



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 01:16 PM JST

PDB ID : 5Z58
EMDB ID : EMD-6891
Title : Cryo-EM structure of a human activated spliceosome (early Bact) at 4.9 angstrom.
Authors : Zhang, X.; Yan, C.; Zhan, X.; Li, L.; Lei, J.; Shi, Y.
Deposited on : 2018-01-17
Resolution : 4.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

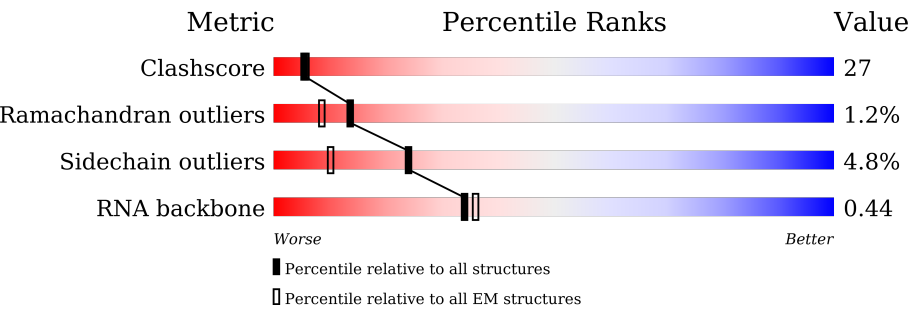
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2335	<div><div>24%</div><div>54%</div><div>36%</div><div>5%</div></div>
2	B	117	<div><div>20%</div><div>28%</div><div>27%</div><div>13%</div><div>28%</div></div>
3	C	972	<div><div>38%</div><div>47%</div><div>33%</div><div>7%</div><div>12%</div></div>
4	D	2136	<div><div>73%</div><div>79%</div><div>19%</div></div>
5	E	357	<div><div>83%</div><div>59%</div><div>21%</div><div>16%</div></div>
6	a	126	<div><div>64%</div><div>64%</div><div>36%</div></div>
6	h	126	<div><div>63%</div><div>63%</div><div>37%</div></div>

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Mol	Chain	Length	Quality of chain
7	b	231	
7	i	231	
8	c	119	
8	j	119	
9	d	118	
9	k	118	
10	f	86	
10	m	86	
11	e	92	
11	l	92	
12	g	76	
12	n	76	
13	F	107	
14	G	274	
15	H	188	
16	o	255	
17	p	225	
18	w	501	
19	u	793	
20	v	464	
21	1	1304	
22	2	895	
23	3	1217	
24	4	424	
25	5	125	

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Mol	Chain	Length	Quality of chain
26	6	110	
27	7	86	
28	J	848	
29	L	802	
30	M	343	
31	P	229	
32	R	540	
33	T	514	
34	V	908	
35	X	396	
36	Y	322	
37	Z	619	
38	z	472	
39	x	1041	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
41	GTP	C	1500	-	-	X	-

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 94673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2211	Total	C	N	O	S	0	0
			18165	11706	3163	3220	76		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	P	0	0
			1768	792	295	597	84		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	860	Total	C	N	O	S	0	0
			6716	4294	1120	1270	32		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1722	Total	C	N	O		0	0
			8528	5084	1722	1722			

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	299	Total	C	N	O	S	0	0
			2338	1470	410	445	13		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	81	Total	C	N	O		0	0
			399	237	81	81			

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	h	80	Total	C	N	O	0	0
			393	233	80	80		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	b	82	Total	C	N	O	0	0
			405	241	82	82		
7	i	86	Total	C	N	O	0	0
			422	250	86	86		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	c	82	Total	C	N	O	0	0
			406	242	82	82		
8	j	82	Total	C	N	O	0	0
			406	242	82	82		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	d	97	Total	C	N	O	0	0
			480	286	97	97		
9	k	85	Total	C	N	O	0	0
			422	252	85	85		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	f	74	Total	C	N	O	0	0
			361	213	74	74		
10	m	74	Total	C	N	O	0	0
			361	213	74	74		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	79	Total	C	N	O	0	0
			391	233	79	79		
11	l	79	Total	C	N	O	0	0
			391	233	79	79		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	g	74	Total	C	N	O	0	0
			363	215	74	74		
12	n	68	Total	C	N	O	0	0
			334	198	68	68		

- Molecule 13 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	93	Total	C	N	O	P	0	0
			1988	889	363	643	93		

- Molecule 14 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	77	Total	C	N	O	P	0	0
			1545	689	240	539	77		

- Molecule 15 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	136	Total	C	N	O	P	0	0
			2886	1289	499	962	136		

- Molecule 16 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	o	162	Total	C	N	O	0	0
			804	480	162	162		

- Molecule 17 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	p	165	Total	C	N	O	0	0
			813	483	165	165		

- Molecule 18 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	437	Total	C	N	O	S	0	0
			2369	1448	460	458	3		

- Molecule 19 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	u	105	Total	C	N	O	0	0
			525	315	105	105		

- Molecule 20 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	v	98	Total	C	N	O	0	0
			486	290	98	98		

- Molecule 21 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1	1038	Total	C	N	O	S	0	0
			7702	4900	1347	1415	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	183	Total	C	N	O	S	0	0
			1252	809	213	226	4		

- Molecule 23 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 24 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	4	78	Total	C	N	O	0	0
			527	345	83	99		

- Molecule 25 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5	108	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 26 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	89	Total	C	N	O	S	0	0
			670	410	119	128	13		

- Molecule 27 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	66	Total	C	N	O	S	0	0
			540	343	94	98	5		

- Molecule 28 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J	522	Total	C	N	O	S	0	0
			3463	2156	653	648	6		

- Molecule 29 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	132	Total	C	N	O	S	0	0
			1077	691	188	194	4		

- Molecule 30 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	M	36	Total	C	N	O	S	0	0
			267	167	45	52	3		

- Molecule 31 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	96	Total	C	N	O	S	0	0
			829	508	162	157	2		

- Molecule 32 is a protein called Skip.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R	309	Total	C	N	O	S	0	0
			2314	1454	413	435	12		

- Molecule 33 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	313	Total	C	N	O	S	0	0
			2457	1552	447	450	8		

- Molecule 34 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	V	451	Total	C	N	O		0	0
			2238	1336	451	451			

- Molecule 35 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	X	158	Total	C	N	O	S	0	0
			1012	645	172	194	1		

- Molecule 36 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Y	104	Total	C	N	O	S	0	0
			737	466	126	143	2		

- Molecule 37 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Z	113	Total	C	N	O		0	0
			755	474	147	134			

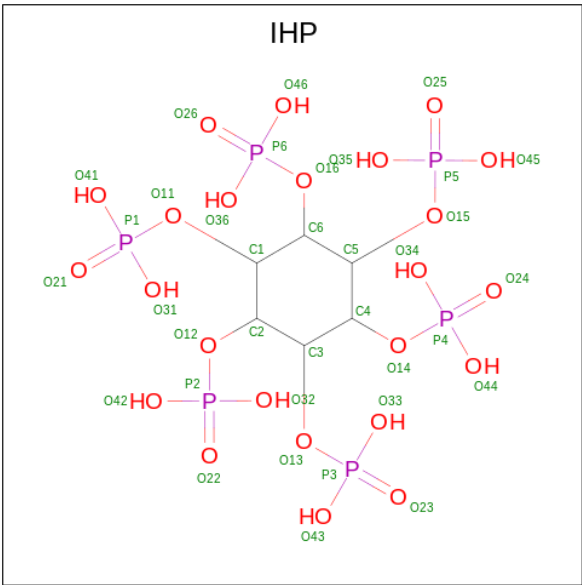
- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	z	177	Total	C	N	O	S	1	0
			1381	869	241	266	5		

- Molecule 39 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

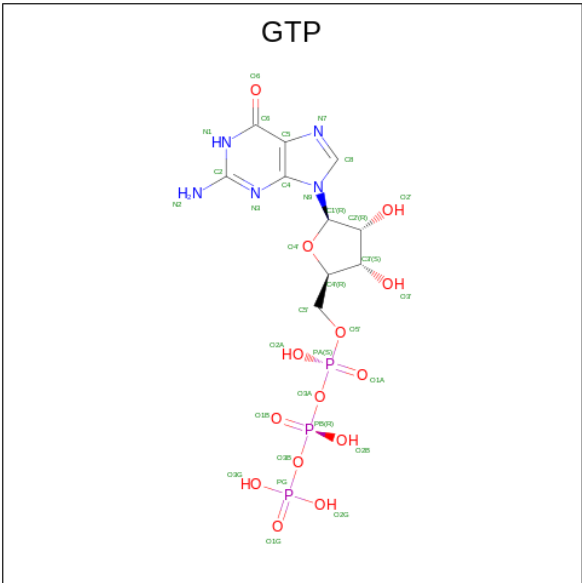
Mol	Chain	Residues	Atoms					AltConf	Trace
39	x	583	Total	C	N	O		0	0
			2882	1715	583	584			

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



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

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
42	C	1	Total 1	Mg 1	0
42	F	5	Total 5	Mg 5	0

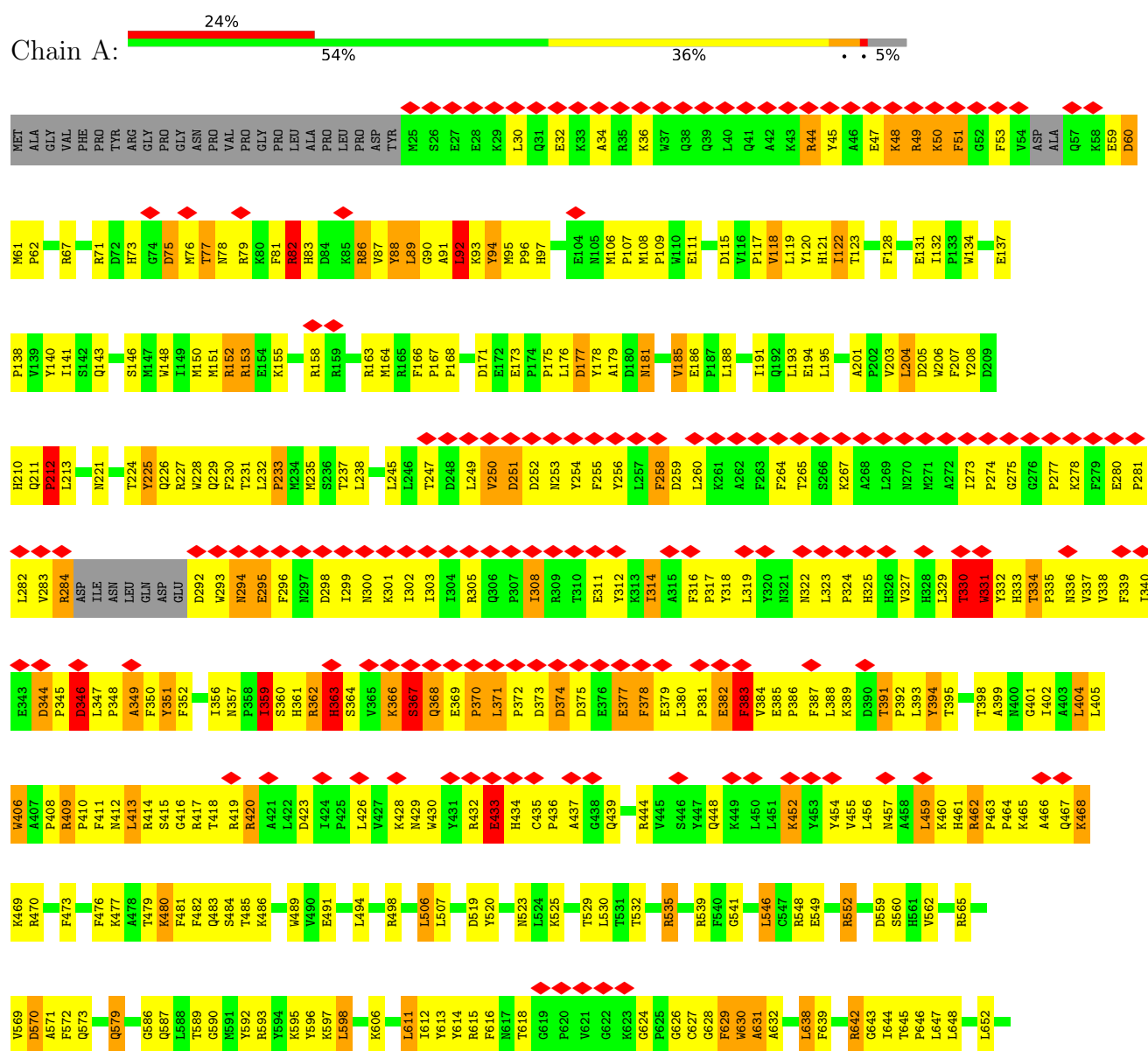
- Molecule 43 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
43	6	3	Total 3	Zn 3	0
43	M	1	Total 1	Zn 1	0

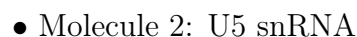
3 Residue-property plots

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

• Molecule 1: Pre-mRNA-processing-splicing factor 8



L856	A857	F860	E861	H864	S865	K866	G867	V868	T871	V872	T873	K874	Q875	R876	E878	S879	R886	M890	H891	D892	I893	L894	D895	M896	P897	E898	G900	I901	K902	K905	A906	R907	L910	Q911	H912	E915	R918	C919	N923	G930	L931	P932	T933	P934	I935	E936								
M937	M938	I939	R941	K944	A945	D948	W949	W950	H955	R958	R962	D968	V971	K974	N975	L976	G977	R978	D979	L982	R983	L986	I987	E988	Q989	I981	K982	L985	Q988	R989	A990	F991	N1013	N1012	M1026	S1027	G1029	I1030	L1034	Q1035	F1036	A1037	S1038	G1045	L1051	V1052	L1055							
P924	I925	P928	P929	S931	Y932	K933	H934	D935	T936	L941	A942	L943	E944	R945	E948	A949	R955	E963	L966	I967	E968	Q969	I981	K982	L985	Q988	R989	A990	F991	N1013	N1012	M1026	S1027	G1029	I1030	L1034	Q1035	F1036	A1037	S1038	G1045	L1051	V1052	L1055										
Y925	R933	P938	K941	P942	D944	P948	L951	N960	Y961	L962	Y965	Y966	E970	G971	E972	C973	N974	Y975	N976	L977	E978	E982	E986	I1000	V1001	K1012	N1013	N1026	S1027	G1029	I1030	L1034	Q1035	F1036	A1037	S1038	G1045	L1051	V1052	L1055														
H1056	R1057	E1060	N1069	D1070	F1071	L1072	S1073	F1074	Q1075	D1076	I1077	P1084	I1085	R1086	L1087	F1088	C1089	R1090	Y1091	I1092	I1097	F1098	F1099	R1100	F1101	I1110	Y1113	L1114	T1115	E1116	H1117	P1118	D1119	P1120	N1121	E1122	E1123	N1124	I1125	V1126	G1127	Y1128	N1129	N1130	K1131	K1132	C1133	W1134	P1135	R1136	D1137			
A1138	R1139	M1140	R1141	K1144	H1145	D1146	V1147	N1148	V1153	I1157	L1161	P1162	R1163	Q1169	Y1178	S1179	K1180	D1181	N1182	P1183	N1184	F1187	N1188	F1192	R1195	K1199	C1200	H1201	T1202	E1205	E1206	F1207	T1208	K1210	D1211	G1212	V1213	W1214	P1215	T1221	K1222	E1223	R1224	T1225	L1230									
R1231	V1232	D1233	D1234	E1235	S1236	M1237	H1241	A1250	S1251	G1252	F1256	T1257	K1258	I1259	N1261	K1262	W1263	L1270	Y1273	F1274	R1275	E1276	V1279	N1280	T1281	L1284	L1285	D1286	L1287	E1292	I1295	Q1296	T1297	R1298	I1301	G1302	L1303	K1306	R1310	F1311	P1312	V1315	T1318	P1319										
K1320	E1321	L1322	G1323	G1324	L1325	L1328	G1331	H1332	V1333	L1334	I1335	PRO	GLN	SER	ASP	LEU	ARG	TRP	SER	LYS	GLN	THR	ASP	VAL	GLY	I1342	R1354	S1355	G1356	M1357	S1358	H1359	E1360	E1361	D1362	Q1363	L1364	N1367	L1368	Y1369	R1370	Q1373	P1374	W1375	E1378	F1379	I1380	D1381	S1382	Q1383	R1384			
V1385	W1386	E1387	E1388	K1392	R1393	I1397	A1398	Q1399	N1400	R1401	R1402	L1403	T1404	L1405	E1406	D1407	D1413	R1414	G1415	T1416	P1417	R1418	L1422	K1425	R1426	R1427	H1428	T1429	L1430	D1433	K1434	G1435	V1436	R1437	V1438	R1439	T1440	D1441	F1442	K1443	Y1444	Q1445	Q1446	V1447	L1448	K1449	Q1450	W1451	P1452	F1453	Y1454	W1455	L1456	
H1457	Q1458	R1459	H1460	D1461	G1462	K1463	L1464	Y1470	A1477	L1489	G1492	L1501	F1502	W1503	E1504	K1505	ALA	SER	GLY	PHE	GLU	GLU	SER	MET	L1519	T1520	TRP	L1521	L1522	L1523	L1524	GLN	ARG	SER	GLY	N1527	Q1528	I1529	P1530	N1531	R1532	R1533	S1539	P1540	W1541	R1544	Y1548	V1549	G1550	F1551				
Q1552	V1553	Q1554	L1555	D1556	L1557	T1558	G1559	F1561	H1562	H1563	S1572	H1580	L1581	M1591	F1597	L1604	E1605	I1606	E1607	T1608	K1611	K1618	S1619	G1620	K1621	M1622	N1623	C1626	I1629	L1630	L1631	F1632	A1633	S1634	L1645	K1649	D1653	Y1660	W1661	I1662	R1667	W1668	D1672											
S1673	H1674	Y1679	D1690	N1691	S1697	G1700	V1701	A1704	L1709	A1714	Y1715	G1716	N1717	W1718	K1723	L1724	L1725	I1726	M1730	I1733	N1734	K1735	A1736	N1737	R1746	L1751	Q1752	L1753	Y1754	E1757	P1758	L1759	E1760	P1761	Y1762	L1763	S1764	S1765	Q1766	N1767	Y1768	G1769	E1770	L1771	F1772	S1773								
N1774	Q1775	I1776	I1777	W1778	F1779	V1780	D1781	D1782	T1783	N1784	V1785	R1787	V1788	I1789	I1790	H1791	K1792	N1793	F1794	E1795	Q1796	N1797	L1798	T1799	T1800	K1801	P1802	I1803	N1804	G1805	A1806	I1807	F1808	I1809	F1810	R1813	F1818	L1819	K1820	I1821	I1822	H1823	T1824	S1825	V1826	W1827	A1828	K1829	Q1830	K1831	R1832	G1834	L1835	A1837

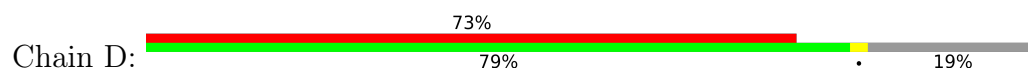
[illegible]

- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

MET	ASP	THR	ASP	ASP	LEU	TYR	ASP	GLU	PHE	GLY	ASN	TYR	ILE	GLY	PRO	GLU	LEU	ASP	SER	ASP	GLU	ASP	ASP	ASP	GLU	LEU	GLY	ARG	GLU	THR	LYS	ASP	LEU	ASP	GLU	MET	MET	ASP	ASP	ASP	ASP	ASP	ASP	VAL	GLY	ASP	HIS	ASP	ASP	ASP	ASP	HIS	PRO	GLY	MET	E56	V57	A58	L59
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TYR PRO MET	P908 G909 D910 P911 L912 D913 K914 S915 I916 V917 I918 R919 P920 L921 E922 P923 Q924 P925 A926 P927 H928 L929 A930 R931 E932 F933 M934	R803 G804 G805 G806 Q807 I808 I809 P810 T811 Y817 S818 M822 A823 T824 P825 R826 E829 P830 V846 R852 R853 R854 G855 R856 I863 P864 G865 S866 P867 I871	T740 G741 P742 L745 D748 T749 L750 P751 S752 E753 V754 D755 K756 T757 L758 L759 G760 S761 V762 K763 D764 S765 T766 V767 Q768 G769 F770 Q771 W772 G773 T774 R775 E776 L779 G780 D781 E782 L783 I784 R785 D786 V787 D788 L789 K788 F789 K790 I791 L792 D793 A794 V795 V796 A797 Q798 E799 P800 L801 H802 H903	T678 P679 N680 K681 K682 N683 K684 T685 T686 H687 L688 A689 E690 P691 L692 E693 K694 G695 L696 I700 E701 N702 E703 V704 V705 Q706 I707 T708 G709 N710 R711 K712 K713 L714 G715 E716 F717 F718 Q719 T720 K721 Y722 D723 W724 D725 L726 L727 A728 A729 R730 S731 I732 L733 K734 A735 F736 P737 D738 A739	P545 A546 G547 N548 W549 L551 L552 E553 G554 V555 D556 Q557 P558 I559 V560 K561 T562 A563 T564 I565 E566 F567 F568 R569 G570 N571 E572 E573 A574 Q575 I576 F577 R578 P579 L580 K581 F582 N583 T584 T585 S586 V587 K588 I589 I590 A591 V592 E593 P594 V595 N596 P597 S598 L600 P601 R602 H603	T484 D485 D486 G487 V488 Q489 F490 H491 A492 F493 G494 R495 V496 L497 S498 G499 T500 I501 G502 A503 G504 Q505 P506 V507 K508 V509 L510 G511 E512 N513 Y514 T515 L516 E517 D518 E519 E520 D521 S522 Q523 I524 C525 T526 V527 G528 R529 L530 H531 I532 S533 V534 A535 R536 Y537 E540 V541 N542 R543 V544	L418 V419 C420 F423 F424 G425 E426 F427 T428 C434 H437 I438 A439 S440 P441 K442 V443 G444 A445 K446 P447 K448 I449 E450 H451 Y453 T454 G455 G456 V457 D458 S459 D460 L461 G462 E463 A464 M465 S466 D467 C468 D469 P470 D471 G472 P473 L474 M475 C476 H477 T478 T479 K480 M481 Y482 S483	L343 W344 G345 Y348 F349 N350 P351 K352 T353 R354 K355 F356 K359 A360 P361 T362 S363 S364 S365 Q366 E371 F372 E375 P376 L377 Y378 L380 L381 A382 Q383 V384 V385 G386 D387 V388 D389 T390 S391 L392 P393 L399 G400 I401 L408 K409 L410 H411 I412 R413 P414 L415 L416 R417	I257 N258 K259 I260 D261 R262 L265 E266 P270 P271 Y275 R279 D283 E284 G287 L288 S289 M291 S293 Y292 E295 E296 N297 K299 L298 I299 L300 G302 L303 G304 N305 V307 C308 S312 F323 I326 G327 T330 F331 G332 D333 I334 N335 Y336 F339	T184 P185 V186 T187 V188 V189 L190 P191 D192 T193 K194 C195 G195 L199 F200 N201 I202 M203 D204 H208 V215 T216 A217 G218 T219 R220 I221 S222 D223 G224 V225 V226 L227 F228 I229 D230 A231 A232 E233 G234 V235 M236 T239 E240 R241 L242 I243 K244 H245 A246 R250 V253 T254 V255 C256	M123 D124 N125 S126 E127 L128 I129 N131 V132 T133 L134 C135 G136 H137 L138 H139 H140 G141 K142 T143 C144 F145 V146 D147 C148 L149 I150 E151 Q152 P155 E156 I157 ARG LYS ARG T127 F128 I229 D230 ASP ASP GLN LYS PHE THR LEU MET GLU GLN THR LEU LEU PHE T173 E174 Q175 E176 G177 E178 V179 G180 I181 K182 S183	E61 D62 K63 K64 Y65 P66 P67 T68 A69 E70 E71 V72 Y73 E76 V77 E78 T79 I80 V81 Q82 E83 E84 D85 T86 Q87 P88 L89 T90 E91 P92 I93 I94 K95 P96 V97 K98 T99 LYS LYS PHE THR LEU MET GLU GLN THR LEU LEU PRO VAL T112 V113 Y114 E115 M116 D117 F118 L119 L122
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● Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

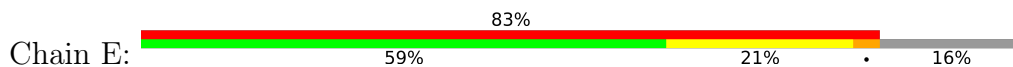


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V810	S811	T812	A813	T814	L815	A816	N817	G818	V819	N820	L821	P822	A823	H824	T825	N826	T831	Y834	S835	P836	E837	N841	T842	E843	L844	G845	A846	L847	L850	Q851	N852	L853	G854	R855	P859	Q860	Y861	D862	T863	K864	G865	E866	G867	T871	E875	L876	Y879	L880	S881	L882																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
D746	T747	L748	G749	L750	F751	L752	R753	E754	G755	S756	A757	S758	T759	E760	V761	L762	R763	T764	E765	A766	E767	Q768	C769	K770	N771	L772	E773	L774	K775	D776	L777	L778	Q779	H780	G781	F782	A783	L784	A787	G788	N789	T790	R791	V792	D793	R794	T795	L796	V797	E798	D799	L800	F801	A802	D803	K804	H805	L806																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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T606	Q607	L608	V609	R610	L611	I612	L613	L614	D615	E616	I617	D622	D623	D624	V627	L628	E629	A630	L631	V632	A633	R634	A635	I636	R637	N638	L639	E640	M641	T642	Q643	E644	D645	V646	I649	G650	P656	N657	Y658	E659	D660	V661	F664	L665	R666	V667	D668	P669	K671	G672	L673	F674	Y675																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
S546	L547	V548	Q549	E550	M551	V552	G553	P554	F555	G556	K557	R558	L559	A560	T561	Y562	G563	I564	T565	V566	A567	E568	L569	T570	G571	D572	H573	Q574	L575	C576	K577	E578	E579	I580	S581	A582	T583	Q584	I585	I586	V587	Y588	C588	E589	P590	E591	K592	M593	D594	I595	I596	T597	R598	K599	G600	G601	E602	R603	T604	Y605																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
Q485	S486	K487	L488	Y489	R490	A491	A492	L493	E494	T495	D496	A497	N498	L499	L500	L501	C502	A503	P504	T505	G506	A507	G508	K509	T510	A513	L514	M515	C516	M517	L518	R519	E520	I521	G522	K523	H524	I525	N526	M527	D528	G529	T530	I531	N532	V533	D534	D535	F536	K537	I538	I539	Y540	I541	A542	P543	M544	R545																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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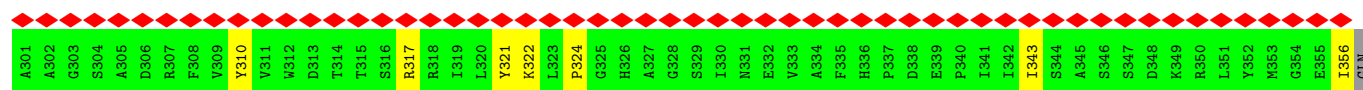
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S1507	A1508	T1509	S1510	T1511	F1512	M1513	F1514	H1515	P1516	M1517	V1518	R1519	P1520	V1521	P1522	L1523	E1524	L1525	H1526	I1527	Q1528	G1529	F1530	M1531	I1532	S1533	H1534	T1535	Q1536	T1537	R1538	L1539	L1540	S1541	M1542	A1543	K1544	P1545	V1546	I1547	H1548	A1549	I1550	T1551	K1552	H1553	S1554	P1555	K1556	L1557	P1558	V1559	L1560	V1561	F1562	P1563	V1564	S1565	R1566
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M1081	V1082	Y1083	V1084	T1085	Q1086	S1087	G1088	G1089	R1090	L1091	M1092	R1093	A1094	I1095	F1096	E1097	I1098	V1099	L1100	N1101	R1102	G1103	W1104	A1105	Q1106	L1107	T1108	D1109	K1110	T1111	L1112	K1116	M1117	I1118	D1119	K1120	R1121	M1122	W1123	Q1124	M1125	C1126	C1127	P1128	L1129	R1130	Q1131	F1132	R1133	K1134	L1135	P1136	E1137	E1138	V1139	V1140	K1141	L1142	
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Q1749	D1809	R1869	V1929	E1989	M2109
D1750	V1810	Q1870	L1930	D1990	S2110
A1751	A1811	L1871	S1931	E1991	D2111
V1752	P1812	A1872	S1932	E1992	A2112
D1753	L1813	Q1873	N1933	R1993	Y2113
Y1754	N1814	K1874	G1934	N1994	M2114
L1755	L1815	V1875	W1935	A1995	G2115
T1756	G1816	P1876	L1936	L1996	C2116
W1757	M1817	H1877	S1937	L1997	D2117
T1758	I1818	K1878	P1938	Q1998	Q2118
F1759	A1819	L1879	A1939	L1999	Y2119
L1760	A1820	N1880	L1940	T2000	Y2120
Y1761	Y1821	M1881	A1941	D2001	E2061
R1762	Y1822	P1882	A1942	S2002	E2062
R1763	Y1823	K1883	M1943	Q2003	S2123
M1764	Y1824	F1884	E1944	T2004	V2124
T1765	N1825	M1885	L1945	A2005	W2065
Q1766	Y1826	D1886	A1946	D2006	W2066
L1767	T1827	P1887	Q1947	V2007	V2067
P1768	T1828	L1888	M1948	A2008	L2068
M1769	I1829	V1889	V1949	R2009	G2069
Y1770	E1830	K1890	T1950	F2010	D2070
Y1771	L1831	T1891	Q1951	C2011	A2071
M1772	F1832	N1892	A1952	N2012	G2072
L1773	S1833	L1893	M1953	R2013	S2073
Q1774	M1834	L1894	W1954	Y2014	N2074
G1775	S1835	L1895	S1955	P2015	S2075
T1776	L1836	Q1896	L1956	N2016	L2076
S1777	N1837	A1897	D1957	T2017	T2077
H1778	A1838	H1898	S1958	E2018	S2078
R1779	K1839	L1899	Y1959	L2019	T2079
H1780	T1840	S1900	L1960	S2020	K2080
L1781	K1841	R1901	K1961	Y2021	R2081
S1782	V1842	M1902	Q1962	E2022	L2082
D1783	R1843	Q1903	L1963	V2023	T2083
H1784	G1844	L1904	P1964	V2024	L2084
L1785	L1845	S1905	H1965	D2025	Q2085
S1786	L1846	A1906	F1966	K2026	Q2086
L1787	E1847	L1907	T1967	D2027	K2087
L1788	I1848	L1908	S1968	S2028	A2088
V1789	I1849	Q1909	E1969	L2029	K2089
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Q1791	N1851	D1911	I1971	S2031	K2091
T1792	A1852	T1912	K1972	G2032	L2092
L1793	A1853	E1913	R1973	G2033	D2093
S1794	E1854	E1914	G1974	P2034	F2094
D1795	Y1855	L1915	T1975	V2035	A2095
L1796	L1856	L1916	D1976	V2036	A2096
E1797	N1857	S1917	K1977	V2037	P2097
Q1798	I1858	K1918	G1978	L2038	A2098
S1799	P1859	A1919	V1979	V2039	T2099
K1800	I1860	E1980	Q2040	Q2040	G2100
C1801	R1861	R1921	S1981	L2041	A2101
T1802	H1862	L1922	V1982	E2042	H2102
S1803	H1863	I1923	F1983	R2043	N2103
L1804	E1864	Q1924	I1984	E2044	Y2104
E1805	D1865	A1925	I1985	E2045	T2105
D1806	N1866	C1926	M1986	E2046	L2106

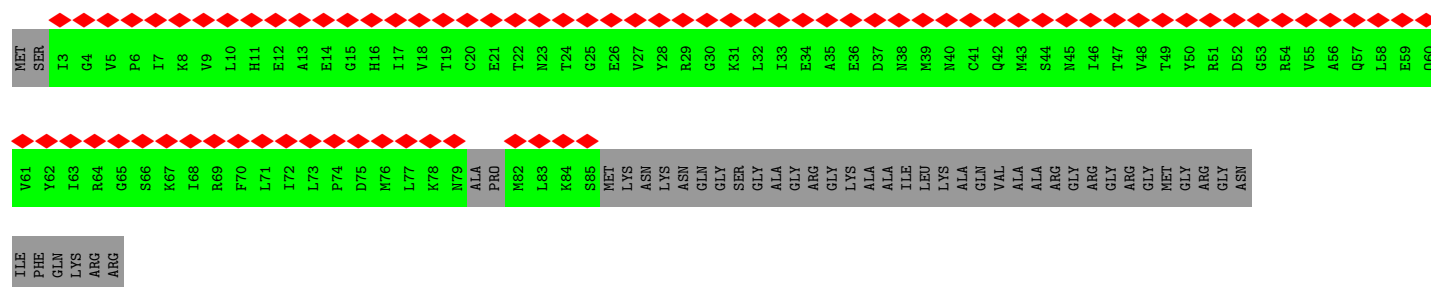
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein



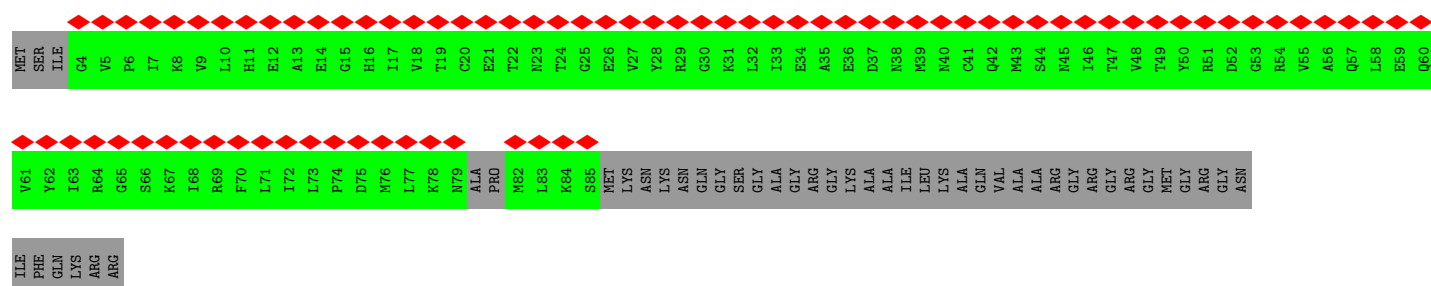
MET	L61	G121	I181	L241
ILE	L62	S122	R182	S242
GLU	S63	M123	K183	L243
GLN	G64	L124	K184	S244
LYS	H65	F125	A185	S245
ARG	E66	S126	A186	E246
GLY	G67	A127	L187	G247
PRO	E68	S128	Q188	S248
LEU	V69	T129	T189	Y249
LEU	Y70	D130	F190	L250
LEU	C71	K131	Q191	L251
VAL	C72	T132	N192	S252
PRO	K73	V133	L193	M253
VAL	F74	A134	Y194	A254
ARG	H75	V135	Q195	M255
GLN	P76	W136	V196	D256
ARG	N77	D137	L197	N257
HIS	G78	S138	A198	T258
GLU	S79	E139	V199	V259
LEU	T80	T140	T200	R260
LEU	L81	G141	F201	V261
GLY	E82	E142	N202	W262
ALA	S83	R143	D203	D263
GLY	A84	V144	T204	V264
THR	G85	K145	S205	R265
ASP	F86	R146	D206	P266
SER	D87	L147	Q207	F267
SER	B88	K148	T208	A268
ASP	L89	G149	T209	P269
ALA	I90	H150	S210	X270
GLN	L91	T151	G211	E271
THR	L92	S152	G212	R272
PRO	W93	F153	T213	C273
ALA	N94	V154	D214	V274
LEU	V95	N155	N215	K275
LEU	Y96	S156	D216	T276
GLN	G97	C157	T217	F277
PRO	D98	Y158	K218	Q278
PRO	C99	P159	V219	G279
ARG	D100	A160	W220	N280
CYS	N101	R161	D221	V281
SER	I102	R162	L222	H282
LEU	A103	G163	R223	N283
GLN	T104	P164	Q224	F284
ALA	L105	Q165	N225	E285
P58	K106	L166	K226	K286
I59	G107	V167	L227	N287
M60	H108	C168	T228	L288
	S109	T169	Y229	L289
	G110	G170	T230	R290
	A111	S171	N231	C291
	V112	D172	R232	S292
	M113	D173	G233	W293
	E114	G174	H234	S294
	L115	T175	A235	P295
	H116	V176	D236	D296
	Y117	K177	S237	G297
	N118	L178	V238	S298
	T119	W179	T239	K299
	D120	D180	G240	I300



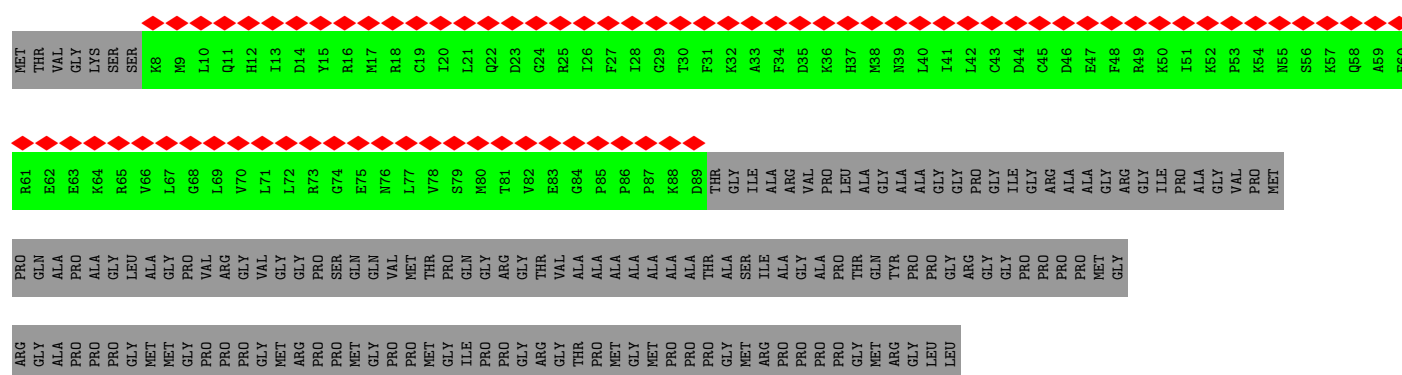
• Molecule 6: Small nuclear ribonucleoprotein Sm D3



• Molecule 6: Small nuclear ribonucleoprotein Sm D3

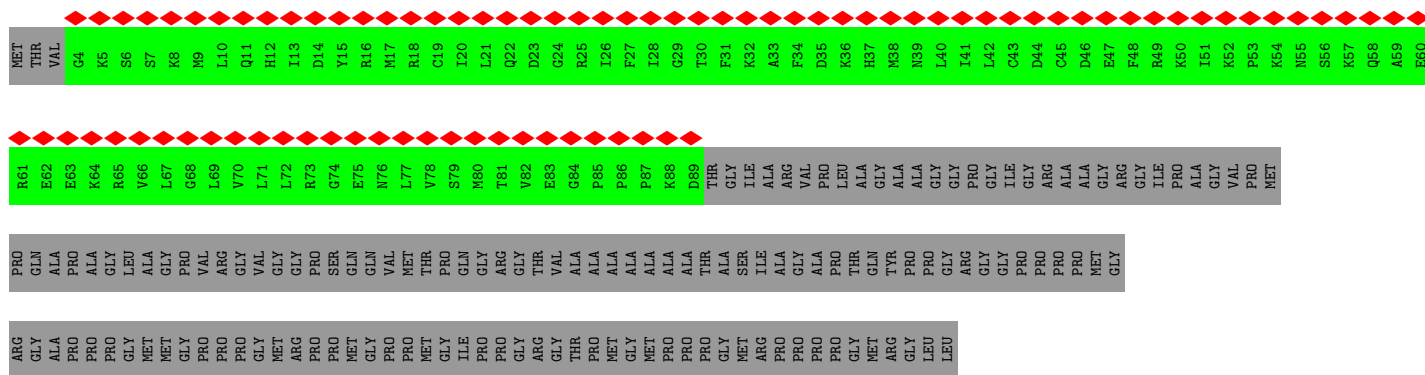


• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'

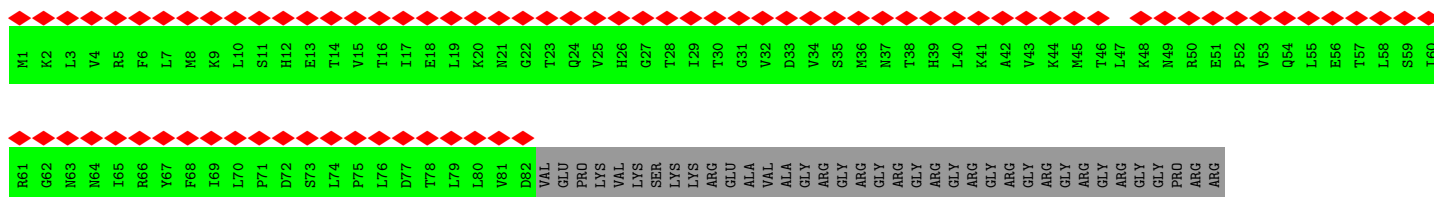


• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'





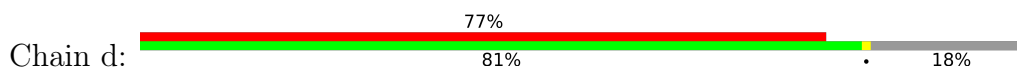
- Molecule 8: Small nuclear ribonucleoprotein Sm D1



- Molecule 8: Small nuclear ribonucleoprotein Sm D1

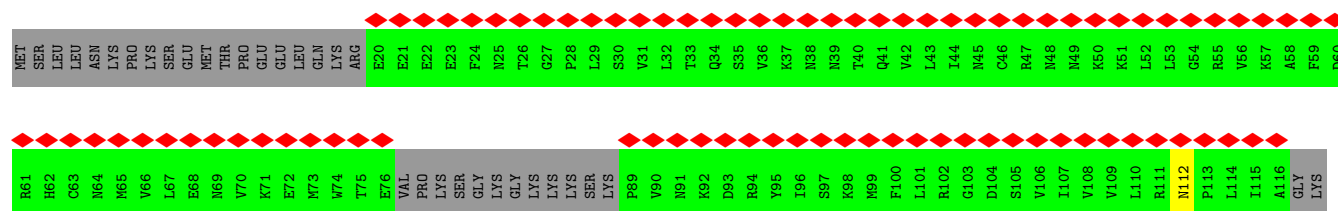


- Molecule 9: Small nuclear ribonucleoprotein Sm D2

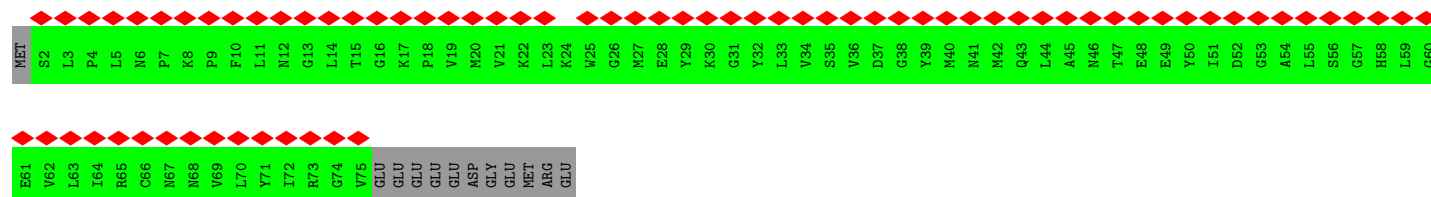
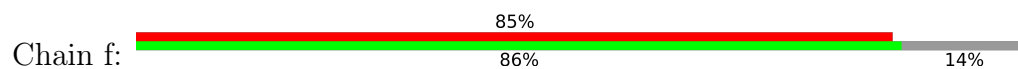


- Molecule 9: Small nuclear ribonucleoprotein Sm D2

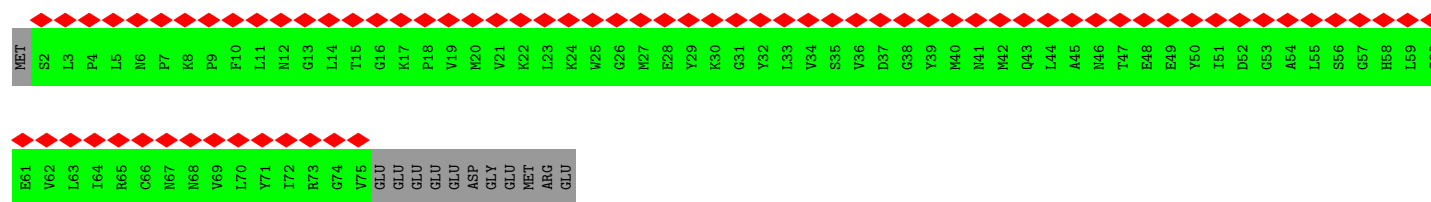
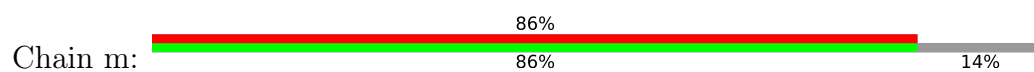




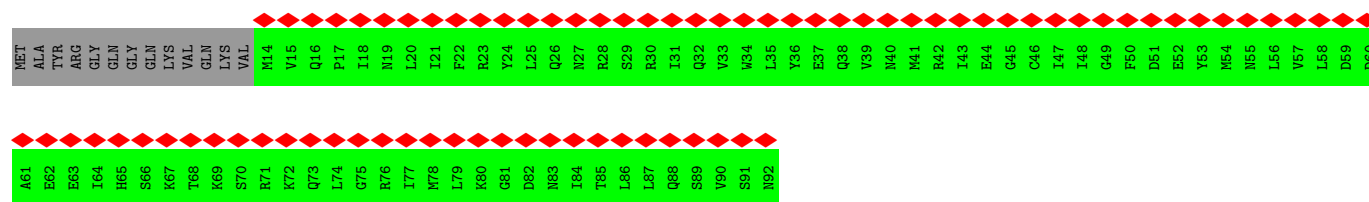
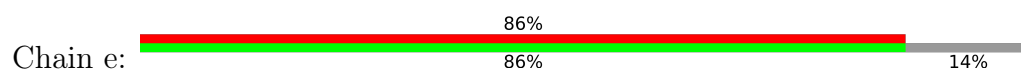
• Molecule 10: Small nuclear ribonucleoprotein F



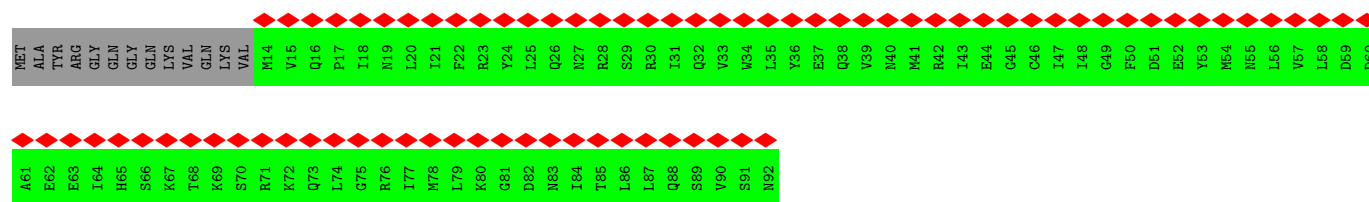
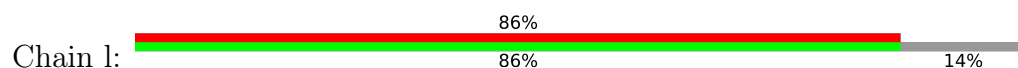
• Molecule 10: Small nuclear ribonucleoprotein F



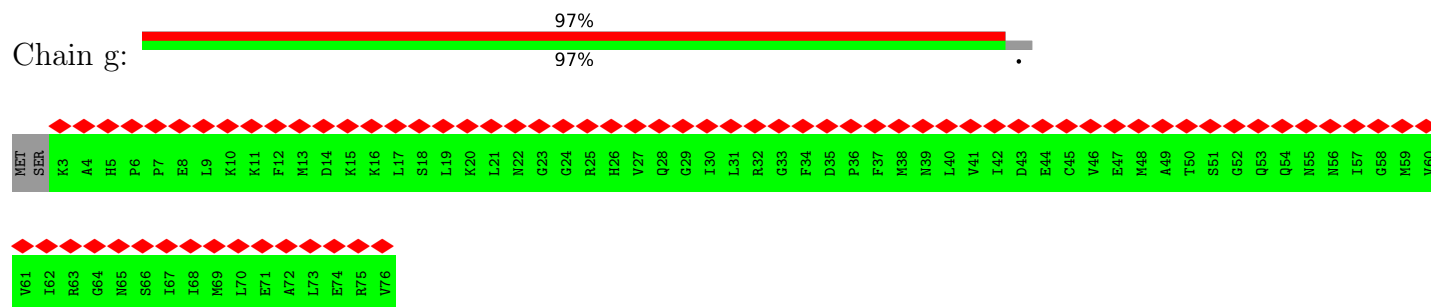
• Molecule 11: Small nuclear ribonucleoprotein E



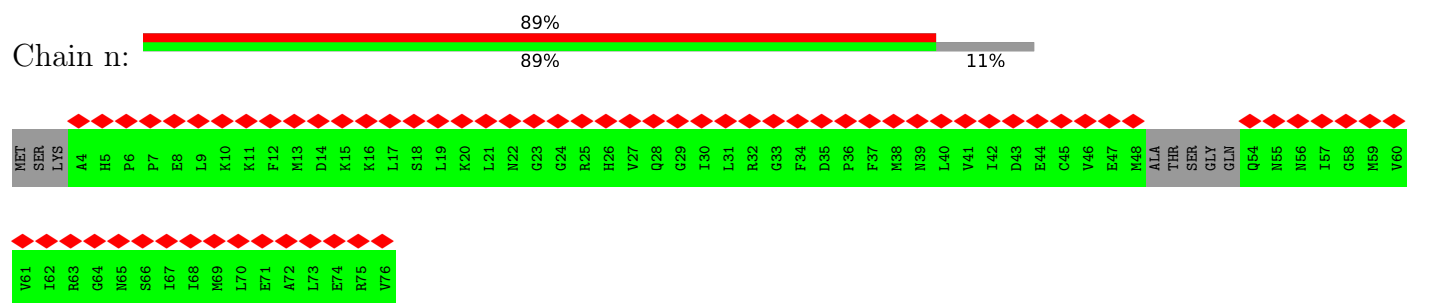
• Molecule 11: Small nuclear ribonucleoprotein E



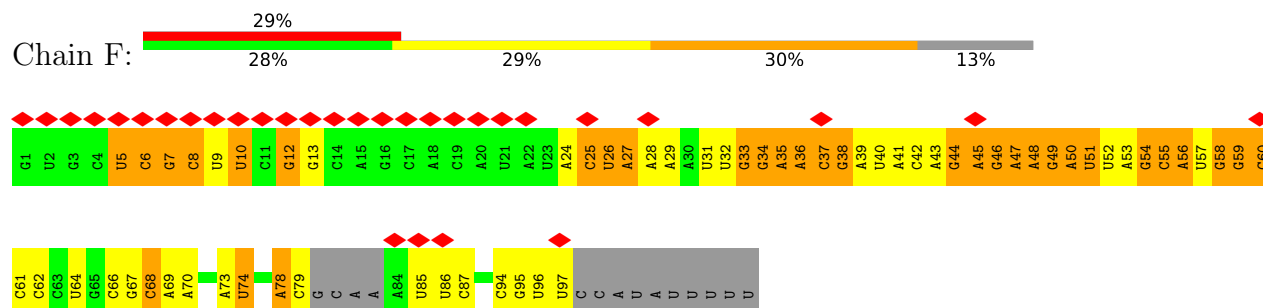
Chain g:



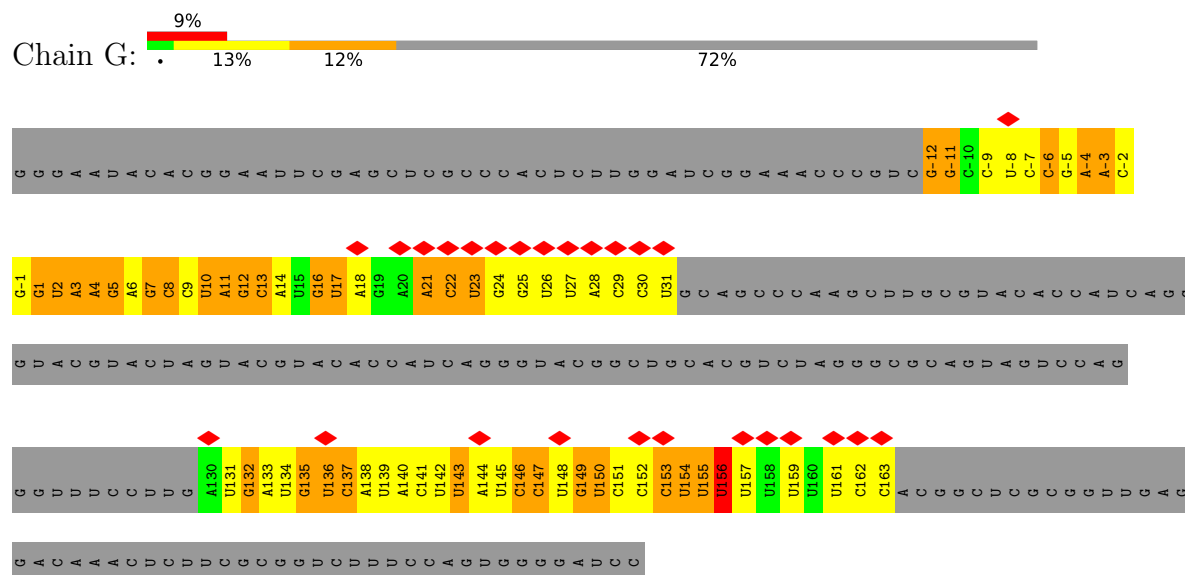
Chain n:



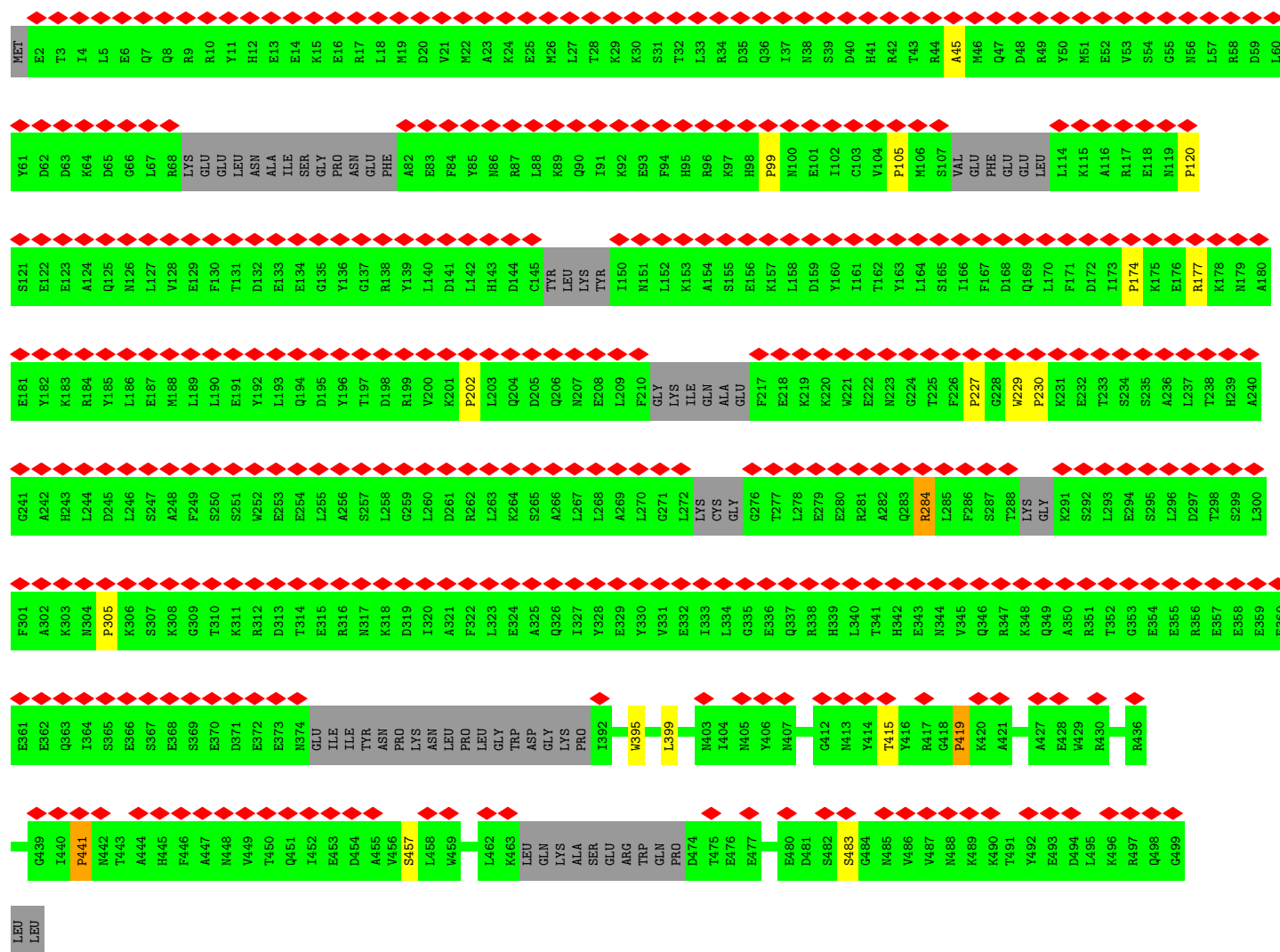
Chain F:



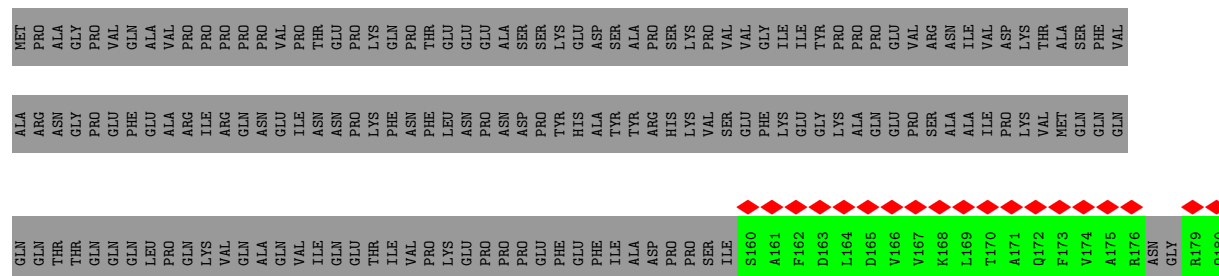
Chain G:



Chain w: 78% 83% 13%

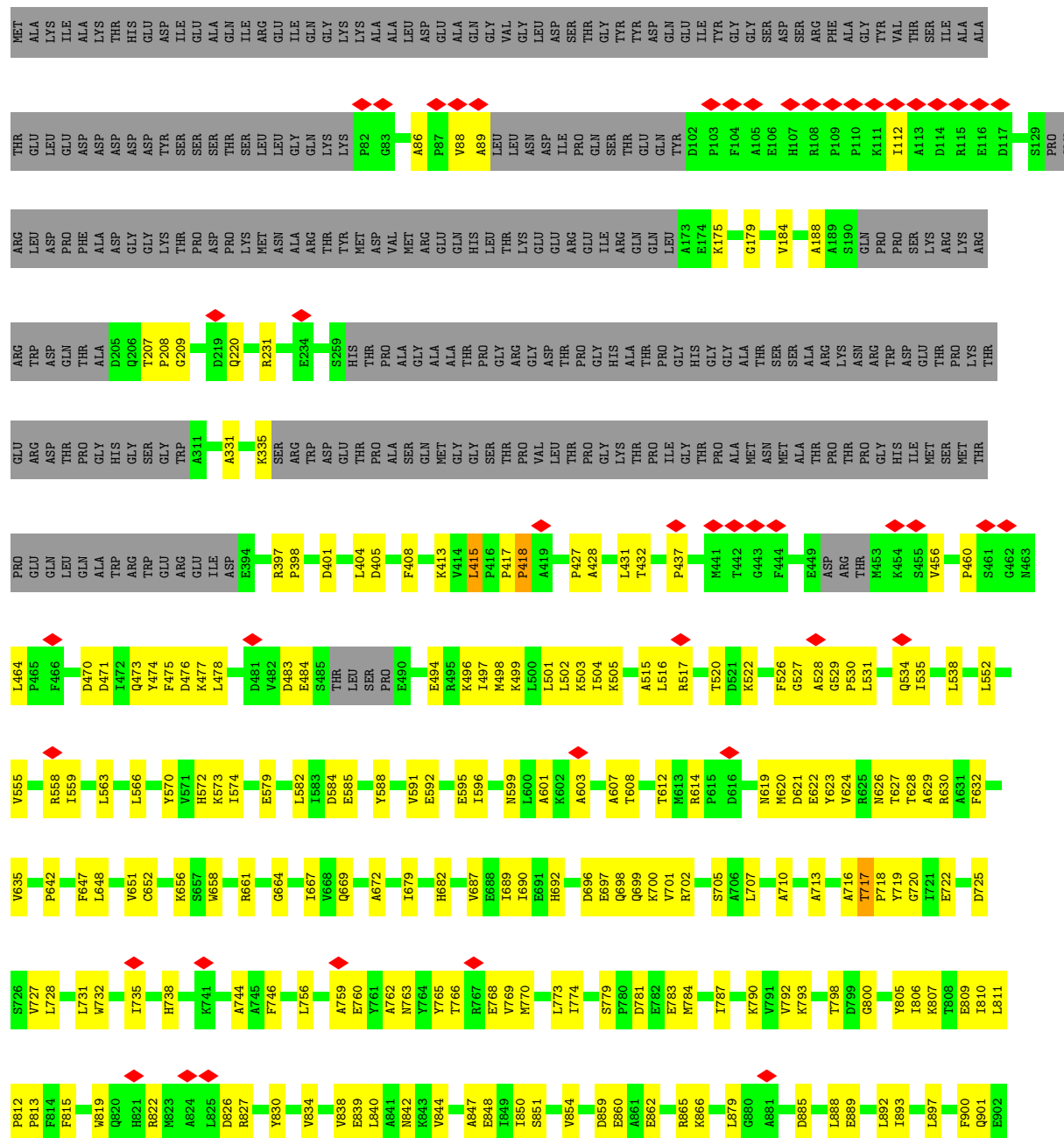


Chain u: 13% 13% 87%

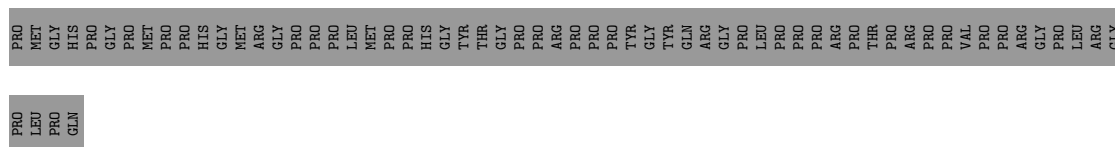


VAL	HIS	PRO	GLN	PRO	PRO	GLY	VAL	HIS	PRO	SER	ASN	PRO	GLY	VAL	HIS	PRO	PRO	THR	PRO	MET	PRO	PRO	MET	LEU	ARG	PRO	PRO	PRO	LEU	PRO	SER	GLU	GLY	PRO	GLY	ASN	ILE	PRO	PRO	PRO	PRO	THR	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

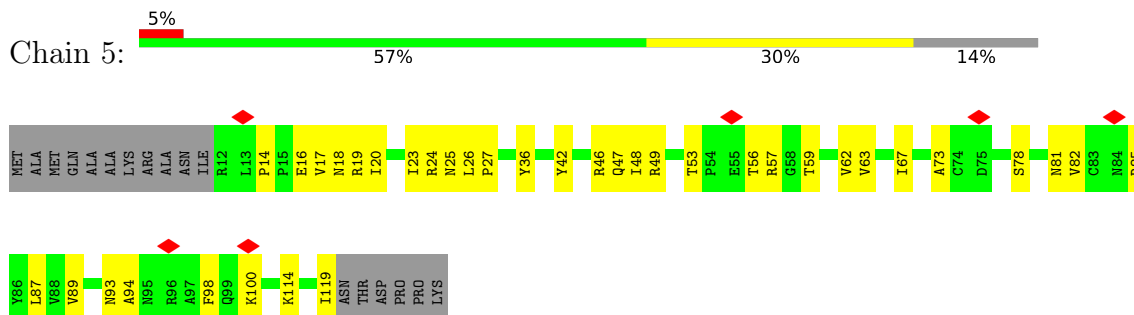
- Molecule 21: Splicing factor 3B subunit 1



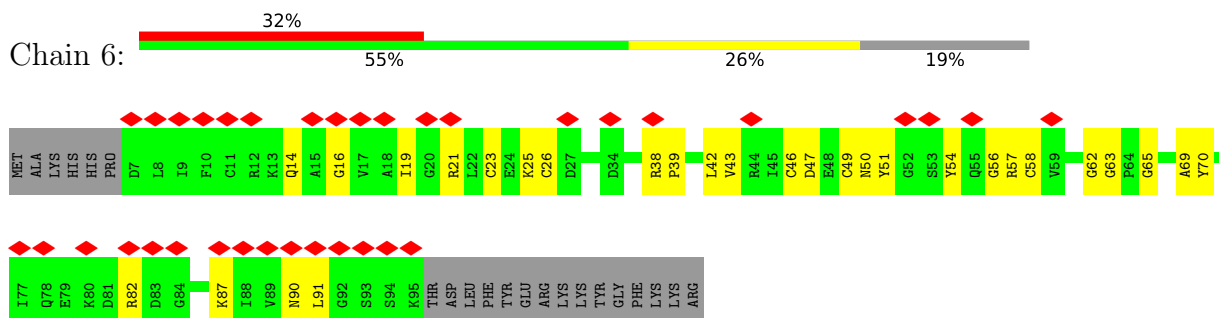




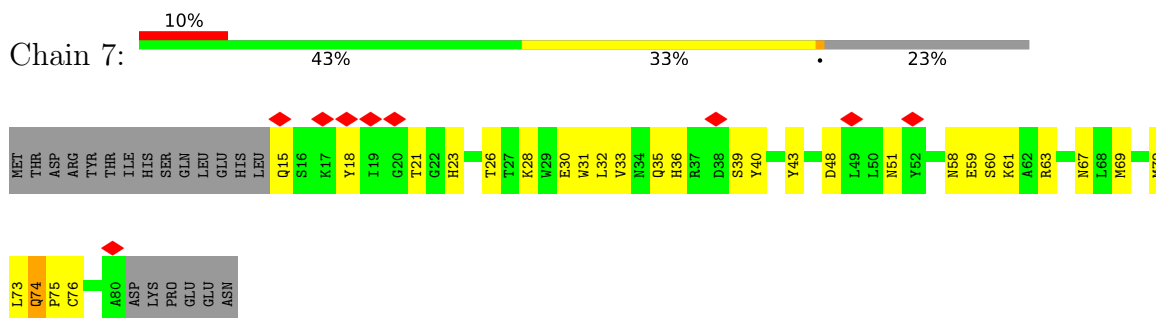
• Molecule 25: Splicing factor 3B subunit 6



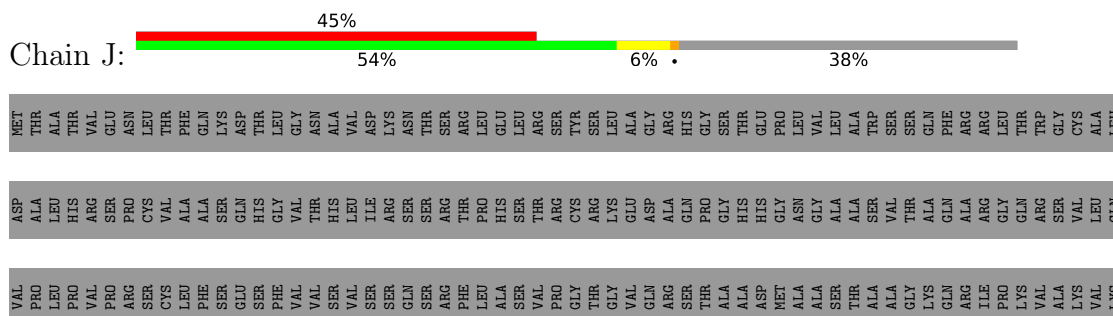
• Molecule 26: PHD finger-like domain-containing protein 5A

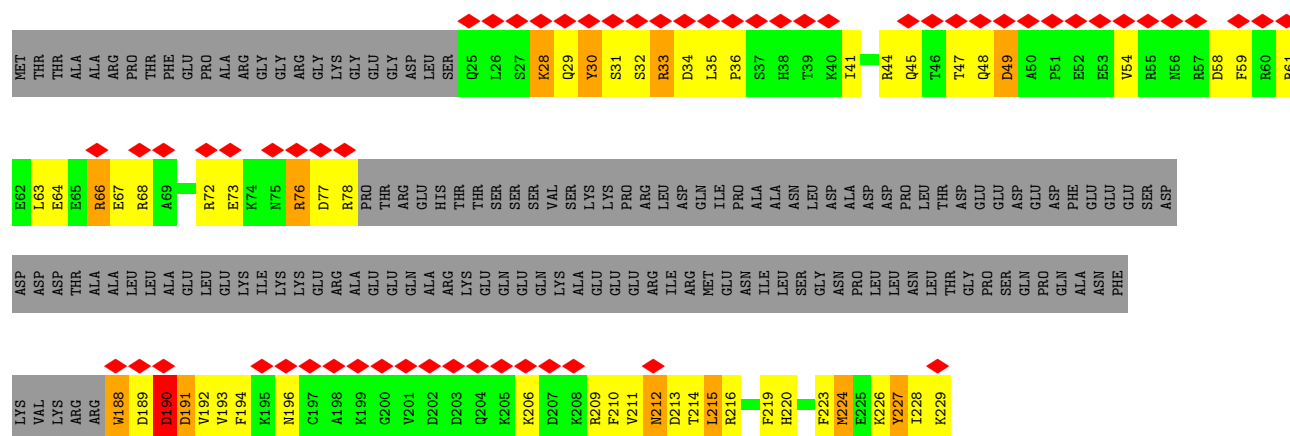
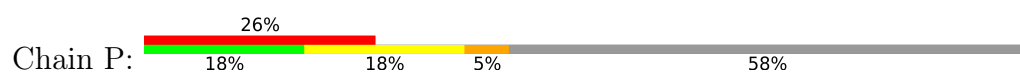


• Molecule 27: Splicing factor 3B subunit 5

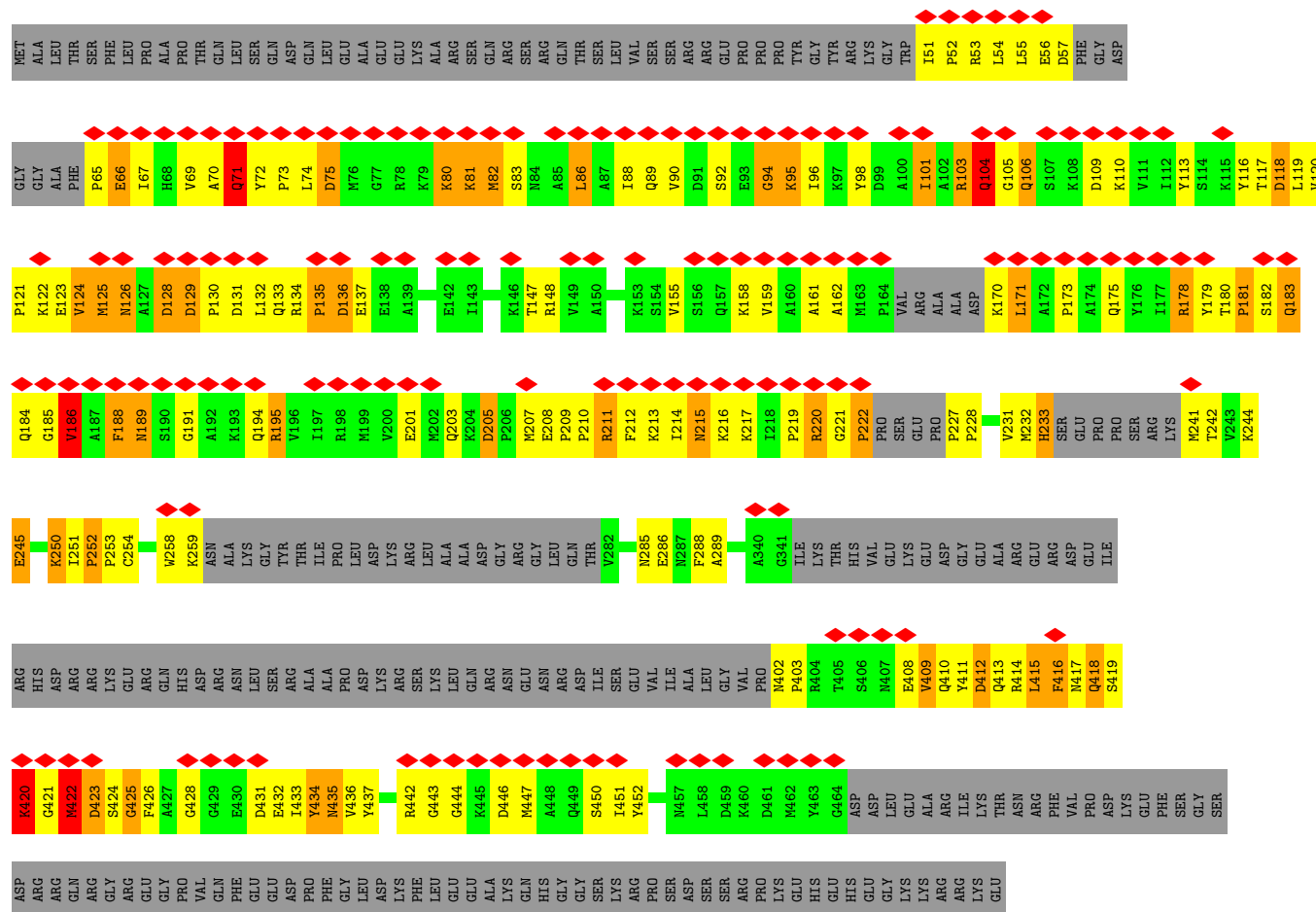
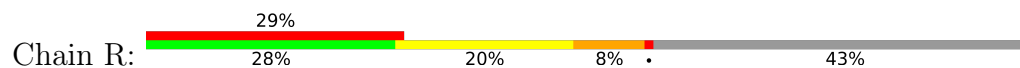


• Molecule 28: Crooked neck-like protein 1

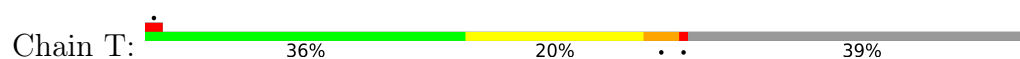




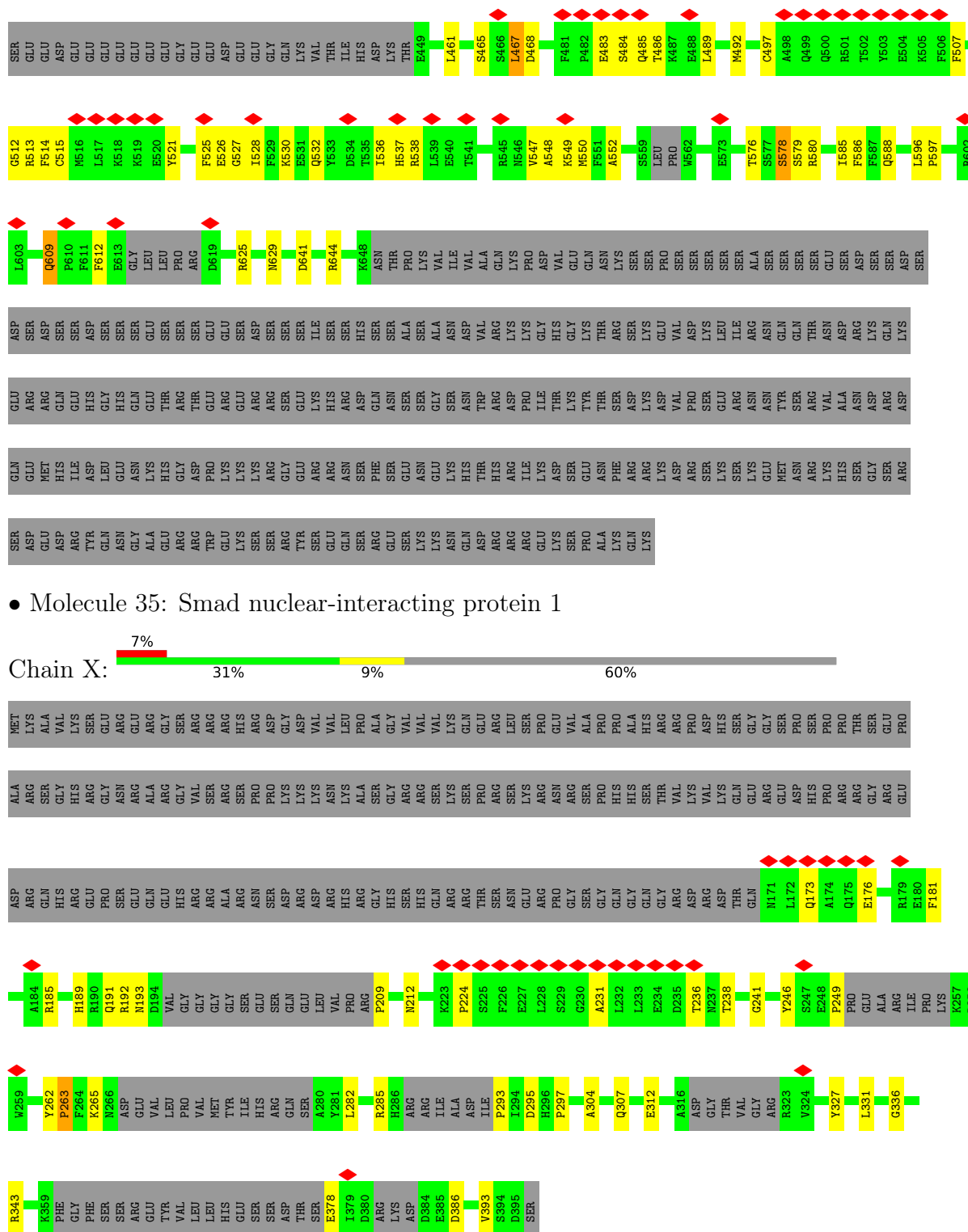
• Molecule 32: Skip



• Molecule 33: Pleiotropic regulator 1

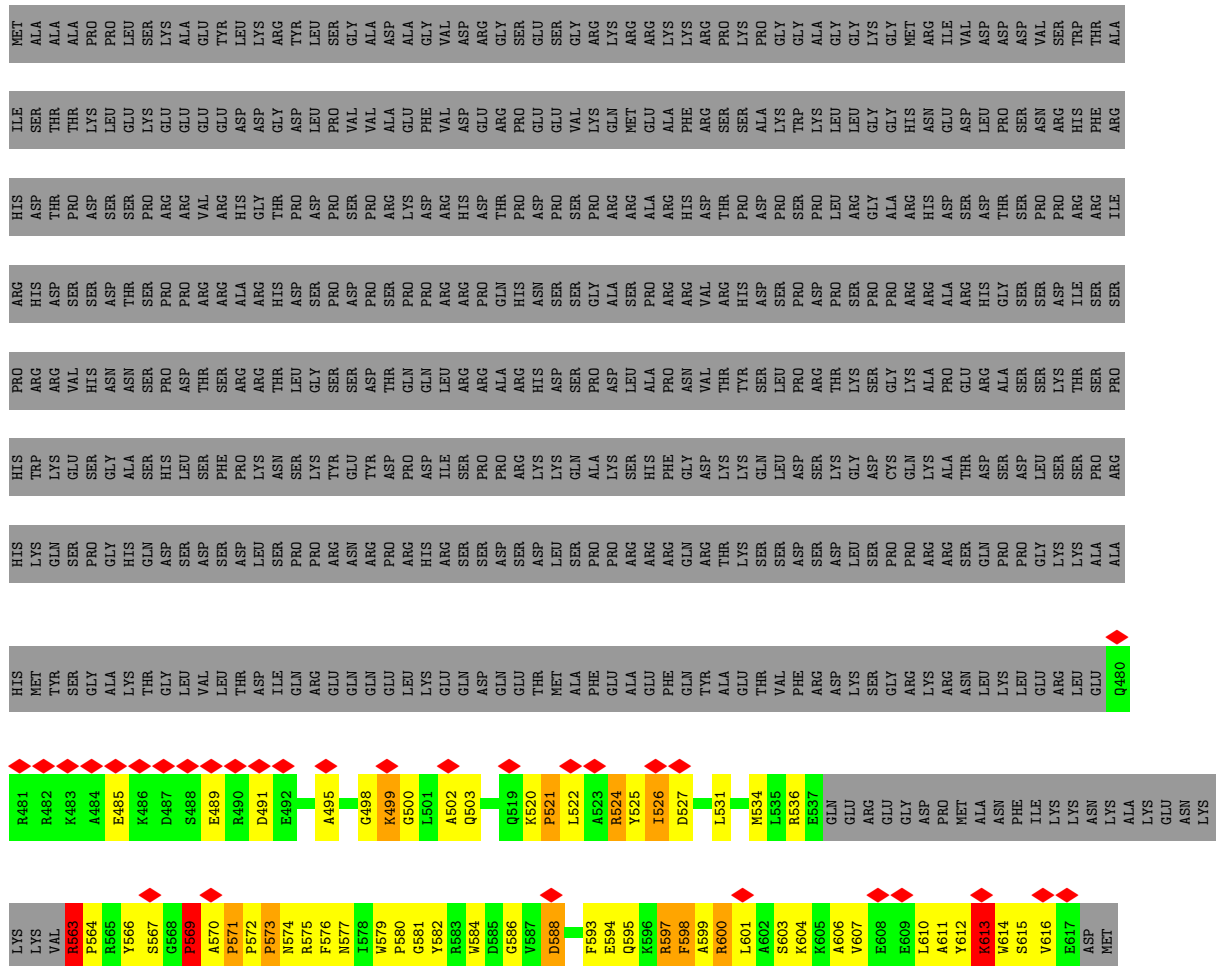






• Molecule 35: Smad nuclear-interacting protein 1

• Molecule 36: RNA-binding motif protein, X-linked 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96523	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0346	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.69	10/18665 (0.1%)	0.77	26/25340 (0.1%)
2	B	0.73	2/1970 (0.1%)	0.91	7/3060 (0.2%)
3	C	0.79	1/6864 (0.0%)	0.96	10/9334 (0.1%)
4	D	0.33	0/8527	0.59	0/11887
5	E	0.64	0/2392	0.79	0/3242
6	a	0.47	0/397	0.61	0/549
6	h	0.46	0/391	0.61	0/540
7	b	0.49	0/404	0.72	0/561
7	i	0.50	0/421	0.73	0/583
8	c	0.57	0/405	0.73	0/563
8	j	0.57	0/405	0.73	0/563
9	d	0.68	0/479	0.84	0/666
9	k	0.70	0/420	0.85	0/583
10	f	0.75	0/360	0.81	0/497
10	m	0.75	0/360	0.81	0/497
11	e	0.65	0/390	0.80	0/542
11	l	0.64	0/390	0.80	0/542
12	g	0.54	0/362	0.71	0/501
12	n	0.54	0/332	0.72	0/458
13	F	0.39	0/2224	0.86	0/3462
14	G	0.35	0/1717	0.95	1/2664 (0.0%)
15	H	0.59	7/3217 (0.2%)	1.06	18/4997 (0.4%)
16	o	0.61	0/803	1.41	2/1119 (0.2%)
17	p	1.01	1/810 (0.1%)	1.46	4/1122 (0.4%)
18	w	0.53	5/2376 (0.2%)	0.67	13/3269 (0.4%)
19	u	0.23	0/519	0.62	4/717 (0.6%)
20	v	0.36	0/482	0.81	7/666 (1.1%)
21	1	0.33	0/7826	0.51	0/10617
22	2	0.52	3/1277 (0.2%)	0.73	7/1724 (0.4%)
23	3	0.32	0/9408	0.53	0/12767
24	4	0.83	2/535 (0.4%)	0.98	4/724 (0.6%)
25	5	0.29	0/823	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	6	0.29	0/678	0.51	0/909
27	7	0.31	0/556	0.45	0/751
28	J	0.62	0/3500	0.73	0/4750
29	L	0.41	0/1103	0.57	0/1487
30	M	0.29	0/272	0.49	0/363
31	P	0.83	1/841 (0.1%)	1.01	2/1117 (0.2%)
32	R	0.66	5/2351 (0.2%)	0.86	7/3163 (0.2%)
33	T	1.05	1/2522 (0.0%)	1.11	4/3438 (0.1%)
34	V	0.55	0/2234	0.67	1/3111 (0.0%)
35	X	0.27	0/1011	0.48	0/1348
36	Y	0.31	0/747	0.48	0/1006
37	Z	0.57	2/772 (0.3%)	0.79	7/1056 (0.7%)
38	z	0.29	0/1414	0.51	0/1916
39	x	0.35	0/2871	0.53	3/3981 (0.1%)
All	All	0.57	40/96823 (0.0%)	0.76	127/133875 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
3	C	0	3
4	D	0	1
9	d	0	1
9	k	0	1
21	1	0	9
22	2	0	1
23	3	0	4
27	7	0	1
30	M	0	1
32	R	0	1
33	T	0	2
35	X	0	1
All	All	0	33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	w	457	SER	CB-OG	8.21	1.52	1.42
18	w	483	SER	CB-OG	7.46	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	142	C	C1'-N1	7.35	1.59	1.48
22	2	655	SER	CB-OG	7.35	1.51	1.42
1	A	406	TRP	CB-CG	-7.08	1.37	1.50

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	83	PRO	CA-CB-CG	10.19	124.17	104.80
22	2	636	MET	CG-SD-CE	9.28	115.05	100.20
37	Z	569	PRO	CA-N-CD	-8.56	99.52	111.50
37	Z	573	PRO	CA-N-CD	-8.45	99.67	111.50
1	A	404	LEU	CB-CG-CD1	8.13	124.82	111.00

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	PHE	Peptide
1	A	346	ASP	Peptide
1	A	408	PRO	Peptide
1	A	433	GLU	Peptide
1	A	697	MET	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18165	0	17930	1529	0
2	B	1768	0	897	123	0
3	C	6716	0	6691	968	0
4	D	8528	0	3745	69	0
5	E	2338	0	2272	136	0
6	a	399	0	173	0	0
6	h	393	0	170	0	0
7	b	405	0	170	0	0
7	i	422	0	177	0	0
8	c	406	0	170	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	j	406	0	170	0	0
9	d	480	0	200	0	0
9	k	422	0	175	0	0
10	f	361	0	158	0	0
10	m	361	0	158	0	0
11	e	391	0	163	0	0
11	l	391	0	163	0	0
12	g	363	0	160	0	0
12	n	334	0	143	0	0
13	F	1988	0	1005	133	0
14	G	1545	0	786	121	0
15	H	2886	0	1463	239	0
16	o	804	0	350	0	0
17	p	813	0	365	0	0
18	w	2369	0	1298	0	0
19	u	525	0	216	0	0
20	v	486	0	206	0	0
21	1	7702	0	7389	291	0
22	2	1252	0	1040	56	0
23	3	9220	0	9139	481	0
24	4	527	0	438	40	0
25	5	807	0	729	27	0
26	6	670	0	654	21	0
27	7	540	0	509	25	0
28	J	3463	0	2544	106	0
29	L	1077	0	1067	54	0
30	M	267	0	225	23	0
31	P	829	0	814	187	0
32	R	2314	0	2189	405	0
33	T	2457	0	2416	251	0
34	V	2238	0	969	49	0
35	X	1012	0	731	18	0
36	Y	737	0	608	67	0
37	Z	755	0	591	155	0
38	z	1381	0	1298	0	0
39	x	2882	0	1308	0	0
40	A	36	0	6	0	0
41	C	32	0	12	11	0
42	C	1	0	0	0	0
42	F	5	0	0	0	0
43	6	3	0	0	0	0
43	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	94673	0	74250	4461	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 4461 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Y:37:TRP:CH2	37:Z:498:GLY:HA2	1.23	1.65
1:A:2270:PHE:HB3	4:D:1264:PRO:CB	1.34	1.57
1:A:2270:PHE:CG	4:D:1264:PRO:CB	1.89	1.56
3:C:149:LEU:HD13	3:C:427:PHE:CD2	1.38	1.54
3:C:77:VAL:HG11	33:T:196:LEU:CG	1.39	1.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2199/2335 (94%)	2049 (93%)	117 (5%)	33 (2%)	8	39
3	C	854/972 (88%)	777 (91%)	57 (7%)	20 (2%)	5	28
4	D	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	44	78
5	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	22
6	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
6	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
7	b	80/231 (35%)	78 (98%)	2 (2%)	0	100	100
7	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
8	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
9	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
9	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
10	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
10	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
11	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
12	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
16	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10	42
17	p	159/225 (71%)	138 (87%)	9 (6%)	12 (8%)	1	10
18	w	419/501 (84%)	379 (90%)	37 (9%)	3 (1%)	19	56
19	u	93/793 (12%)	87 (94%)	4 (4%)	2 (2%)	5	29
20	v	90/464 (19%)	67 (74%)	16 (18%)	7 (8%)	1	10
21	1	1022/1304 (78%)	897 (88%)	119 (12%)	6 (1%)	22	59
22	2	171/895 (19%)	154 (90%)	17 (10%)	0	100	100
23	3	1165/1217 (96%)	1086 (93%)	78 (7%)	1 (0%)	48	83
24	4	76/424 (18%)	69 (91%)	6 (8%)	1 (1%)	10	42
25	5	106/125 (85%)	90 (85%)	16 (15%)	0	100	100
26	6	87/110 (79%)	80 (92%)	7 (8%)	0	100	100
27	7	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
28	J	483/848 (57%)	452 (94%)	24 (5%)	7 (1%)	9	40
29	L	128/802 (16%)	119 (93%)	8 (6%)	1 (1%)	16	54
30	M	34/343 (10%)	30 (88%)	3 (9%)	1 (3%)	3	23
31	P	92/229 (40%)	82 (89%)	8 (9%)	2 (2%)	5	29
32	R	295/540 (55%)	249 (84%)	31 (10%)	15 (5%)	1	15
33	T	311/514 (60%)	282 (91%)	17 (6%)	12 (4%)	2	18
34	V	443/908 (49%)	412 (93%)	26 (6%)	5 (1%)	12	46
35	X	142/396 (36%)	131 (92%)	11 (8%)	0	100	100
36	Y	102/322 (32%)	91 (89%)	11 (11%)	0	100	100
37	Z	109/619 (18%)	93 (85%)	10 (9%)	6 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	z	176/472 (37%)	170 (97%)	6 (3%)	0	100	100
39	x	561/1041 (54%)	536 (96%)	20 (4%)	5 (1%)	14	50
All	All	12645/20929 (60%)	11680 (92%)	812 (6%)	153 (1%)	14	44

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	92	LEU
1	A	167	PRO
1	A	188	LEU
1	A	331	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1954/2108 (93%)	1850 (95%)	104 (5%)	19	41
3	C	745/866 (86%)	677 (91%)	68 (9%)	7	25
5	E	256/300 (85%)	244 (95%)	12 (5%)	22	44
18	w	49/446 (11%)	47 (96%)	2 (4%)	26	48
21	1	735/1104 (67%)	735 (100%)	0	100	100
22	2	94/776 (12%)	90 (96%)	4 (4%)	25	47
23	3	1018/1051 (97%)	1017 (100%)	1 (0%)	92	94
24	4	39/336 (12%)	37 (95%)	2 (5%)	20	42
25	5	74/109 (68%)	74 (100%)	0	100	100
26	6	76/95 (80%)	76 (100%)	0	100	100
27	7	57/77 (74%)	57 (100%)	0	100	100
28	J	205/751 (27%)	194 (95%)	11 (5%)	18	40
29	L	110/709 (16%)	105 (96%)	5 (4%)	23	45
30	M	25/294 (8%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	P	90/203 (44%)	77 (86%)	13 (14%)	2	13
32	R	220/463 (48%)	170 (77%)	50 (23%)	0	5
33	T	268/441 (61%)	251 (94%)	17 (6%)	15	36
35	X	50/349 (14%)	44 (88%)	6 (12%)	4	17
36	Y	57/291 (20%)	56 (98%)	1 (2%)	54	71
37	Z	47/545 (9%)	39 (83%)	8 (17%)	1	10
38	z	146/416 (35%)	146 (100%)	0	100	100
39	x	1/897 (0%)	1 (100%)	0	100	100
All	All	6316/12627 (50%)	6012 (95%)	304 (5%)	24	43

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	R	89	GLN
33	T	461	SER
32	R	122	LYS
32	R	245	GLU
37	Z	597	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
23	3	264	GLN
30	M	198	GLN
23	3	304	GLN
23	3	1087	GLN
32	R	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	91/107 (85%)	37 (40%)	12 (13%)
14	G	76/274 (27%)	48 (63%)	9 (11%)
15	H	130/188 (69%)	33 (25%)	4 (3%)
2	B	82/117 (70%)	21 (25%)	10 (12%)
All	All	379/686 (55%)	139 (36%)	35 (9%)

5 of 139 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	G	151	C
14	G	153	C
15	H	46	U
13	F	25	C
13	F	7	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 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	$\# Z > 2$
40	IHP	A	3000	-	36,36,36	1.01	2 (5%)	54,60,60	1.62	12 (22%)
41	GTP	C	1500	42	26,34,34	1.18	1 (3%)	32,54,54	1.81	8 (25%)

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
40	IHP	A	3000	-	-	6/30/54/54	0/1/1/1
41	GTP	C	1500	42	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	C	1500	GTP	C6-N1	-3.52	1.32	1.37
40	A	3000	IHP	P5-O45	-2.86	1.43	1.54
40	A	3000	IHP	P2-O12	2.65	1.64	1.59

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	3000	IHP	O45-P5-O35	4.10	123.30	107.64
40	A	3000	IHP	O35-P5-O15	-3.97	88.19	105.99
41	C	1500	GTP	C5-C6-N1	3.79	120.64	113.95
41	C	1500	GTP	PA-O3A-PB	-3.79	119.84	132.83
41	C	1500	GTP	O6-C6-C5	-3.73	117.08	124.37

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	A	3000	IHP	C4-C5-O15-P5
40	A	3000	IHP	C6-C5-O15-P5
41	C	1500	GTP	PB-O3B-PG-O3G
41	C	1500	GTP	C5'-O5'-PA-O3A
41	C	1500	GTP	C5'-O5'-PA-O1A

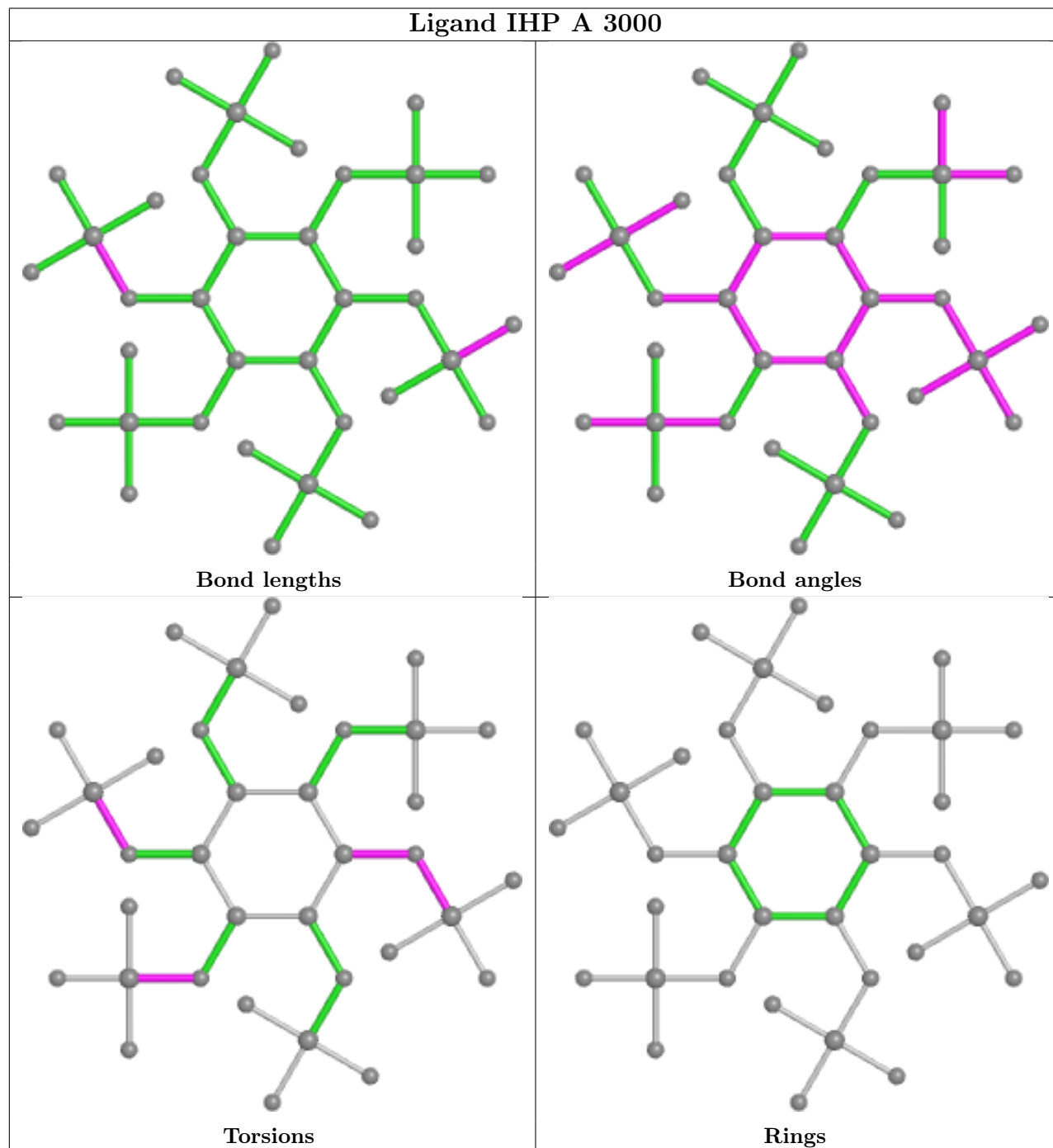
There are no ring outliers.

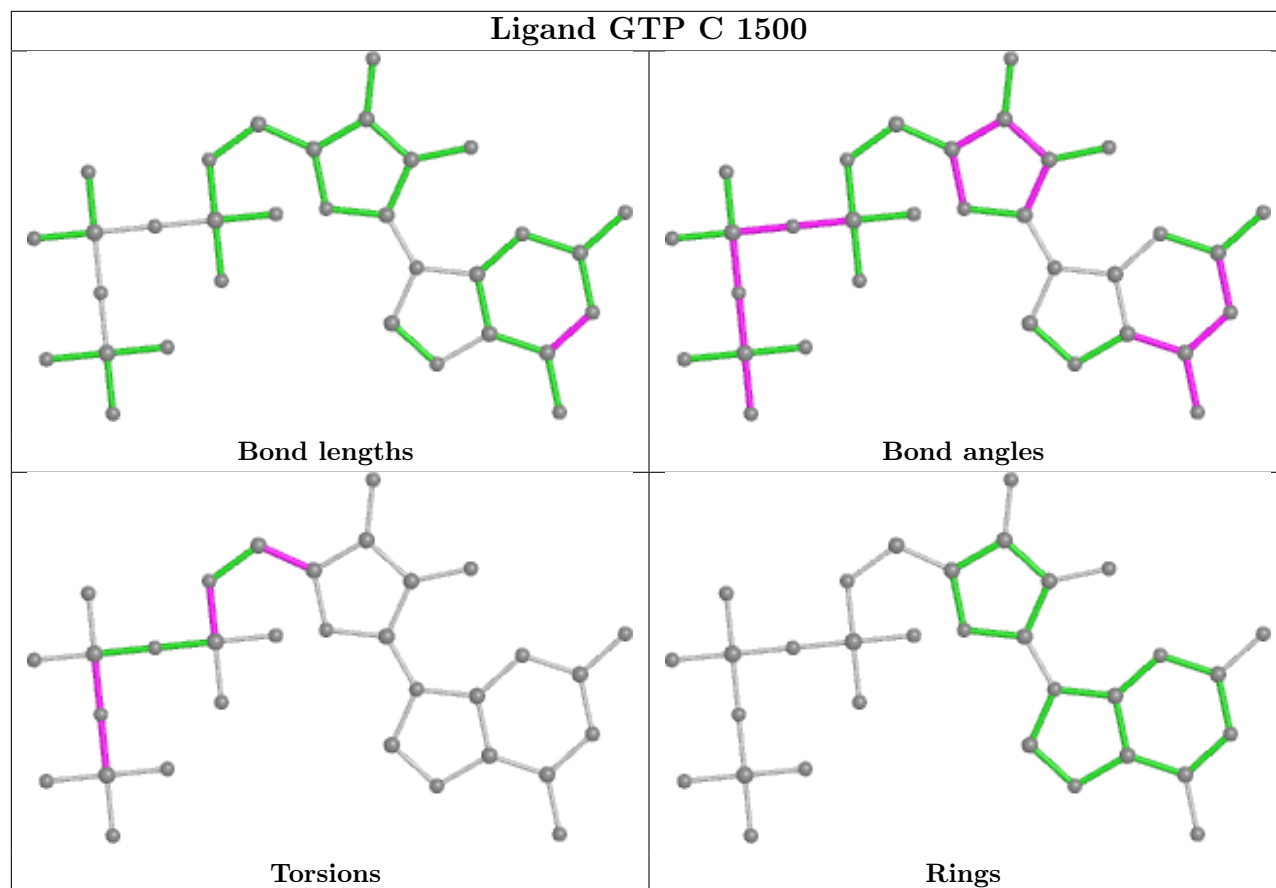
1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	C	1500	GTP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

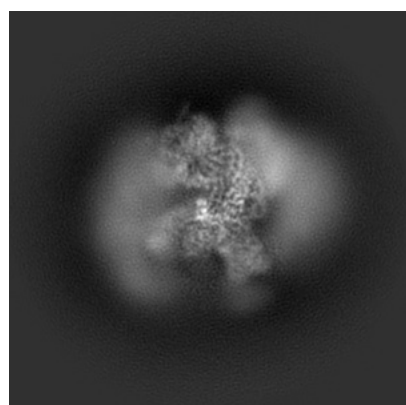
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6891. These allow visual inspection of the internal detail of the map and identification of artifacts.

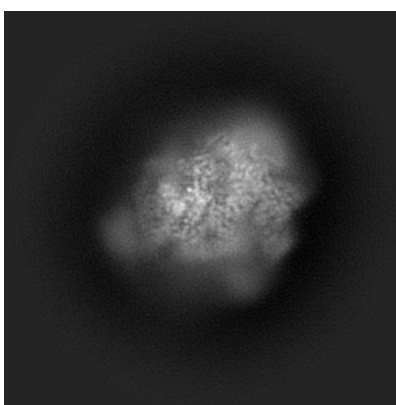
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

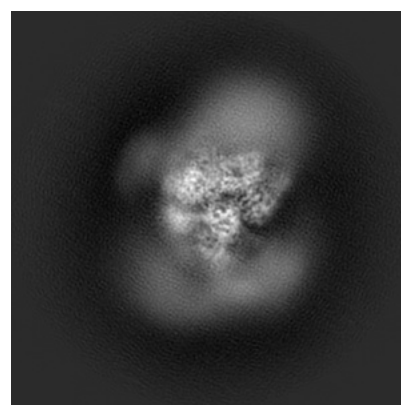
6.1.1 Primary map



X



Y

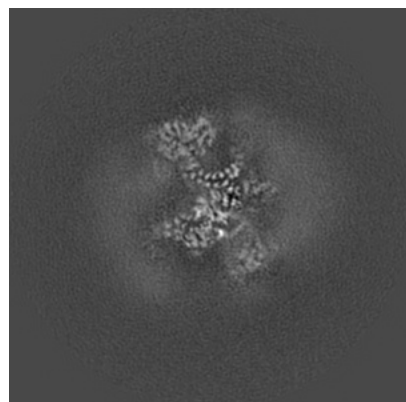


Z

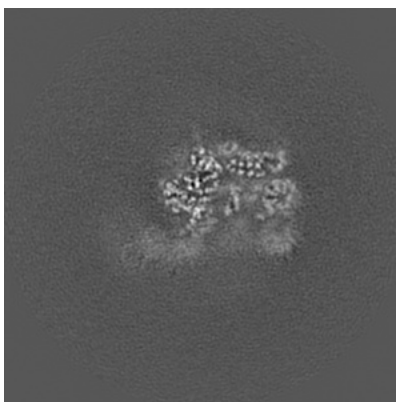
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

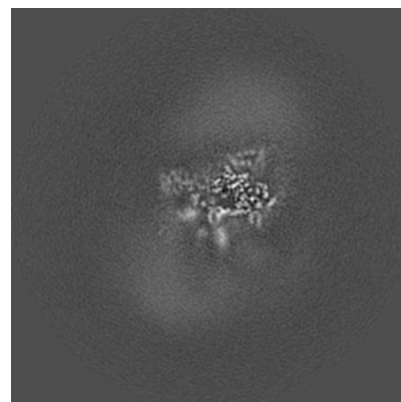
6.2.1 Primary map



X Index: 200



Y Index: 200

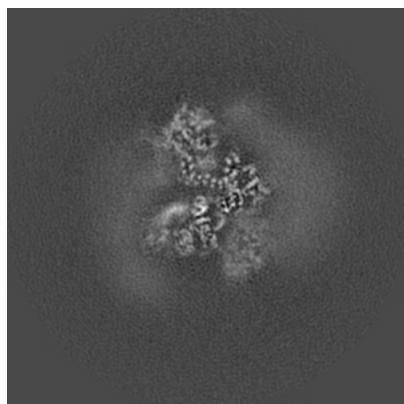


Z Index: 200

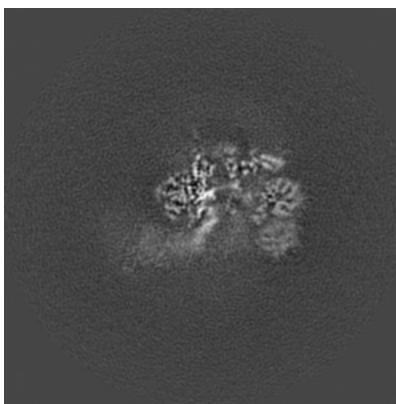
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

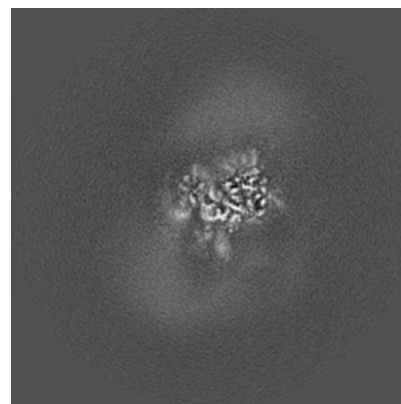
6.3.1 Primary map



X Index: 210



Y Index: 195

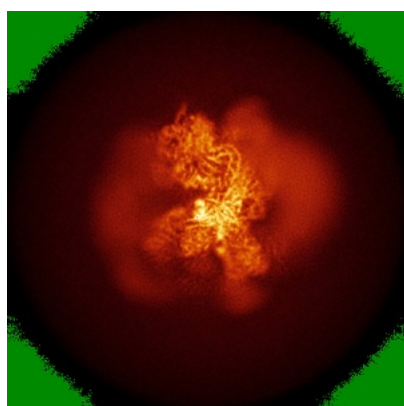


Z Index: 193

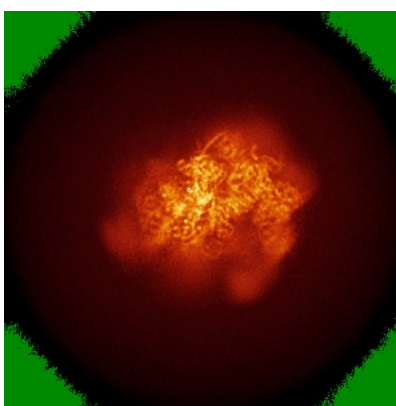
The images above show the largest variance slices of the map in three orthogonal directions.

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

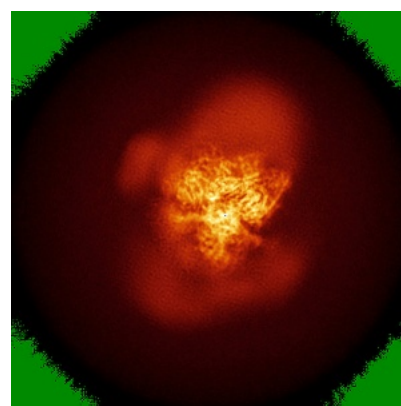
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0346. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

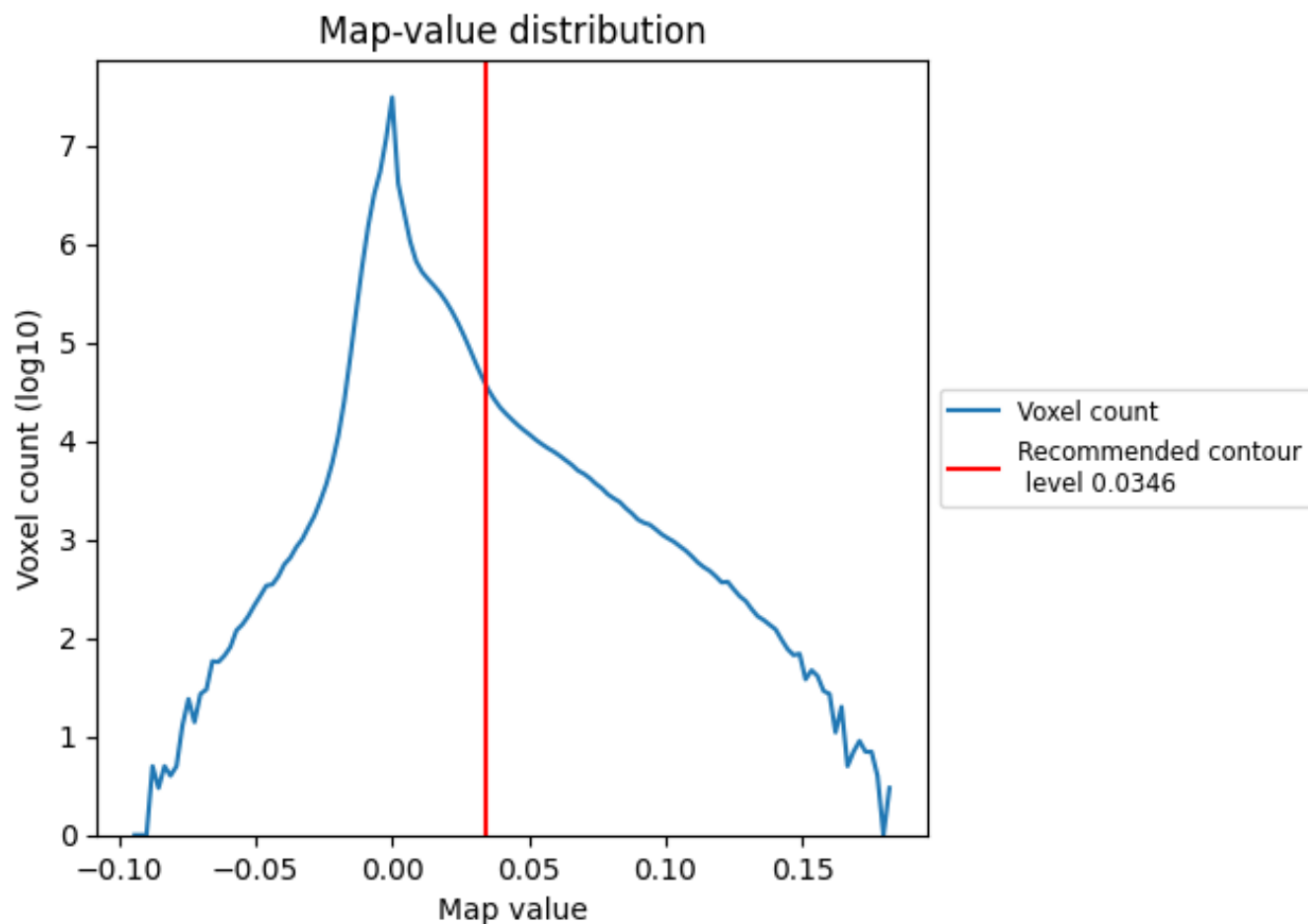
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

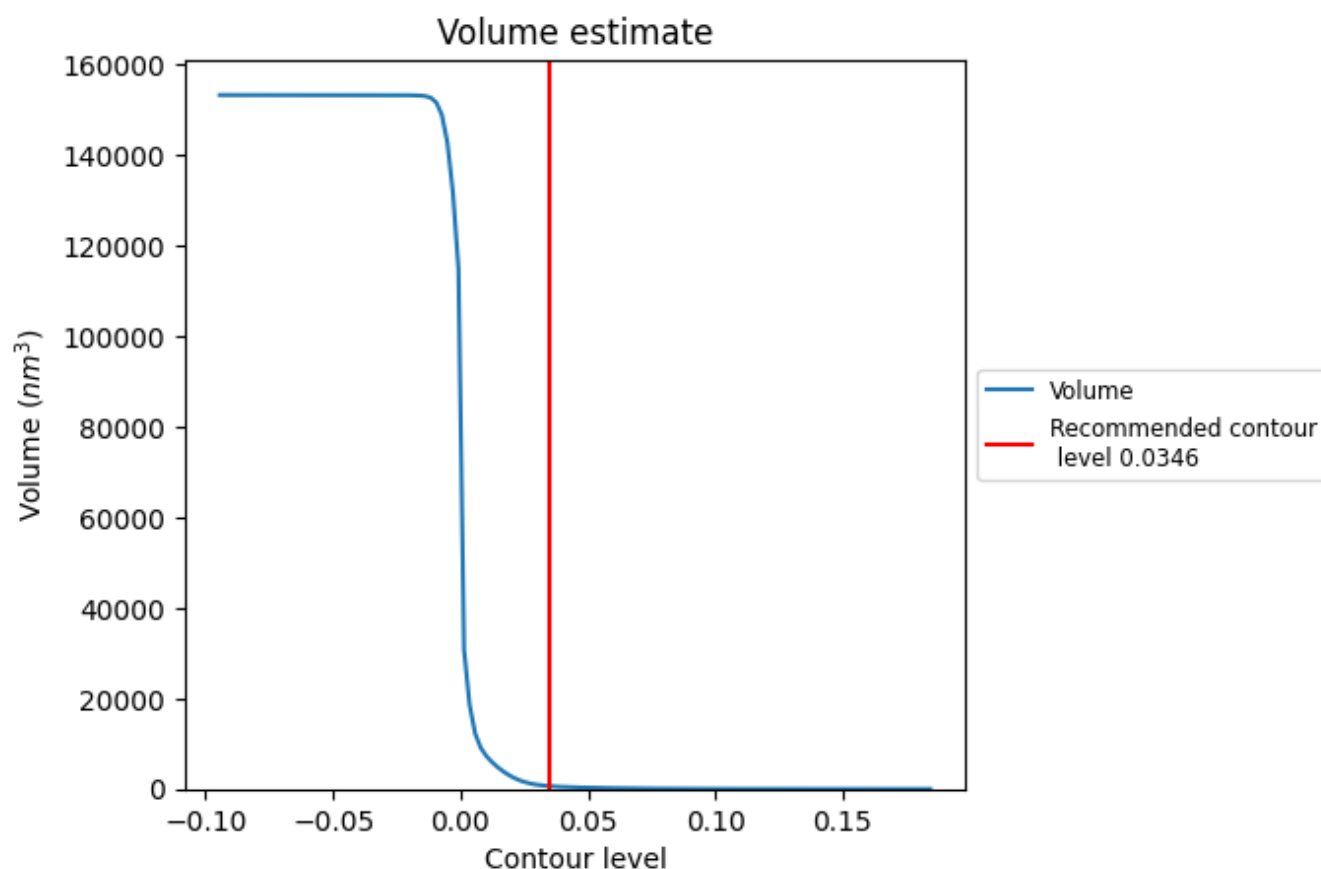
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

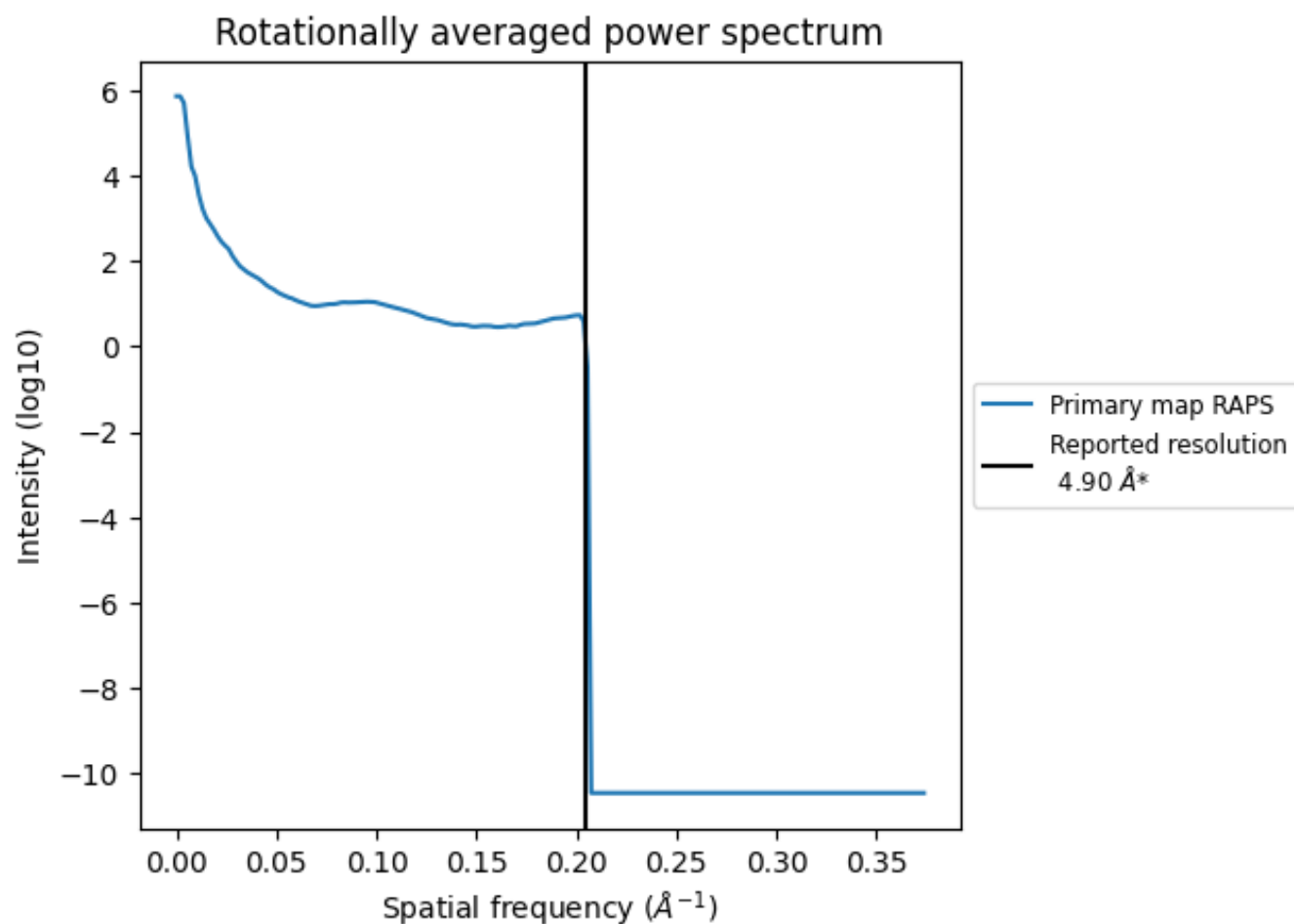
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 nm^3 ; this corresponds to an approximate mass of 580 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

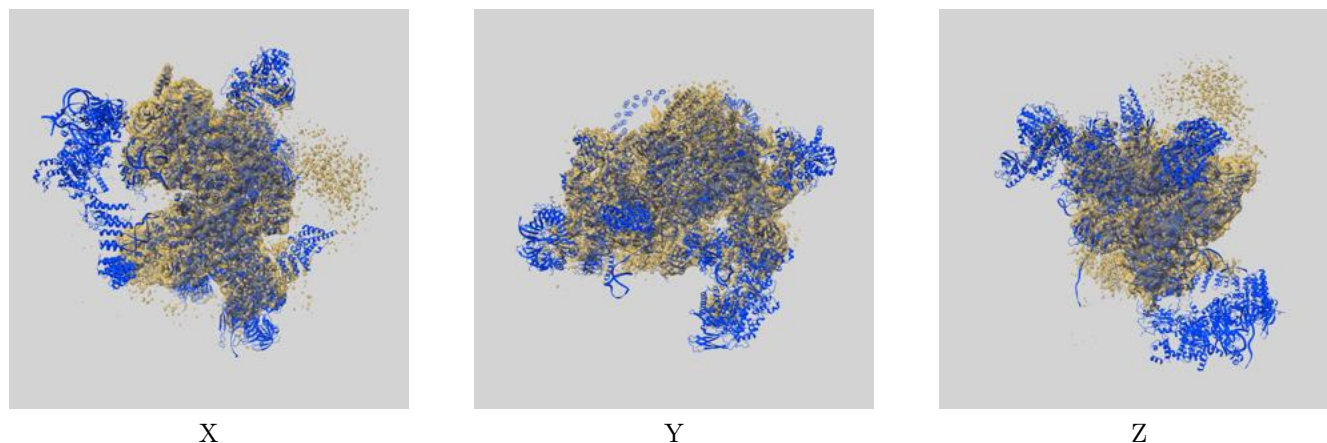
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

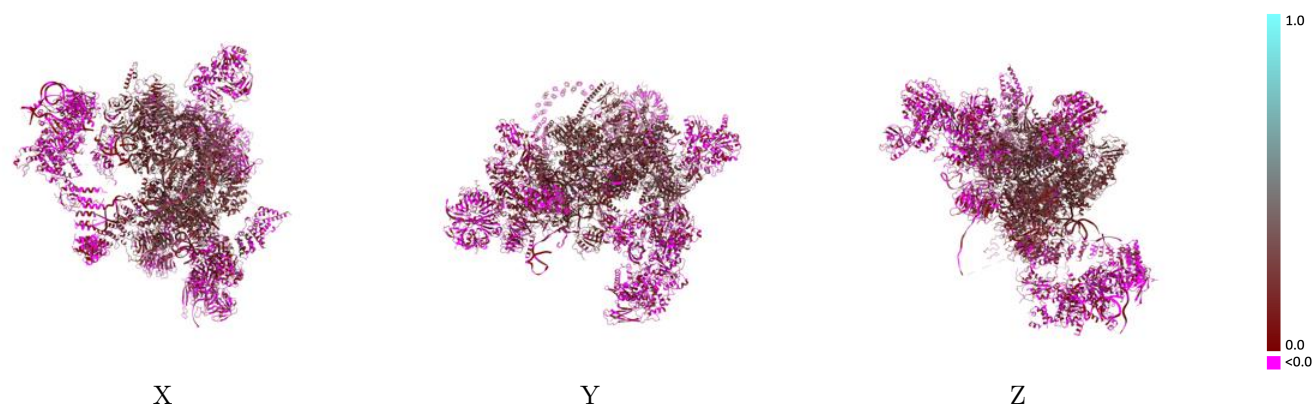
This section contains information regarding the fit between EMDB map EMD-6891 and PDB model 5Z58. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



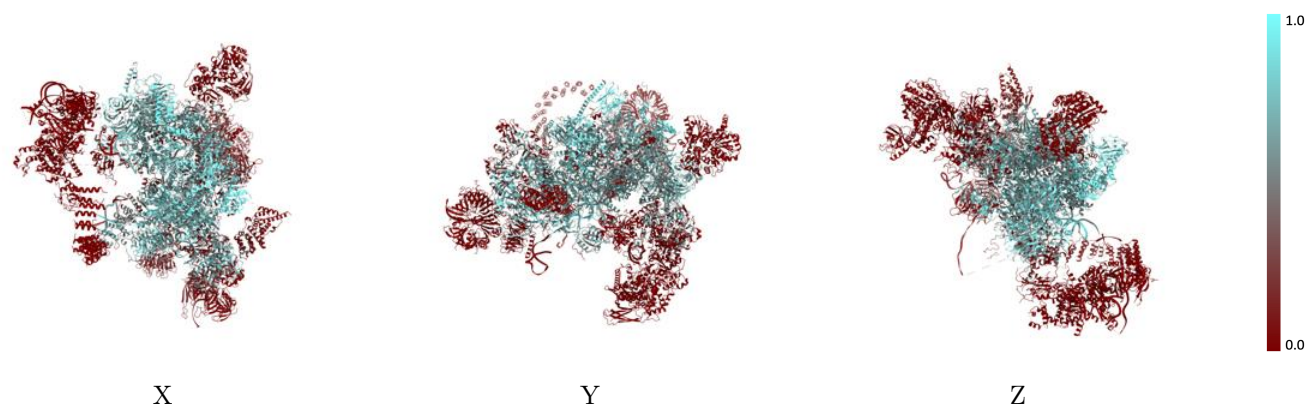
The images above show the 3D surface view of the map at the recommended contour level 0.0346 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



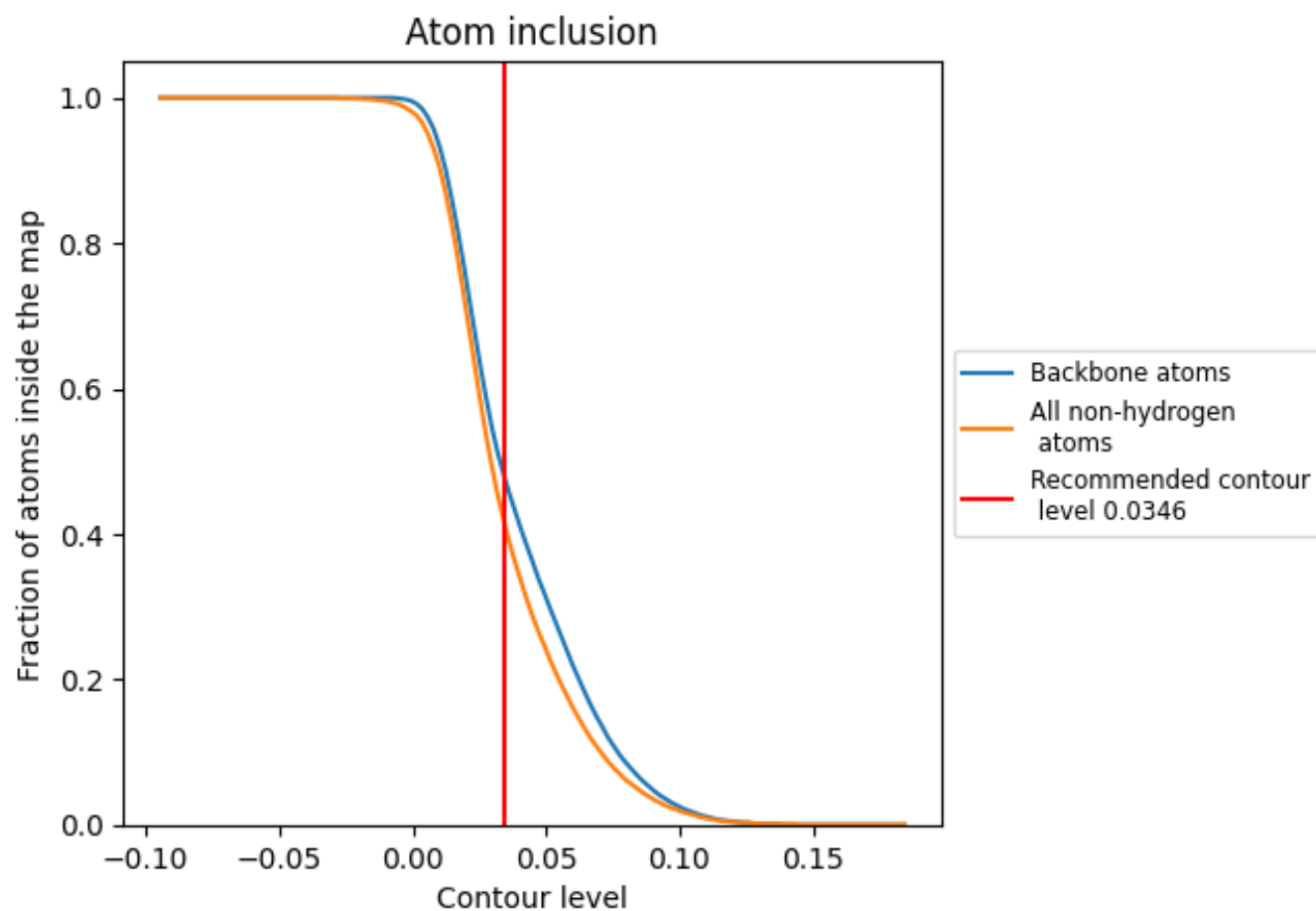
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0346).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 41% 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 (0.0346) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4120	 0.1310
1	 0.6670	 0.2300
2	 0.2970	 0.1480
3	 0.6080	 0.1670
4	 0.0730	 0.0080
5	 0.7300	 0.2390
6	 0.5060	 0.1590
7	 0.6800	 0.2240
A	 0.5570	 0.1970
B	 0.5980	 0.1040
C	 0.4530	 0.0950
D	 0.1160	 0.0400
E	 0.0260	 0.0260
F	 0.5990	 0.1470
G	 0.6230	 0.1490
H	 0.3420	 0.0880
J	 0.2790	 0.0660
L	 0.4750	 0.2070
M	 0.7170	 0.2530
P	 0.3090	 0.1160
R	 0.4080	 0.1660
T	 0.7530	 0.2280
V	 0.3420	 0.1200
X	 0.7090	 0.2160
Y	 0.6250	 0.2470
Z	 0.5950	 0.2670
a	 0.0000	 0.0170
b	 0.0050	 0.0410
c	 0.0220	 0.0060
d	 0.0940	 -0.0040
e	 0.0050	 0.0020
f	 0.0170	 -0.0230
g	 0.0000	 0.0030
h	 0.0000	 0.0340
i	 0.0000	 0.0210



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Chain	Atom inclusion	Q-score
j	 0.0000	 -0.0440
k	 0.0000	 0.0110
l	 0.0000	 0.0140
m	 0.0000	 -0.0500
n	 0.0000	 0.0110
o	 0.0000	 0.0280
p	 0.0000	 0.0160
u	 0.0000	 0.0040
v	 0.0000	 0.0460
w	 0.1150	 0.0420
x	 0.0290	 0.0110
z	 0.4980	 0.1870