN
25	4D	150	LYS
25	4D	163	THR
25	4D	168	SER
25	4D	181	GLU
25	4D	211	ARG
25	4D	214	PHE
25	4D	260	SER
25	4D	311	SER
25	4D	350	GLN
25	4D	362	MET
25	4D	395	SER
25	4D	398	HIS
25	4D	419	ARG
25	4D	421	SER
25	4D	426	ARG
25	4D	430	LYS
25	4D	431	GLN
26	4E	15	ASP
26	4E	81	VAL
26	4E	85	SER
26	4E	108	GLU
26	4E	122	SER
27	4F	25	VAL
27	4F	33	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	4F	80	THR
27	4F	94	LEU
27	4F	132	SER
27	4F	138	THR
27	4F	141	ARG
28	4G	6	LYS
28	4G	32	SER
28	4G	39	ASP
28	4G	102	ASP
28	4G	110	LYS
28	4G	154	GLU
28	4G	155	GLU
28	4G	159	SER
28	4G	175	ARG
28	4G	197	HIS
28	4G	199	SER
28	4G	356	ASP
28	4G	357	THR
28	4G	373	VAL
28	4G	383	GLU
28	4G	714	MET
28	4G	725	MET
28	4G	750	SER
28	4G	788	TYR
28	4G	855	ARG
28	4G	881	PHE
28	4G	892	GLU
28	4G	896	GLU
28	4G	907	ARG
28	4G	912	TRP
28	4G	918	ASP
28	4G	921	ASN
28	4G	928	ASP
30	4I	8	GLN
30	4I	23	ASN
30	4I	29	PHE
30	4I	34	LYS
30	4I	42	LYS
31	4J	149	GLU
31	4J	168	ARG
31	4J	250	SER
31	4J	255	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	4J	267	ARG
31	4J	347	HIS
31	4J	350	ARG
31	4J	352	GLU
32	4K	349	MET
32	4K	351	GLU
32	4K	359	ASP
32	4K	374	LEU
32	4K	376	LYS
32	4K	400	THR
33	4L	4	ARG
33	4L	7	LYS
33	4L	24	ILE
33	4L	60	VAL
33	4L	72	CYS
33	4L	74	THR
33	4L	75	LEU
33	4L	76	LYS
33	4L	96	PHE
33	4L	108	ARG
33	4L	118	LYS
33	4L	124	TYR
33	4L	172	GLU
34	4M	3	GLU
34	4M	9	ARG
34	4M	21	ASP
34	4M	23	THR
34	4M	49	THR
34	4M	73	GLN
35	4N	58	LEU
35	4N	59	GLU
35	4N	60	SER
35	4N	61	LYS
35	4N	70	LYS
35	4N	84	VAL
35	4N	88	VAL
35	4N	102	LYS
35	4N	119	LEU
35	4N	133	MET
40	2D	482	THR
44	2H	800	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36)

such sidechains are listed below:

Mol	Chain	Res	Type
3	5B	65	HIS
3	5B	73	HIS
3	5B	105	ASN
3	5B	361	HIS
3	5B	434	HIS
3	5B	509	HIS
3	5B	542	ASN
3	5B	545	HIS
3	5B	1450	GLN
3	5B	1487	HIS
3	5B	1552	GLN
3	5B	1563	HIS
3	5B	1944	HIS
3	5B	1966	HIS
3	5B	2166	HIS
4	5C	140	HIS
4	5C	245	HIS
4	5C	627	HIS
5	5D	785	HIS
5	5D	911	GLN
5	5D	1515	HIS
23	4B	511	HIS
23	4B	668	HIS
24	4C	282	HIS
24	4C	322	HIS
24	4C	421	HIS
25	4D	111	HIS
25	4D	270	HIS
26	4E	17	HIS
26	4E	28	GLN
26	4E	87	GLN
27	4F	89	HIS
28	4G	741	HIS
28	4G	773	ASN
31	4J	261	HIS
33	4L	81	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	62/144 (43%)	37 (59%)	12 (19%)

*Continued on next page...*

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	6A	56/107 (52%)	10 (17%)	1 (1%)
2	5A	114/117 (97%)	30 (26%)	5 (4%)
22	4A	124/145 (85%)	33 (26%)	2 (1%)
37	2A	105/188 (55%)	22 (20%)	3 (2%)
All	All	461/701 (65%)	132 (28%)	23 (4%)

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	10	C
1	A	11	C
1	A	12	U
1	A	13	U
1	A	15	A
1	A	20	U
1	A	21	U
1	A	22	C
1	A	25	G
1	A	29	A
1	A	30	C
1	A	31	C
1	A	32	C
1	A	33	U
1	A	34	G
1	A	35	U
1	A	36	C
1	A	37	C
1	A	39	U
1	A	41	U
1	A	42	U
1	A	44	U
1	A	46	U
1	A	47	C
1	A	48	C
1	A	100	C
1	A	102	U
1	A	103	A
1	A	106	A
1	A	108	G
1	A	110	G

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	111	A
1	A	116	G
1	A	117	G
1	A	118	A
2	5A	8	G
2	5A	10	U
2	5A	17	U
2	5A	21	A
2	5A	22	U
2	5A	24	G
2	5A	25	C
2	5A	26	A
2	5A	28	A
2	5A	35	U
2	5A	36	C
2	5A	40	U
2	5A	45	C
2	5A	52	U
2	5A	68	C
2	5A	69	A
2	5A	78	U
2	5A	79	C
2	5A	80	U
2	5A	83	A
2	5A	88	A
2	5A	89	U
2	5A	90	U
2	5A	92	U
2	5A	93	U
2	5A	94	U
2	5A	95	G
2	5A	96	A
2	5A	97	G
2	5A	109	G
14	6A	36	A
14	6A	46	G
14	6A	47	A
14	6A	48	A
14	6A	49	G
14	6A	51	U
14	6A	77	C
14	6A	78	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	6A	103	U
14	6A	104	U
22	4A	2	G
22	4A	25	A
22	4A	26	G
22	4A	37	C
22	4A	38	U
22	4A	39	A
22	4A	40	U
22	4A	45	G
22	4A	53	U
22	4A	54	A
22	4A	62	U
22	4A	71	U
22	4A	73	U
22	4A	74	C
22	4A	75	C
22	4A	76	C
22	4A	84	C
22	4A	85	G
22	4A	90	G
22	4A	100	A
22	4A	103	A
22	4A	109	G
22	4A	114	U
22	4A	115	G
22	4A	118	A
22	4A	119	A
22	4A	120	U
22	4A	121	U
22	4A	124	U
22	4A	125	G
22	4A	126	A
22	4A	127	C
22	4A	144	G
37	2A	31	G
37	2A	37	U
37	2A	40	C
37	2A	45	C
37	2A	47	U
37	2A	51	A
37	2A	65	U

*Continued on next page...*



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Mol	Chain	Res	Type
37	2A	112	G
37	2A	143	A
37	2A	147	G
37	2A	152	G
37	2A	153	A
37	2A	154	C
37	2A	156	U
37	2A	157	G
37	2A	164	C
37	2A	165	A
37	2A	168	A
37	2A	169	C
37	2A	177	A
37	2A	178	A
37	2A	179	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	21	U
1	A	28	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	38	C
1	A	40	U
1	A	41	U
1	A	99	C
1	A	116	G
1	A	117	G
2	5A	67	A
2	5A	78	U
2	5A	79	C
2	5A	94	U
2	5A	96	A
14	6A	77	C
22	4A	99	C
22	4A	114	U
37	2A	156	U
37	2A	164	C
37	2A	168	A

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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
51	GTP	5C	1500	52	26,34,34	1.11	2 (7%)	32,54,54	1.53	7 (21%)
50	IHP	5B	3000	-	36,36,36	0.76	0	54,60,60	1.13	2 (3%)

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
51	GTP	5C	1500	52	-	8/18/38/38	0/3/3/3
50	IHP	5B	3000	-	-	3/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	5C	1500	GTP	C5-C6	-3.96	1.39	1.47
51	5C	1500	GTP	C2-N3	2.20	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	5C	1500	GTP	C5-C6-N1	3.27	119.73	113.95
51	5C	1500	GTP	PB-O3B-PG	-3.15	122.02	132.83
51	5C	1500	GTP	PA-O3A-PB	-3.11	122.14	132.83
51	5C	1500	GTP	C8-N7-C5	3.09	108.87	102.99
51	5C	1500	GTP	C2-N1-C6	-2.91	119.73	125.10
51	5C	1500	GTP	C3'-C2'-C1'	2.79	105.18	100.98
50	5B	3000	IHP	C5-C4-C3	2.47	115.82	110.41
50	5B	3000	IHP	C6-C5-C4	2.25	115.35	110.41
51	5C	1500	GTP	O6-C6-C5	-2.10	120.28	124.37

There are no chirality outliers.

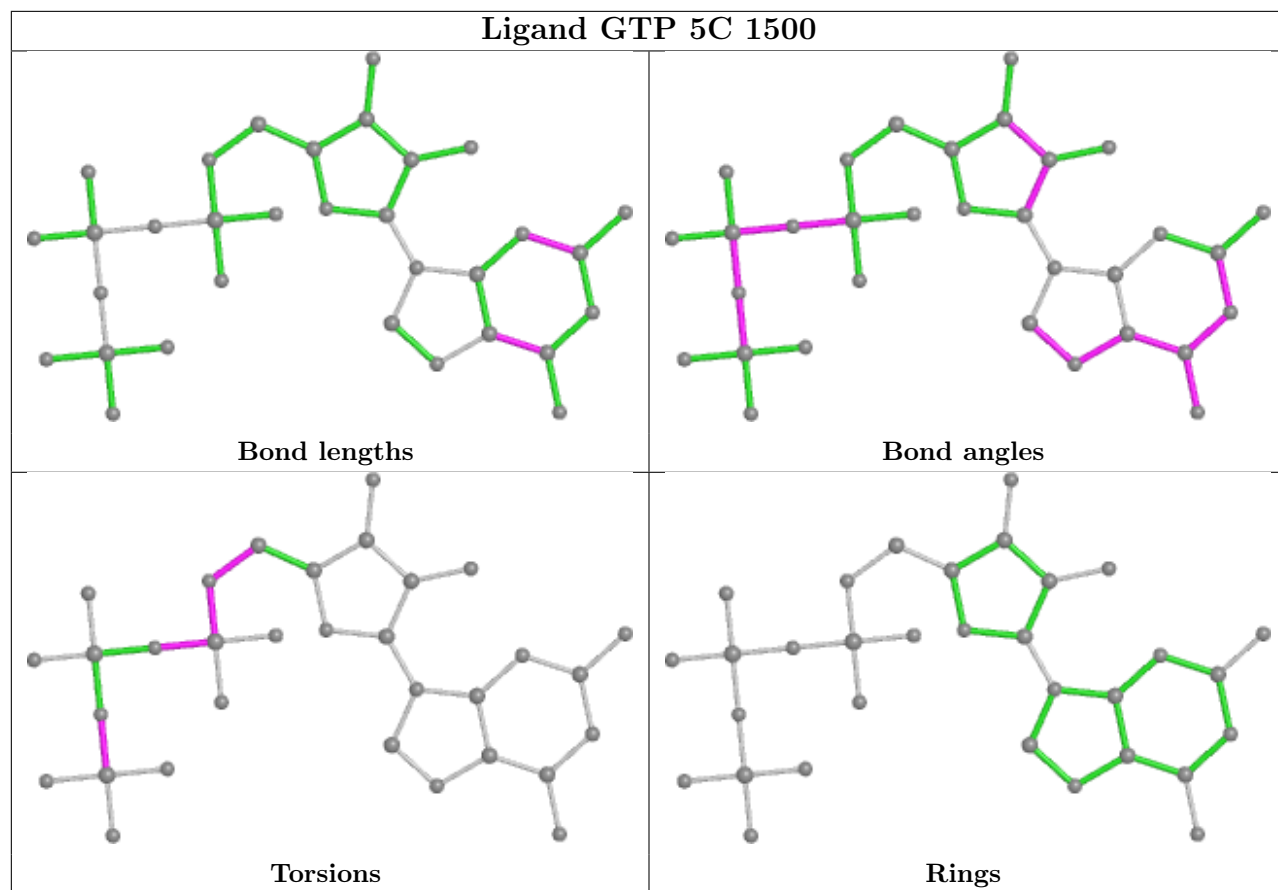
All (11) torsion outliers are listed below:

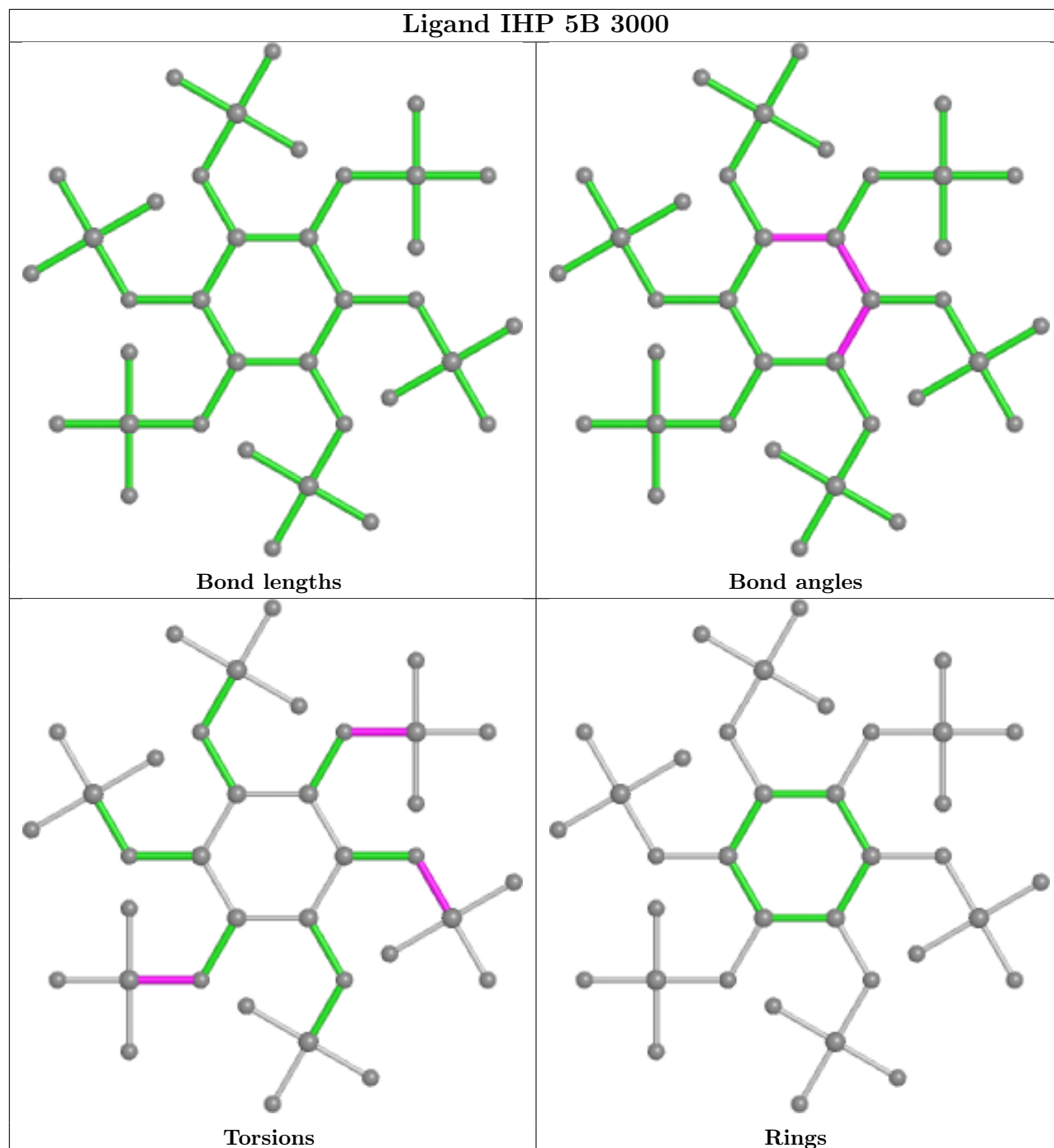
Mol	Chain	Res	Type	Atoms
50	5B	3000	IHP	C4-O14-P4-O44
51	5C	1500	GTP	C5'-O5'-PA-O1A
51	5C	1500	GTP	C5'-O5'-PA-O2A
51	5C	1500	GTP	PB-O3A-PA-O5'
51	5C	1500	GTP	C4'-C5'-O5'-PA
51	5C	1500	GTP	PB-O3B-PG-O1G
51	5C	1500	GTP	PB-O3B-PG-O2G
51	5C	1500	GTP	PB-O3B-PG-O3G
50	5B	3000	IHP	C1-O11-P1-O31
50	5B	3000	IHP	C5-O15-P5-O35
51	5C	1500	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

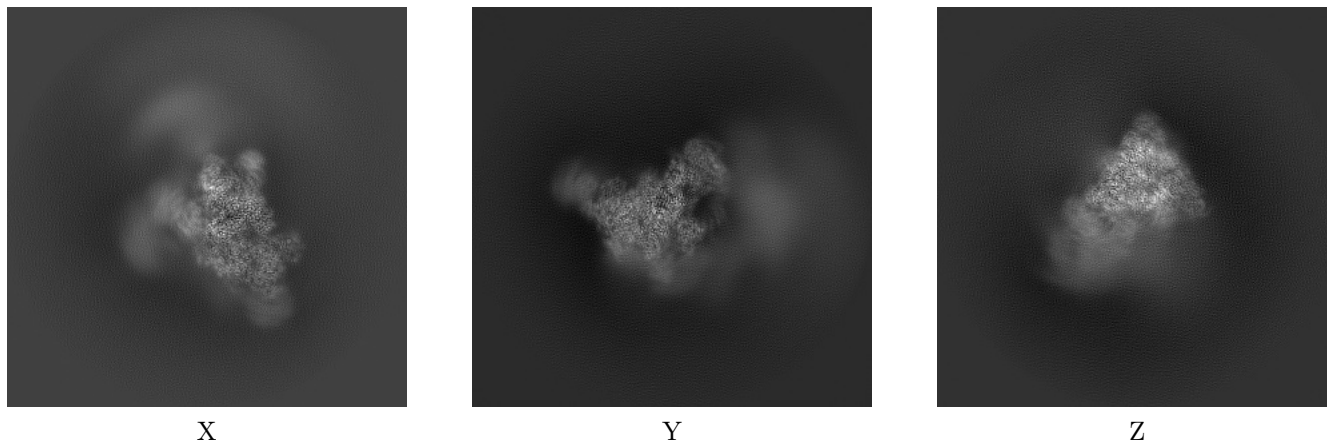
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34507. These allow visual inspection of the internal detail of the map and identification of artifacts.

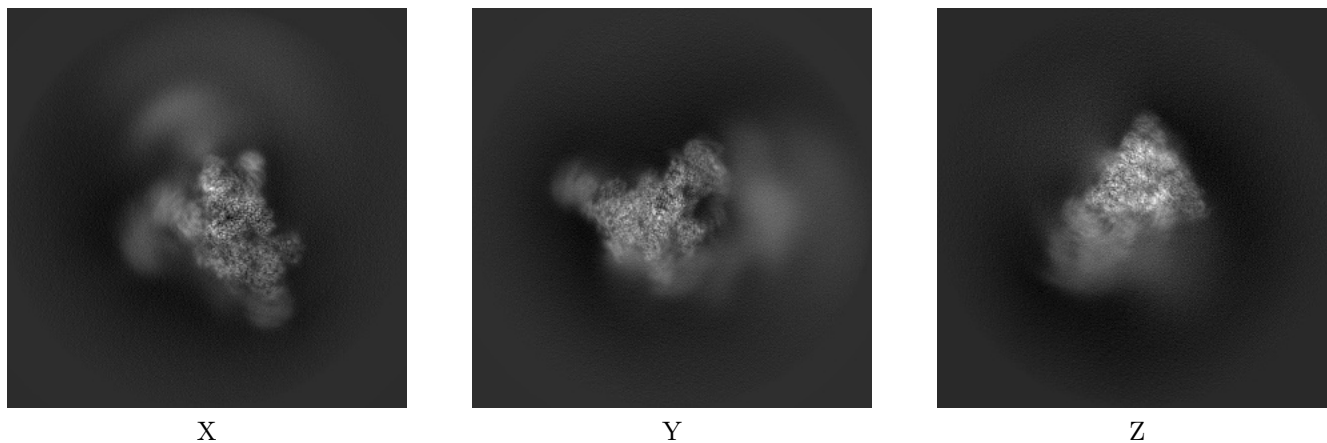
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



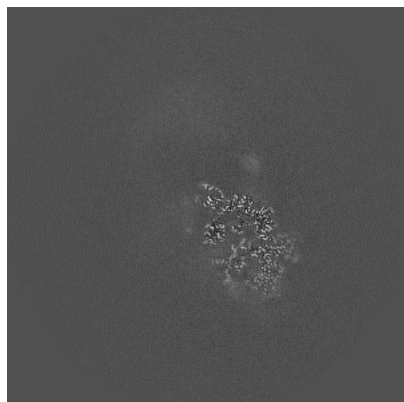
#### 6.1.2 Raw map



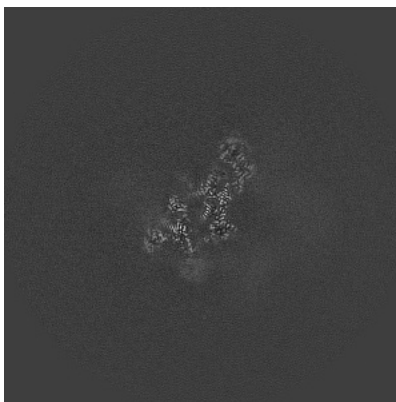
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

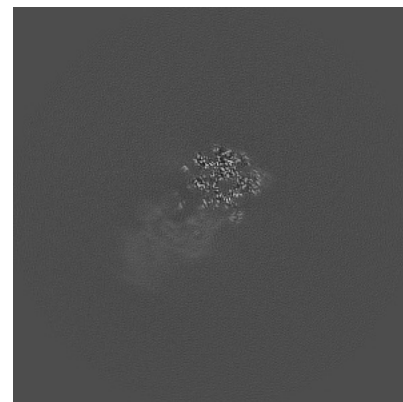
### 6.2.1 Primary map



X Index: 256

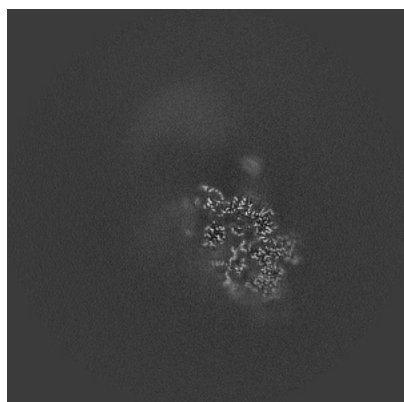


Y Index: 256

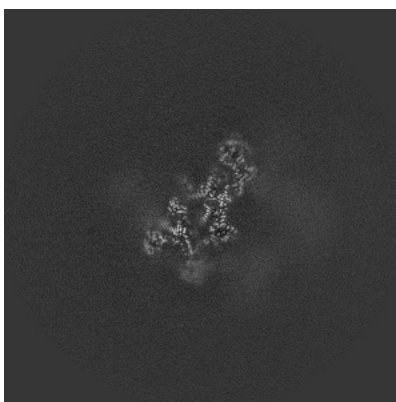


Z Index: 256

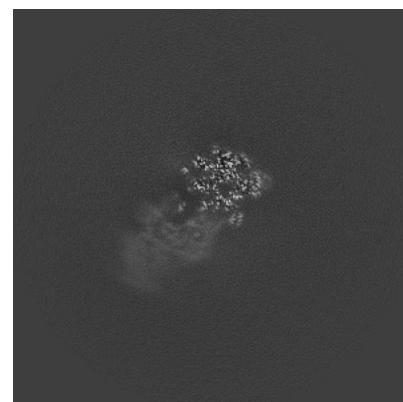
### 6.2.2 Raw map



X Index: 256



Y Index: 256

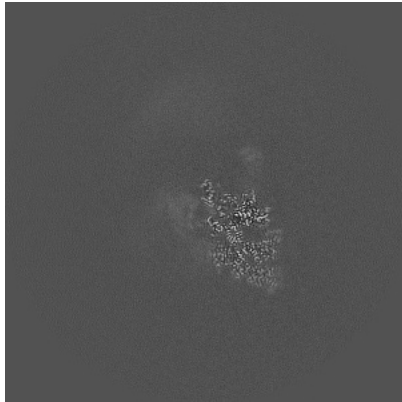


Z Index: 256

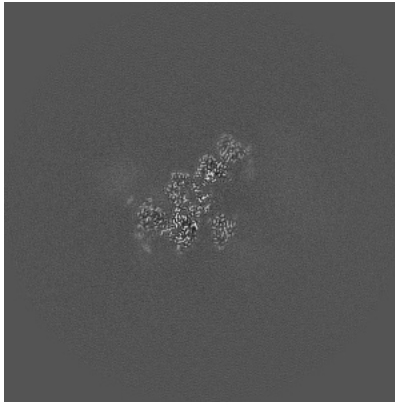
The images above show central slices of the map in three orthogonal directions.

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

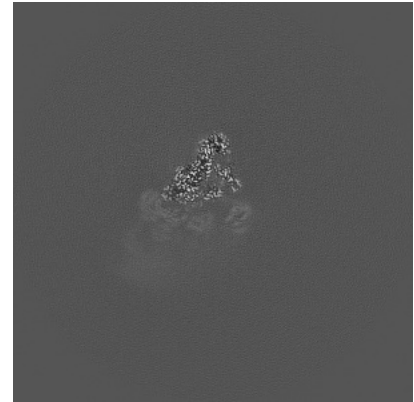
### 6.3.1 Primary map



X Index: 245

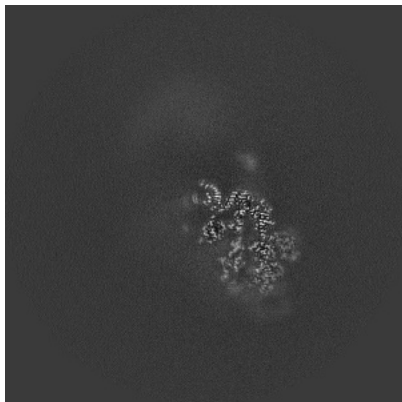


Y Index: 277

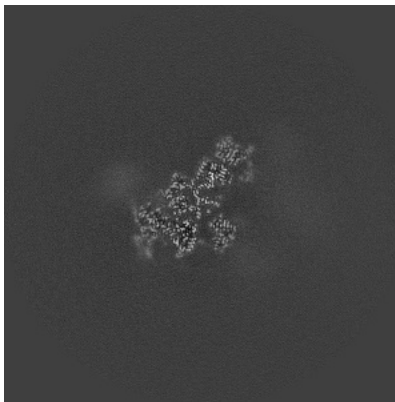


Z Index: 234

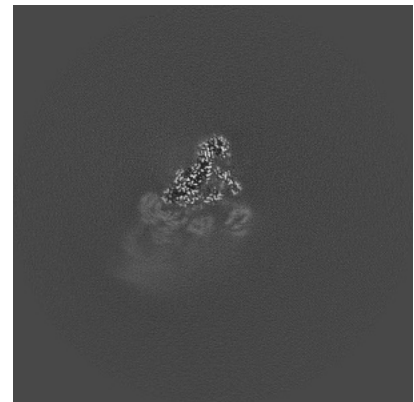
### 6.3.2 Raw map



X Index: 259



Y Index: 274



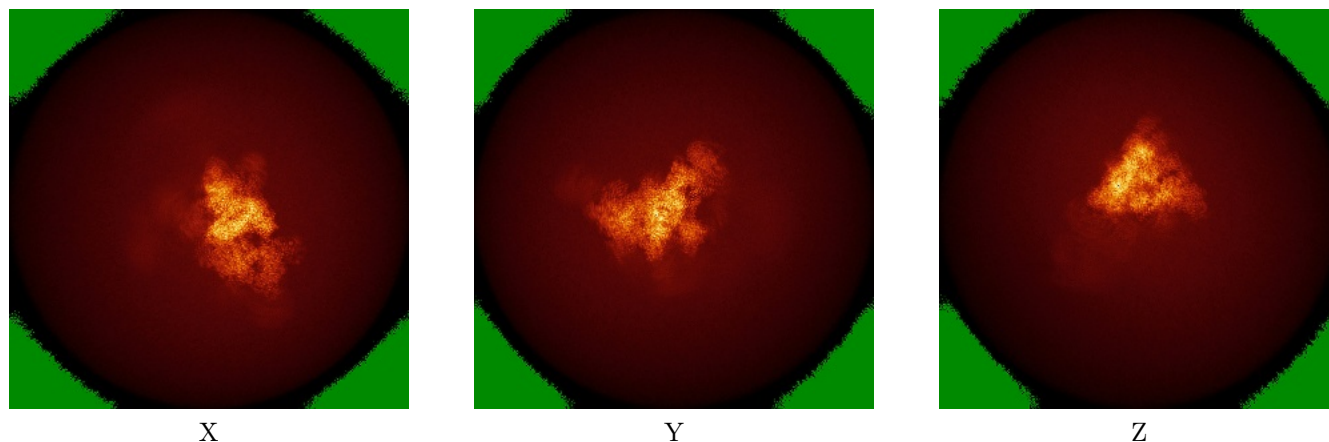
Z Index: 234

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

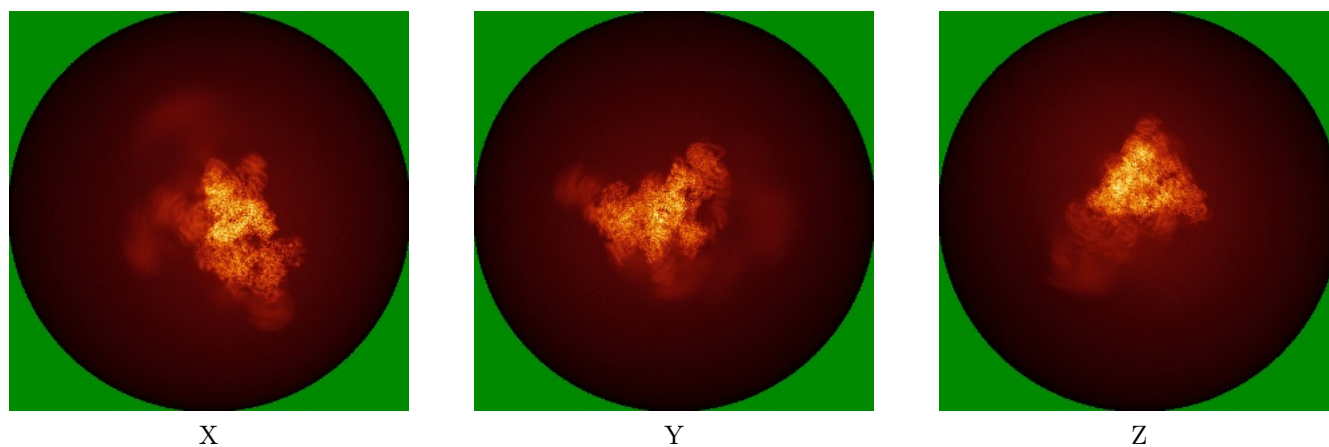


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



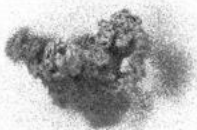
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

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

### 6.5.2 Raw map



X



Y



Z

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

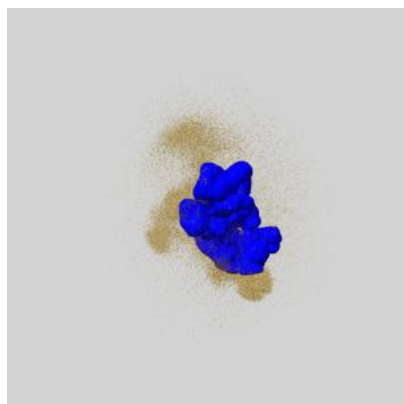
## 6.6 Mask visualisation [i](#)

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

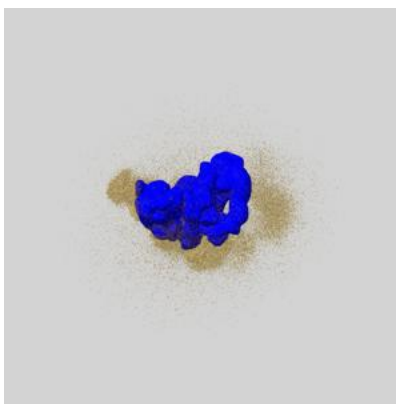
A mask typically either:

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

### 6.6.1 emd\_34507\_msk\_1.map [i](#)



X



Y

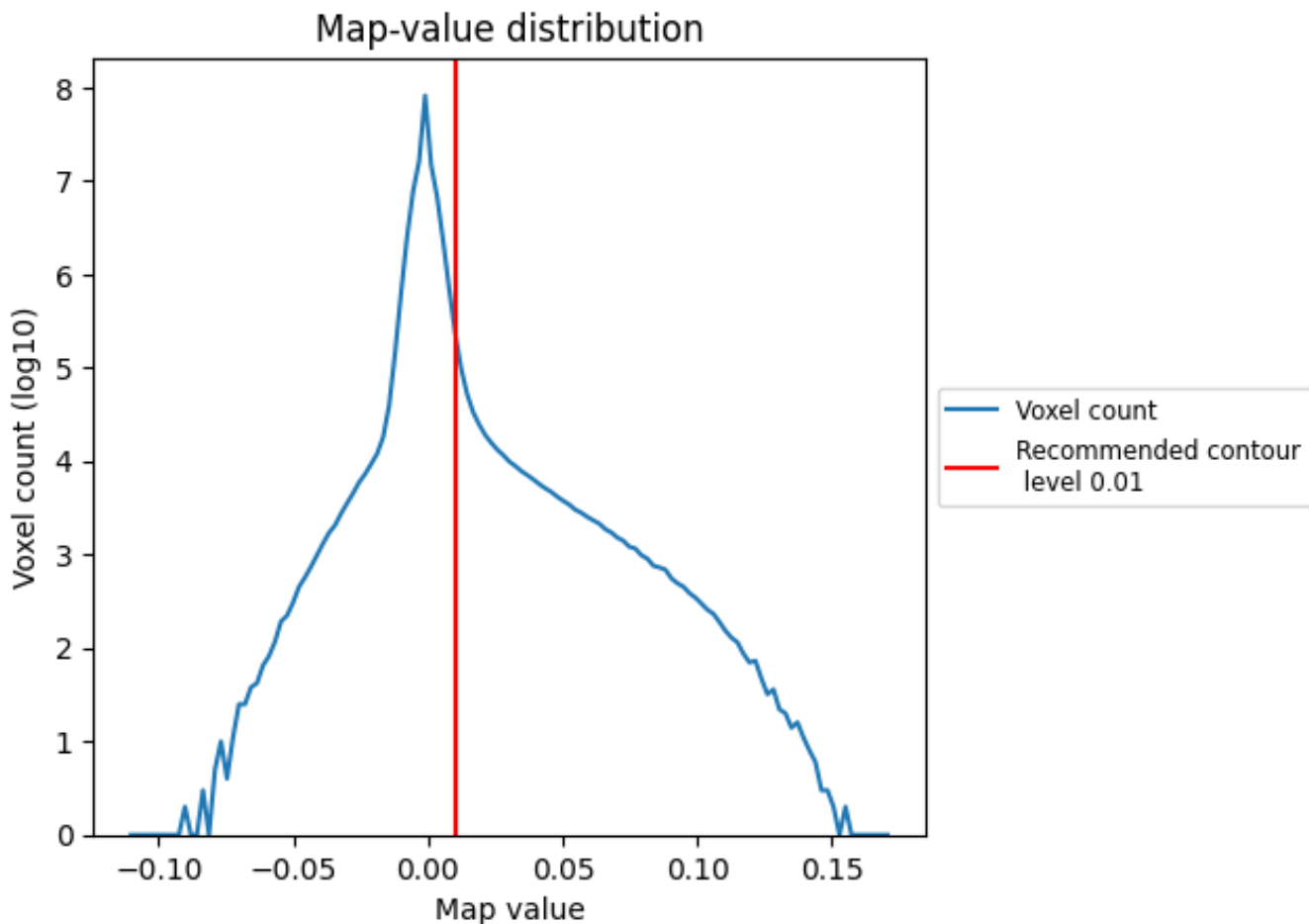


Z

## 7 Map analysis [i](#)

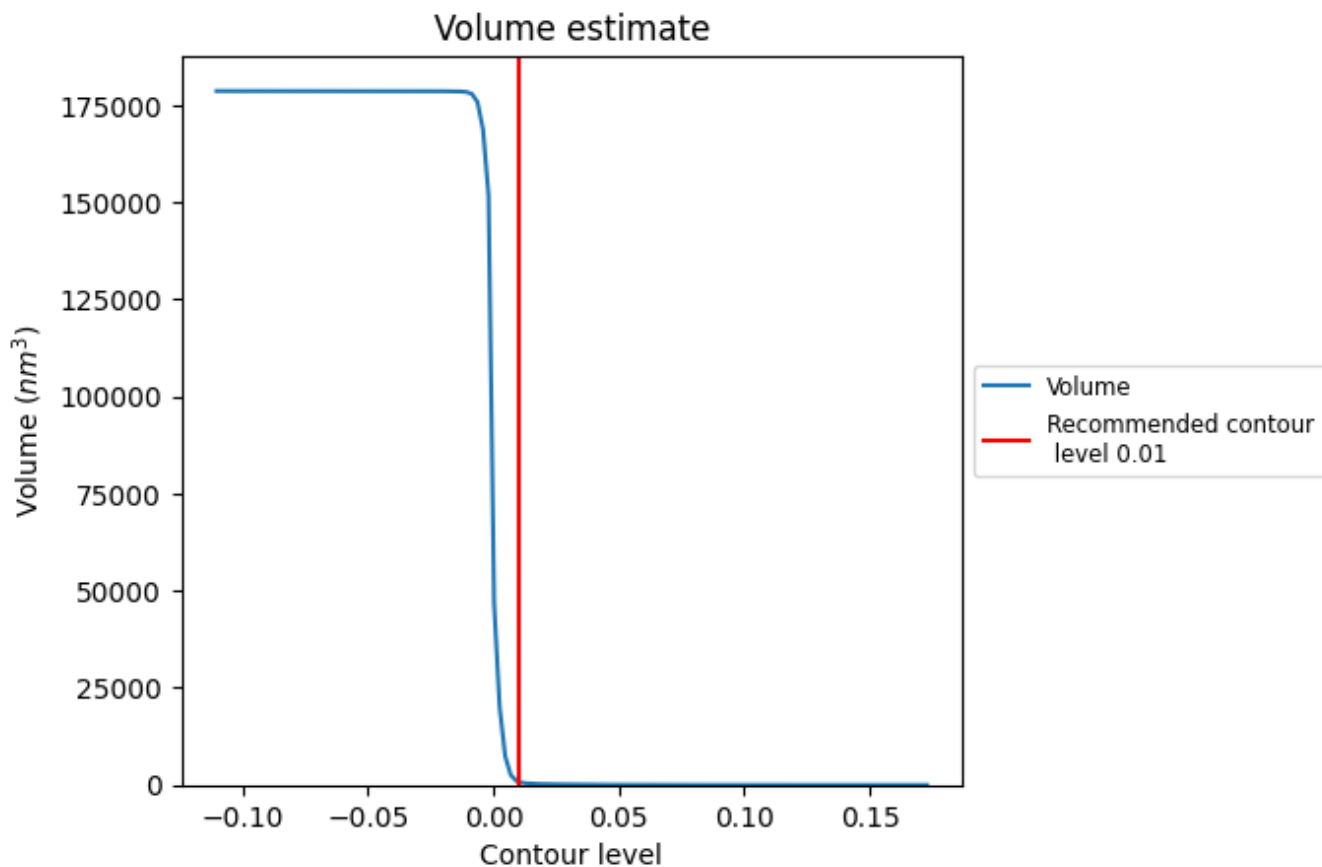
This section contains the results of statistical analysis of the map.

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



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

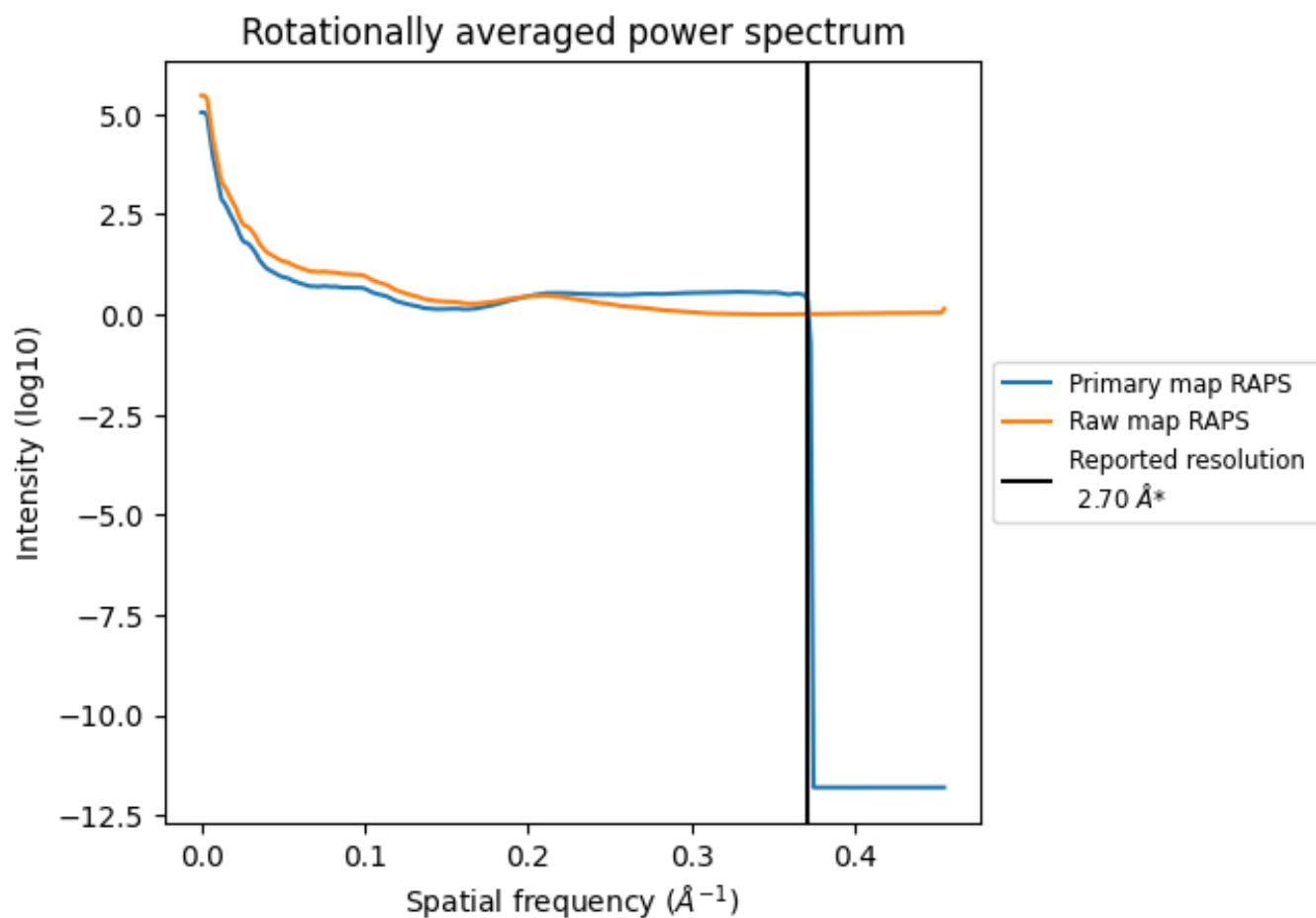
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 875  $\text{nm}^3$ ; this corresponds to an approximate mass of 791 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](#)

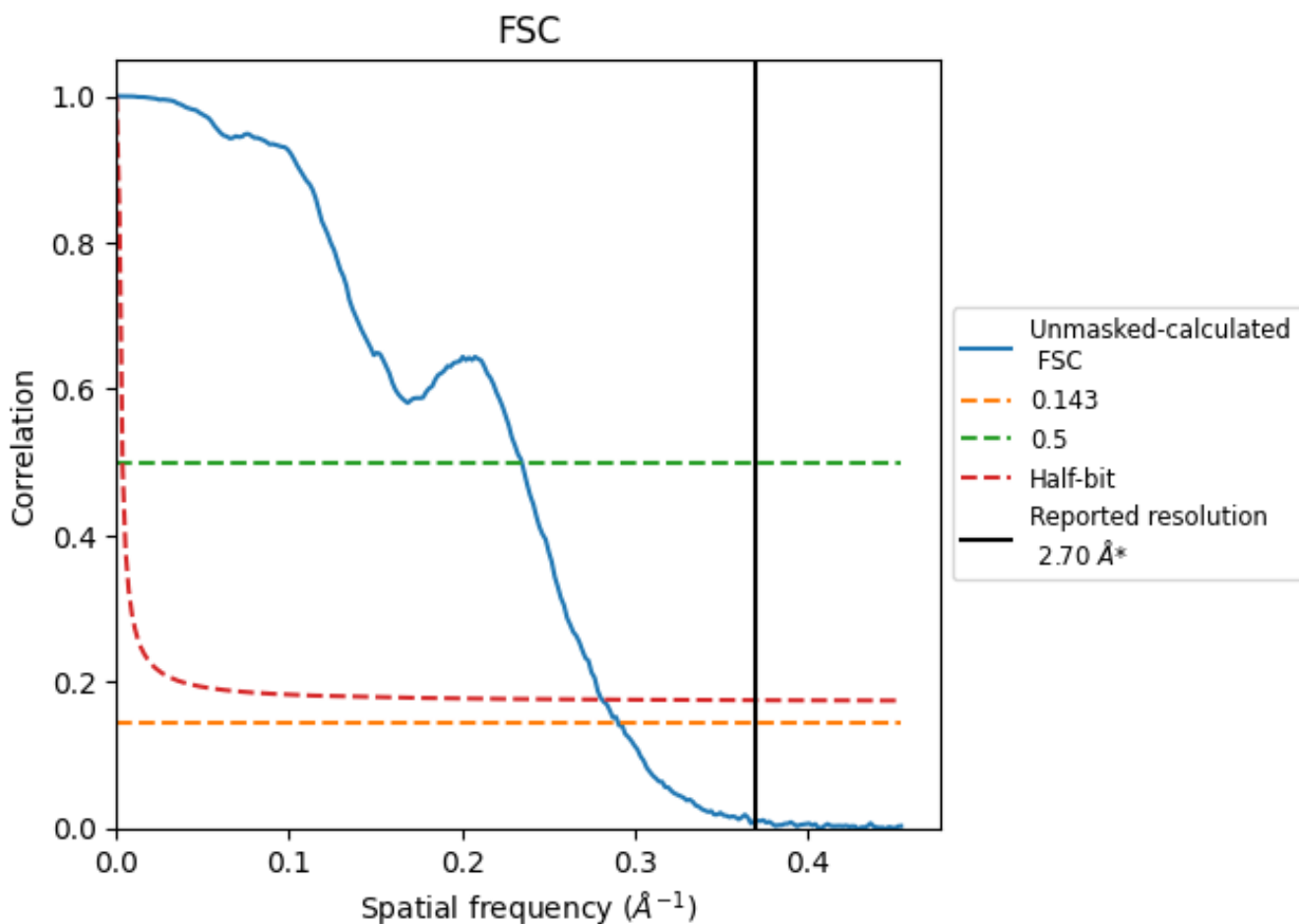


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370 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	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.26	3.55

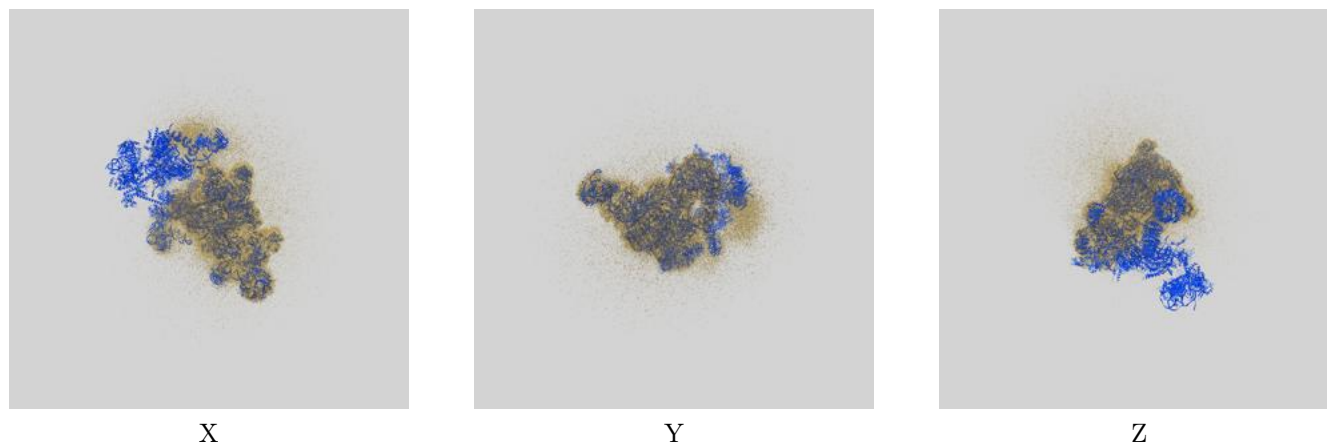
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.7 by more than 10 %



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

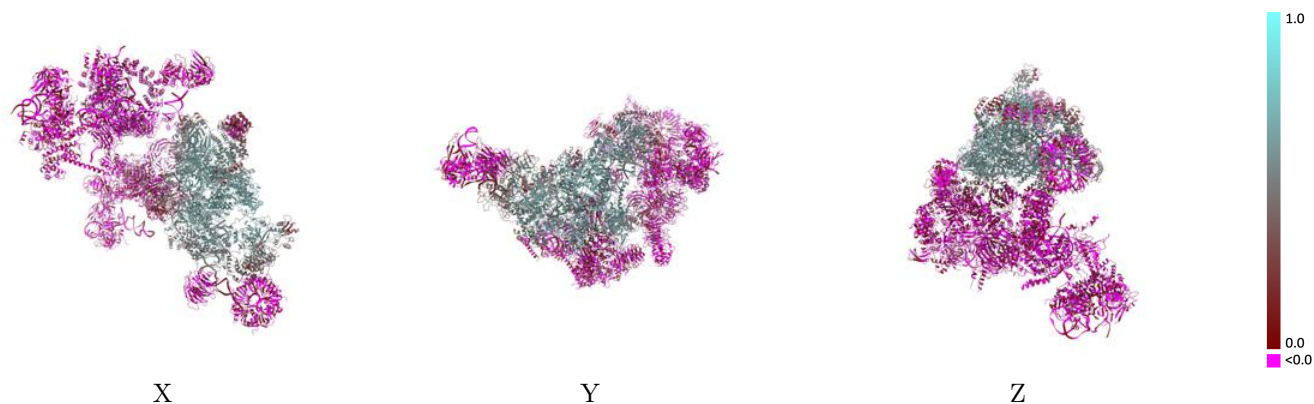
This section contains information regarding the fit between EMDB map EMD-34507 and PDB model 8H6K. Per-residue inclusion information can be found in section 3 on page 16.

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



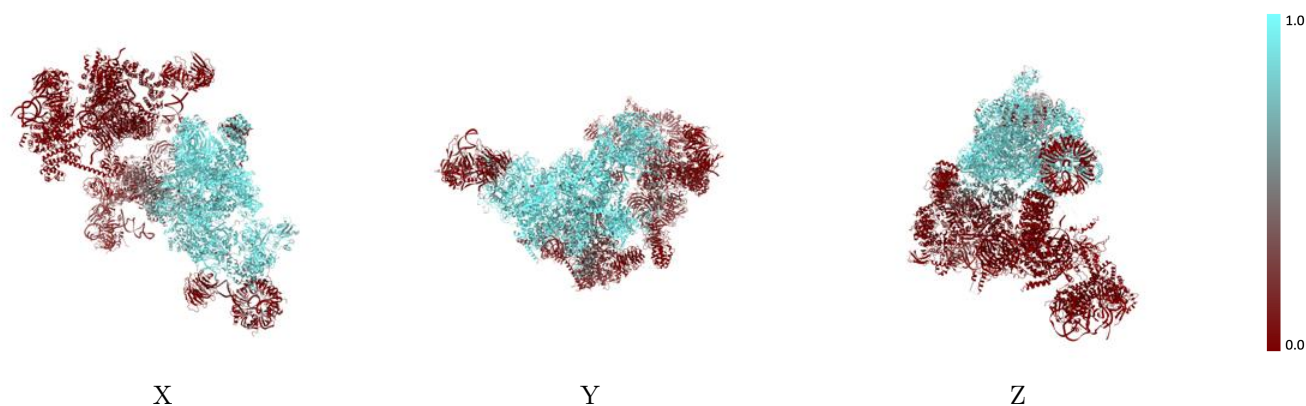
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



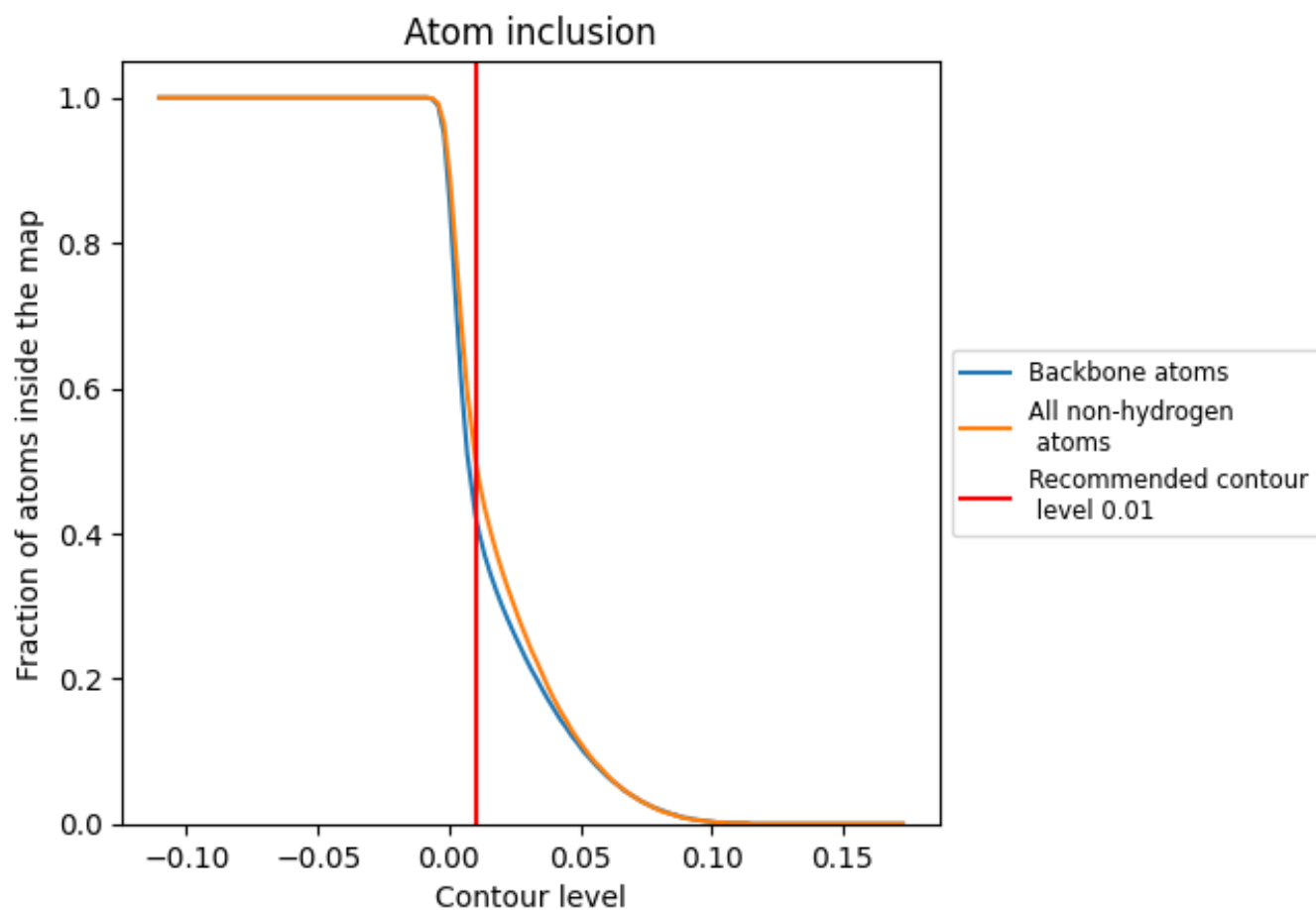
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 43% of all backbone atoms, 50% 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	 0.5030	 0.2790
2A	 0.0020	 -0.0150
2B	 0.0000	 0.0460
2C	 0.0000	 0.0250
2D	 0.4950	 0.2890
2E	 0.0000	 0.0250
2F	 0.0000	 0.0160
2G	 0.0020	 0.0060
2H	 0.2270	 0.1180
2I	 0.0000	 0.0020
2J	 0.0030	 0.0230
2K	 0.0000	 -0.0020
2L	 0.0000	 -0.0190
2M	 0.0000	 -0.0220
2a	 0.0000	 -0.0370
2b	 0.0000	 -0.0030
2c	 0.0000	 -0.0640
2d	 0.0000	 0.0100
2e	 0.0000	 -0.0200
2f	 0.0000	 0.0370
2g	 0.0000	 0.0170
4A	 0.5220	 0.3060
4B	 0.9070	 0.5190
4C	 0.9190	 0.5180
4D	 0.9380	 0.5700
4E	 0.9780	 0.6280
4F	 0.9790	 0.6330
4G	 0.8120	 0.4270
4H	 0.8040	 0.2910
4I	 0.7400	 0.3700
4J	 0.8570	 0.5110
4K	 0.6850	 0.3810
4L	 0.9440	 0.5510
4M	 0.9900	 0.6420
4N	 0.7960	 0.4350



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Chain	Atom inclusion	Q-score
4Z	0.0240	0.0010
4a	0.0120	-0.0050
4b	0.0180	-0.0060
4c	0.0130	-0.0090
4d	0.0410	0.0560
4e	0.0480	0.0060
4f	0.0270	-0.0200
4g	0.0380	-0.0290
5A	0.5990	0.3000
5B	0.8960	0.5420
5C	0.8770	0.4650
5D	0.1830	0.0350
5E	0.0320	-0.0090
5a	0.1370	0.0100
5b	0.0730	0.0010
5c	0.1080	0.0050
5d	0.1010	0.0190
5e	0.0730	-0.0220
5f	0.1250	0.0070
5g	0.1720	-0.0110
6A	0.7020	0.4220
6a	0.0080	0.0260
6b	0.0000	-0.0270
6c	0.0000	-0.0050
6d	0.0000	-0.0560
6e	0.0110	0.0270
6f	0.0000	0.0110
6g	0.0000	-0.0170
A	0.3350	0.1550