



# wwPDB EM Validation Summary Report ⓘ

Oct 22, 2024 – 05:09 AM JST

PDB ID : 8I0S  
EMDB ID : EMD-35108  
Title : The cryo-EM structure of human Bact-II complex  
Authors : Zhan, X.; Lu, Y.; Shi, Y.  
Deposited on : 2023-01-11  
Resolution : 4.20 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:

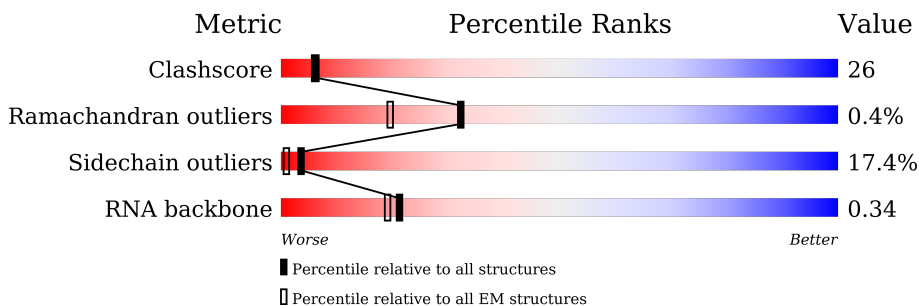
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001) 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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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  $\geq 3$ , 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	2335	
2	B	117	
3	C	972	
4	D	2136	
5	E	357	
6	F	107	
7	G	220	

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Mol	Chain	Length	Quality of chain
8	H	188	
9	I	855	
10	J	848	
11	K	343	
12	L	802	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	166	
19	T	514	
20	U	2752	
21	V	908	
22	X	1041	
23	Y	492	
24	1	1304	
25	3	1217	
26	p	225	
27	w	501	
28	2	895	
29	4	424	
30	7	110	
31	5	86	
32	y	301	

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Mol	Chain	Length	Quality of chain
33	v	464	
34	u	793	
35	9	520	
36	a	240	
36	m	240	
37	b	119	
37	n	119	
38	c	118	
38	h	118	
39	d	86	
39	i	86	
40	e	92	
40	j	92	
41	f	76	
41	k	76	
42	g	126	
42	l	126	
43	o	255	

## 2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 112874 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
			Total	C	N	O	S		
1	A	2230	17607	11288	3122	3129	68	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	98	2066	925	347	696	98	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	860	6724	4298	1122	1272	32	0	0

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

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

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

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

- Molecule 6 is a RNA chain called U6 snRNA.

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

- Molecule 7 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	G	72	1503	673	248	510	72	0	0

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	167	3539	1581	607	1184	167	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	571	2880	1738	571	571	0	0

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	249	2116	1355	380	375	6	0	0

- Molecule 11 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	46	392	246	67	76	3	0	0

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	169	1403	890	262	247	4	0	0

- Molecule 13 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	1174	740	213	209	12	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	287	Total	C	N	O	0	0
			1432	853	289	290		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	101	Total	C	N	O	S	0	0
			876	537	175	162	2		

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1329	Total	C	N	O	0	0
			6730	4072	1329	1329		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
17	R	361	Total	C	N	O	P	S	0	0
			2760	1694	524	529	1	12		

- Molecule 18 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	158	Total	C	N	O	0	0
			770	454	158	158		

- Molecule 19 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	462	2959	1842	537	567	13	0	0

- Molecule 22 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	786	6357	4010	1133	1184	30	0	0

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	320	2556	1616	420	508	12	0	0

- Molecule 24 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1	816	6468	4154	1110	1165	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	3	1177	9210	5849	1563	1753	45	0	0

- Molecule 26 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	p	167	841	507	167	167	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	w	434	2275	1287	491	493	4	0	0

- Molecule 28 is a protein called Splicing factor 3B subunit 2.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	2	250	1803	1132	340	324	7	0	0

- Molecule 29 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	4	161	792	470	161	161	0	0

- Molecule 30 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	7	81	613	376	109	115	13	0	0

- Molecule 31 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	5	77	635	403	110	117	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	y	79	390	232	79	79	0	0

- Molecule 33 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	v	158	964	558	203	200	3	0	0

- Molecule 34 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	u	187	834	460	187	187	0	0

- Molecule 35 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
35	9	338	2307	1429	420	450	8	0	0

- Molecule 36 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
36	a	86	344	172	86	86		0	0
36	m	82	413	249	82	82		0	0

- Molecule 37 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
37	b	82	328	164	82	82		0	0
37	n	80	402	242	80	80		0	0

- Molecule 38 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
38	c	97	388	194	97	97		0	0
38	h	95	482	292	95	95		0	0

- Molecule 39 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
39	d	74	296	148	74	74		0	0
39	i	72	359	215	72	72		0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
40	e	79	316	158	79	79		0	0
40	j	81	403	241	81	81		0	0

- Molecule 41 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	f	74	296	148	74	74	0	0
41	k	73	364	218	73	73	0	0

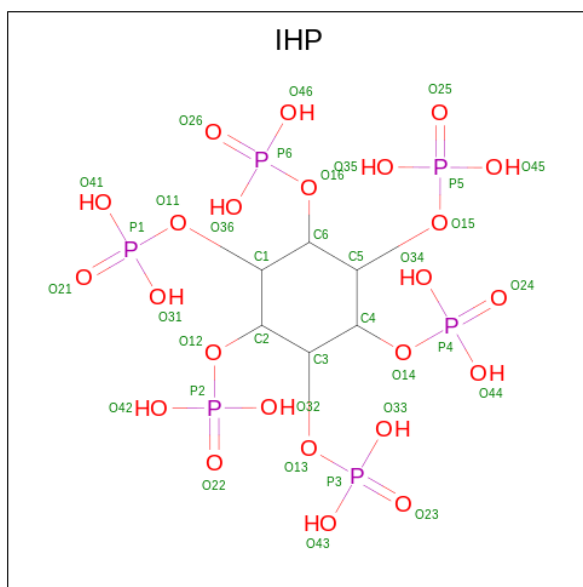
- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	g	81	324	162	81	81	0	0
42	l	83	415	249	83	83	0	0

- Molecule 43 is a protein called U2 small nuclear ribonucleoprotein A'.

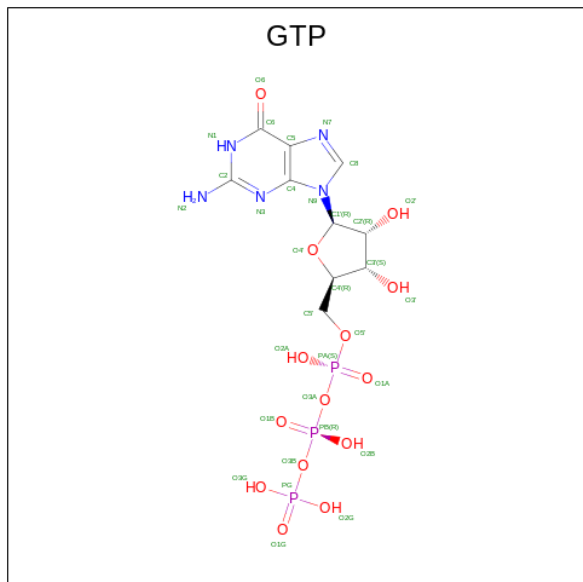
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	o	162	816	492	162	162	0	0

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



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

- Molecule 45 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	
45	C	1	32	10	5	14	3	0

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
46	C	1	1	1	0
46	F	6	6	6	0

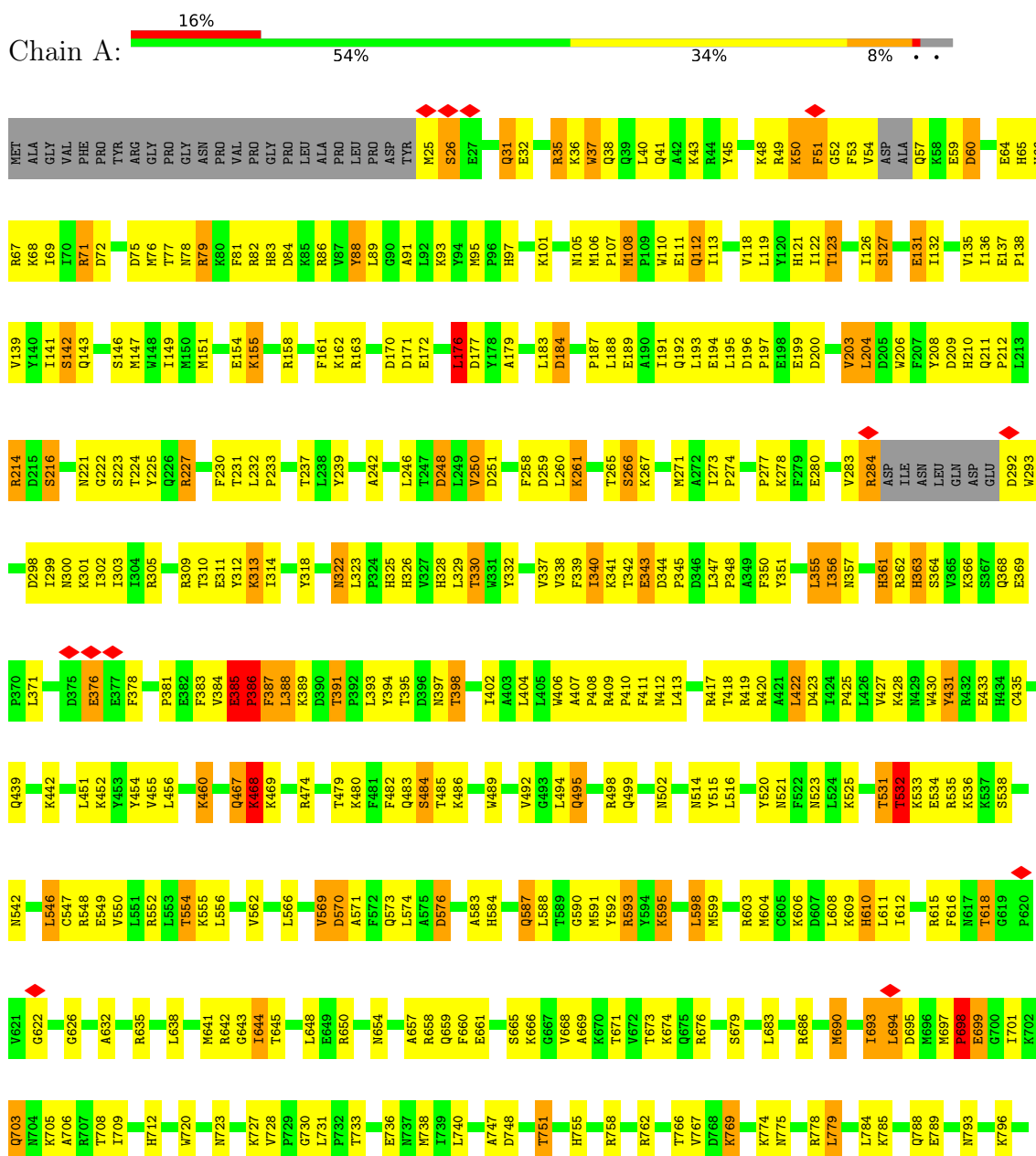
- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
47	K	1	1	1	0
47	N	3	3	3	0
47	7	3	3	3	0

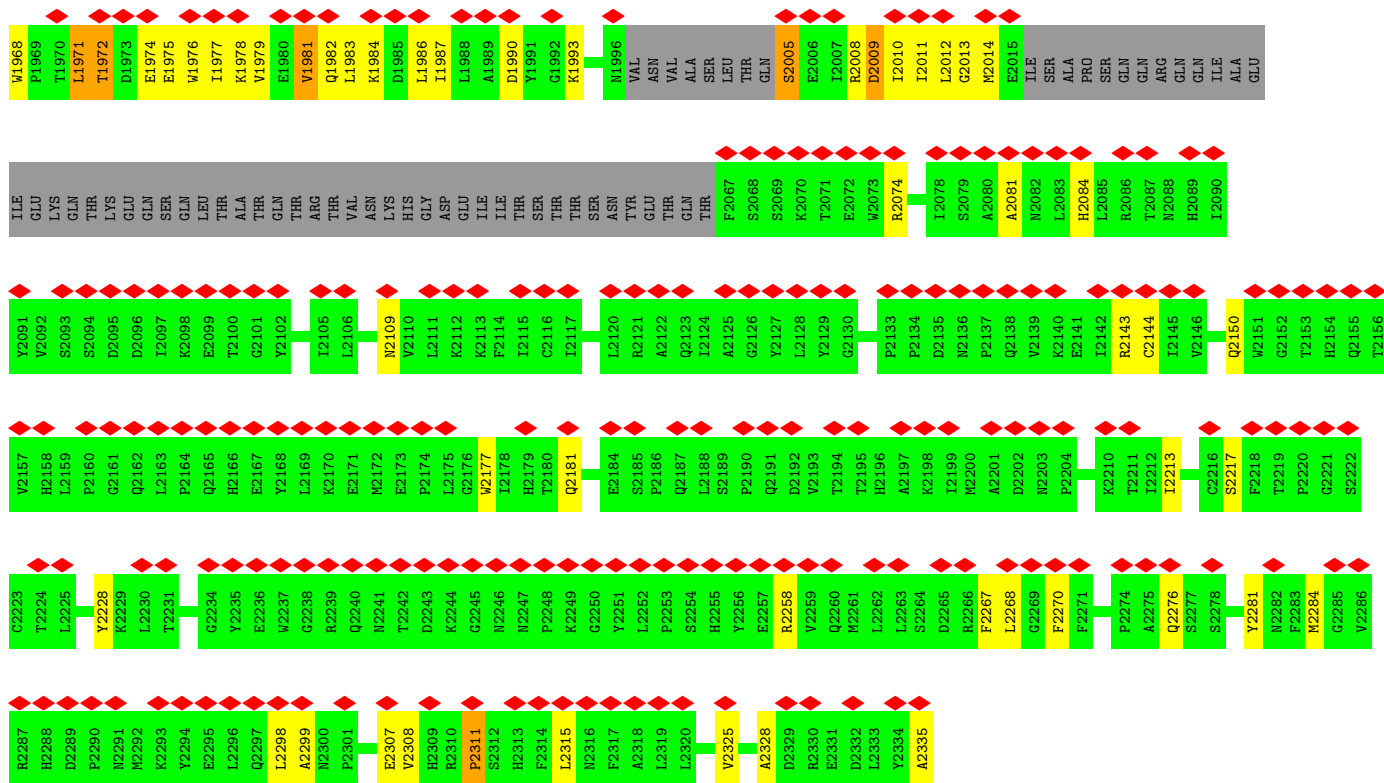
### 3 Residue-property plots [i](#)

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.

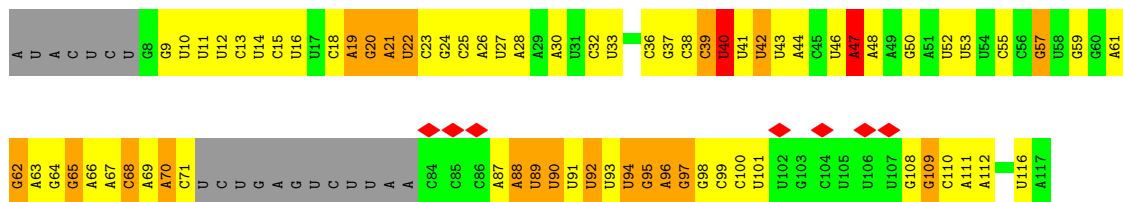
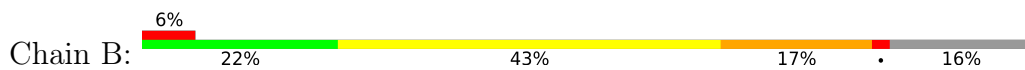
- Molecule 1: Pre-mRNA-processing-splicing factor 8



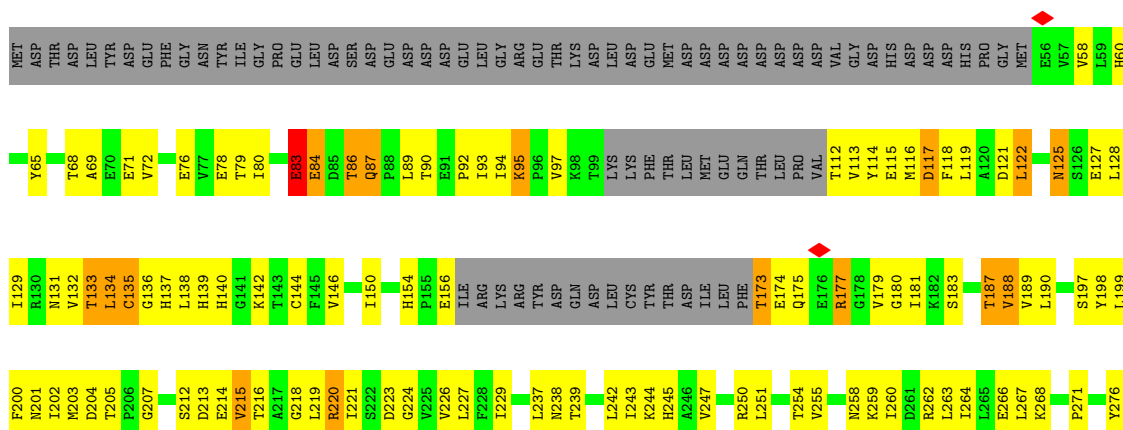
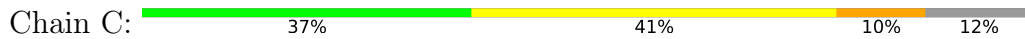
L1907	A1846	V1785	D1706	A1633	V1549	Y1470	L1391	L1303	T1292	N1122	1988	T887	Y800
K1908	A1847	Y1786	H1712	S1634	G1550	Y1473	Q1394	K1306	S1203	E1123	I1000	Q888	I801
A1909	L1848	R1787	H1713	Y1635	F1551	D1473	Q1394	K1306	Y1204	M1124	I1000	R889	T802
T1910	S1713	W1788	A1714	W1637	Q1554	E1482	I1397	S1309	E1205	E1205	E1001	A890	Y810
P1912	R1850	T1789	Y1715	M1638	L1555	E1486	Q1398	S1310	F1207	G1126	D1002	F891	S819
Q1913	S1851	H1791	G1716	S1640	T1558	E1486	Q1399	F1311	T1298	Y1128	D1007	K892	
M1914	L1852	K1792	R1641	G1559	G1559	L1489	M1400	V1315	H1209	M1129	T1010	Y902	P824
V1915	P1853	T1793	W1718	P1642	K1565	L1489	R1401	V1316	M1210	A1011	A1011	L905	F827
L1916	V1854	F1794	F1719	S1643	K1565	F1490	R1402	Y1317	G1212	K1131	A1012	L905	K833
L1917	E1855	F1794	L1644	L1644	G1491	K1491	L1403	T1318	G1213	K1132	M1013	P828	P828
M1918	E1856	G1796	L1645	L1645	G1492	G1492	E1406	K1320	W1214	R1136	M1014	Y809	L830
L1818	Q1857	M1797	K1649	K1649	T1493	T1493	D1407	K1321	M1215	D1137	Y1018	P913	S831
Y1920	P1858	L1798	M1652	M1652	Y1494	Y1494	L1408	E1321	M1218	R1139	Y1019	L914	Y832
D1922	K1859	T1799	M1653	L1725	P1496	P1496	E1409	G1324	E1219	R1138	E1018	Y832	Y832
W1923	Q1860	T1800	Q1575	Q1575	T1497	T1497	E1410	L1325	V1220	M1143	D1021	K916	K834
L1924	I1861	K1801	I1576	I1576	W1498	W1498	S1411	L1328	T1221	K1144	M1022	D923	D835
K1925	T1862	G1802	A1579	A1579	F1502	F1502	D1413	L1328	K1222	H1146	S1027	Y839	L839
T1926	V1863	G1806	H1580	H1580	W1503	W1503	R1414	H1332	E1223	D1146	Y1028	E929	L839
L1927	T1864	A1806	L1581	L1581	I1416	I1416	G1415	H1332	R1224	V1147	G1029	A930	Y832
S1928	R1865	I1807	Q1582	Q1582	Y1416	Y1416	G1415	I1335	E1235	M1148	I1030	D931	L843
S1929	G1867	F1808	W1584	W1584	P1417	P1417	R1418	Q1336	R1243	A1152	I1031	K932	E844
Y1930	I1868	I1747	I1585	I1585	R1418	R1418	M1420	Q1337	Q1246	V1153	R1032	R833	R845
L1931	L1869	R1748	I1589	V1590	ALA	ALA	G1420	S1338	Q1246	K1158	S1038	W939	E848
A1932	D1870	L1751	V1590	L1593	GLU	GLU	Q1424	D1339	S1251	M1159	F1039	P940	A849
P1871	R1812	S1756	L1593	L1593	GLU	GLU	Q1424	D1339	G1252	R1160	I1040	K941	Y850
L1872	R1813	S1756	E1600	E1600	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
E1873	T1814	Y1671	L1601	L1601	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
R1935	G1815	Y1671	L1601	L1601	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
V1874	Q1816	T1759	L1601	L1601	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
H1875	F1817	E1760	L1604	L1604	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
L1876	F1818	E1760	E1605	E1605	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
L1877	F1818	E1760	E1605	E1605	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
D1878	L1819	LEU	E1607	E1607	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
F1879	K1820	SER	T1608	T1608	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
P1880	I1822	SER	Q1766	Q1766	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
M1881	H1823	SER	Q1766	Q1766	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
I1882	H1824	SER	Q1766	Q1766	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
V1883	S1825	SER	Q1766	Q1766	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
I1884	V1826	SER	Q1766	Q1766	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
K1885	W1827	SER	Q1766	Q1766	GLU	GLU	Q1424	D1339	G1252	R1161	I1040	P942	S851
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• Molecule 2: U5 snRNA



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

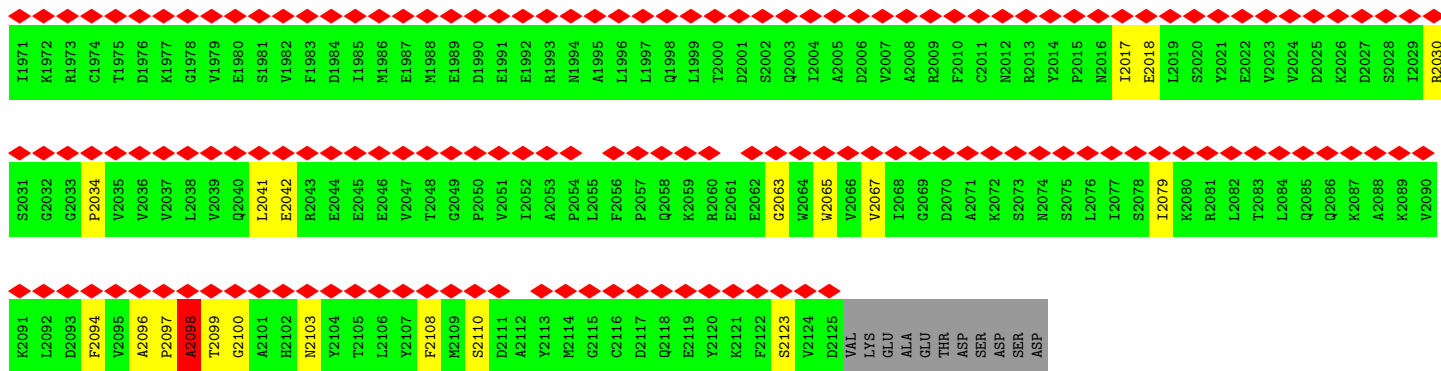




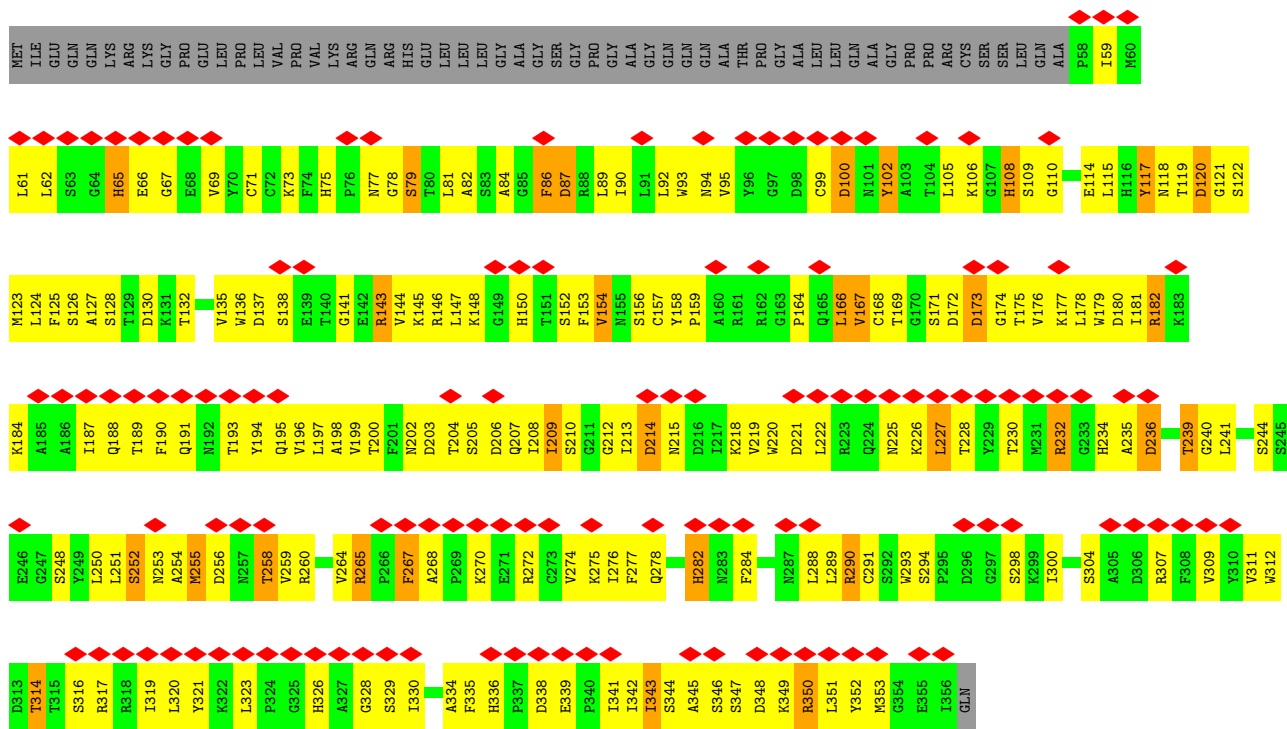


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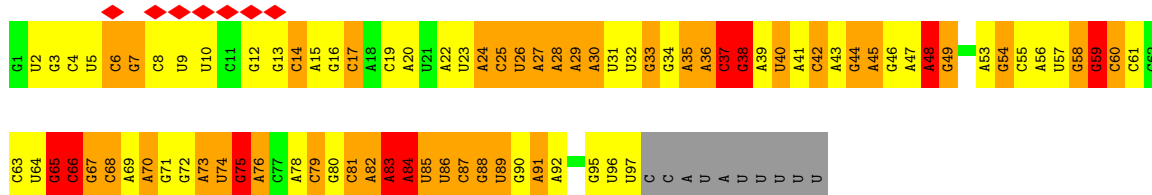
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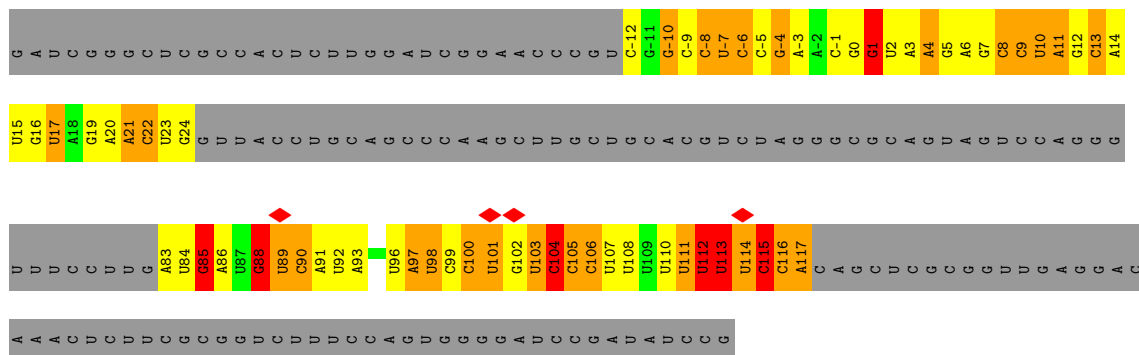
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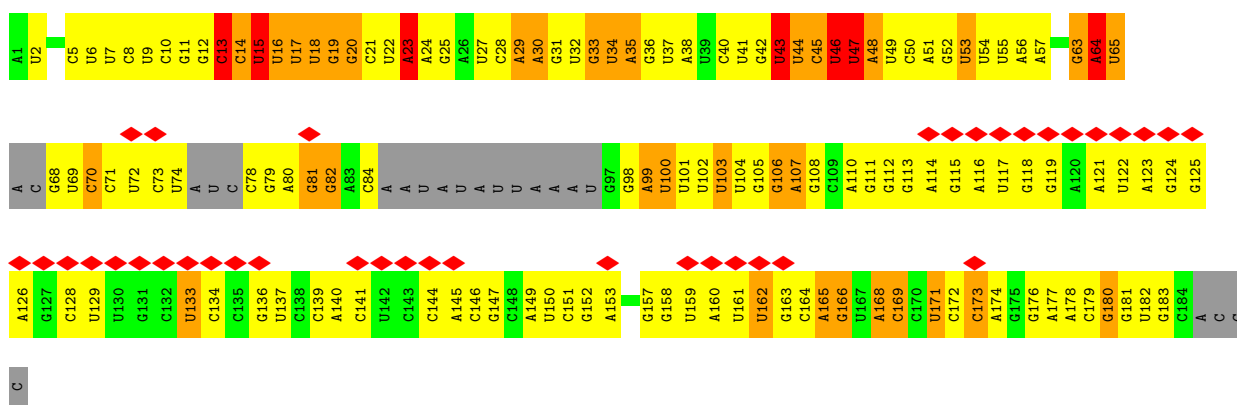
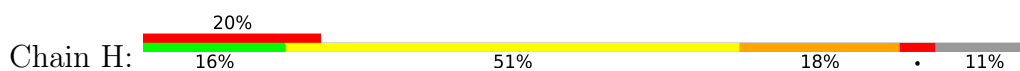
● Molecule 6: U6 snRNA



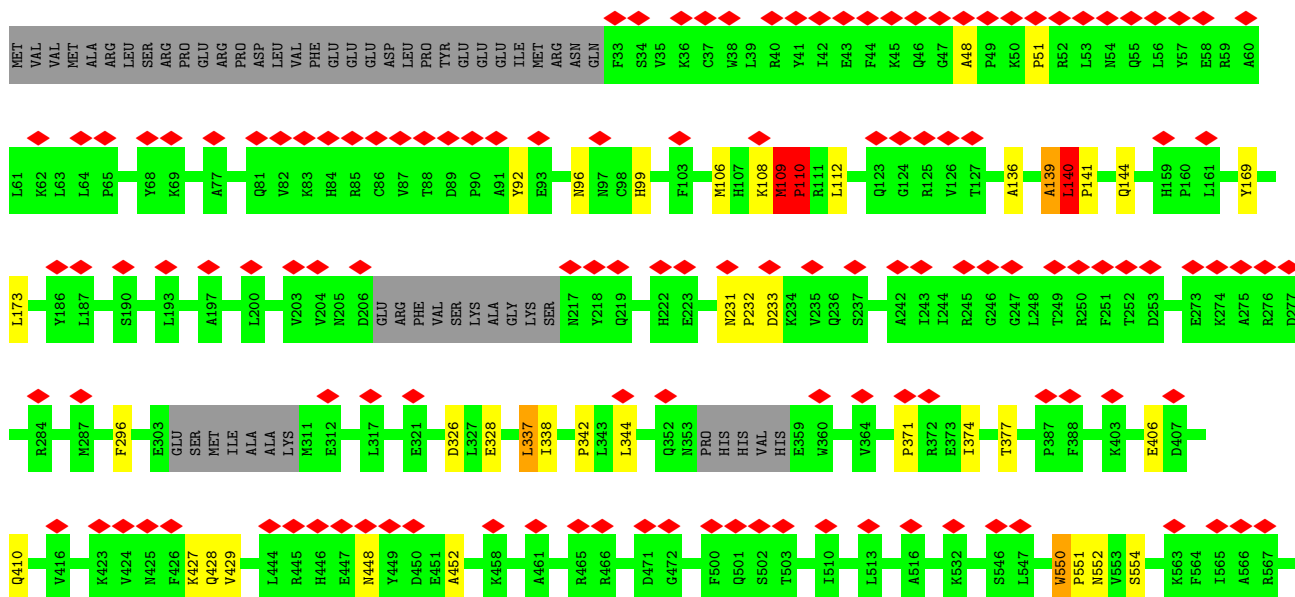
● Molecule 7: pre-mRNA

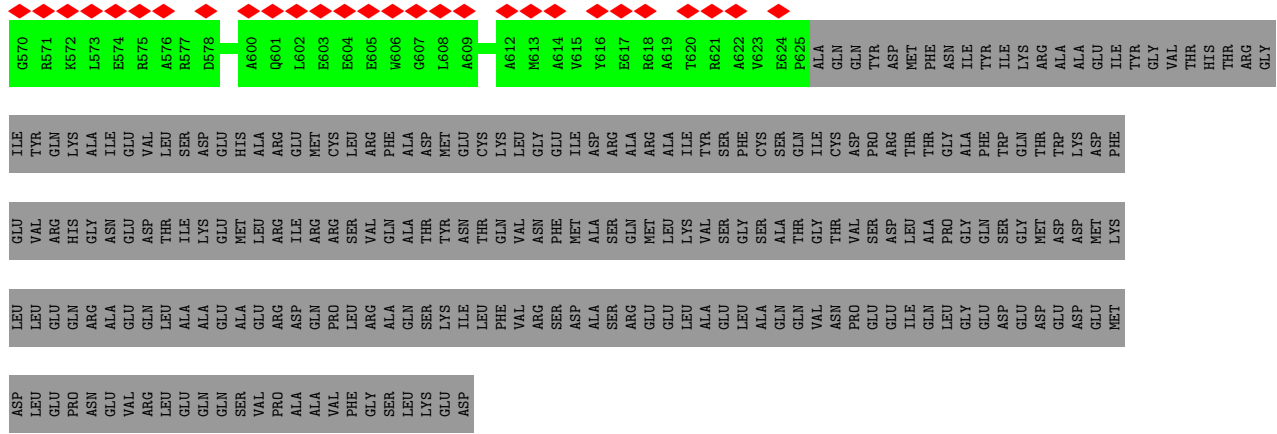


● Molecule 8: U2 snRNA

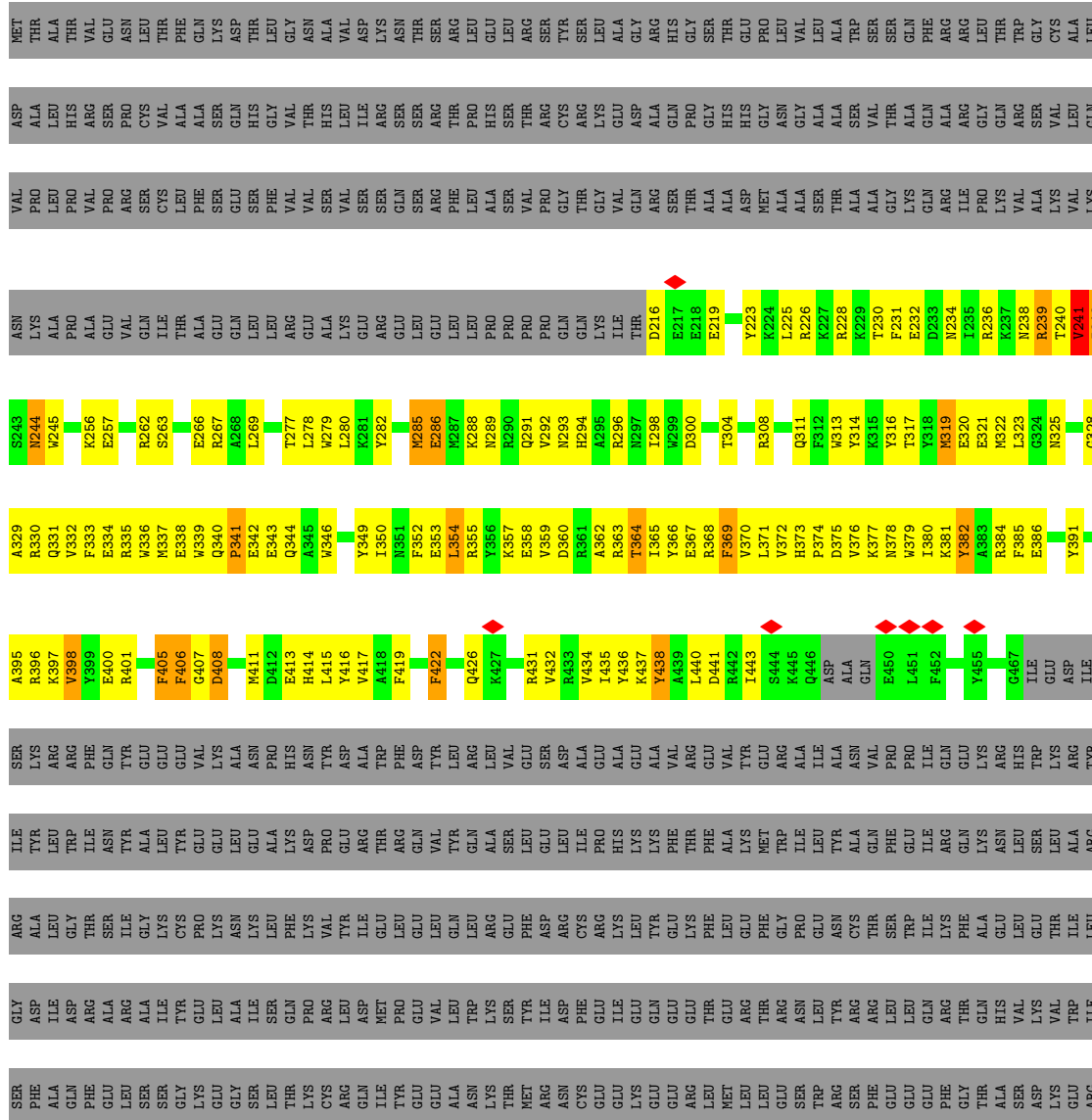


● Molecule 9: Pre-mRNA-splicing factor SYF1



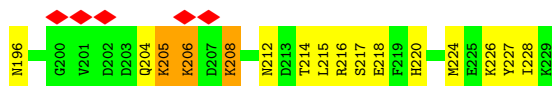
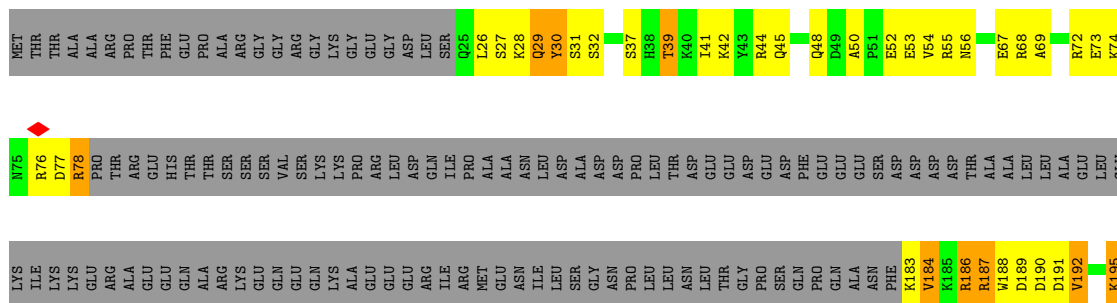


● Molecule 10: Crooked neck-like protein 1

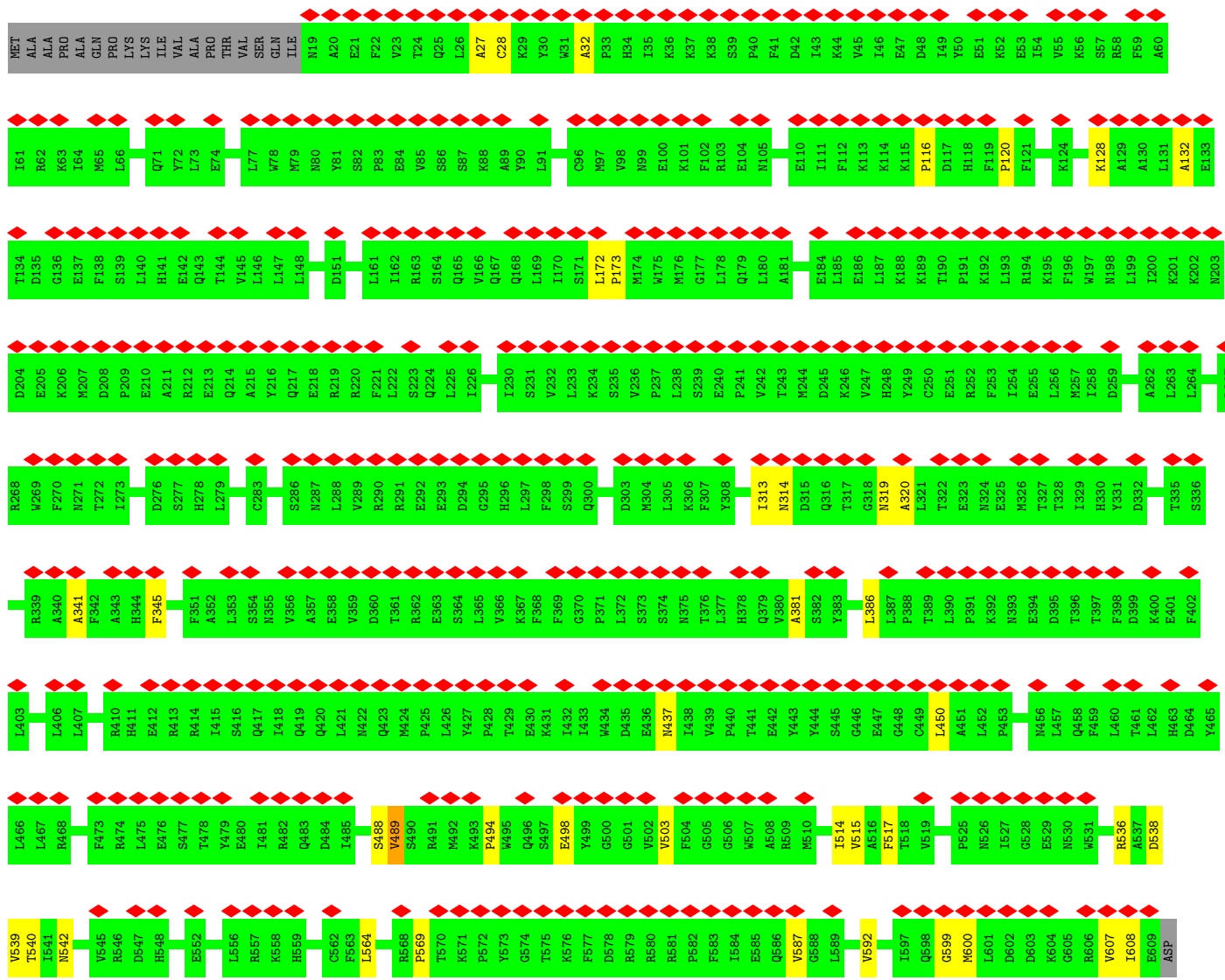
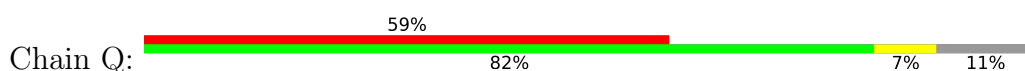




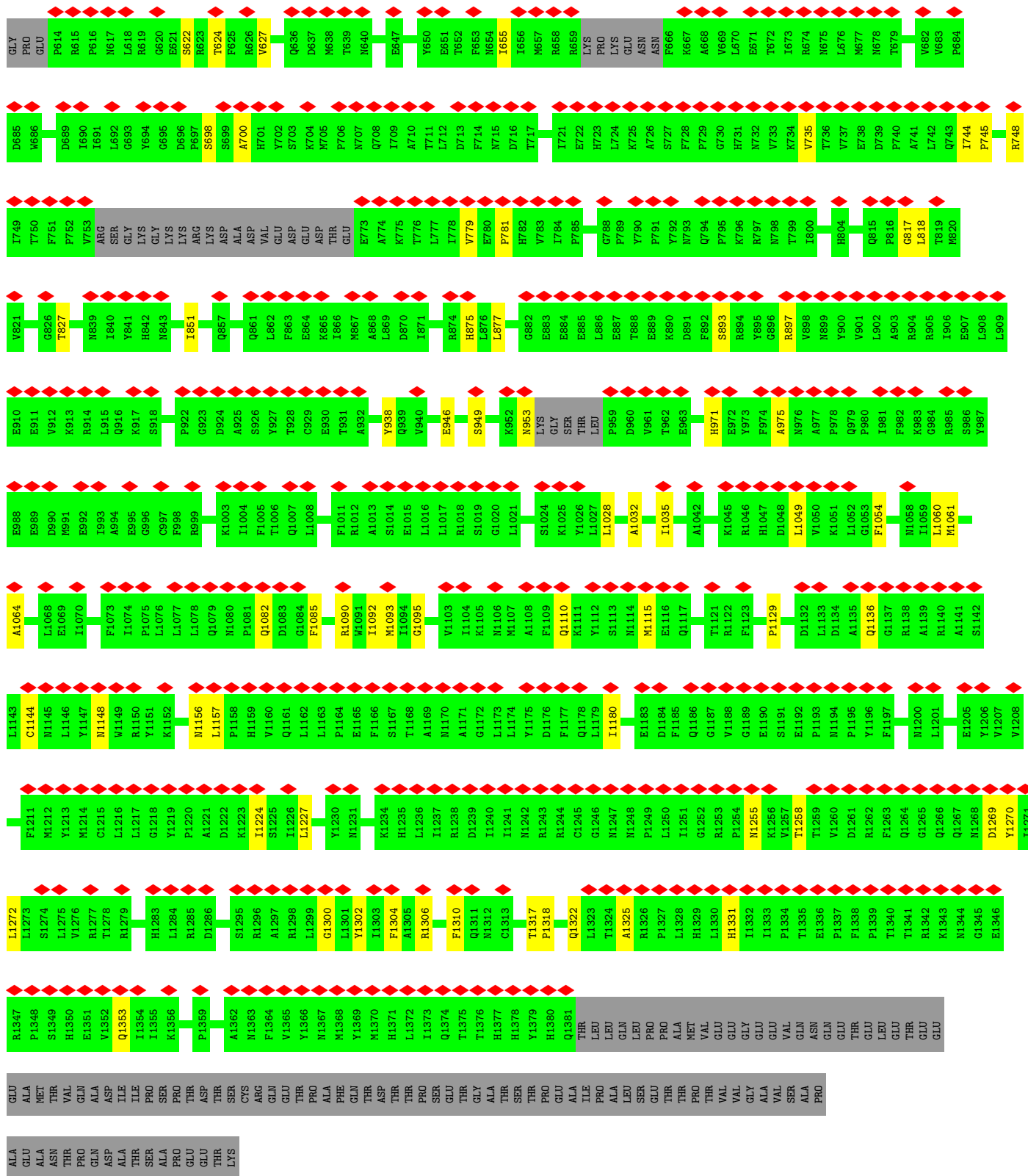




• Molecule 16: RNA helicase aquarius

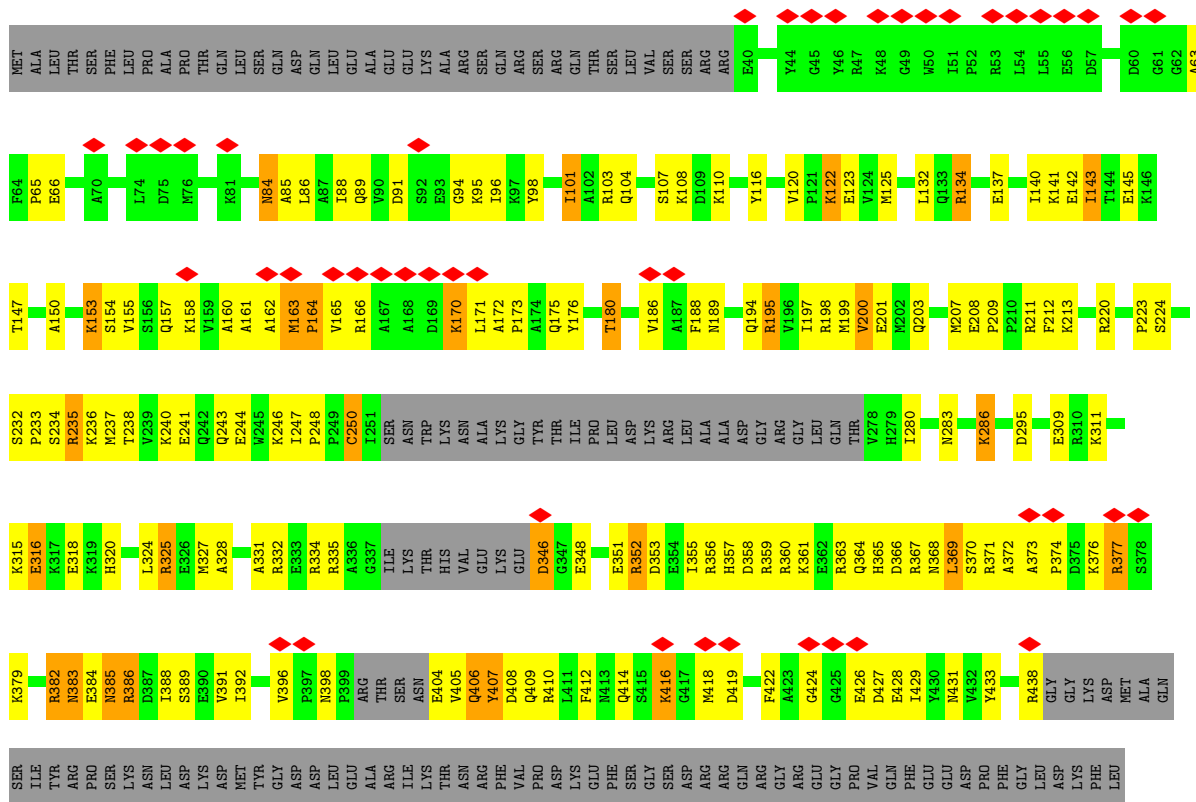




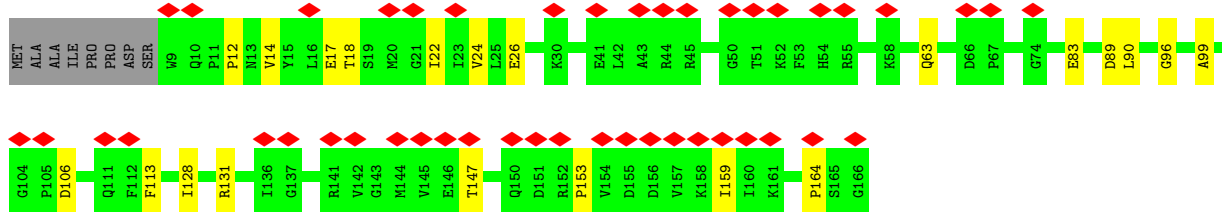
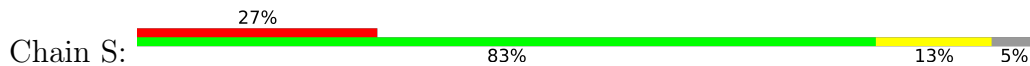


• Molecule 17: SNW domain-containing protein 1

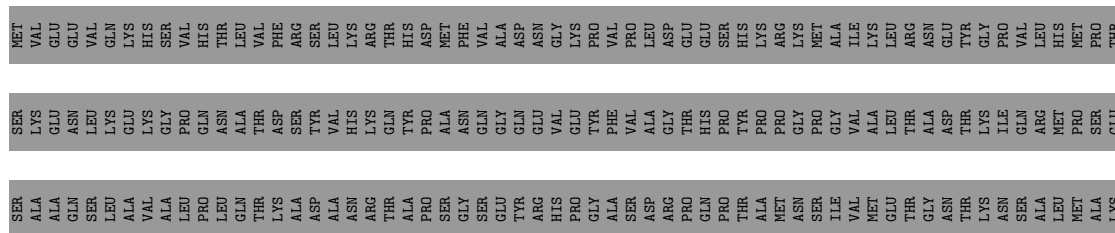
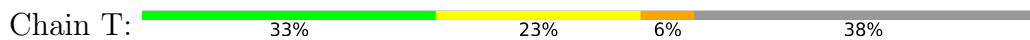


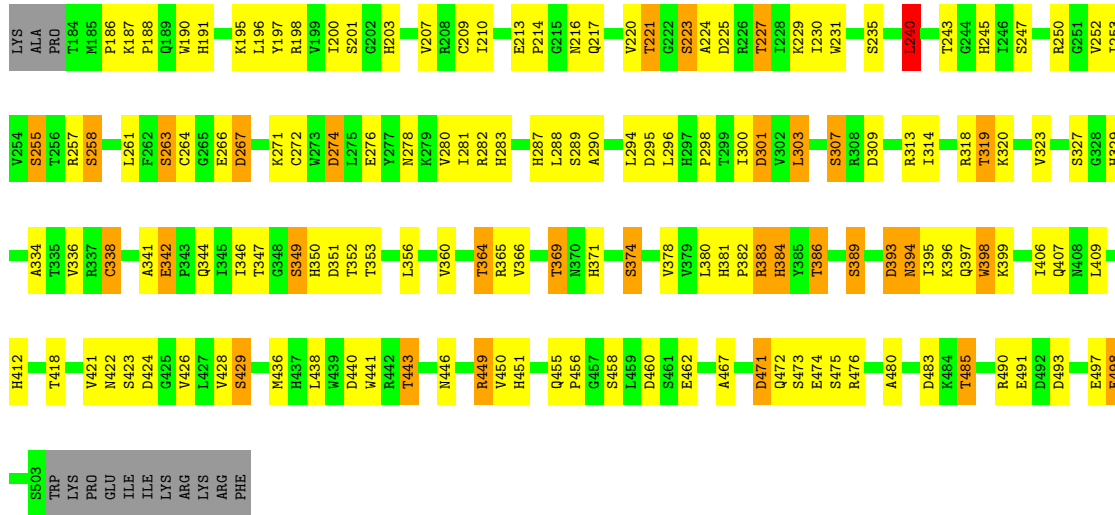


• Molecule 18: Peptidyl-prolyl cis-trans isomerase-like 1

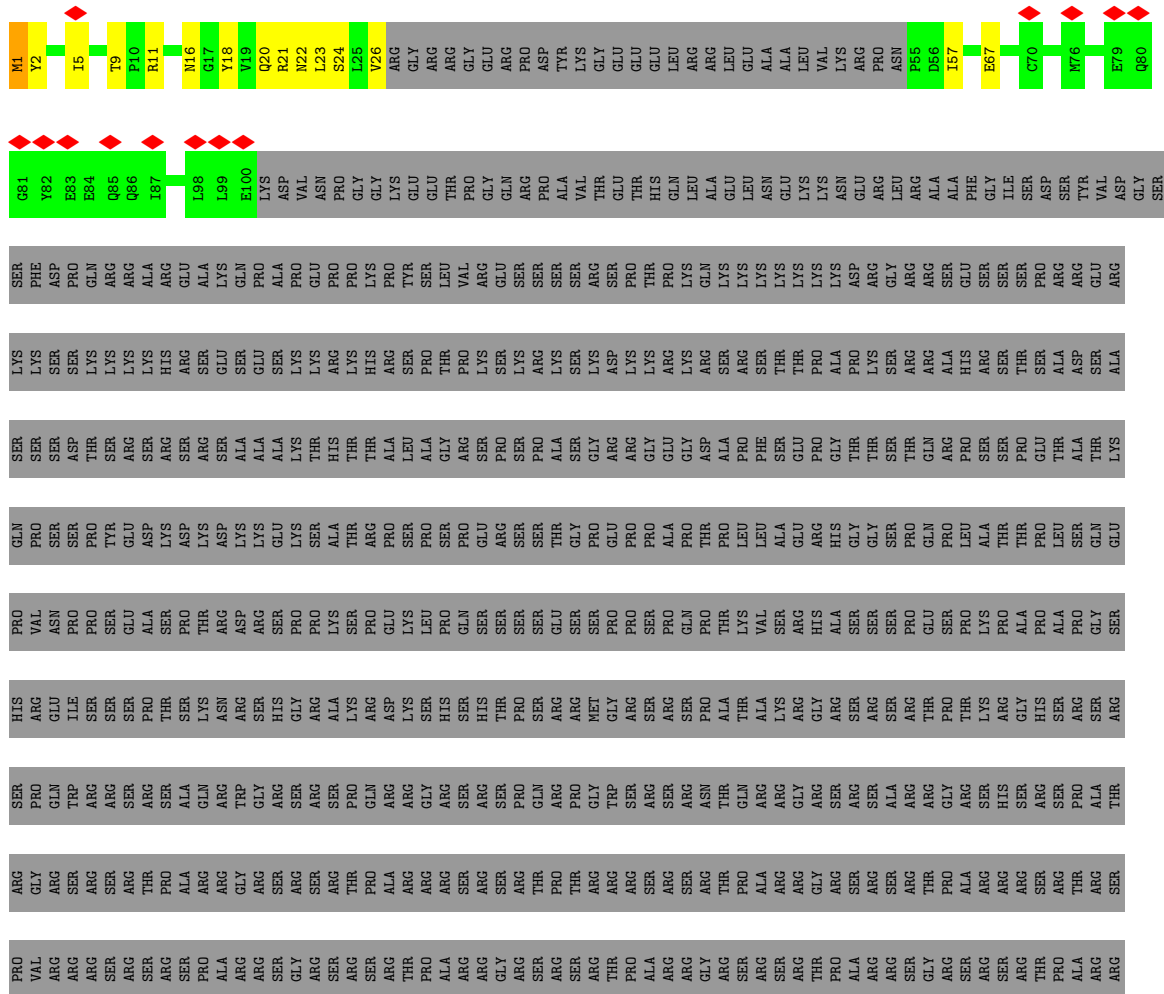


• Molecule 19: Pleiotropic regulator 1



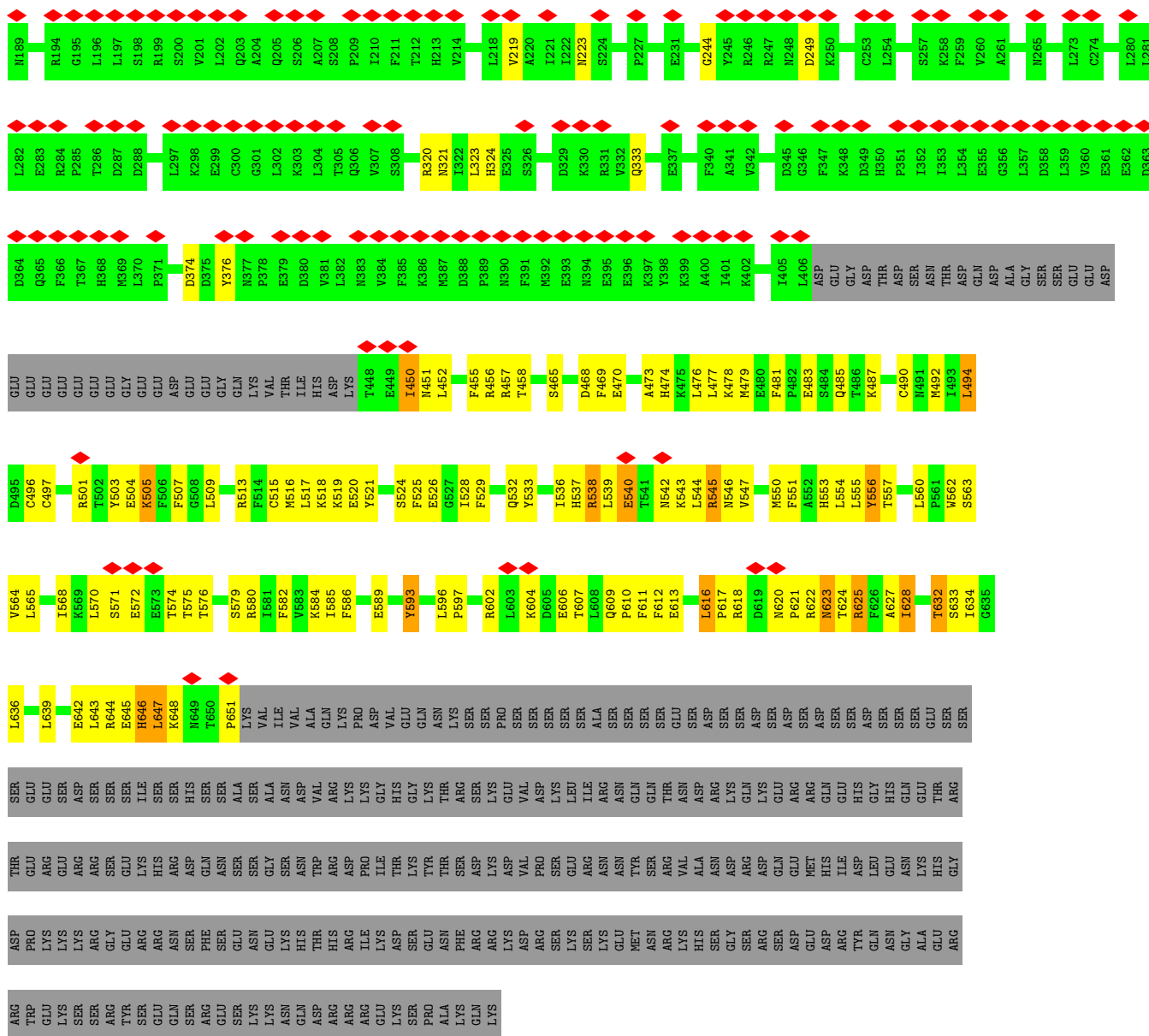


● Molecule 20: Serine/arginine repetitive matrix protein 2



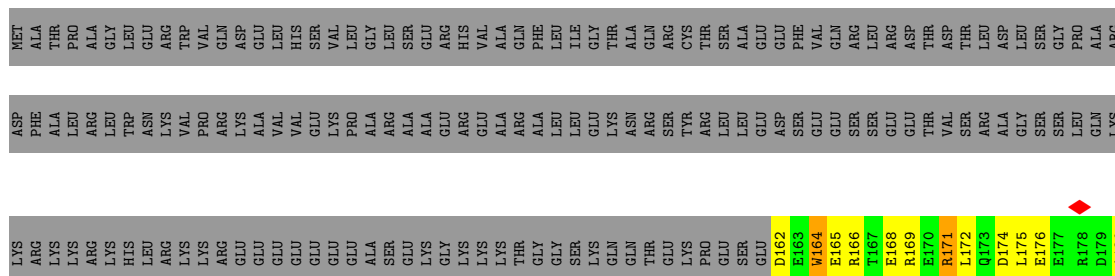






● Molecule 22: Pre-mRNA-splicing factor ATP-dependent RNA helicase DDX16

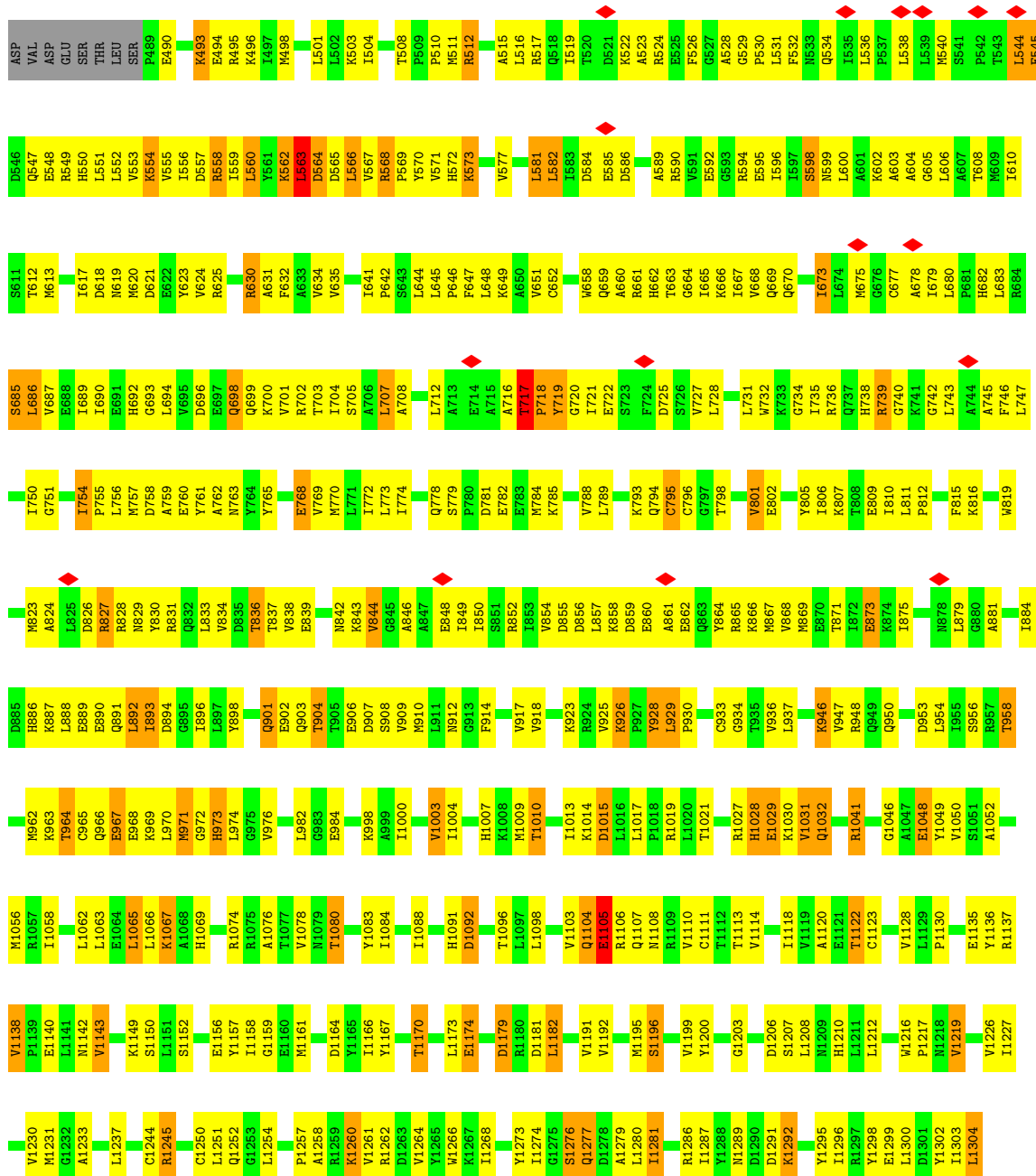
Chain X: 28% 39% 8% 24%



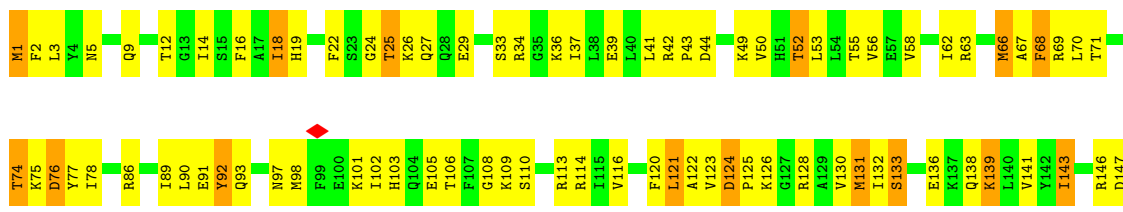
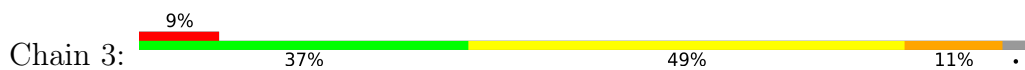




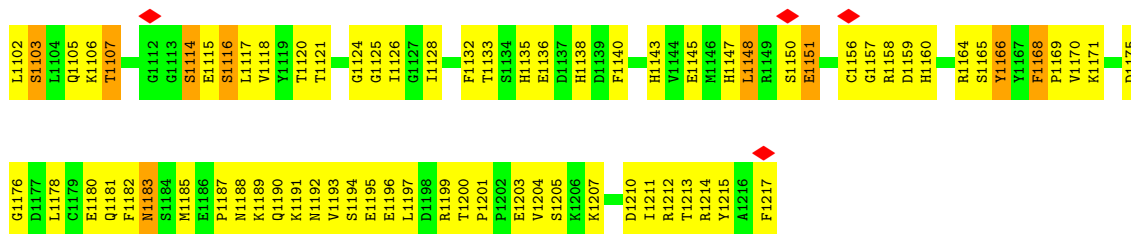




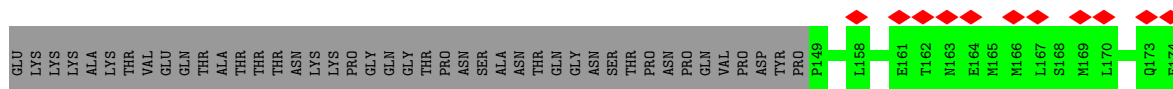
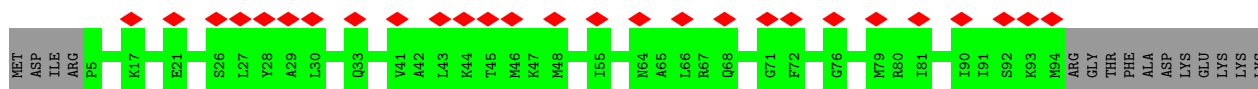
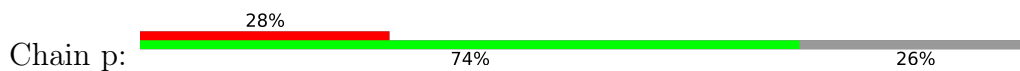
• Molecule 25: Splicing factor 3B subunit 3



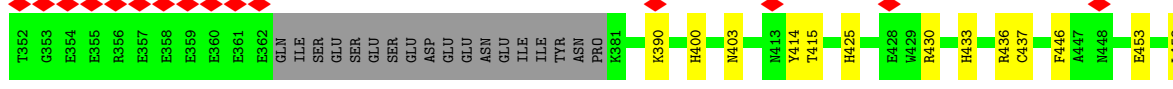
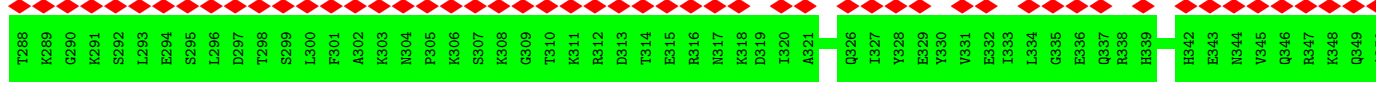
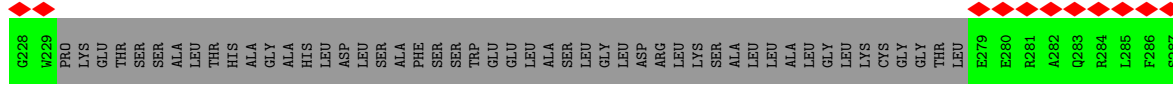
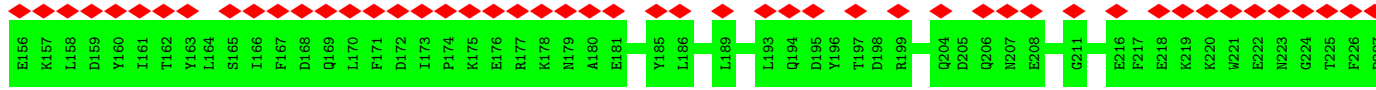
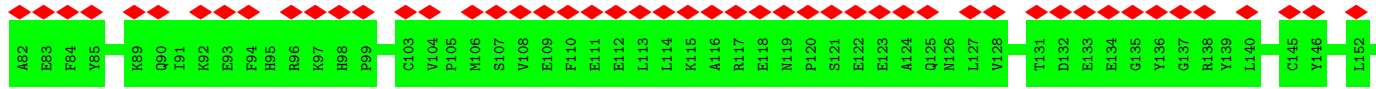
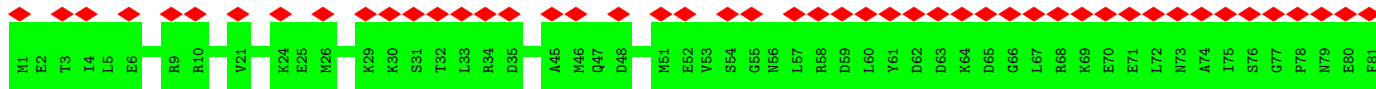
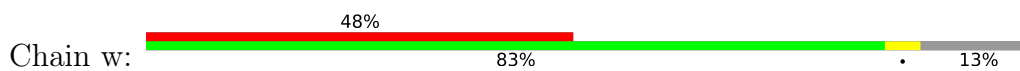
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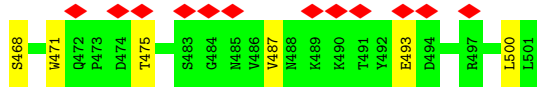


• Molecule 26: U2 small nuclear ribonucleoprotein B”

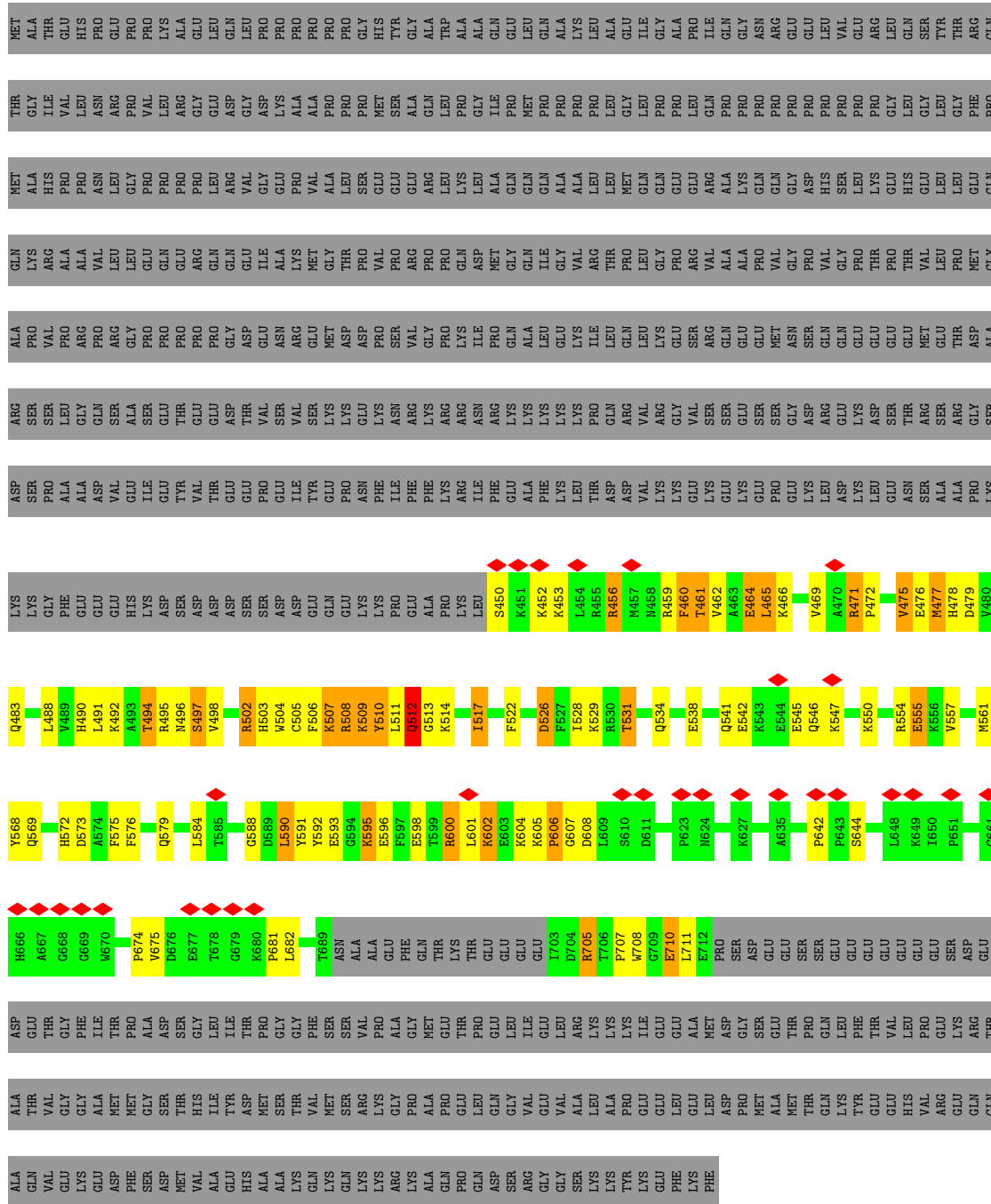


• Molecule 27: Splicing factor 3A subunit 3



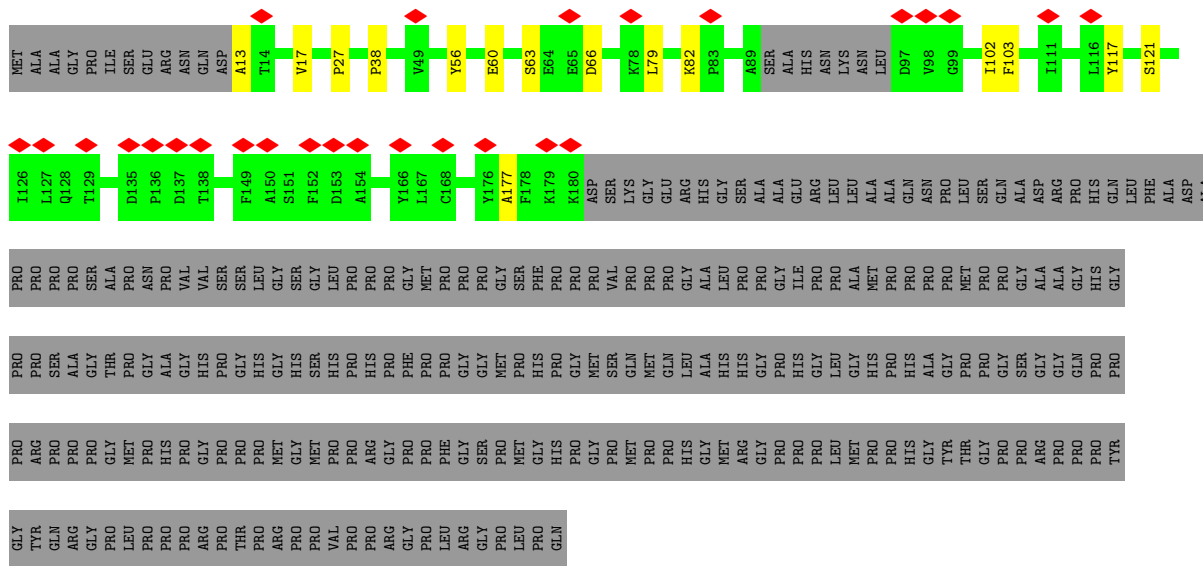


• Molecule 28: Splicing factor 3B subunit 2

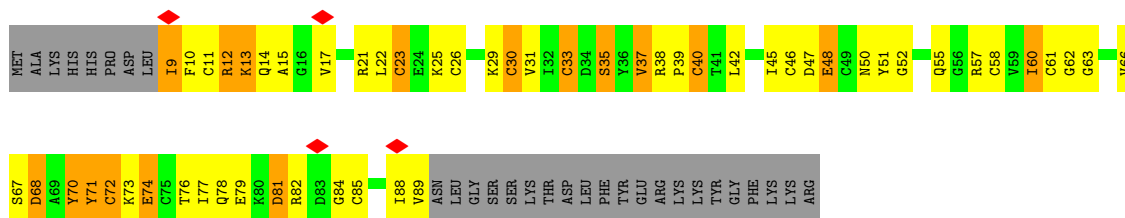
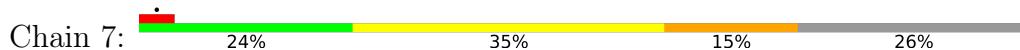


• Molecule 29: Splicing factor 3B subunit 4

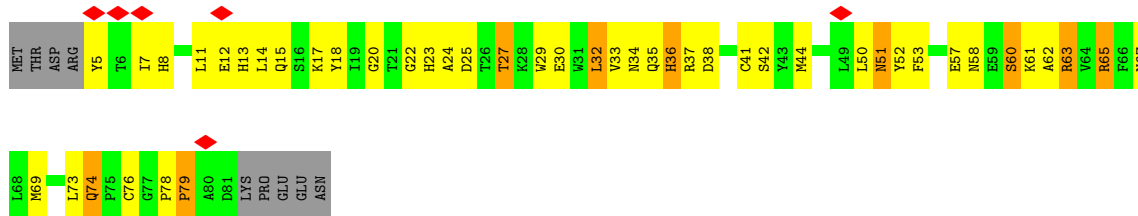




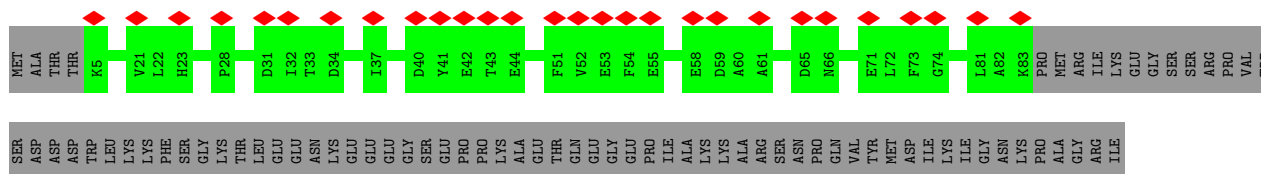
• Molecule 30: PHD finger-like domain-containing protein 5A



• Molecule 31: Splicing factor 3B subunit 5



• Molecule 32: Peptidyl-prolyl cis-trans isomerase E

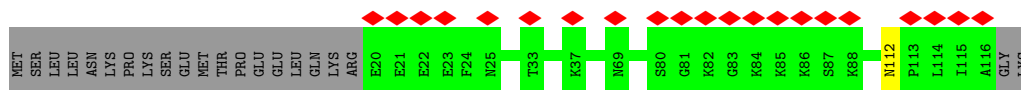




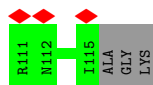
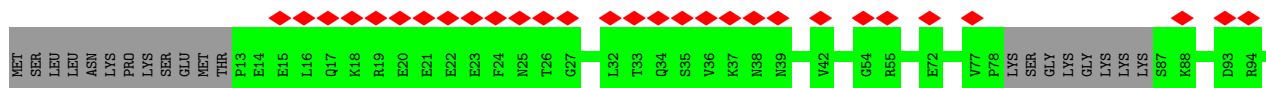
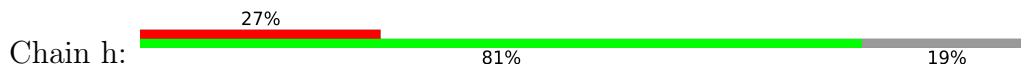




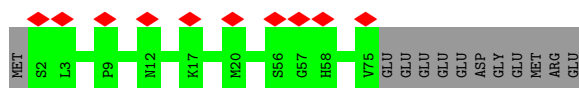
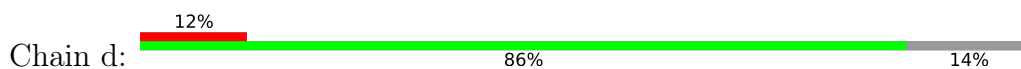




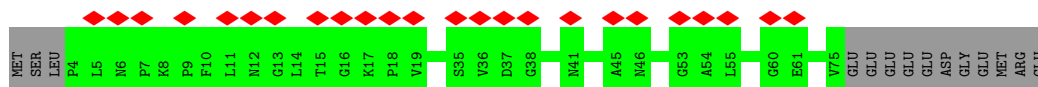
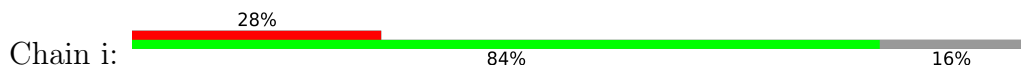
- Molecule 38: Small nuclear ribonucleoprotein Sm D2



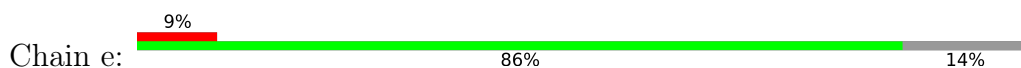
- Molecule 39: Small nuclear ribonucleoprotein F



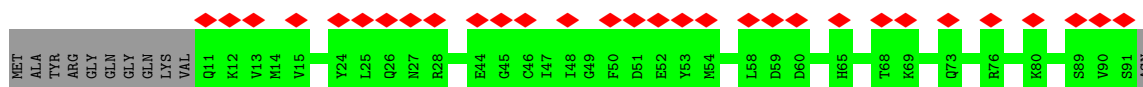
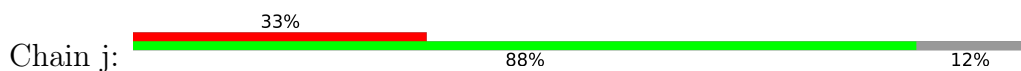
- Molecule 39: Small nuclear ribonucleoprotein F



- Molecule 40: Small nuclear ribonucleoprotein E

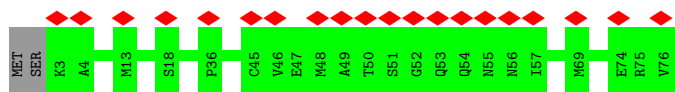


- Molecule 40: Small nuclear ribonucleoprotein E

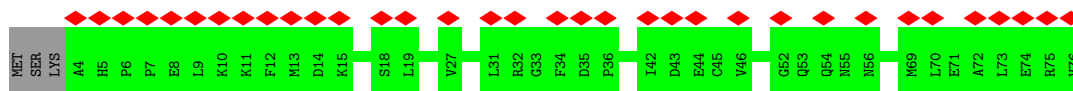
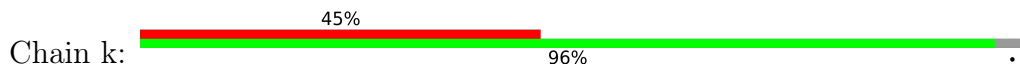


- Molecule 41: Small nuclear ribonucleoprotein G

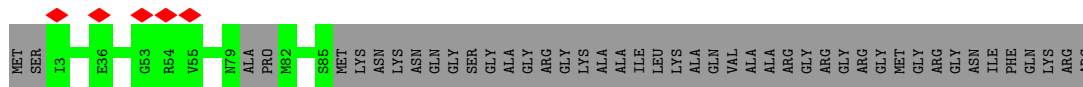




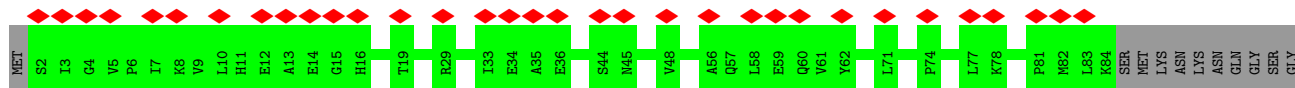
• Molecule 41: Small nuclear ribonucleoprotein G



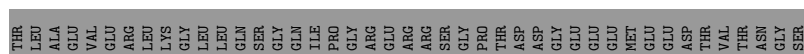
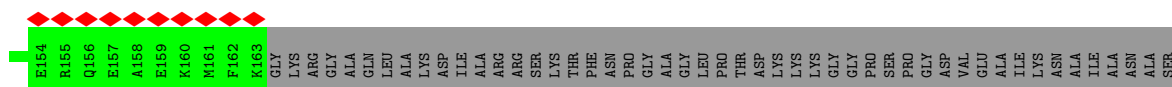
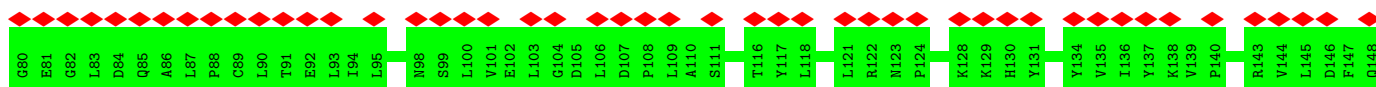
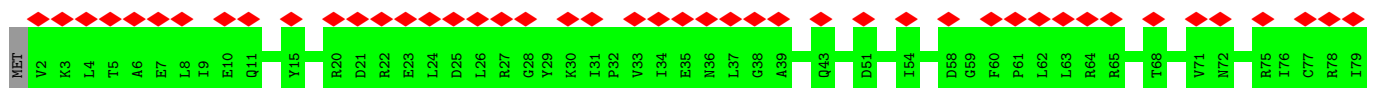
• Molecule 42: Small nuclear ribonucleoprotein Sm D3



• Molecule 42: Small nuclear ribonucleoprotein Sm D3



• Molecule 43: U2 small nuclear ribonucleoprotein A'



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13372	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)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.423	Depositor
Minimum map value	-0.641	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.23	Depositor
Map size ( $\text{\AA}$ )	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.077, 1.077, 1.077	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.94	25/18048 (0.1%)	0.71	14/24520 (0.1%)
2	B	1.13	8/2303 (0.3%)	1.10	7/3579 (0.2%)
3	C	0.39	0/6873	0.59	3/9346 (0.0%)
4	D	0.26	0/8527	0.46	0/11887
5	E	0.32	0/2392	0.60	1/3242 (0.0%)
6	F	1.51	34/2323 (1.5%)	1.32	19/3619 (0.5%)
7	G	0.96	4/1673 (0.2%)	1.28	18/2597 (0.7%)
8	H	0.80	15/3947 (0.4%)	1.12	14/6138 (0.2%)
9	I	0.43	3/2898 (0.1%)	0.51	1/4057 (0.0%)
10	J	0.44	0/2171	0.55	0/2929
11	K	0.60	0/404	0.60	0/541
12	L	0.58	1/1430 (0.1%)	0.63	0/1915
13	N	0.61	2/1200 (0.2%)	0.64	1/1611 (0.1%)
14	O	0.27	0/1432	0.49	0/1992
15	P	0.77	2/888 (0.2%)	0.60	0/1177
16	Q	0.25	0/6796	0.45	0/9527
17	R	0.52	0/2789	0.57	0/3747
18	S	0.27	0/769	0.52	0/1063
19	T	0.86	0/2574	0.71	2/3511 (0.1%)
20	U	0.56	0/424	0.49	0/582
21	V	0.42	0/2993	0.55	1/4088 (0.0%)
22	X	0.42	1/6479 (0.0%)	0.61	1/8747 (0.0%)
23	Y	0.38	0/2605	0.60	2/3522 (0.1%)
24	1	0.62	0/6591	0.64	3/8926 (0.0%)
25	3	0.55	2/9398 (0.0%)	0.69	6/12755 (0.0%)
26	p	0.26	0/847	0.48	0/1181
27	w	0.31	0/2311	0.49	0/3008
28	2	0.50	0/1833	0.63	0/2468
29	4	0.27	0/790	0.48	0/1095
30	7	0.56	0/621	0.61	0/833
31	5	0.72	0/654	0.64	0/885
32	y	0.26	0/389	0.49	0/540

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	v	0.39	0/976	0.57	0/1282
34	u	0.25	0/842	0.42	0/1110
35	9	0.32	0/2342	0.55	0/3182
36	a	0.51	0/343	0.69	0/427
36	m	0.26	0/416	0.54	0/581
37	b	0.56	0/327	0.67	0/407
37	n	0.24	0/404	0.50	0/564
38	c	0.69	0/387	0.72	0/482
38	h	0.24	0/485	0.48	0/677
39	d	0.78	0/295	0.76	0/367
39	i	0.27	0/362	0.53	0/502
40	e	0.65	0/315	0.75	0/392
40	j	0.25	0/403	0.46	0/561
41	f	0.54	0/295	0.61	0/367
41	k	0.26	0/366	0.53	0/509
42	g	0.47	0/322	0.56	0/399
42	l	0.26	0/417	0.51	0/581
43	o	0.24	0/821	0.48	0/1149
All	All	0.63	97/115490 (0.1%)	0.68	93/159167 (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	15
3	C	0	6
4	D	0	2
9	I	0	4
10	J	0	3
11	K	0	1
12	L	0	2
13	N	0	1
15	P	0	2
16	Q	0	2
17	R	0	1
18	S	0	1
22	X	0	1
23	Y	0	3
24	1	0	3
25	3	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	2	0	1
30	7	0	1
31	5	0	1
35	9	0	2
38	c	0	1
All	All	0	58

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	36	PRO	N-CA	14.04	1.71	1.47
9	I	110	PRO	N-CA	13.43	1.70	1.47
25	3	570	PRO	N-CA	10.41	1.65	1.47
1	A	385	GLU	C-N	8.98	1.51	1.34
9	I	140	LEU	C-N	8.80	1.50	1.34

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	570	PRO	N-CA-C	-12.58	79.40	112.10
25	3	570	PRO	CA-N-CD	-10.49	96.81	111.50
9	I	110	PRO	CA-N-CD	-10.42	96.91	111.50
8	H	47	U	P-O3'-C3'	9.41	131.00	119.70
7	G	104	C	N1-C2-O2	9.23	124.44	118.90

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	MET	Peptide
1	A	187	PRO	Peptide
1	A	203	VAL	Peptide
1	A	376	GLU	Peptide
1	A	467	GLN	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	17607	0	16789	923	0
2	B	2066	0	1047	73	0
3	C	6724	0	6697	481	0
4	D	8528	0	3745	121	0
5	E	2338	0	2275	167	0
6	F	2075	0	1048	133	0
7	G	1503	0	766	156	0
8	H	3539	0	1791	178	0
9	I	2880	0	1411	39	0
10	J	2116	0	1977	121	0
11	K	392	0	343	49	0
12	L	1403	0	1431	93	0
13	N	1174	0	1168	100	0
14	O	1432	0	632	25	0
15	P	876	0	875	59	0
16	Q	6730	0	3268	68	0
17	R	2760	0	2639	288	0
18	S	770	0	356	20	0
19	T	2507	0	2451	113	0
20	U	422	0	291	30	0
21	V	2959	0	2237	126	0
22	X	6357	0	6349	559	0
23	Y	2556	0	2492	263	0
24	1	6468	0	6657	402	0
25	3	9210	0	9124	688	0
26	p	841	0	420	0	0
27	w	2275	0	1347	0	0
28	2	1803	0	1618	204	0
29	4	792	0	367	15	0
30	7	613	0	597	51	0
31	5	635	0	595	49	0
32	y	390	0	190	0	0
33	v	964	0	735	0	0
34	u	834	0	325	0	0
35	9	2307	0	1898	149	0
36	a	344	0	93	0	0
36	m	413	0	194	0	0
37	b	328	0	89	0	0
37	n	402	0	184	0	0
38	c	388	0	102	0	0
38	h	482	0	220	0	0
39	d	296	0	87	0	0
39	i	359	0	179	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	e	316	0	85	0	0
40	j	403	0	173	0	0
41	f	296	0	84	0	0
41	k	364	0	176	0	0
42	g	324	0	89	0	0
42	l	415	0	198	0	0
43	o	816	0	386	0	0
44	A	36	0	6	8	0
45	C	32	0	12	8	0
46	C	1	0	0	0	0
46	F	6	0	0	0	0
47	7	3	0	0	0	0
47	K	1	0	0	0	0
47	N	3	0	0	0	0
All	All	112874	0	88308	4869	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 26.

The worst 5 of 4869 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)
1:A:2084:HIS:CB	4:D:1008:THR:CB	1.79	1.56
13:N:37:HIS:HB2	13:N:41:ARG:CB	1.10	1.52
1:A:2335:ALA:HA	4:D:592:LYS:CB	1.44	1.45
1:A:1889:LEU:HD12	1:A:2014:MET:N	1.21	1.44
15:P:184:VAL:HG11	23:Y:50:ILE:CD1	1.43	1.43

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	2216/2335 (95%)	1957 (88%)	246 (11%)	13 (1%)	22	59
3	C	854/972 (88%)	737 (86%)	110 (13%)	7 (1%)	16	54
4	D	1720/2136 (80%)	1585 (92%)	124 (7%)	11 (1%)	22	59
5	E	297/357 (83%)	271 (91%)	26 (9%)	0	100	100
9	I	563/855 (66%)	479 (85%)	79 (14%)	5 (1%)	14	50
10	J	245/848 (29%)	214 (87%)	28 (11%)	3 (1%)	11	44
11	K	44/343 (13%)	39 (89%)	5 (11%)	0	100	100
12	L	165/802 (21%)	142 (86%)	23 (14%)	0	100	100
13	N	141/144 (98%)	124 (88%)	17 (12%)	0	100	100
14	O	285/420 (68%)	239 (84%)	46 (16%)	0	100	100
15	P	97/229 (42%)	86 (89%)	9 (9%)	2 (2%)	5	32
16	Q	1319/1485 (89%)	1208 (92%)	111 (8%)	0	100	100
17	R	352/536 (66%)	314 (89%)	36 (10%)	2 (1%)	22	59
18	S	156/166 (94%)	147 (94%)	9 (6%)	0	100	100
19	T	318/514 (62%)	289 (91%)	29 (9%)	0	100	100
20	U	68/2752 (2%)	62 (91%)	6 (9%)	0	100	100
21	V	458/908 (50%)	430 (94%)	28 (6%)	0	100	100
22	X	778/1041 (75%)	692 (89%)	82 (10%)	4 (0%)	25	62
23	Y	318/492 (65%)	277 (87%)	41 (13%)	0	100	100
24	1	814/1304 (62%)	706 (87%)	104 (13%)	4 (0%)	25	62
25	3	1165/1217 (96%)	991 (85%)	172 (15%)	2 (0%)	44	77
26	p	163/225 (72%)	147 (90%)	15 (9%)	1 (1%)	22	59
27	w	428/501 (85%)	381 (89%)	47 (11%)	0	100	100
28	2	246/895 (28%)	210 (85%)	31 (13%)	5 (2%)	6	34
29	4	157/424 (37%)	138 (88%)	19 (12%)	0	100	100
30	7	79/110 (72%)	65 (82%)	14 (18%)	0	100	100
31	5	75/86 (87%)	64 (85%)	11 (15%)	0	100	100
32	y	77/301 (26%)	64 (83%)	13 (17%)	0	100	100
33	v	150/464 (32%)	134 (89%)	16 (11%)	0	100	100
34	u	183/793 (23%)	170 (93%)	13 (7%)	0	100	100
35	9	330/520 (64%)	292 (88%)	38 (12%)	0	100	100
36	a	84/240 (35%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	m	80/240 (33%)	72 (90%)	8 (10%)	0	100	100
37	b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
37	n	78/119 (66%)	67 (86%)	11 (14%)	0	100	100
38	c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
38	h	91/118 (77%)	82 (90%)	9 (10%)	0	100	100
39	d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
39	i	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
40	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
40	j	79/92 (86%)	73 (92%)	6 (8%)	0	100	100
41	f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
41	k	71/76 (93%)	63 (89%)	8 (11%)	0	100	100
42	g	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
42	l	81/126 (64%)	70 (86%)	11 (14%)	0	100	100
43	o	160/255 (63%)	136 (85%)	24 (15%)	0	100	100
All	All	15528/26144 (59%)	13822 (89%)	1647 (11%)	59 (0%)	32	67

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1258	VAL
9	I	139	ALA
17	R	164	PRO
17	R	223	PRO
24	1	1106	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1762/2108 (84%)	1465 (83%)	297 (17%)	1	11
3	C	747/866 (86%)	611 (82%)	136 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	256/300 (85%)	209 (82%)	47 (18%)	1	9
9	I	22/749 (3%)	22 (100%)	0	100	100
10	J	205/751 (27%)	175 (85%)	30 (15%)	2	14
11	K	41/294 (14%)	35 (85%)	6 (15%)	2	14
12	L	141/709 (20%)	119 (84%)	22 (16%)	2	13
13	N	128/130 (98%)	104 (81%)	24 (19%)	1	8
14	O	3/361 (1%)	3 (100%)	0	100	100
15	P	95/203 (47%)	75 (79%)	20 (21%)	1	5
16	Q	71/1336 (5%)	71 (100%)	0	100	100
17	R	268/458 (58%)	214 (80%)	54 (20%)	1	7
19	T	273/441 (62%)	224 (82%)	49 (18%)	1	9
20	U	21/2432 (1%)	17 (81%)	4 (19%)	1	8
21	V	188/838 (22%)	159 (85%)	29 (15%)	2	13
22	X	682/897 (76%)	564 (83%)	118 (17%)	1	10
23	Y	286/451 (63%)	243 (85%)	43 (15%)	2	13
24	1	697/1104 (63%)	597 (86%)	100 (14%)	2	14
25	3	1016/1051 (97%)	804 (79%)	212 (21%)	1	6
26	p	8/195 (4%)	8 (100%)	0	100	100
27	w	112/446 (25%)	93 (83%)	19 (17%)	1	10
28	2	151/776 (20%)	120 (80%)	31 (20%)	1	6
30	7	69/95 (73%)	47 (68%)	22 (32%)	0	2
31	5	68/77 (88%)	53 (78%)	15 (22%)	1	5
33	v	73/382 (19%)	63 (86%)	10 (14%)	3	16
34	u	10/709 (1%)	10 (100%)	0	100	100
35	9	185/456 (41%)	148 (80%)	37 (20%)	1	7
36	m	4/177 (2%)	4 (100%)	0	100	100
37	n	3/101 (3%)	3 (100%)	0	100	100
38	h	5/110 (4%)	5 (100%)	0	100	100
39	i	4/74 (5%)	4 (100%)	0	100	100
40	j	1/84 (1%)	1 (100%)	0	100	100
41	k	3/66 (4%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1	3/101 (3%)	3 (100%)	0	100	100
43	o	6/218 (3%)	6 (100%)	0	100	100
All	All	7607/19546 (39%)	6282 (83%)	1325 (17%)	3	10

5 of 1325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	1	925	VAL
25	3	931	VAL
24	1	1067	LYS
24	1	904	THR
25	3	318	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
24	1	763	ASN
25	3	709	GLN
24	1	1028	HIS
25	3	179	ASN
25	3	861	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	29 (30%)	3 (3%)
6	F	96/107 (89%)	48 (50%)	4 (4%)
7	G	71/220 (32%)	44 (61%)	9 (12%)
8	H	163/188 (86%)	73 (44%)	6 (3%)
All	All	426/632 (67%)	194 (45%)	22 (5%)

5 of 194 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	U
2	B	20	G
2	B	21	A
2	B	22	U

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	G	111	U
8	H	18	U
8	H	13	C
8	H	43	U
6	F	58	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	SEP	R	224	17	8,9,10	1.41	1 (12%)	8,12,14	2.09	2 (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
17	SEP	R	224	17	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	224	SEP	P-O1P	3.11	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	224	SEP	P-OG-CB	-4.46	106.00	118.30
17	R	224	SEP	OG-CB-CA	3.45	111.50	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 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
44	IHP	A	3000	-	36,36,36	0.93	0	54,60,60	1.52	10 (18%)
45	GTP	C	1500	46	26,34,34	1.14	1 (3%)	32,54,54	1.90	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	IHP	A	3000	-	-	9/30/54/54	0/1/1/1
45	GTP	C	1500	46	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C5-C6	-4.12	1.39	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1500	GTP	PA-O3A-PB	-5.11	115.28	132.83
45	C	1500	GTP	PB-O3B-PG	-5.08	115.38	132.83
44	A	3000	IHP	C6-C5-C4	3.76	118.65	110.41
44	A	3000	IHP	C5-C4-C3	3.70	118.52	110.41
45	C	1500	GTP	C5-C6-N1	3.42	119.99	113.95

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

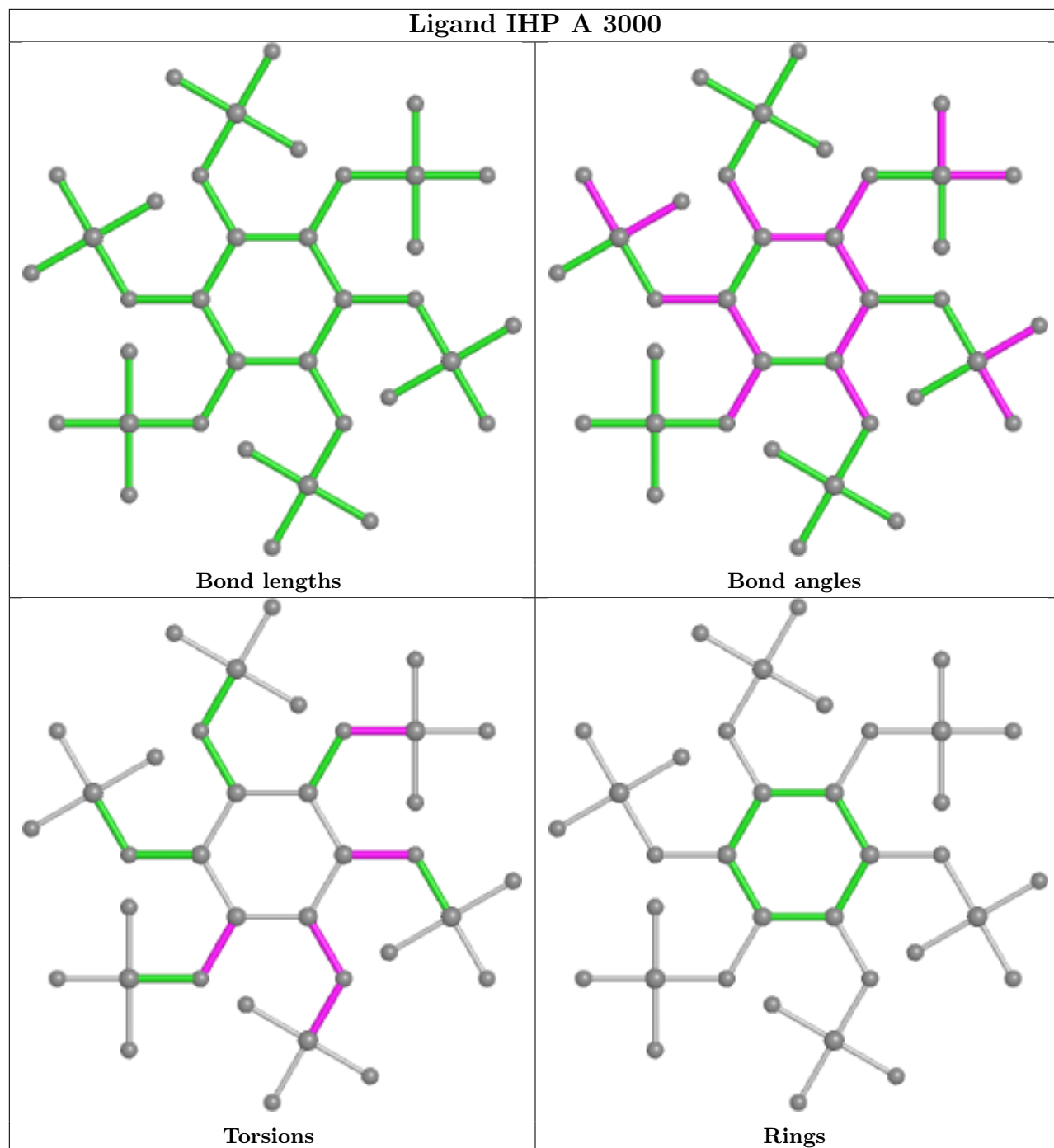
Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C2-C1-O11-P1
44	A	3000	IHP	C4-C5-O15-P5
44	A	3000	IHP	C6-C5-O15-P5
45	C	1500	GTP	C4'-C5'-O5'-PA
45	C	1500	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

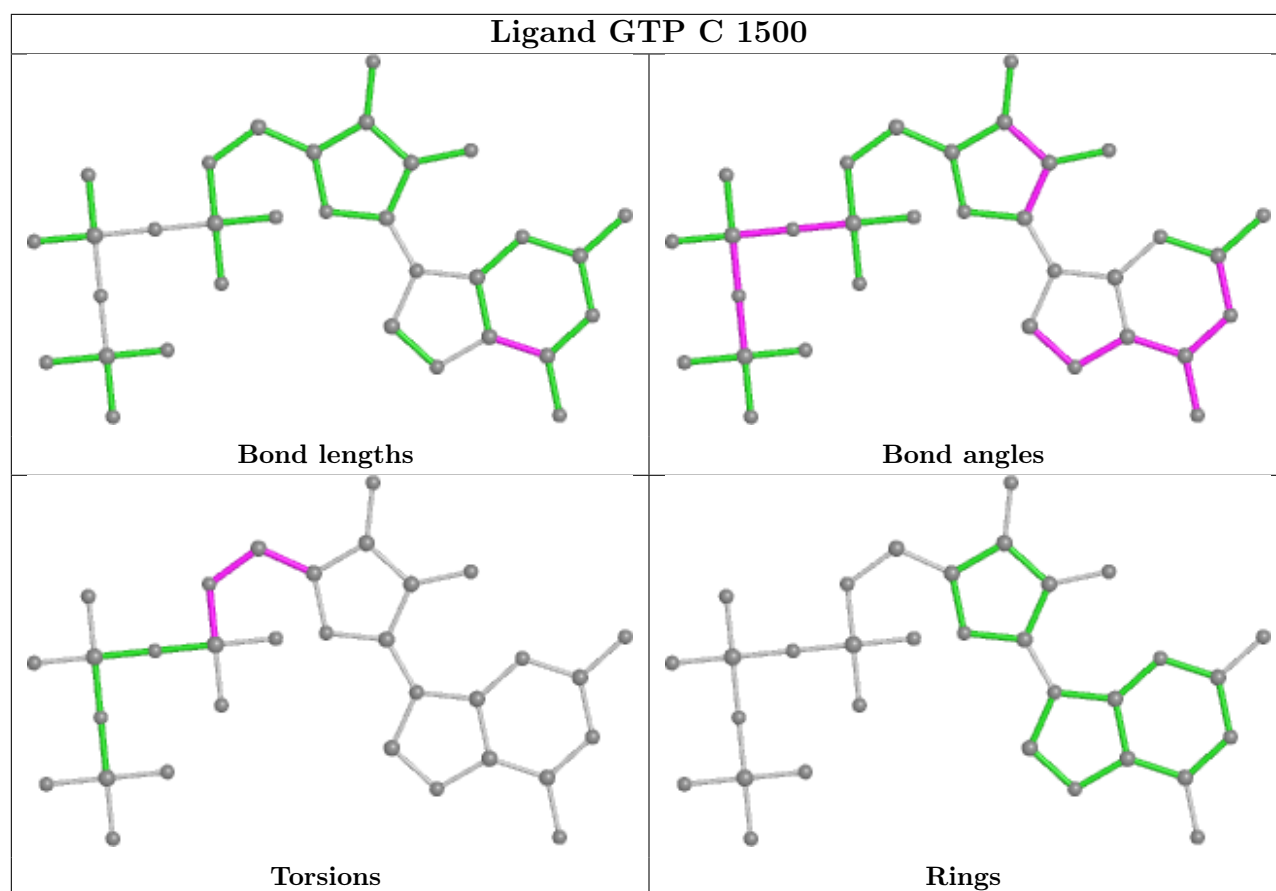
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	A	3000	IHP	8	0
45	C	1500	GTP	8	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.

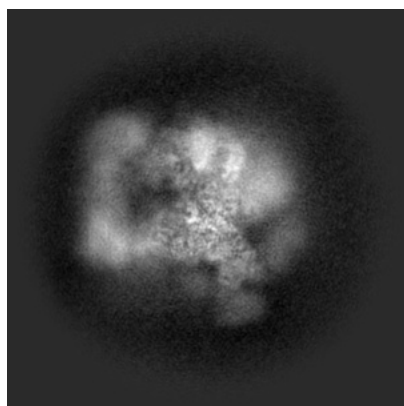
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35108. These allow visual inspection of the internal detail of the map and identification of artifacts.

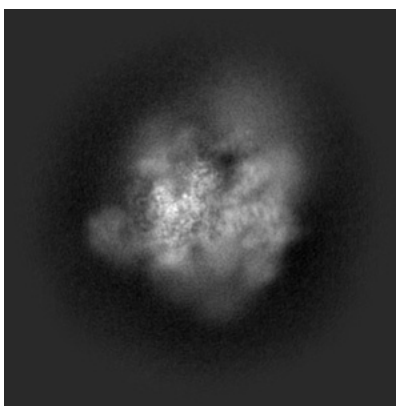
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

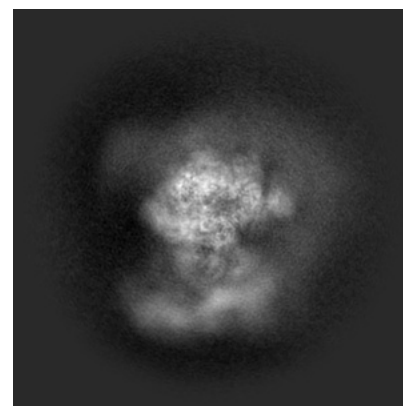
#### 6.1.1 Primary map



X

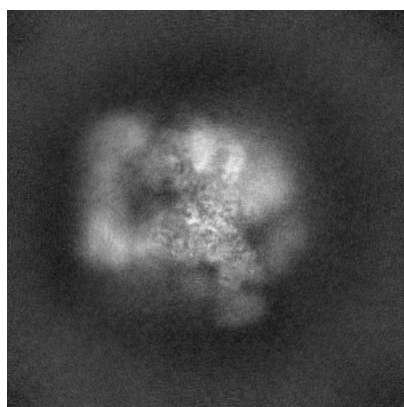


Y

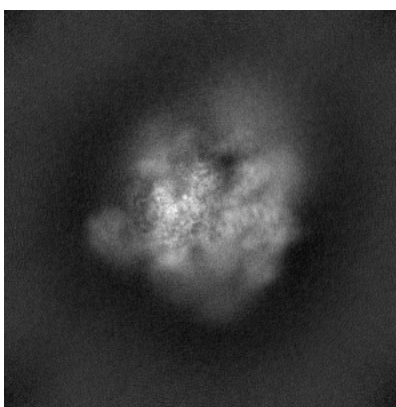


Z

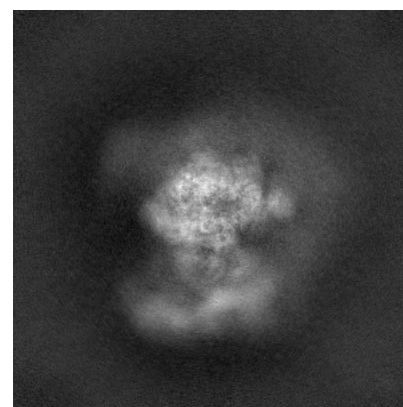
#### 6.1.2 Raw map



X



Y

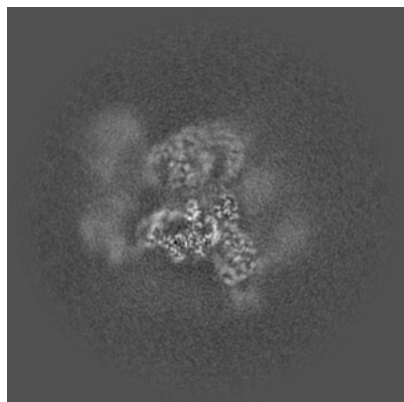


Z

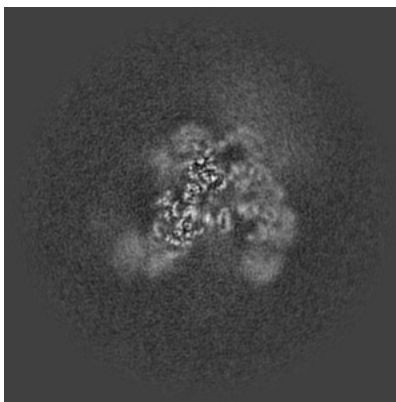
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

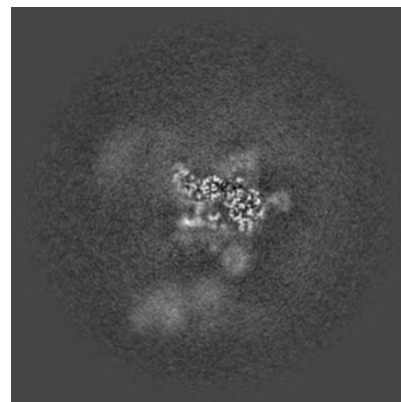
### 6.2.1 Primary map



X Index: 240

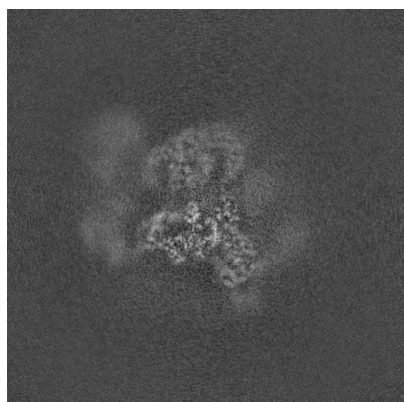


Y Index: 240

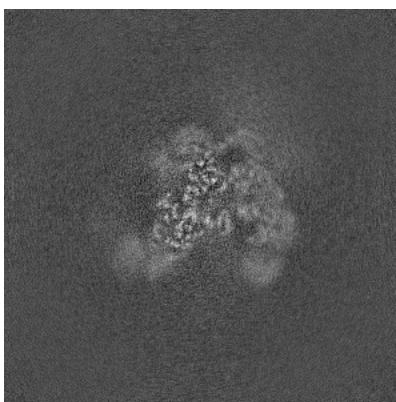


Z Index: 240

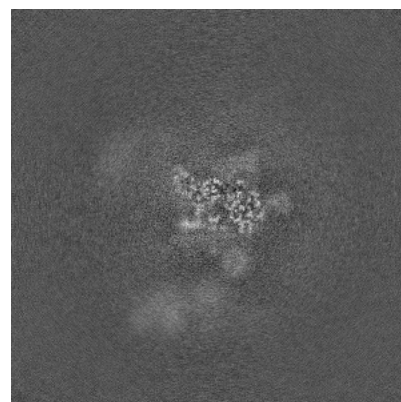
### 6.2.2 Raw map



X Index: 240



Y Index: 240

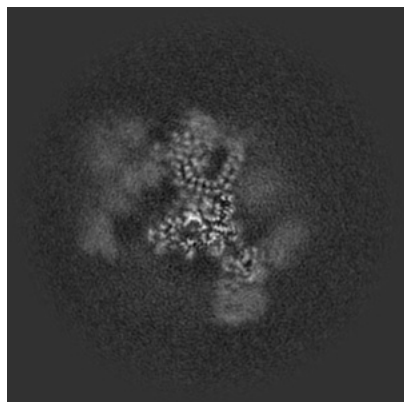


Z Index: 240

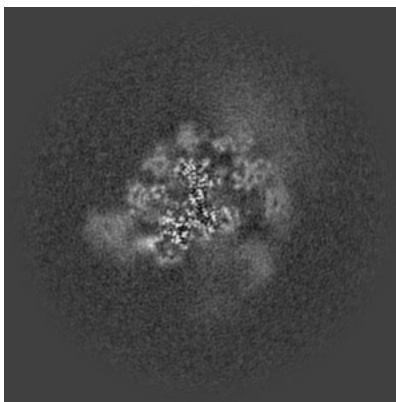
The images above show central slices of the map in three orthogonal directions.

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

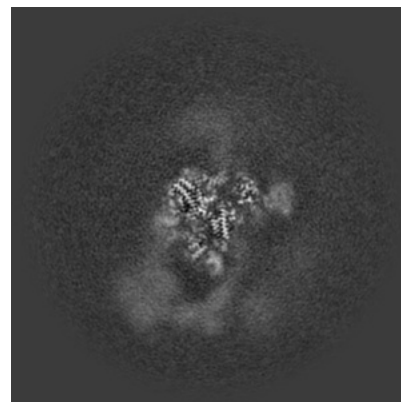
### 6.3.1 Primary map



X Index: 226

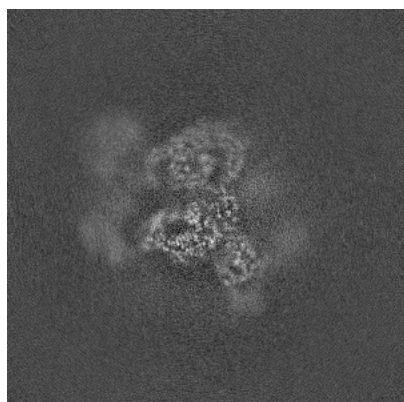


Y Index: 258

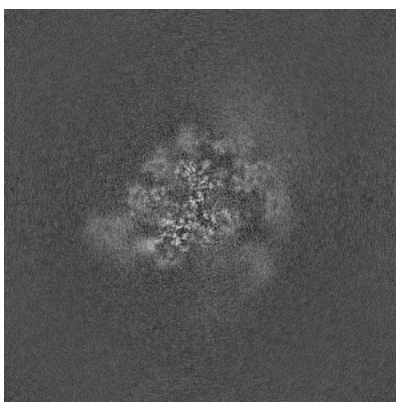


Z Index: 216

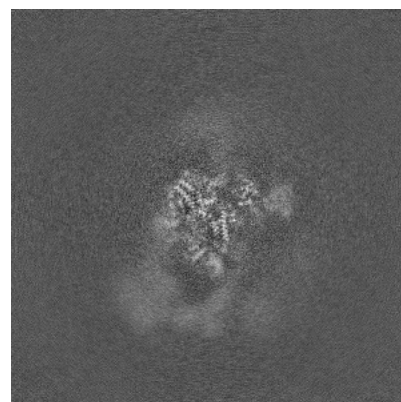
### 6.3.2 Raw map



X Index: 238



Y Index: 258

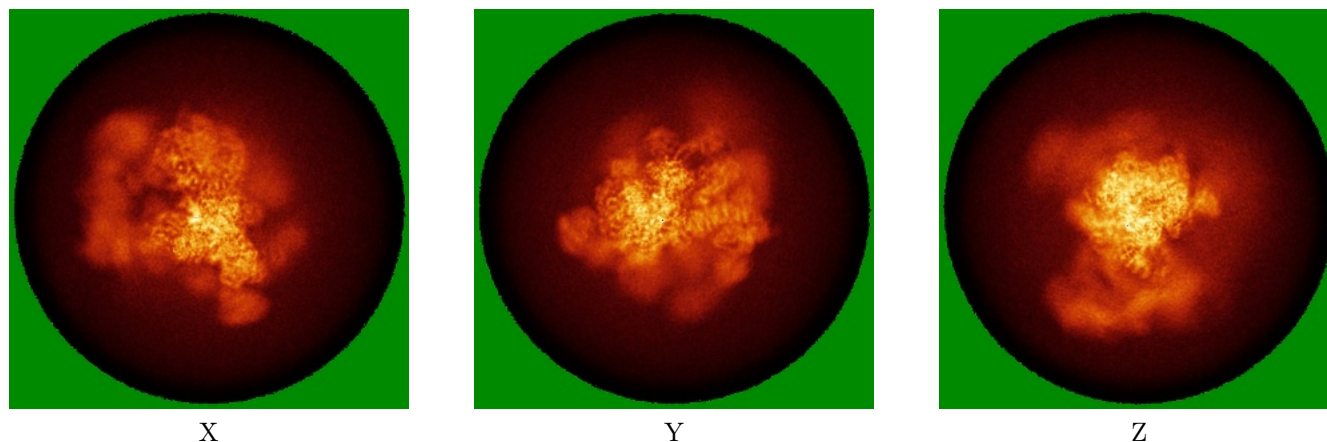


Z Index: 216

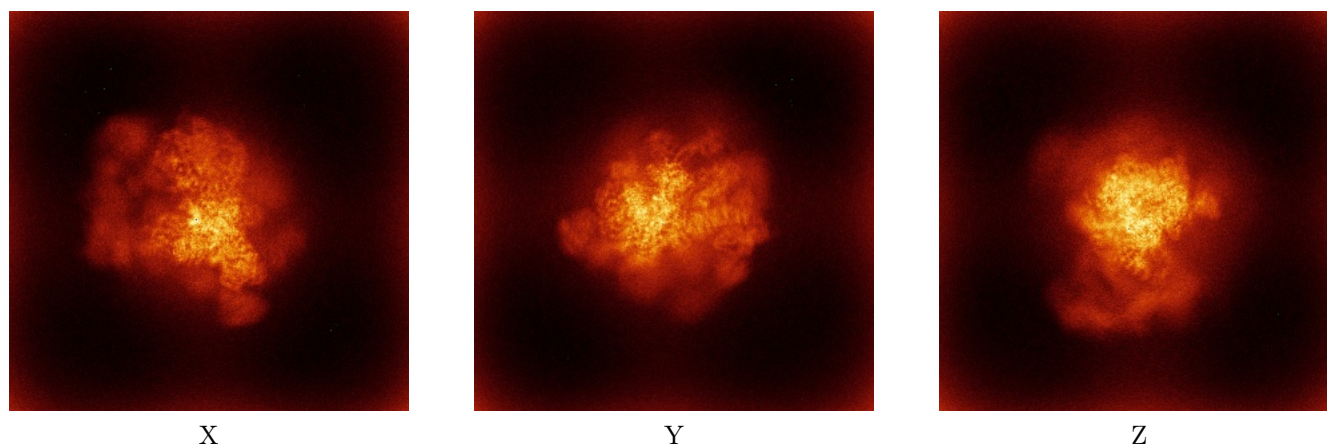
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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

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

### 6.5.1 Primary map



X



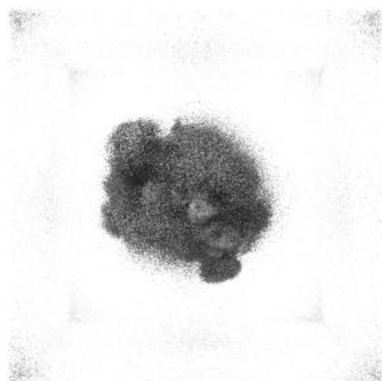
Y



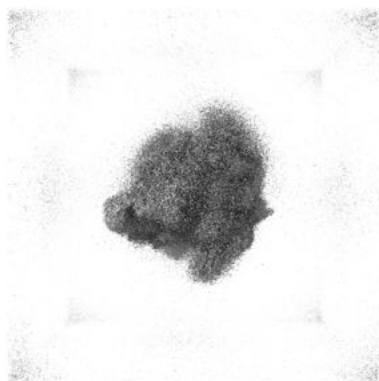
Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

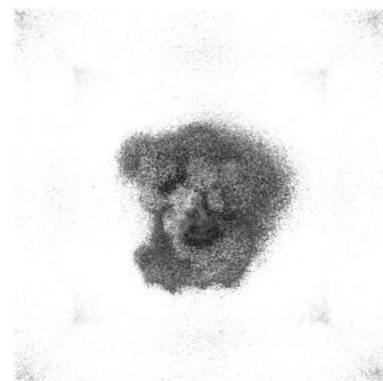
### 6.5.2 Raw map



X



Y



Z

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

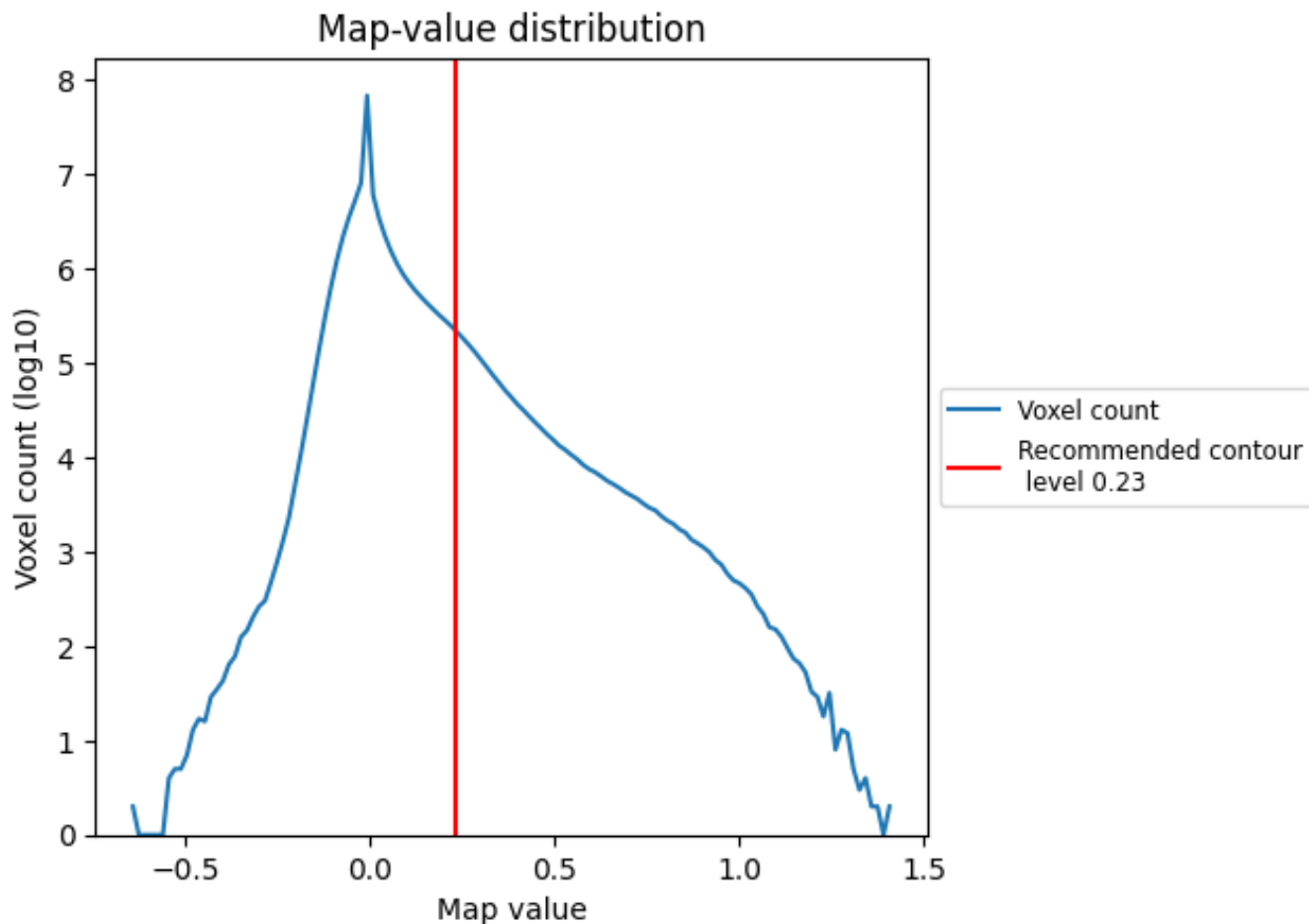
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

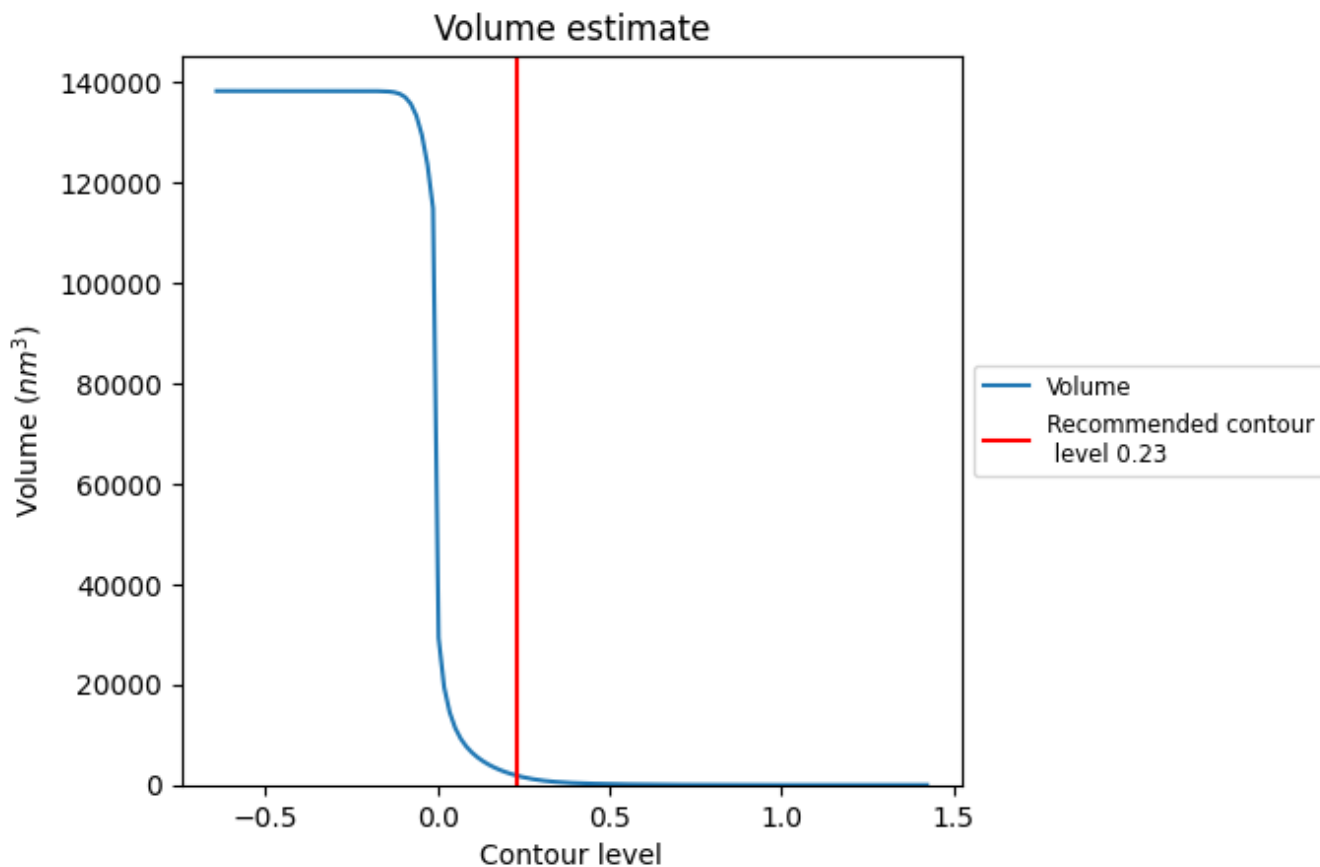
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

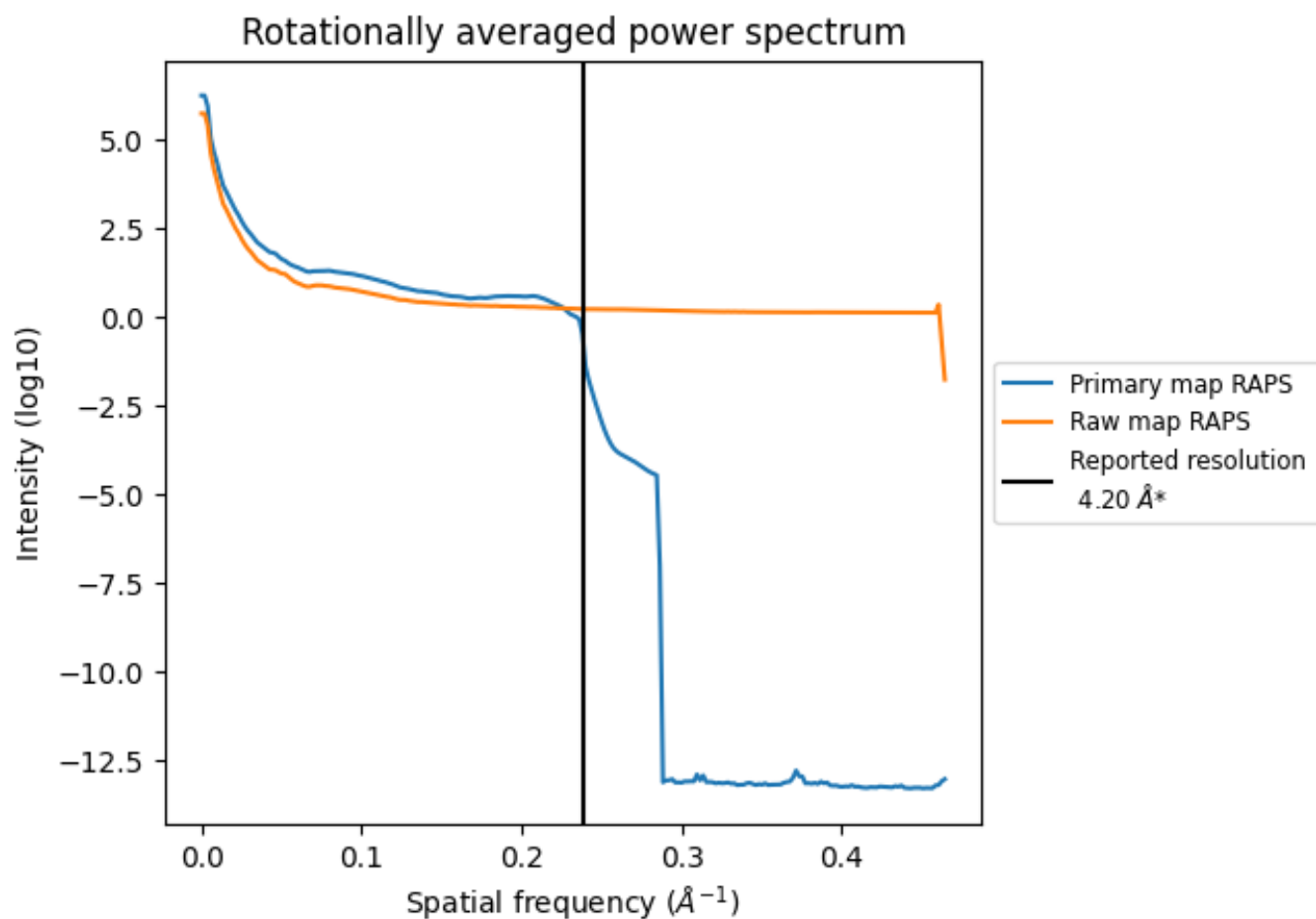


The volume at the recommended contour level is 1882 nm<sup>3</sup>; this corresponds to an approximate mass of 1700 kDa.

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](#)

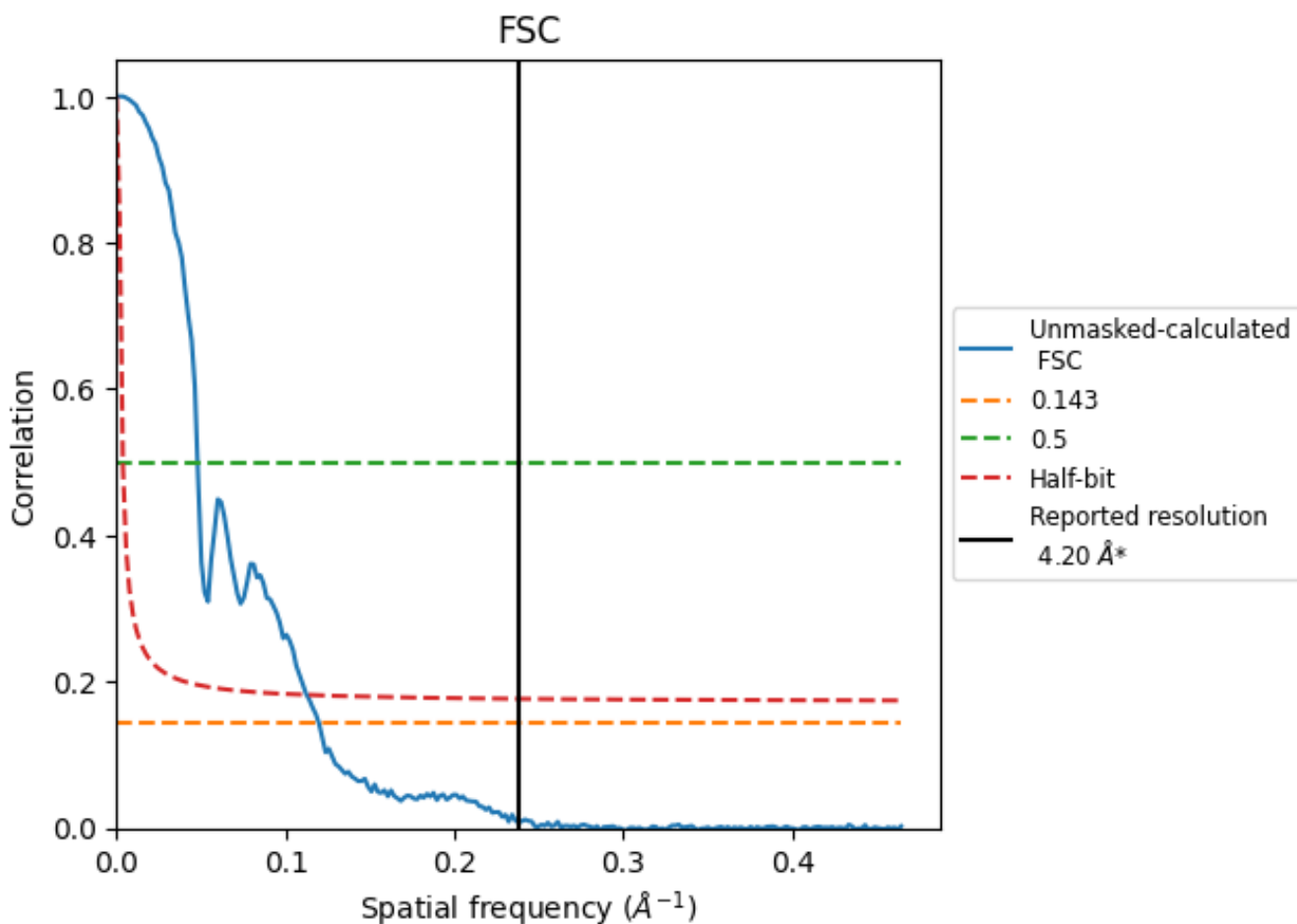


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.238 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

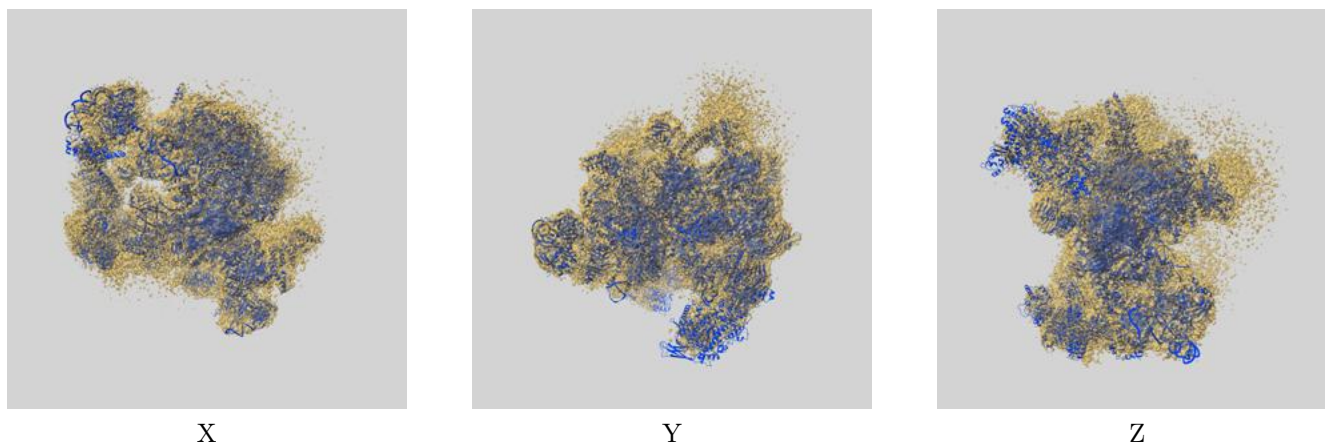
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.35	20.83	8.88

\*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 8.35 differs from the reported value 4.2 by more than 10 %

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

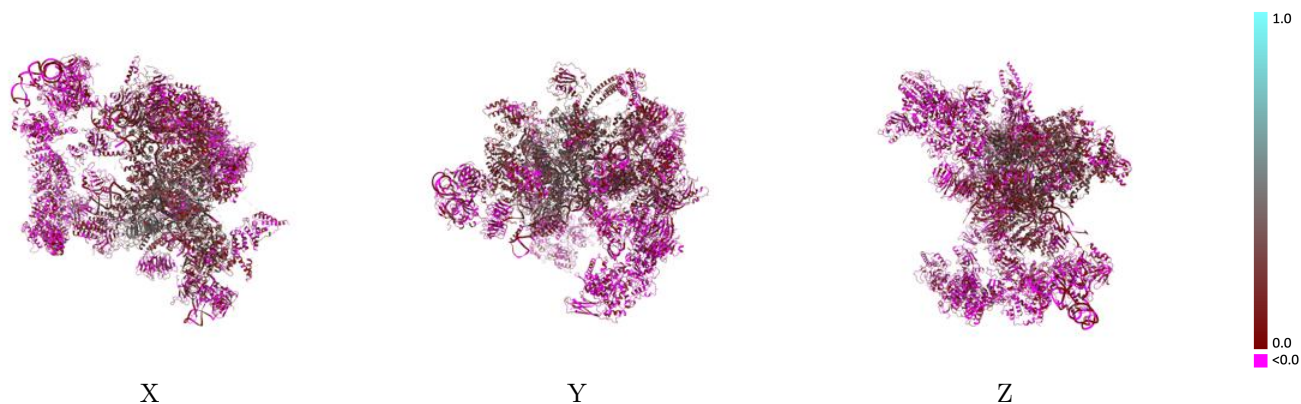
This section contains information regarding the fit between EMDB map EMD-35108 and PDB model 8I0S. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



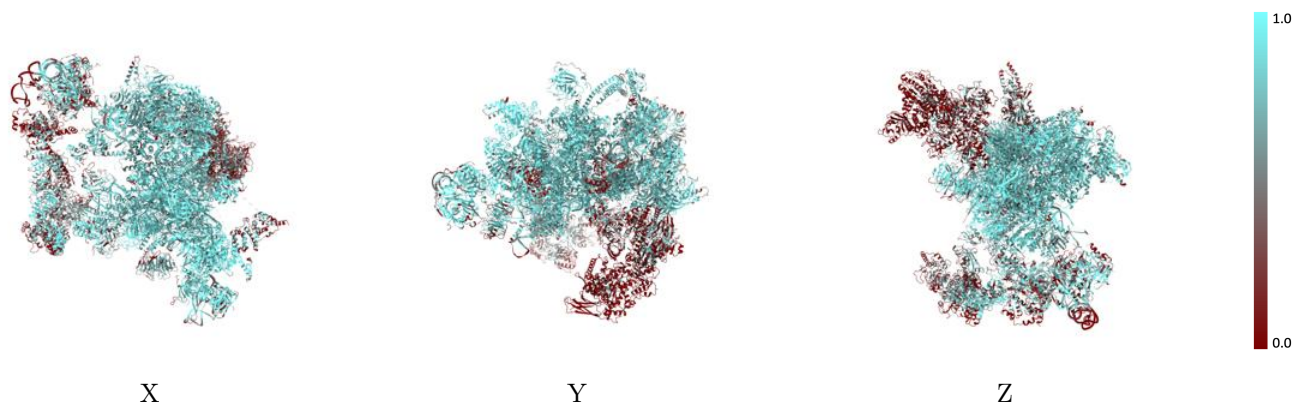
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



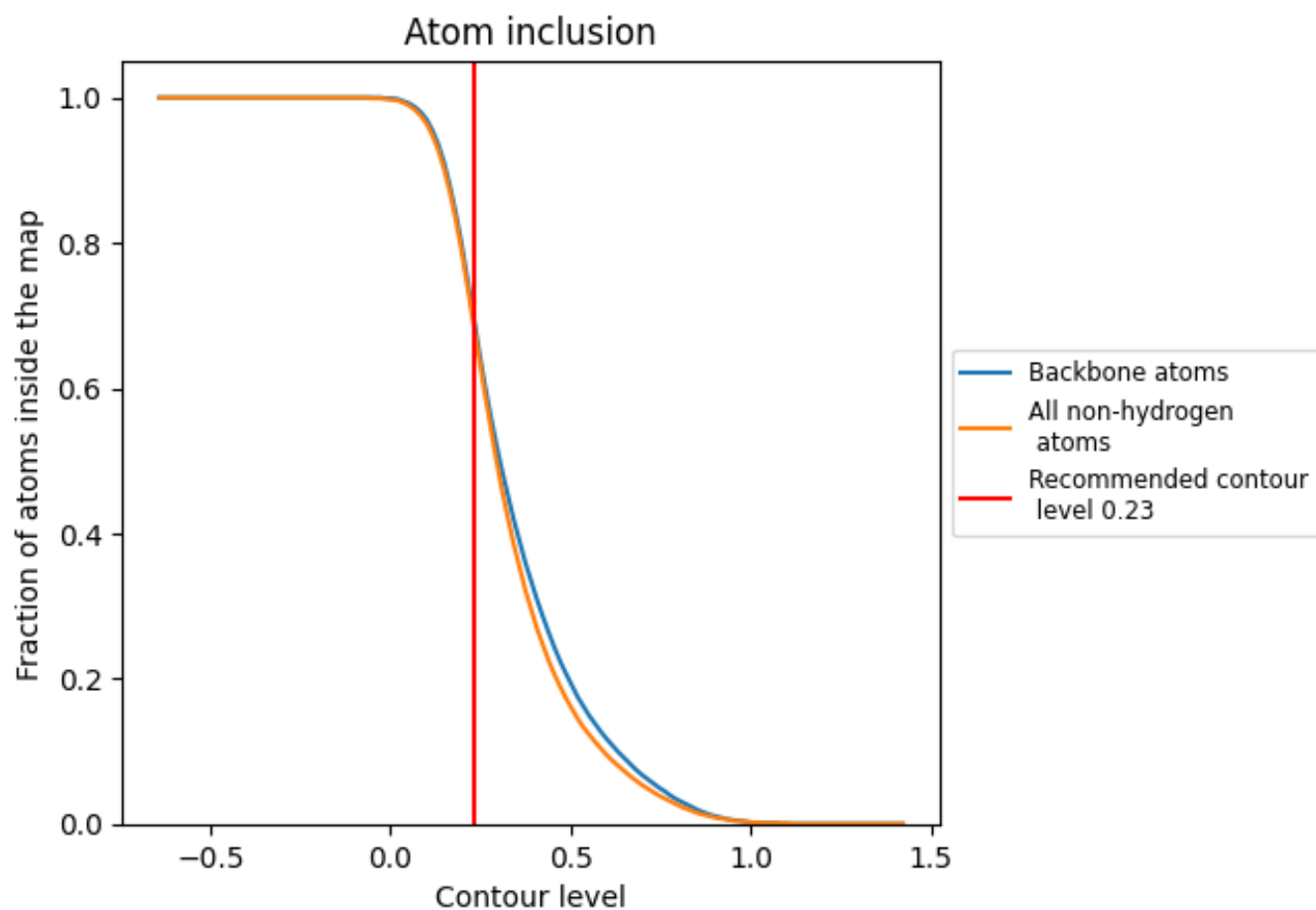
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.1500
1	 0.8260	 0.1670
2	 0.7660	 0.1690
3	 0.8130	 0.1010
4	 0.7950	 0.1090
5	 0.7970	 0.1510
7	 0.8350	 0.1360
9	 0.7080	 0.1070
A	 0.7710	 0.2800
B	 0.8870	 0.2130
C	 0.8870	 0.2460
D	 0.1440	 0.0090
E	 0.5050	 0.0060
F	 0.8820	 0.2120
G	 0.8800	 0.1740
H	 0.6840	 0.0940
I	 0.6980	 0.0410
J	 0.8680	 0.2330
K	 0.7200	 0.1860
L	 0.7620	 0.2020
N	 0.7390	 0.1910
O	 0.7870	 0.1710
P	 0.8120	 0.2930
Q	 0.3560	 0.0320
R	 0.7710	 0.2270
S	 0.6420	 0.0810
T	 0.9300	 0.4050
U	 0.7620	 0.2050
V	 0.6430	 0.1150
X	 0.8030	 0.1600
Y	 0.8260	 0.1320
a	 0.7090	 0.0930
b	 0.8480	 0.0790
c	 0.7290	 0.0670
d	 0.7740	 0.0580



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Chain	Atom inclusion	Q-score
e	 0.8290	 0.0740
f	 0.6990	 0.0610
g	 0.8270	 0.0670
h	 0.6390	 0.0150
i	 0.6320	 0.0050
j	 0.6280	 0.0460
k	 0.5190	 0.0200
l	 0.5660	 0.0070
m	 0.5810	 0.0300
n	 0.6140	 -0.0020
o	 0.3680	 0.0010
p	 0.5760	 0.0540
u	 0.4830	 0.0420
v	 0.5610	 0.1100
w	 0.4710	 0.0410
y	 0.6460	 0.0790