



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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

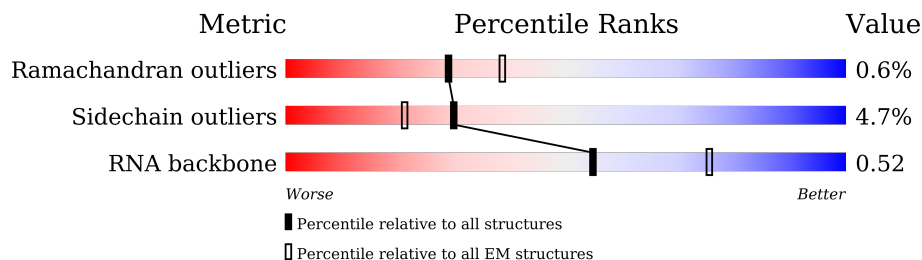
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
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>18%</p> <p>82%</p>
47	2K	125	<p>86%</p> <p>83%</p> <p>14%</p>
48	2L	110	<p>81%</p> <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		

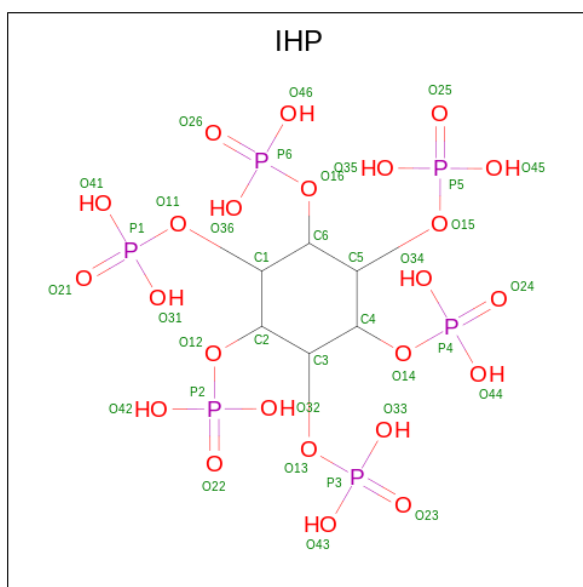
- Molecule 48 is a protein called PHD finger-like domain-containing protein 5A.

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.

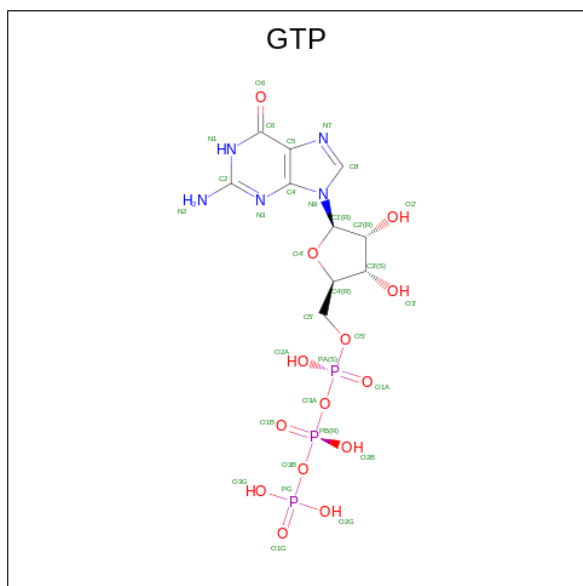
Mol	Chain	Residues	Atoms				AltConf	Trace
49	2M	66	Total	C	N	O	0	0
			264	132	66	66		

- 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	

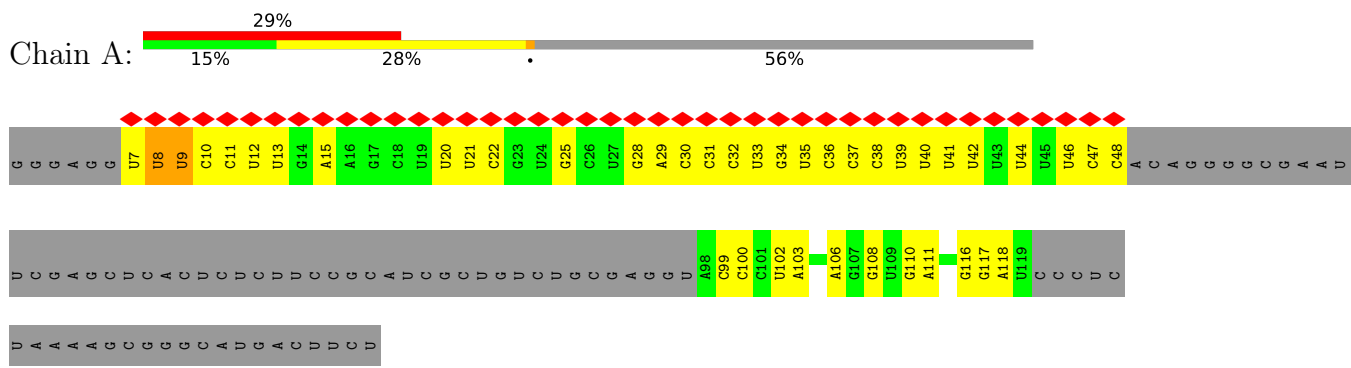
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

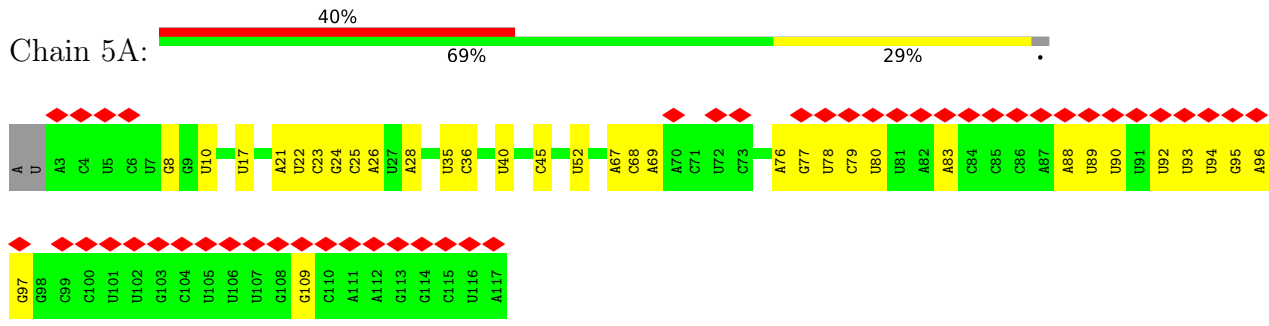
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

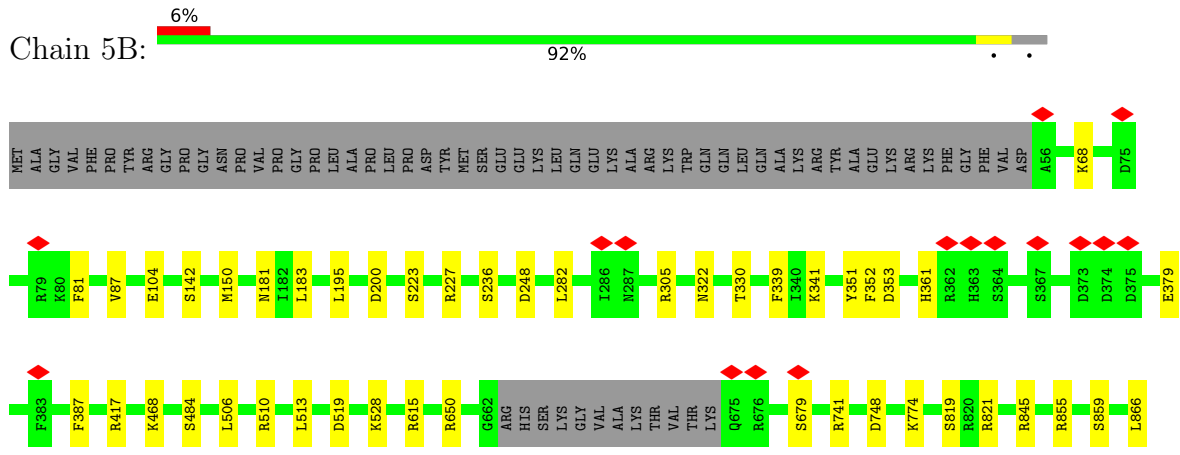
• Molecule 1: pre-mRNA



• Molecule 2: U5 snRNA



• Molecule 3: Pre-mRNA-processing-splicing factor 8

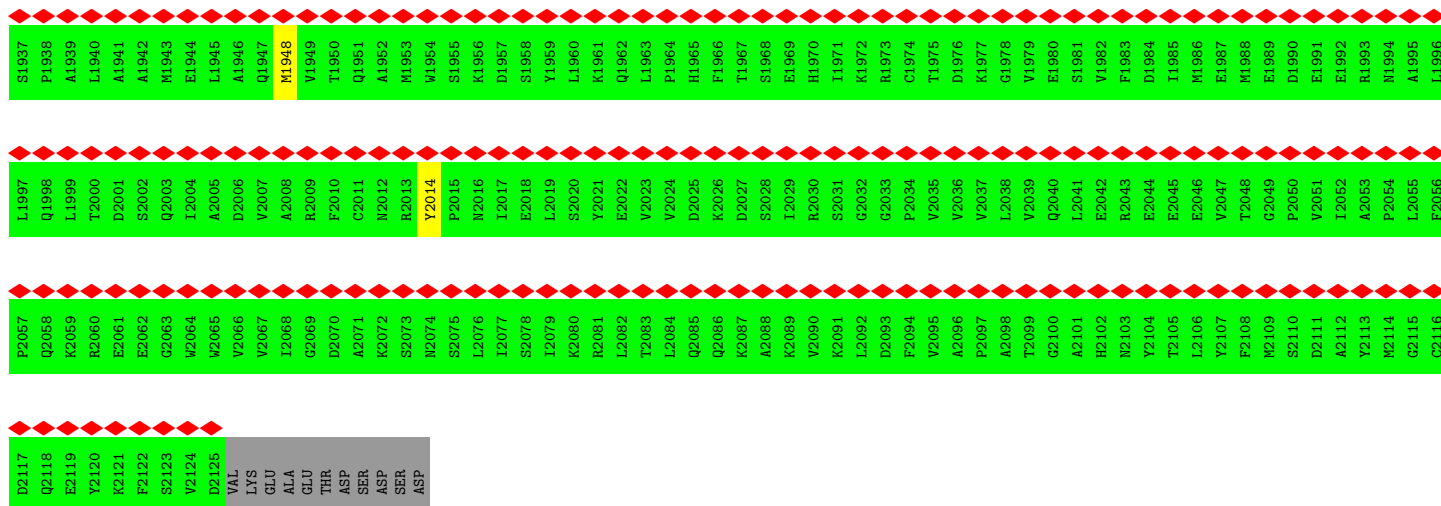




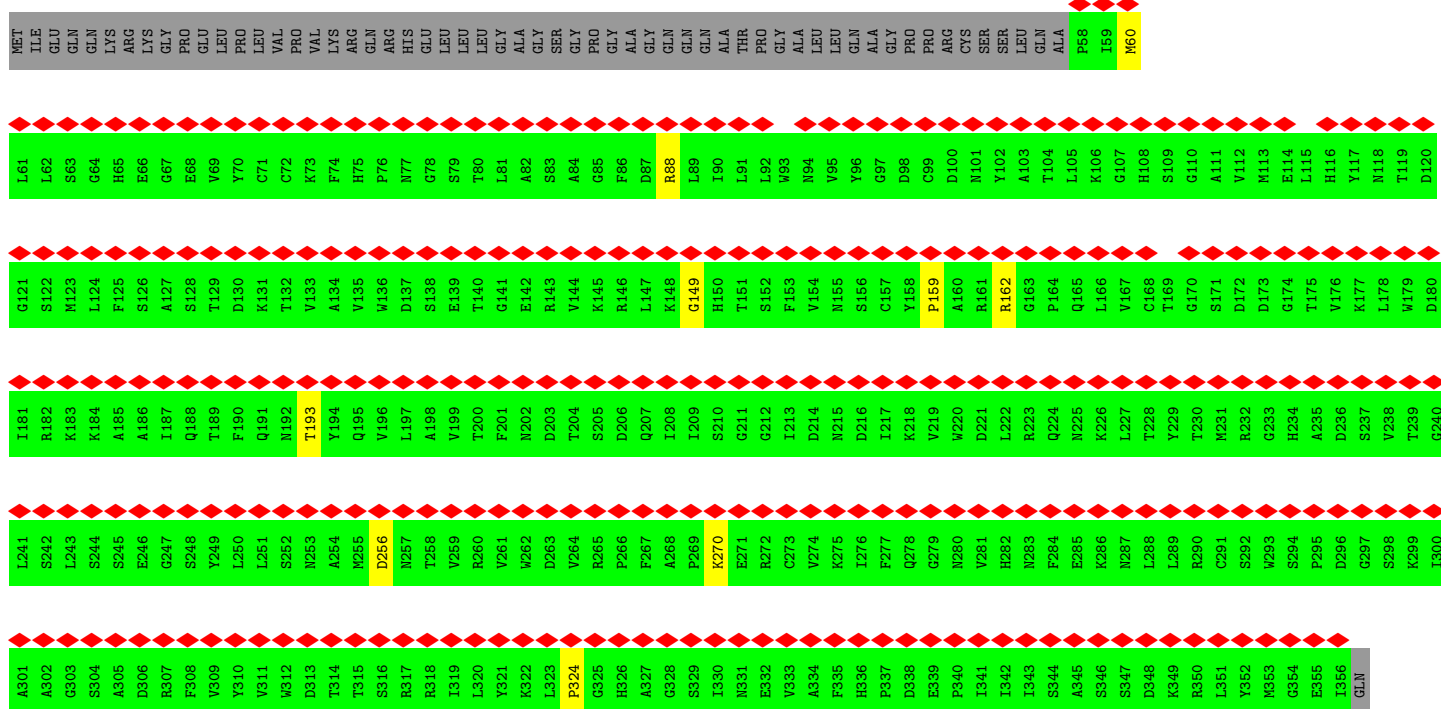
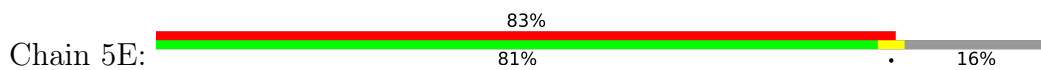




L1153	L1154	D1155	L1156	M1157	M1159	E1160	I1161	G1162	E1163	L1164	I1165	D1166	M1167	P1168	K1169	M1170	G1171	K1172	I1173	I1174	H1175	K1176	H1179	L1180	F1181	P1182	K1183	L1184	E1185	L1186	S1187	E1188	H1189	Q1191	P1192	I1193	T1194	R1195	S1196	T1197	L1198	K1199	L1202	T1203	I1204	T1205	P1206	D1207	F1208	Q1209	M1210	D1211	E1212	K1213	V1214				
H1215	G1216	S1217	S1218	E1219	F1221	V1222	L1223	E1226	D1227	V1228	D1229	S1230	E1231	V1232	I1233	L1234	H1235	H1236	E1237	Y1238	F1239	L1240	L1241	K1242	L1243	Q1244	Y1245	A1246	Q1247	D1248	E1249	H1250	L1251	I1252	T1253	F1254	F1255	V1256	P1257	V1258	F1259	E1260	P1261	L1262	P1263	Q1264	Y1265	Y1266	F1267	I1268	R1269	Y1270	V1271	S1272	D1273	V1275			
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	L1320	Y1321	Q1322	D1323	K1324	F1325	P1326	F1327	F1328	M1329	P1330	I1331	Q1332	T1333	Q1334	V1335	F1336		
M1337	T1338	V1339	Y1340	M1341	S1342	D1343	D1344	M1345	V1346	F1347	V1348	G1349	A1350	P1351	T1352	G1353	S1354	G1355	K1356	T1357	I1358	C1359	A1360	E1361	F1362	A1363	I1364	L1365	M1366	M1367	L1368	L1369	Q1370	S1371	S1372	E1373	G1374	R1375	C1376	V1377	I1378	I1379	T1380	P1381	L1382	E1383	A1384	L1385	L1386	E1387	Q1388	Y1389	V1390	M1391	T1392	M1393	Y1394	E1395	K1396
F1397	Q1398	D1399	R1400	L1401	M1402	K1403	K1404	V1405	V1406	L1407	L1408	T1409	G1410	E1411	T1412	S1413	T1414	D1415	L1416	K1417	L1418	L1419	G1420	K1421	G1422	M1423	I1424	I1425	I1426	S1427	T1428	P1429	E1430	K1431	W1432	D1433	I1434	L1435	S1436	R1437	R1438	W1439	K1440	Q1441	L1442	K1443	M1444	V1445	Q1446	M1447	I1448	M1449	L1450	F1451	V1452	V1453	D1454	E1455	V1456
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M1517	V1518	R1519	P1520	V1521	P1522	L1523	E1524	L1525	I1526	I1527	Q1528	F1529	M1531	I1532	S1533	H1534	T1535	Q1536	T1537	L1538	I1539	P1539	L1540	S1541	M1542	A1543	K1544	P1545	D1546	Y1547	H1548	A1549	I1550	T1551	K1552	H1553	P1555	K1556	K1557	P1558	V1559	I1560	V1561	F1562	G1563	P1564	S1565	R1566	K1567	E1568	R1569	R1570	L1571	V1572	E1573	Q1574	D1575	I1576	
L1577	T1578	T1579	C1580	A1581	A1582	D1583	I1584	Q1585	R1586	Q1587	R1588	F1589	L1590	H1591	C1592	T1593	E1594	K1595	D1596	L1597	I1598	P1599	L1600	L1601	E1602	K1603	L1604	S1605	D1606	S1607	T1608	L1609	K1610	E1611	T1612	L1613	L1614	M1615	G1616	V1617	G1618	Y1619	H1620	I1621	E1622	G1623	L1624	S1625	P1626	M1627	E1628	R1629	R1630	L1631	V1632	E1633	Q1634	L1635	F1636
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D1697	D1698	E1699	G1700	M1701	C1702	V1703	I1704	M1705	C1706	Q1707	G1708	S1709	K1710	K1711	D1712	F1713	F1714	K1715	K1716	F1717	A1718	Y1719	E1720	P1721	L1722	P1723	V1724	D1725	E1726	H1727	L1728	D1729	H1730	M1731	M1732	H1733	I1734	H1735	F1736	M1737	I1738	E1739	I1740	V1741	I1742	K1743	T1744	L1745	E1746	M1747	K1748	Q1749	M1750	A1751	V1752	D1753	P1754	L1755	T1756
V1757	T1758	F1759	L1760	Y1761	R1762	R1763	M1764	T1765	T1766	M1767	P1768	Y1769	Y1770	Y1771	M1772	L1773	Q1774	G1775	I1776	S1777	H1778	R1779	H1780	L1781	V1782	D1783	H1784	L1785	S1786	E1787	L1788	V1789	E1790	Q1791	T1792	L1793	S1794	D1795	L1796	E1797	Q1798	S1799	K1800	C1801	I1802	S1803	I1804	E1805	L1806	E1807	M1808	D1809	V1810	A1811	P1812	L1813	V1814	L1815	G1816
M1817	I1818	A1819	A1820	Y1821	Y1822	Y1823	I1824	M1825	Y1826	T1827	T1828	E1829	E1830	L1831	F1832	S1833	M1834	S1835	L1836	M1837	A1838	K1839	T1840	K1841	R1842	R1843	G1844	L1845	I1846	E1847	I1848	I1849	S1850	M1851	A1852	A1853	E1854	Y1855	E1856	M1857	I1858	P1859	I1860	R1861	H1862	H1863	E1864	D1865	M1866	L1867	L1868	R1869	Q1870	L1871	A1872	Q1873	K1874	V1875	P1876
H1877	K1878	L1879	M1880	M1881	P1882	F1883	F1884	D1885	D1886	P1887	H1888	V1889	K1890	T1891	M1892	L1893	L1894	L1895	Q1896	L1897	H1898	L1899	S1900	M1901	M1902	Q1903	L1904	S1905	A1906	E1907	L1908	Q1909	S1910	D1911	T1912	E1913	E1914	I1915	E1916	S1917	K1918	P1919	I1920	R1921	L1922	I1923	Q1924	A1925	C1926	V1927	D1928	L1929	V1930	S1931	S1932	M1933	G1934	W1935	L1936



• Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

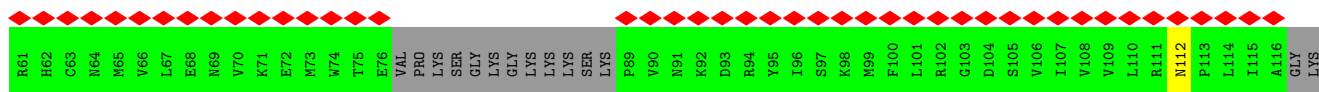


• Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

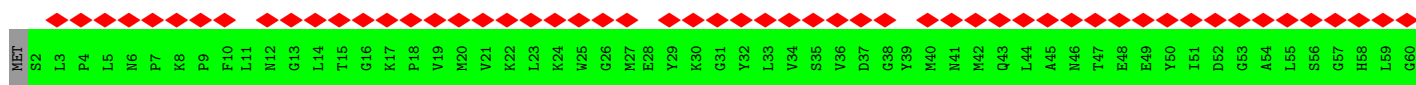
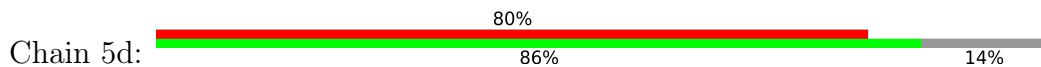




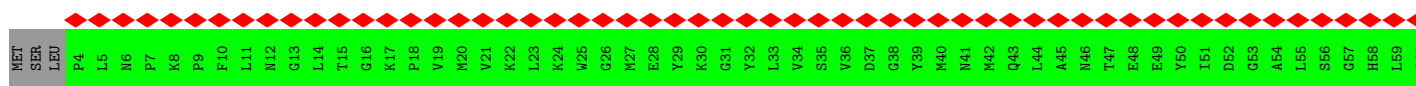
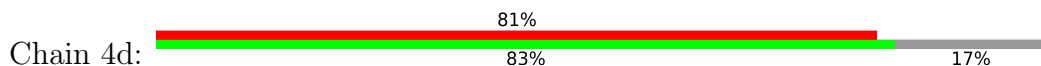




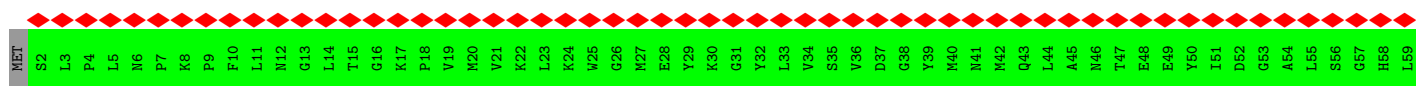
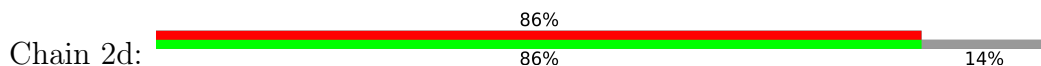
• Molecule 10: Small nuclear ribonucleoprotein F



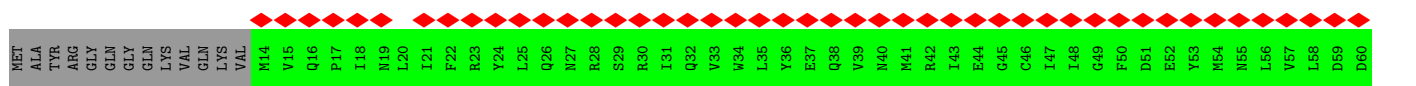
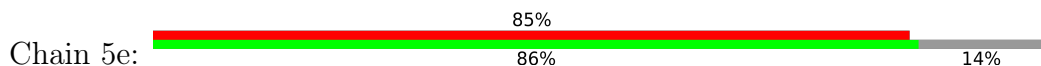
• Molecule 10: Small nuclear ribonucleoprotein F



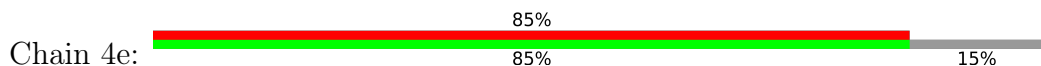
• Molecule 10: Small nuclear ribonucleoprotein F



• Molecule 11: Small nuclear ribonucleoprotein E

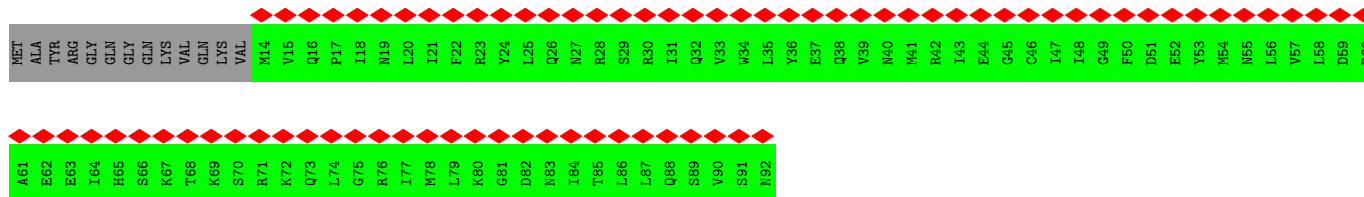
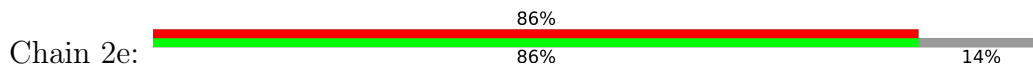


• Molecule 11: Small nuclear ribonucleoprotein E

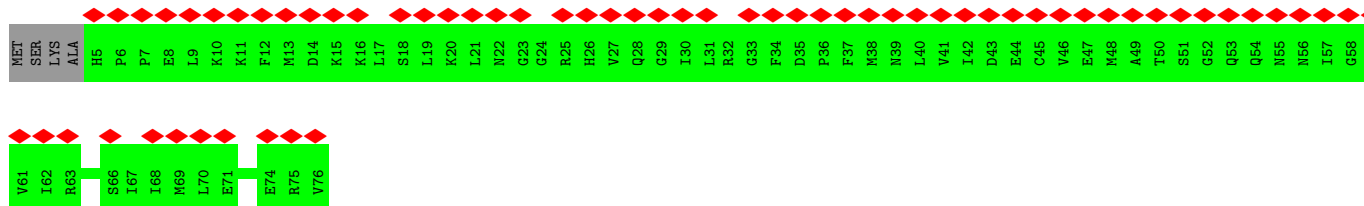
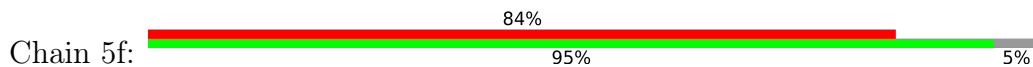




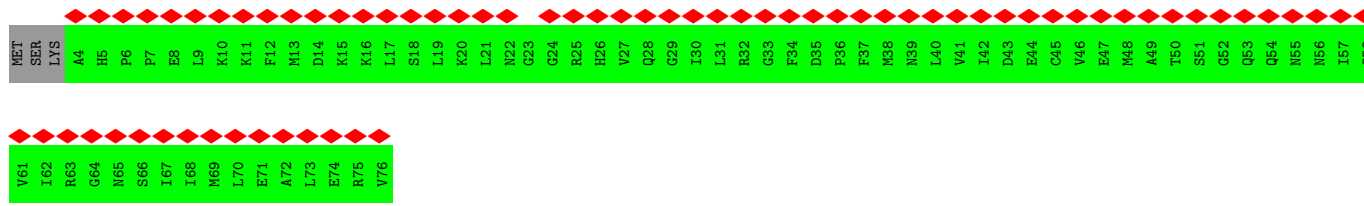
• Molecule 11: Small nuclear ribonucleoprotein E



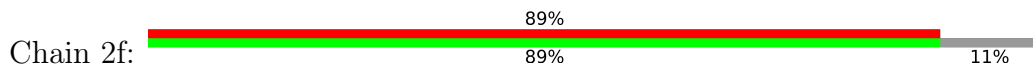
• Molecule 12: Small nuclear ribonucleoprotein G



• Molecule 12: Small nuclear ribonucleoprotein G

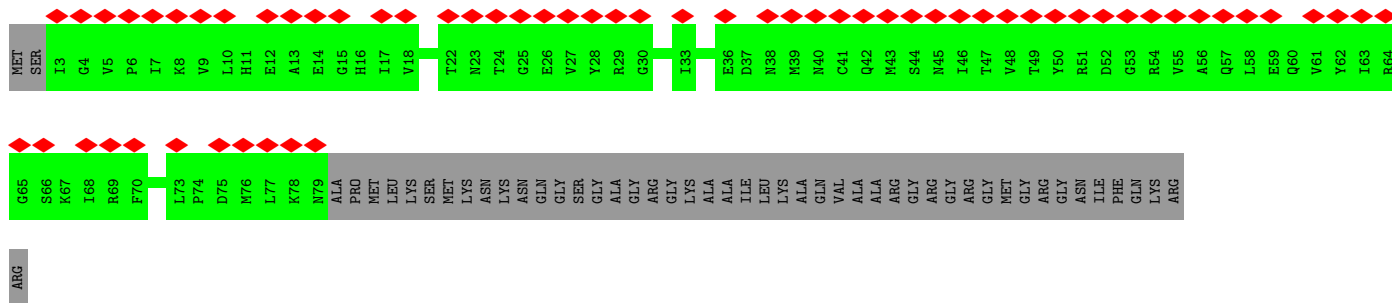


• Molecule 12: Small nuclear ribonucleoprotein G

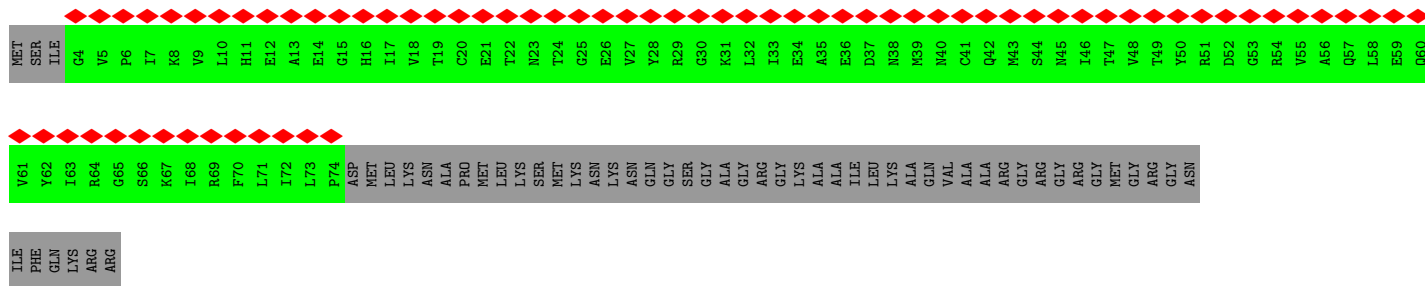




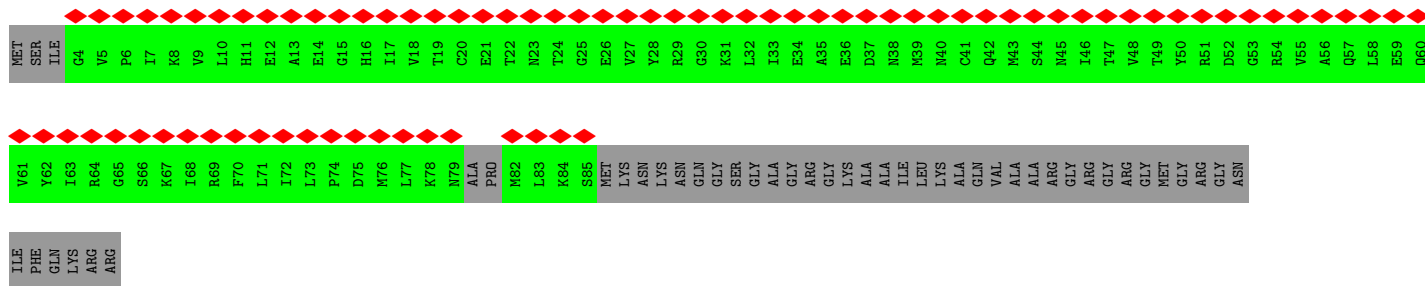
• Molecule 13: Small nuclear ribonucleoprotein Sm D3



• Molecule 13: Small nuclear ribonucleoprotein Sm D3

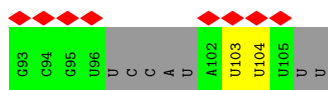


• Molecule 13: Small nuclear ribonucleoprotein Sm D3

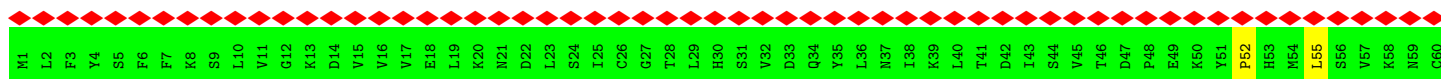
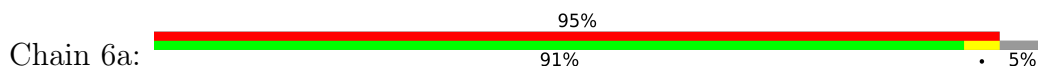


• Molecule 14: U6 snRNA

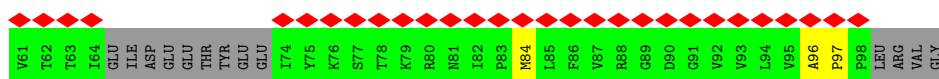
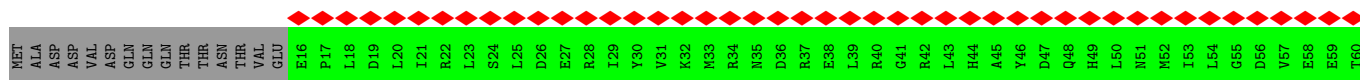




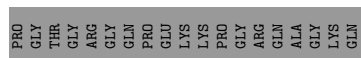
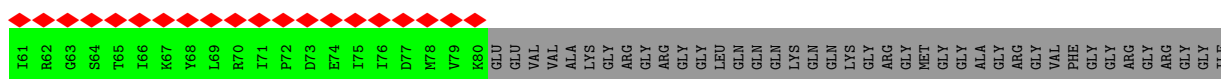
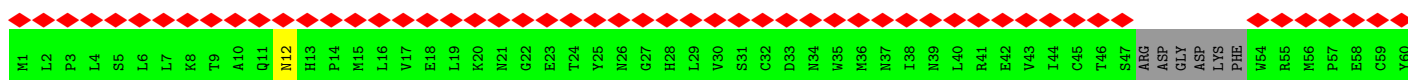
- Molecule 15: U6 snRNA-associated Sm-like protein LSm2



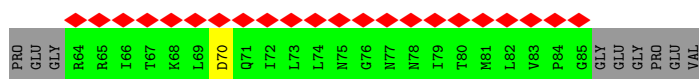
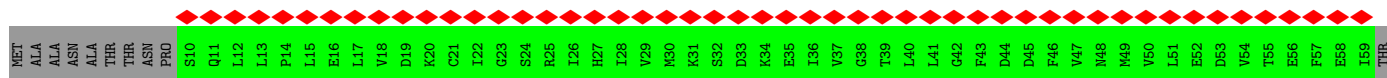
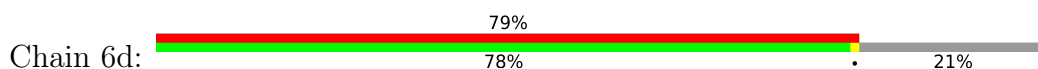
- Molecule 16: U6 snRNA-associated Sm-like protein LSm3



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



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

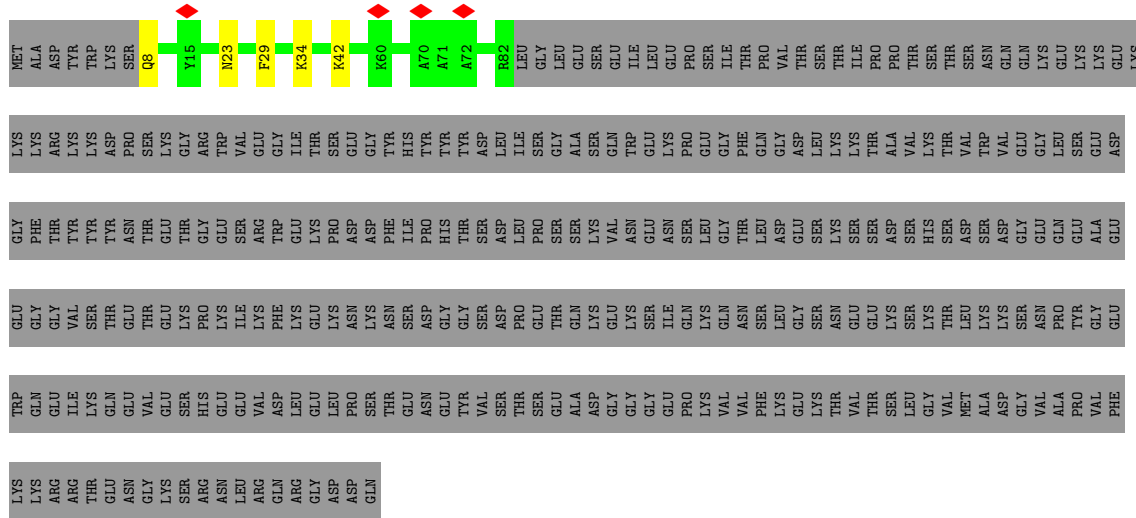


- Molecule 19: U6 snRNA-associated Sm-like protein LSm6

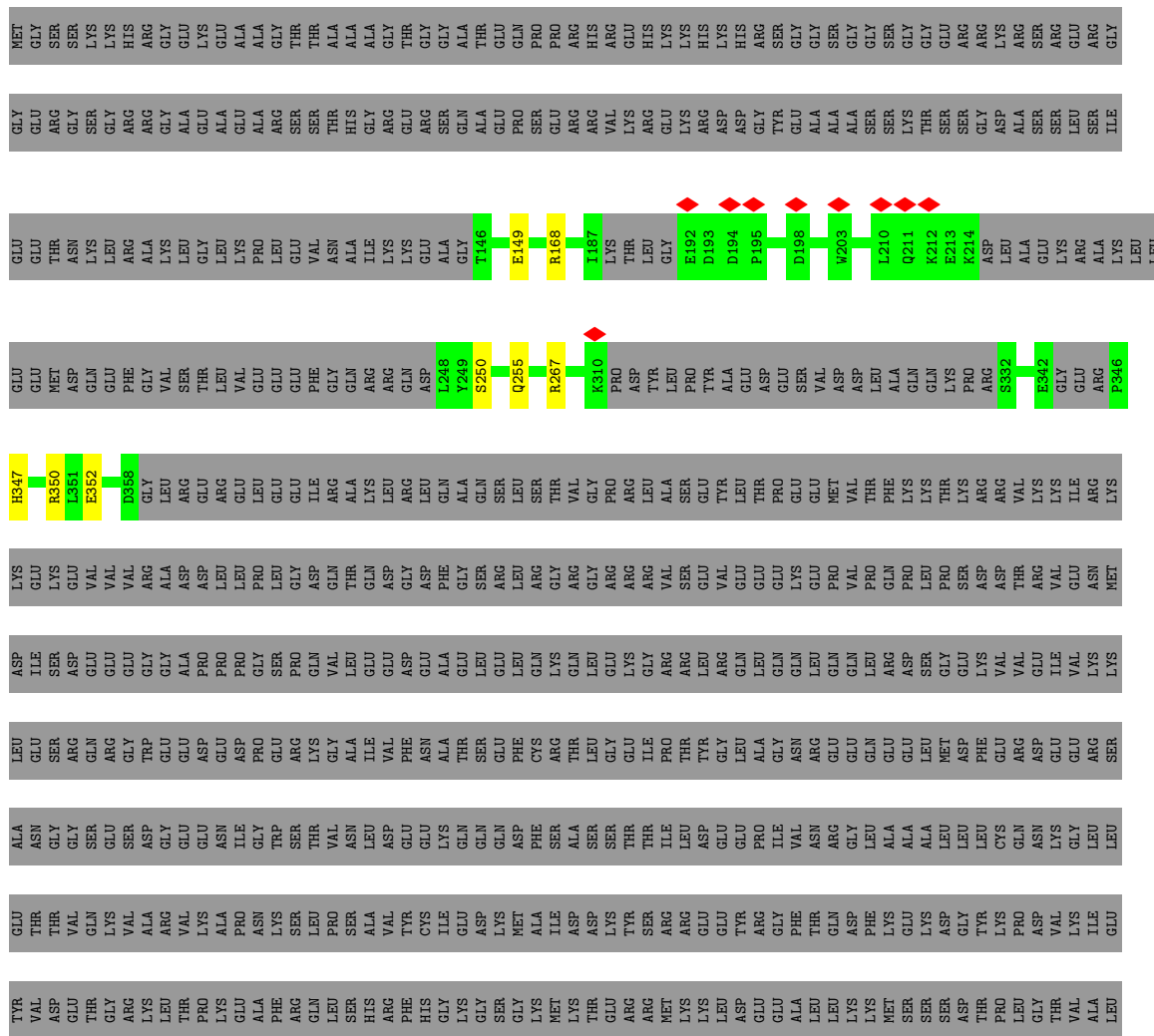




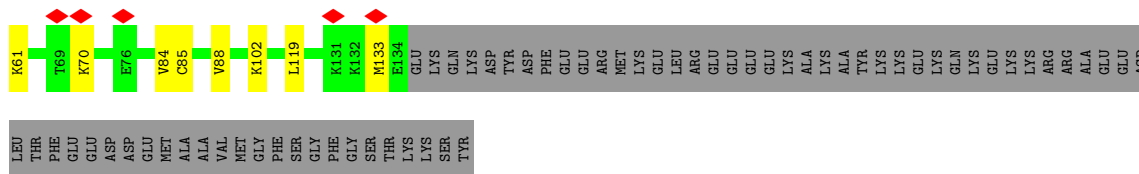




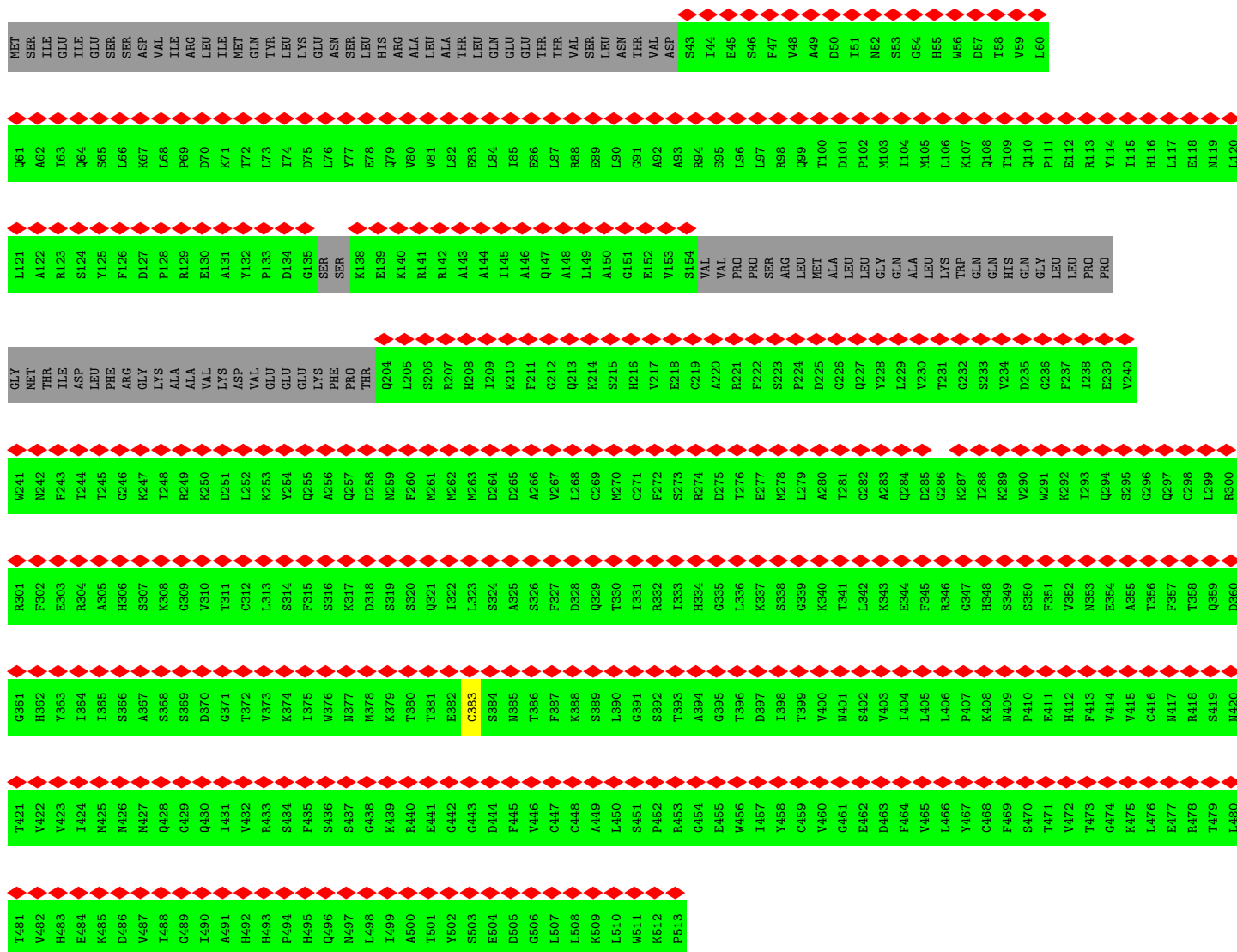
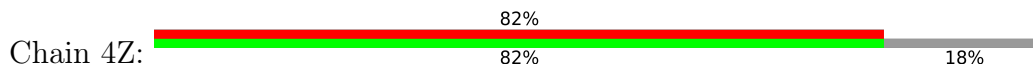
● Molecule 31: U4/U6.U5 tri-snRNP-associated protein 1



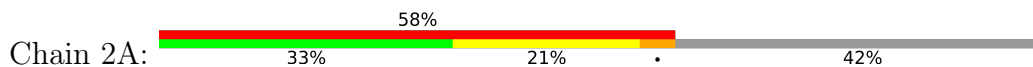




• Molecule 36: WD40 repeat-containing protein SMU1



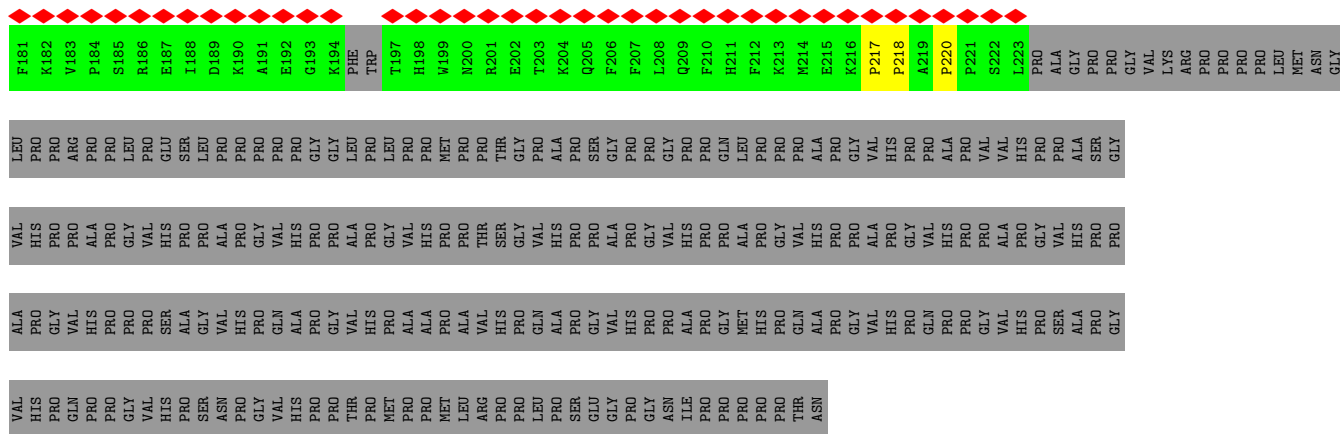
• Molecule 37: U2 snRNA



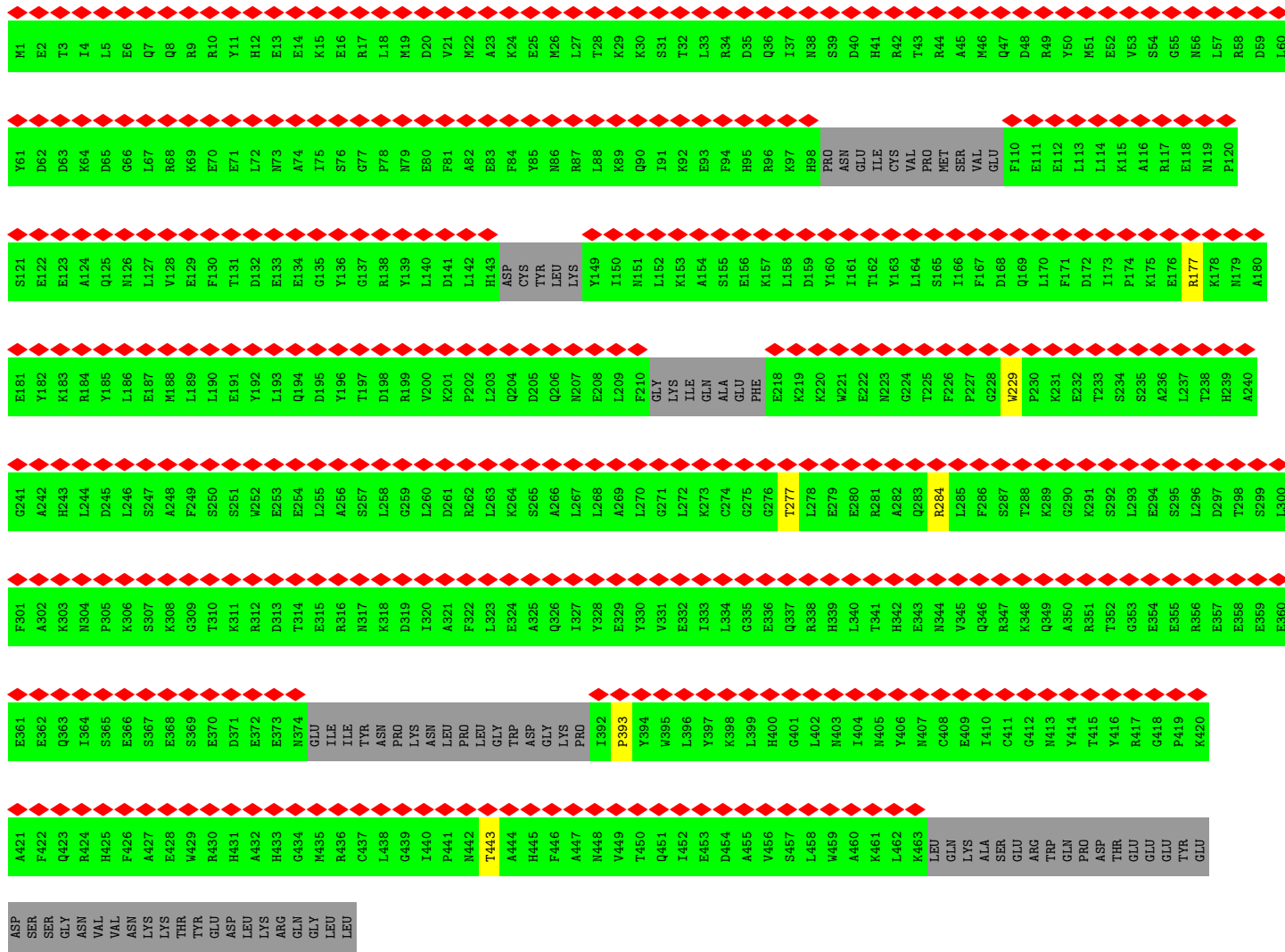
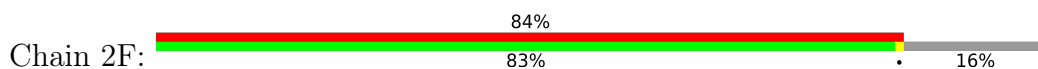








• Molecule 42: Splicing factor 3A subunit 3



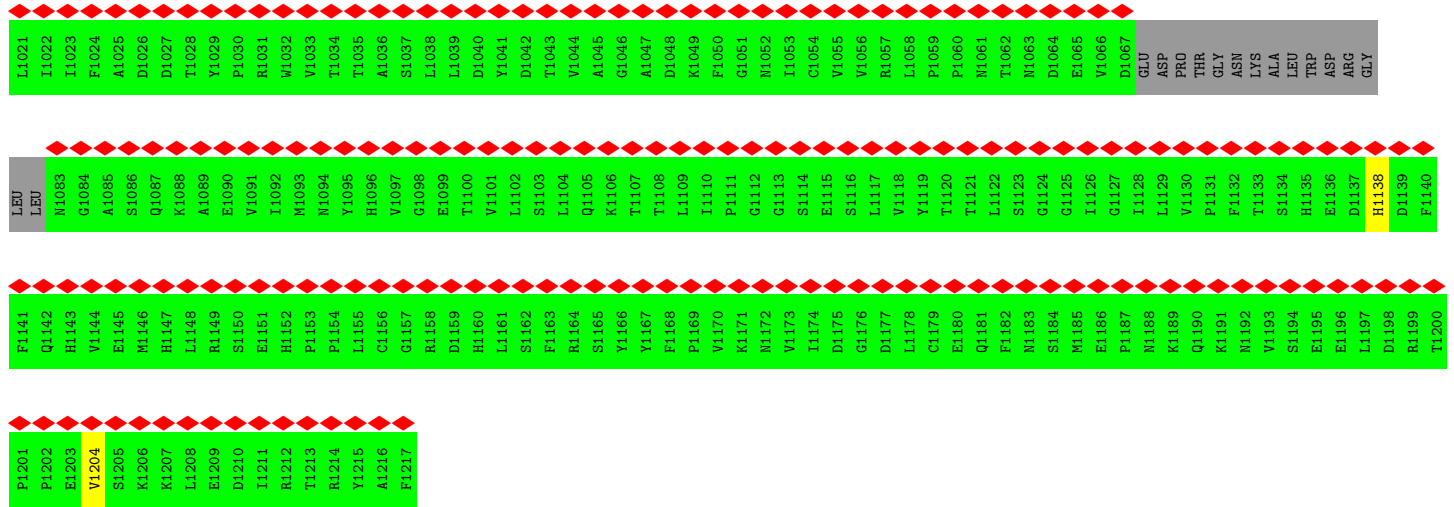
• Molecule 43: Splicing factor 3B subunit 1



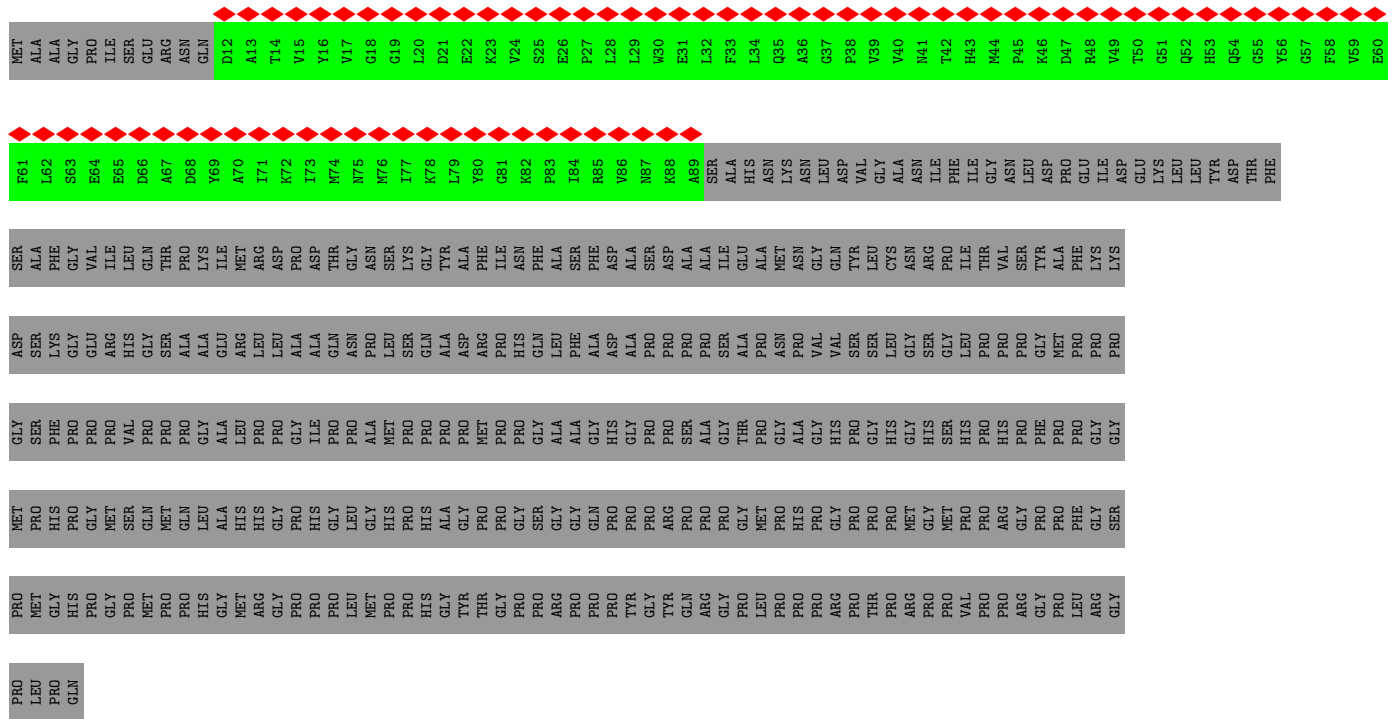




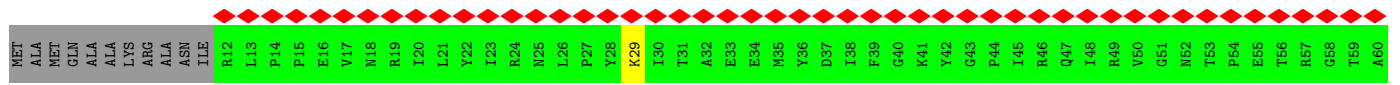
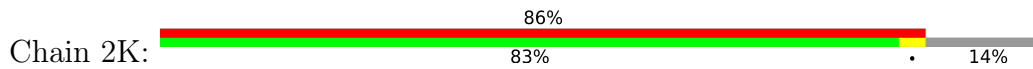




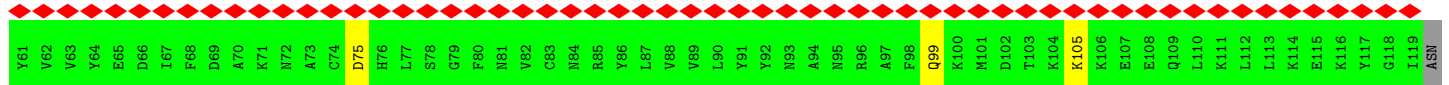
● Molecule 46: Splicing factor 3B subunit 4



● Molecule 47: Splicing factor 3B subunit 6

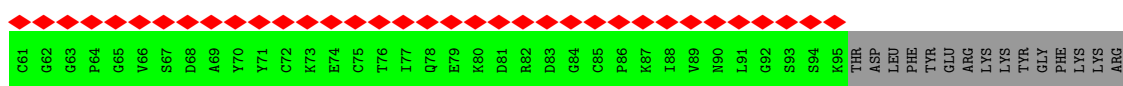
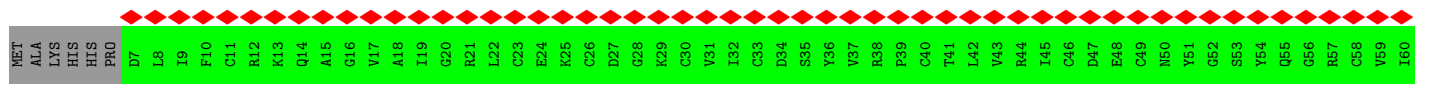
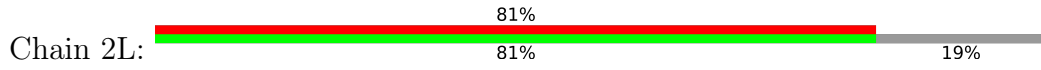




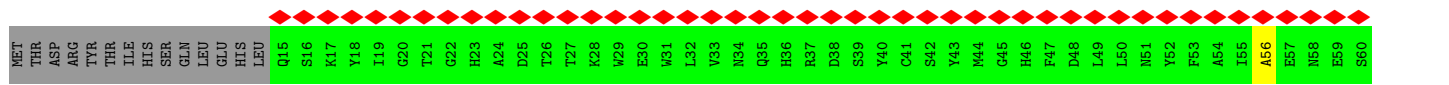
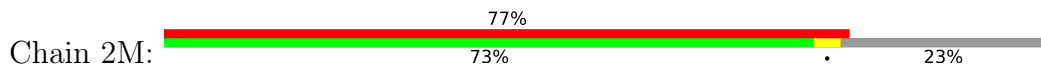


THR  
ASP  
PRO  
LYS

• 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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	2F	443	THR	Peptide
43	2G	220	GLN	Peptide
43	2G	415	LEU	Mainchain
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

### 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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	4G	110	LYS
33	4L	172	GLU
28	4G	356	ASP
31	4J	149	GLU
35	4N	102	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
26	4E	17	HIS
33	4L	81	GLN
26	4E	28	GLN
28	4G	741	HIS
3	5B	1944	HIS

### 5.3.3 RNA [i](#)

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

5 of 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

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5A	79	C
14	6A	77	C
2	5A	96	A
22	4A	99	C
1	A	38	C

#### 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

The worst 5 of 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

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

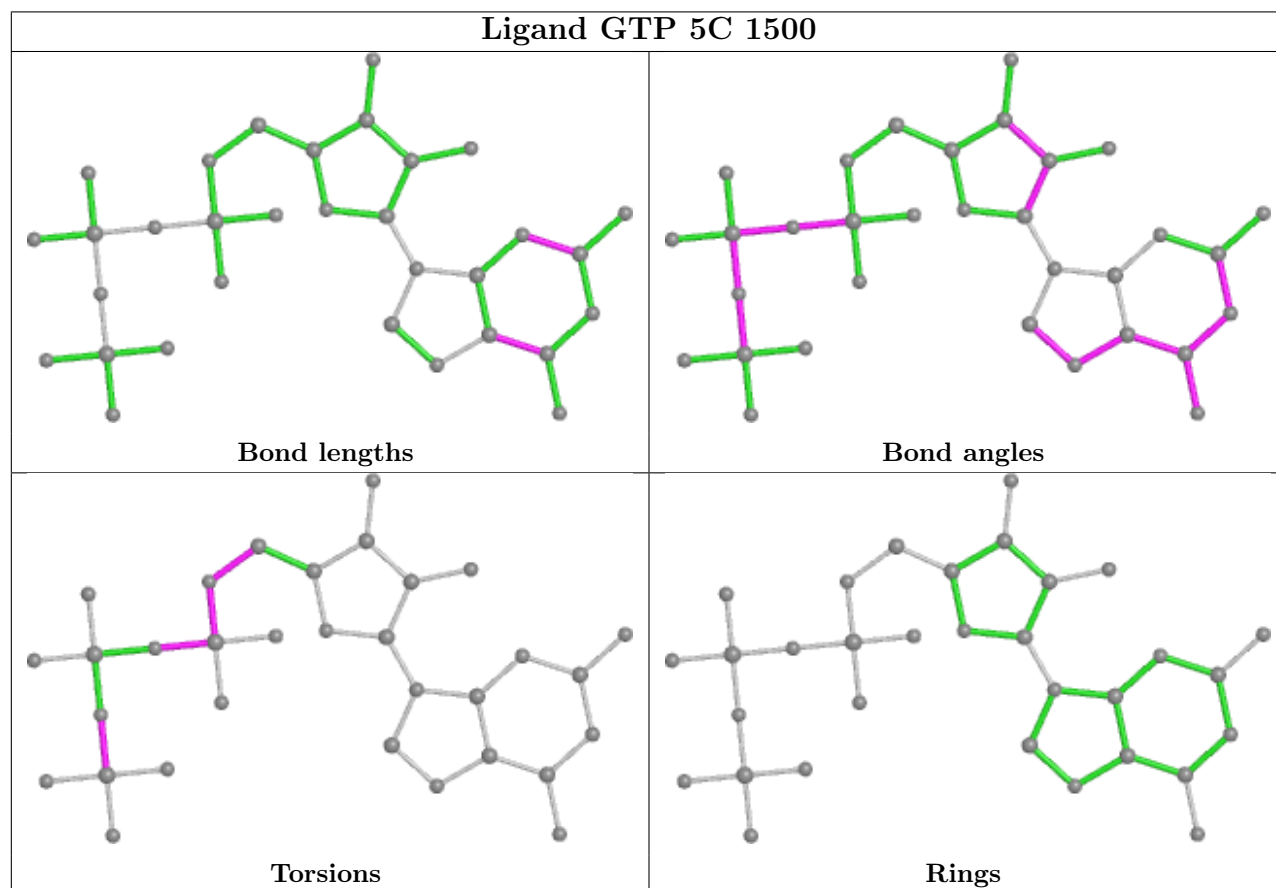
Mol	Chain	Res	Type	Atoms
50	5B	3000	IHP	C4-O14-P4-O44
51	5C	1500	GTP	C5'-O5'-PA-O1A
51	5C	1500	GTP	C5'-O5'-PA-O2A
51	5C	1500	GTP	PB-O3A-PA-O5'
51	5C	1500	GTP	C4'-C5'-O5'-PA

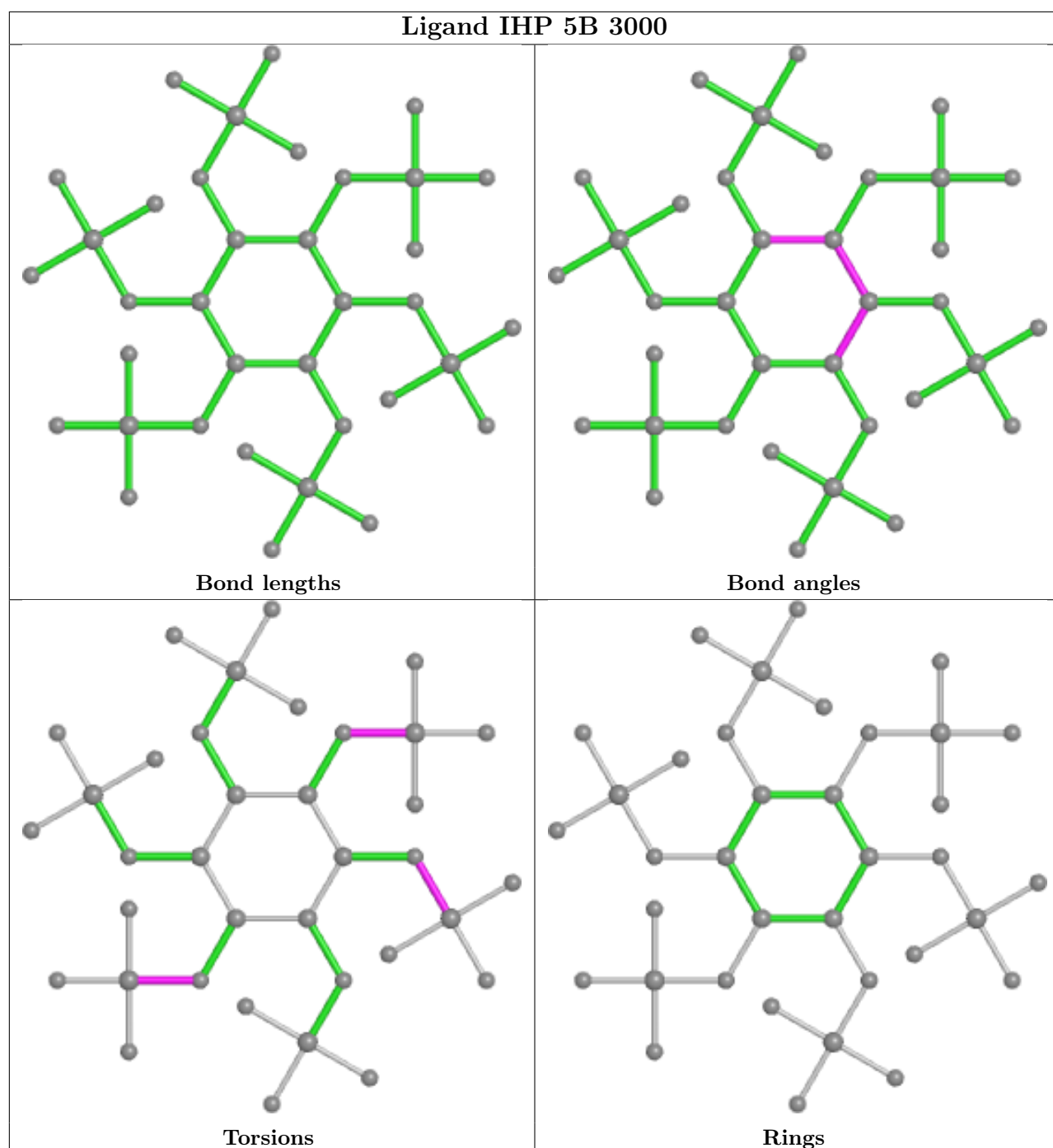
There are no ring outliers.

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.

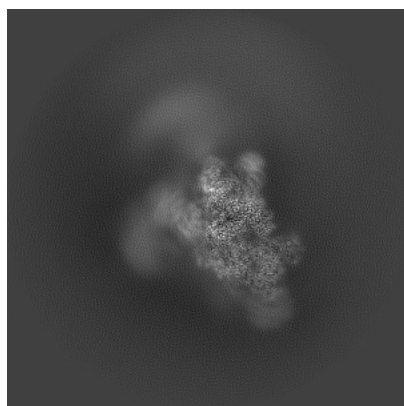
## 6 Map visualisation [i](#)

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.

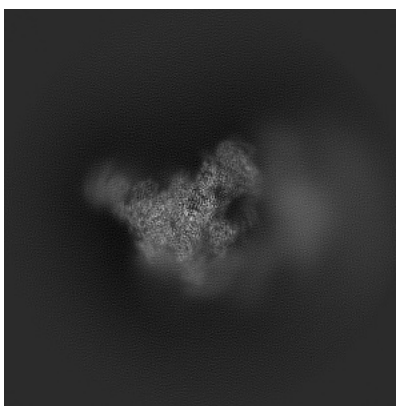
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

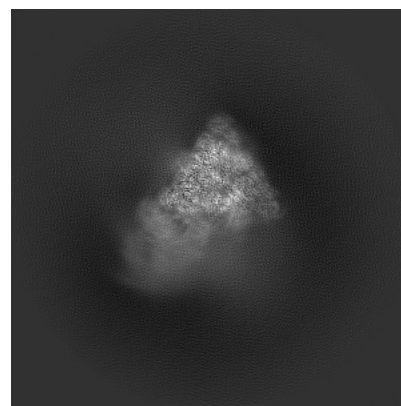
#### 6.1.1 Primary map



X

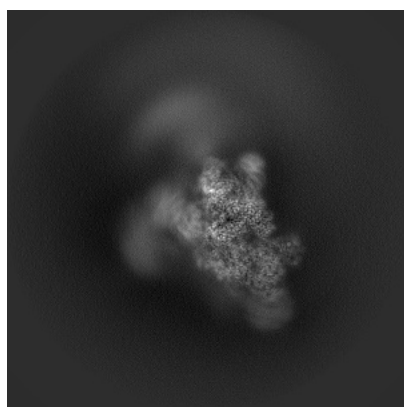


Y

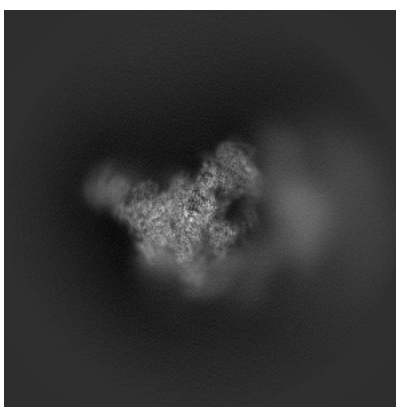


Z

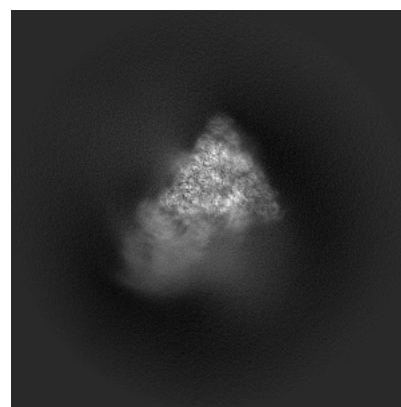
#### 6.1.2 Raw map



X



Y

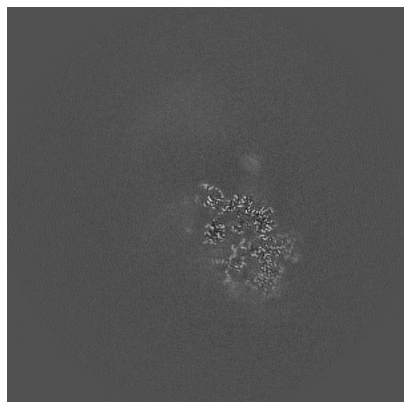


Z

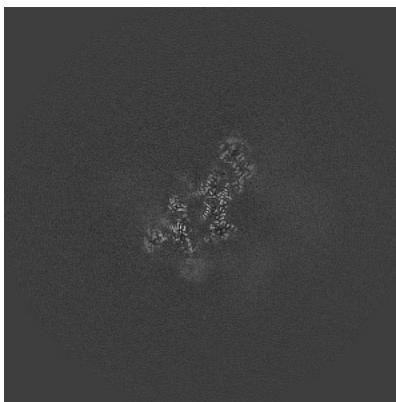
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

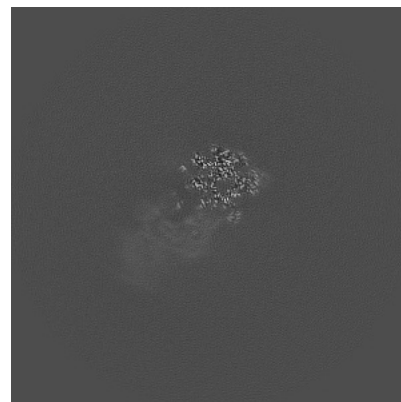
### 6.2.1 Primary map



X Index: 256

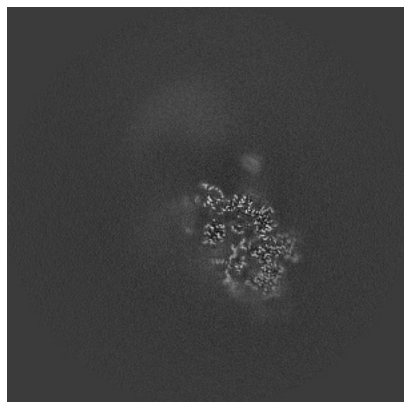


Y Index: 256

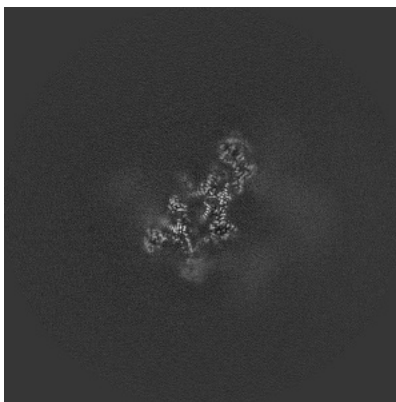


Z Index: 256

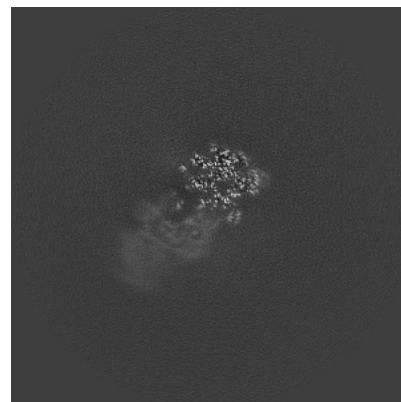
### 6.2.2 Raw map



X Index: 256



Y Index: 256

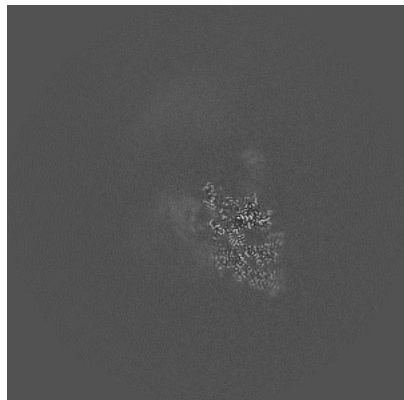


Z Index: 256

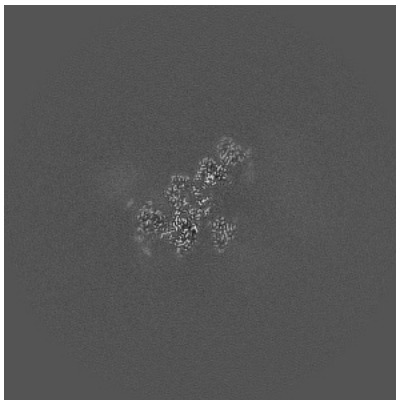
The images above show central slices of the map in three orthogonal directions.

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

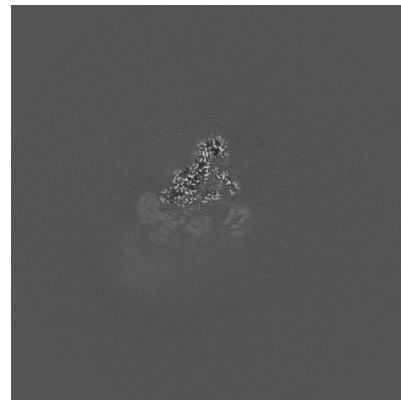
### 6.3.1 Primary map



X Index: 245

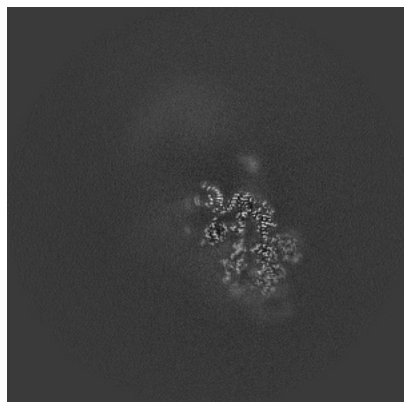


Y Index: 277

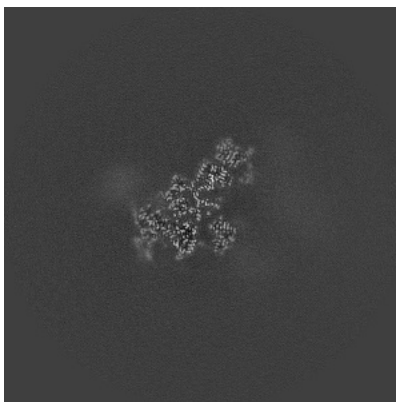


Z Index: 234

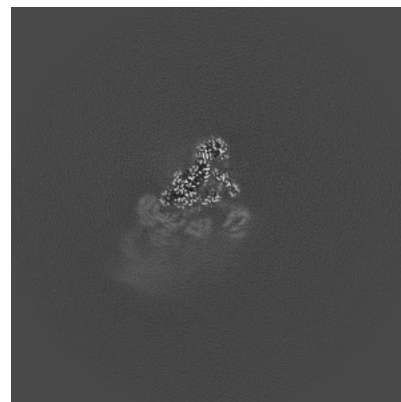
### 6.3.2 Raw map



X Index: 259



Y Index: 274



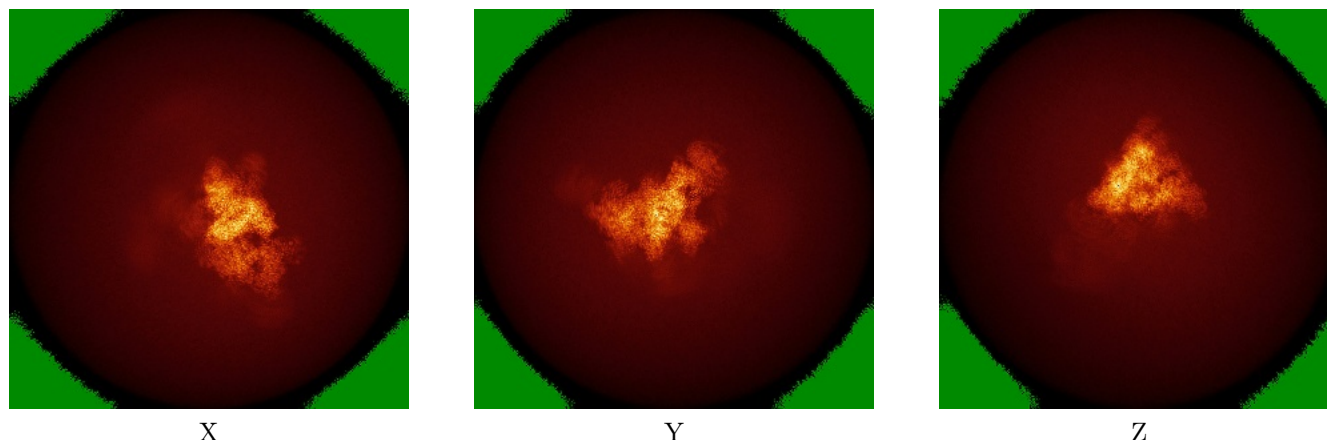
Z Index: 234

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

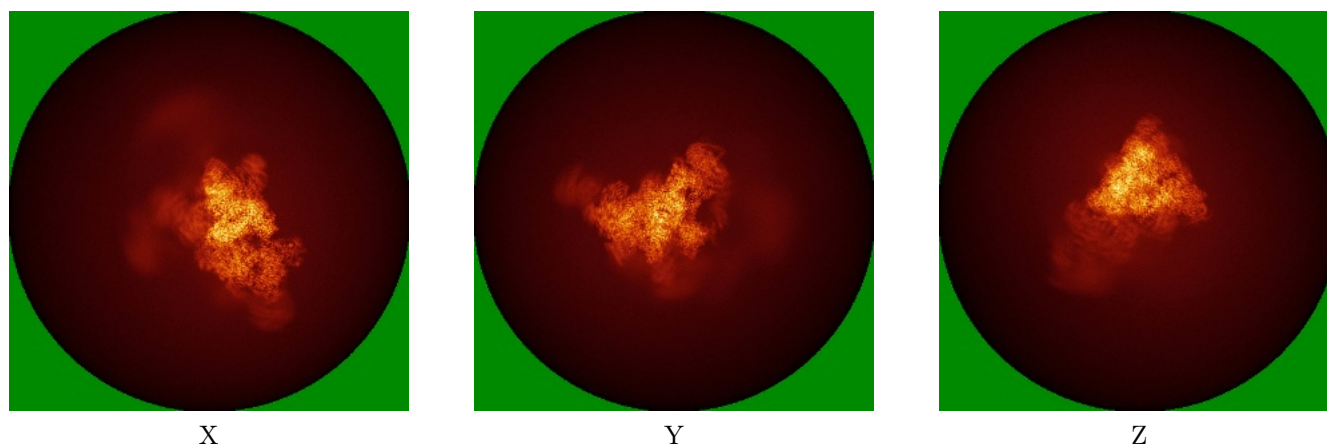


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



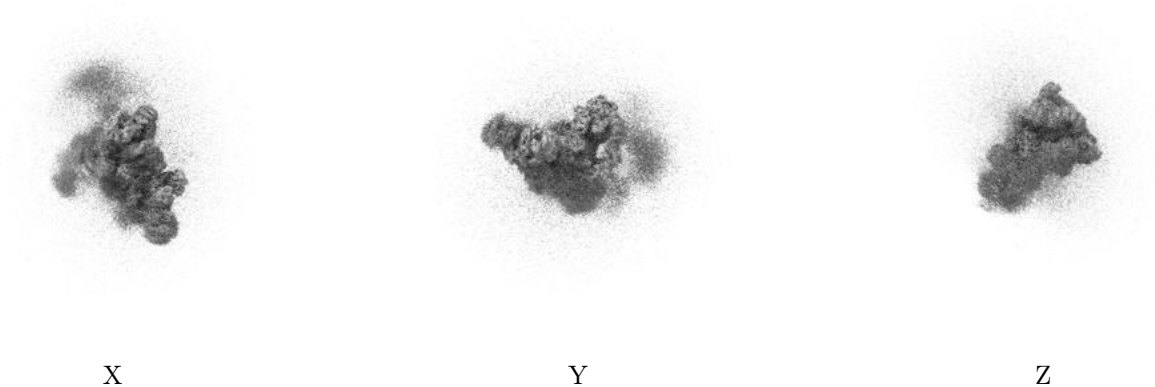
### 6.4.2 Raw map



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.

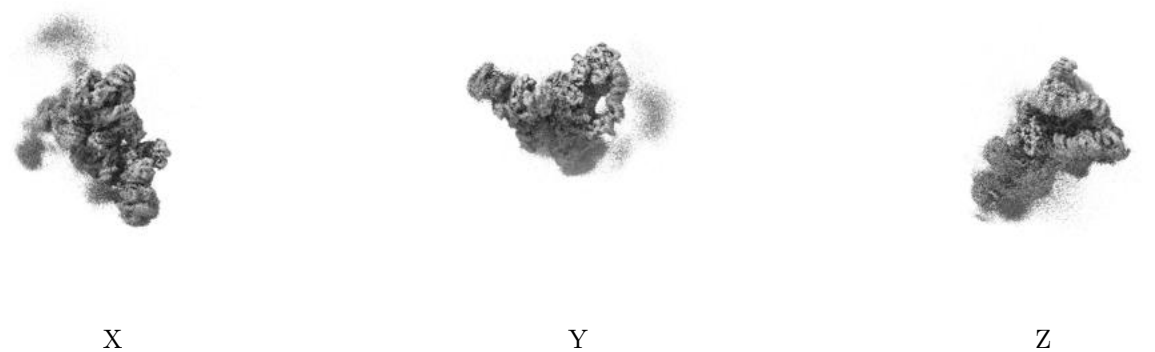
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



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.

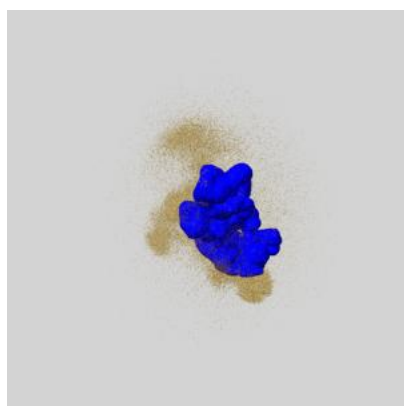
## 6.6 Mask visualisation [i](#)

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

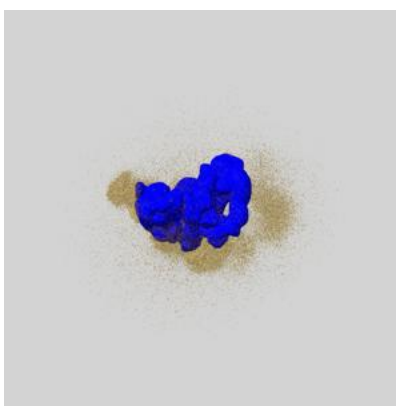
A mask typically either:

- 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

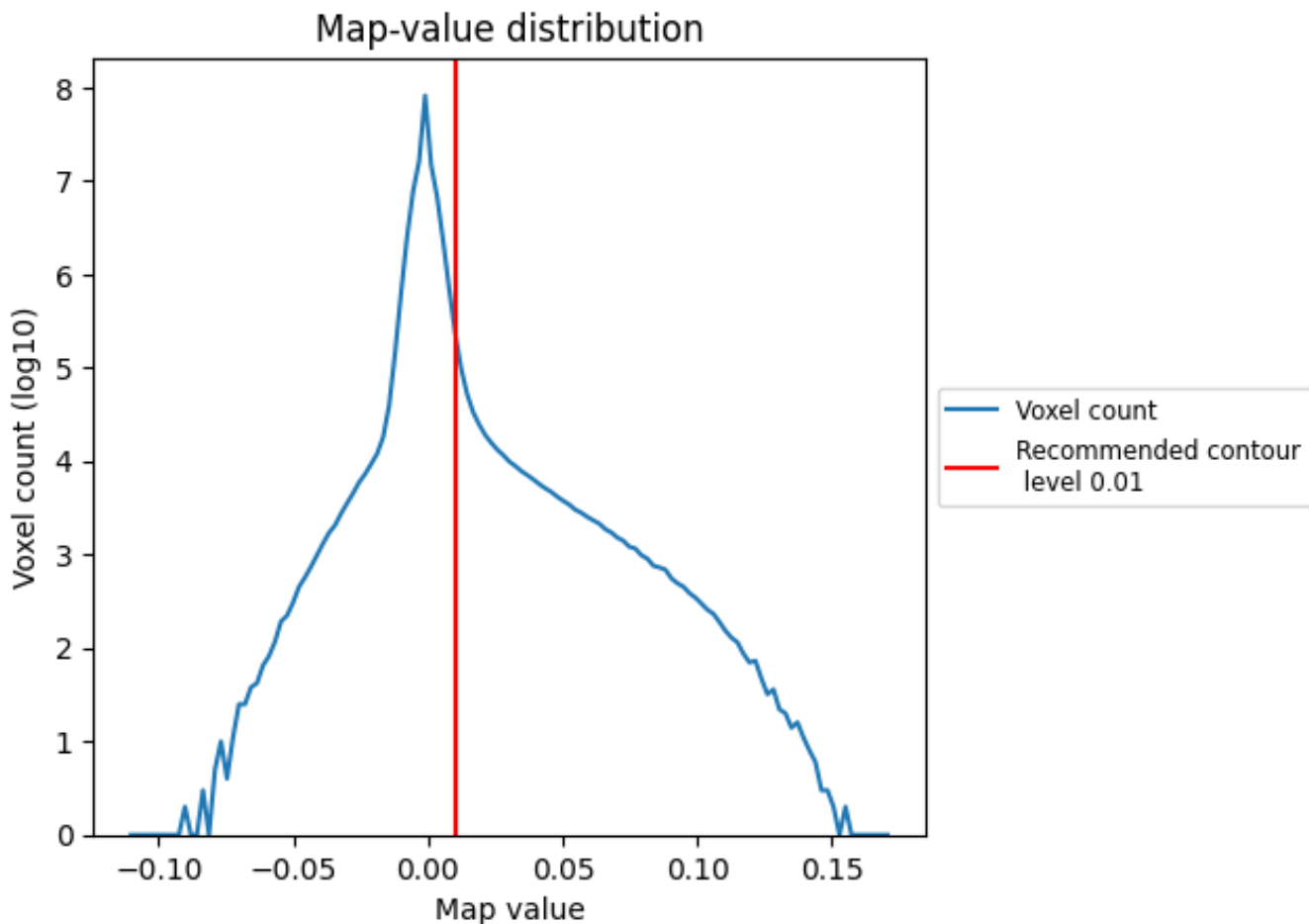


Z

## 7 Map analysis [i](#)

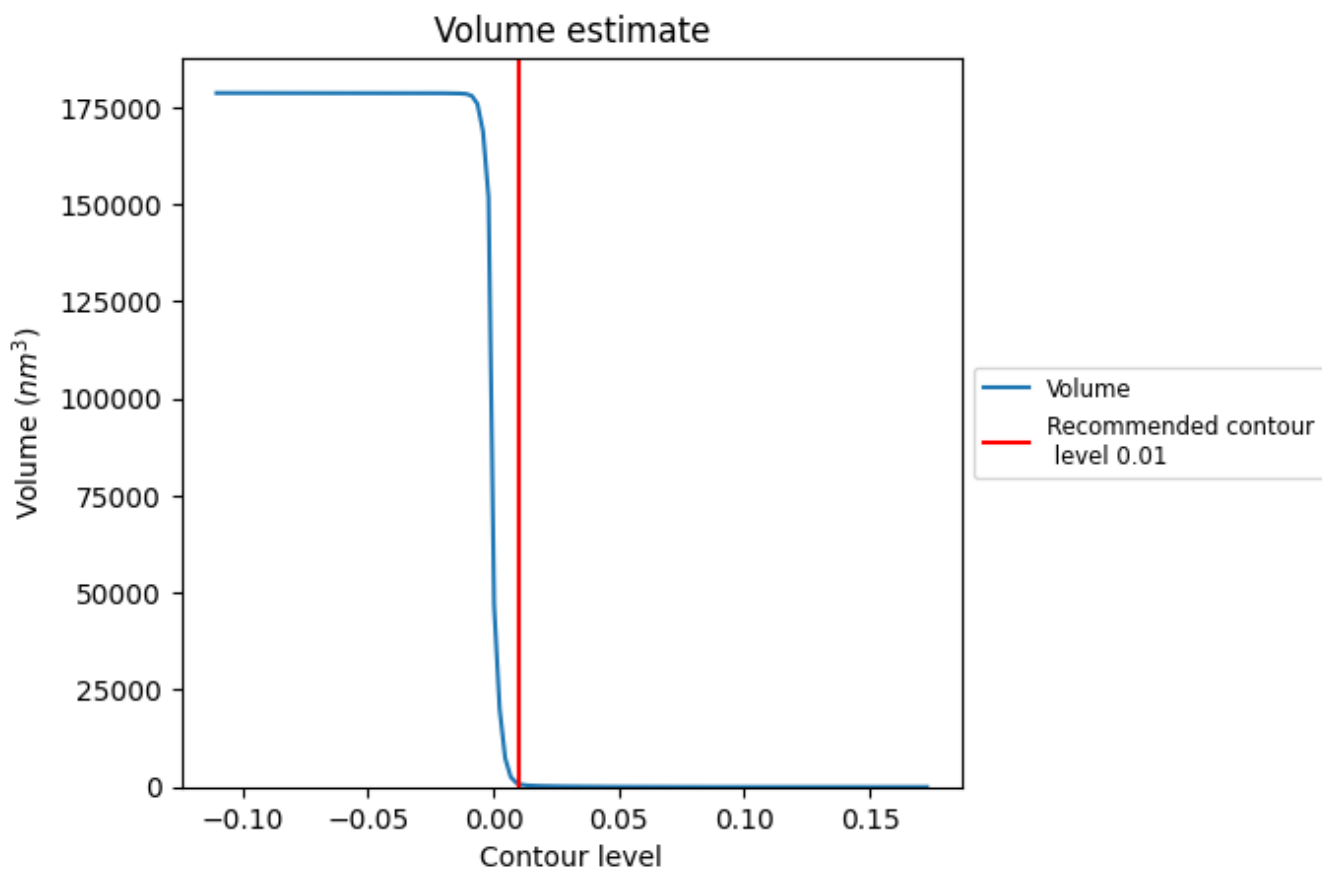
This section contains the results of statistical analysis of the map.

### 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.

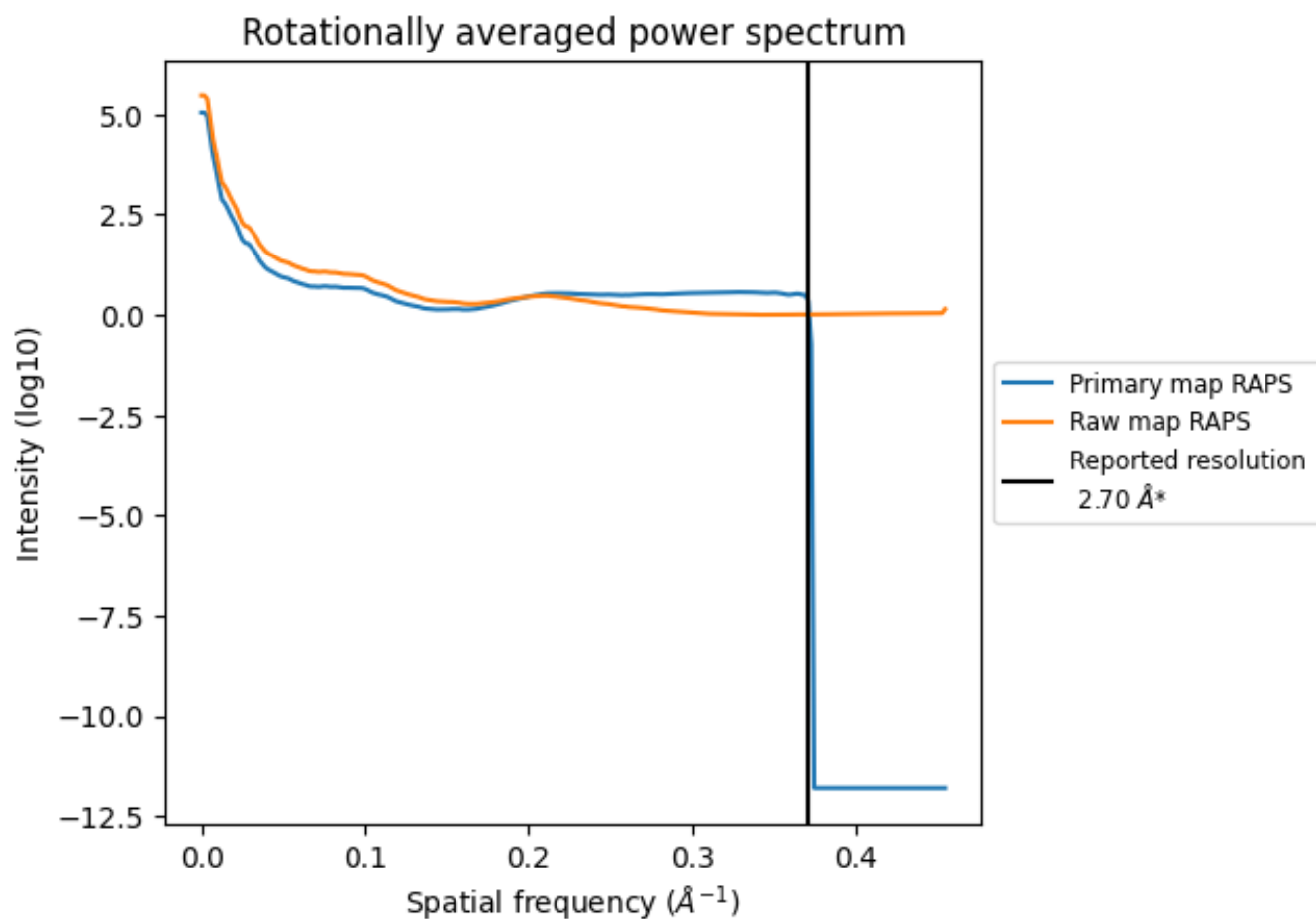
## 7.2 Volume estimate [i](#)



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](#)

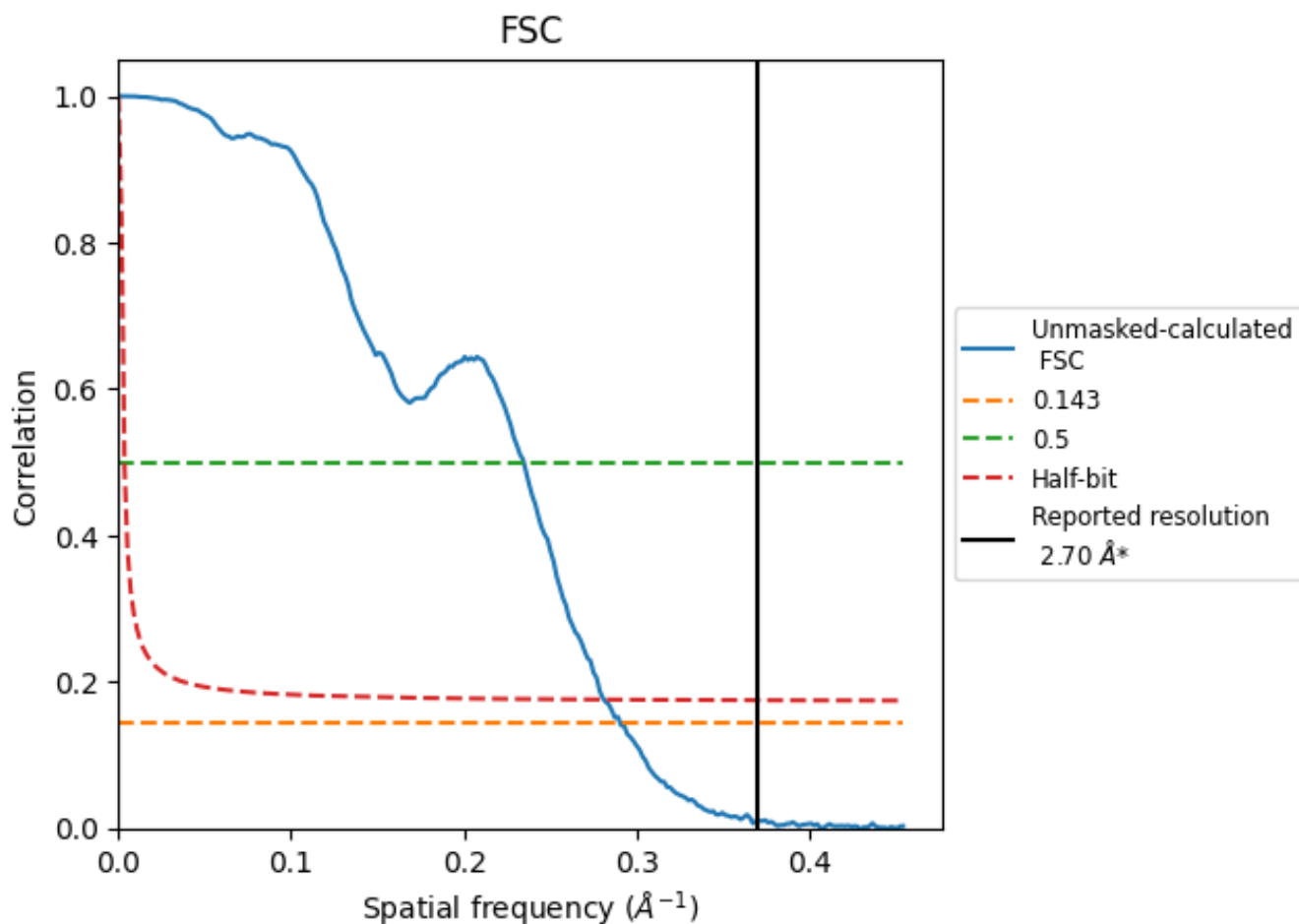


\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.370 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

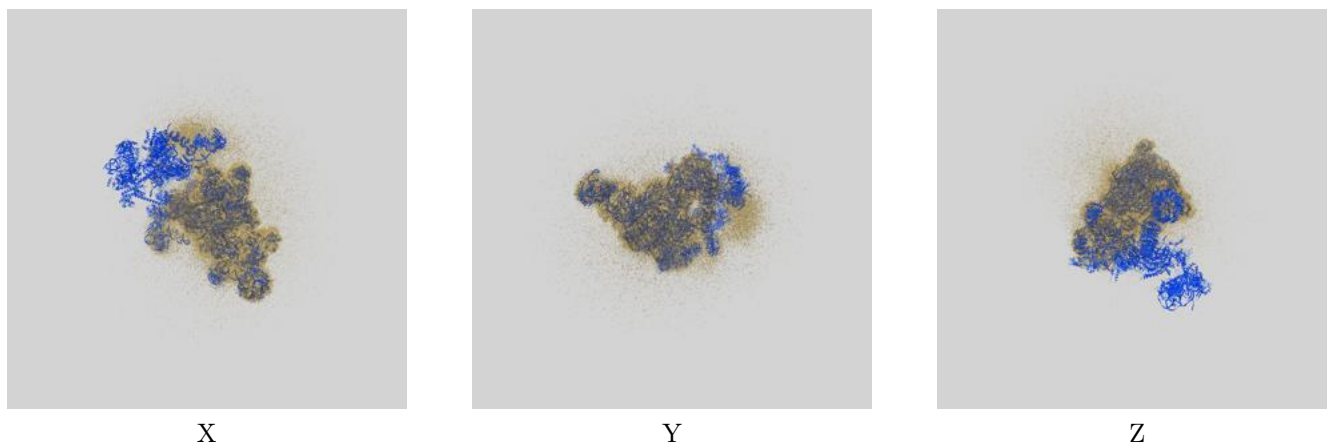
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.7 by more than 10 %



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

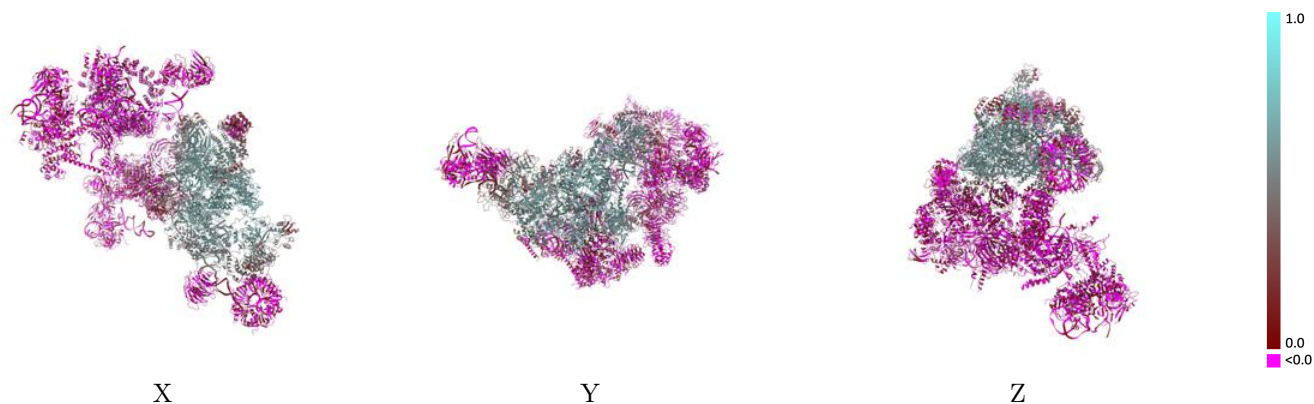
This section contains information regarding the fit between EMDB map EMD-34507 and PDB model 8H6K. Per-residue inclusion information can be found in section 3 on page 16.

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



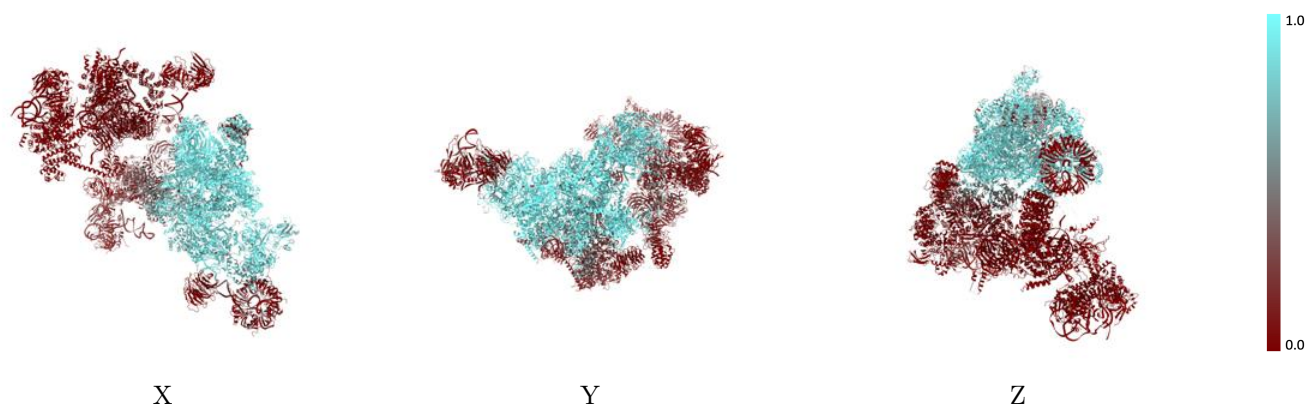
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



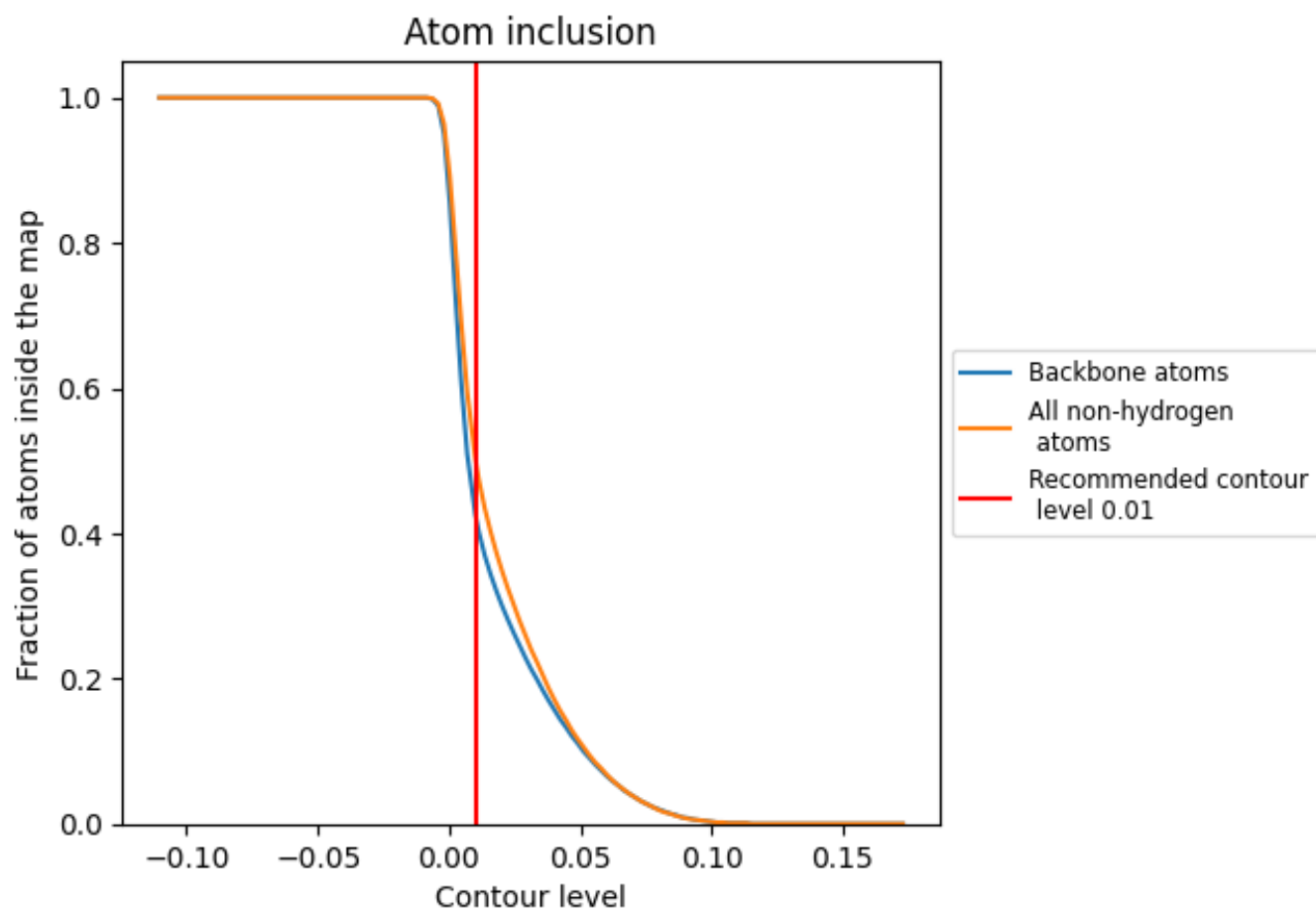
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



*Continued on next page...*

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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