



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 01:48 AM JST

PDB ID : 8I0R
EMDB ID : EMD-35107
Title : The cryo-EM structure of human Bact-I complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2023-01-11
Resolution : 3.00 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:

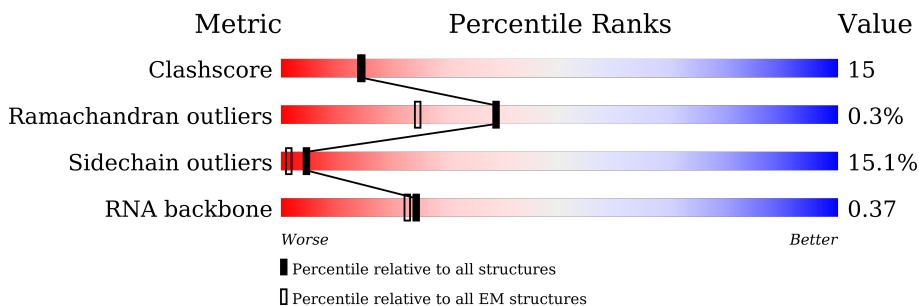
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.00 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	 58% 31% 6%
2	B	117	 29% 39% 14% 16%
3	C	972	 45% 36% 7% 12%
4	D	2136	 20% 77% 19%
5	E	357	 28% 38% 38% 8% 16%
6	F	107	 7% 13% 41% 34% 9%
7	G	220	 5% 10% 15% 68%

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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	1041	
19	T	514	
20	U	2752	
21	V	908	
22	W	122	
23	X	396	
24	Y	322	
25	Z	619	
26	1	1304	
27	3	1217	
28	p	225	
29	w	501	
30	u	793	
31	2	895	
32	4	424	

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Mol	Chain	Length	Quality of chain
33	6	125	
34	7	110	
35	5	86	
36	9	520	
37	8	904	
38	y	301	
39	v	464	
40	o	255	
41	c	118	
41	h	118	
42	d	86	
42	i	86	
43	a	240	
43	m	240	
44	g	126	
44	l	126	
45	f	76	
45	k	76	
46	e	92	
46	j	92	
47	b	119	
47	n	119	
48	z	472	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 115060 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	2242	18543	11943	3241	3280	79	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	71	1481	663	243	504	71	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	593	2991	1805	593	593	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	128	1059	660	190	204	5	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	99	829	532	149	144	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	1184	746	217	209	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	O	290	1433	853	290	290	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	42	362	231	63	66	2	0	0

- Molecule 16 is a protein called RNA helicase aquarius.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	237	1889	1171	347	360	11	0	0

- Molecule 18 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	S	643	3180	1894	643	643	0	0

- Molecule 19 is a protein called Pleiotropic regulator 1.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	468	Total	C	N	O	S	0	0
			3008	1873	546	576	13		

- Molecule 22 is a protein called Unknown polymer.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			229	140	46	43		

- Molecule 23 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	154	Total	C	N	O	S	0	0
			1279	819	231	227	2		

- Molecule 24 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	118	Total	C	N	O	S	0	0
			948	605	163	176	4		

- Molecule 25 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	137	Total	C	N	O	S	0	0
			1142	708	213	216	5		

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	993	Total	C	N	O	P	S	0	0
			7866	5018	1363	1438	1	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	169	Total	C	N	O	0	0
			851	513	169	169		

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

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

- Molecule 30 is a protein called Splicing factor 3A subunit 1.

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

- Molecule 31 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	250	Total	C	N	O	S	0	0
			1807	1134	340	326	7		

- Molecule 32 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4	161	Total	C	N	O	0	0
			792	470	161	161		

- Molecule 33 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	109	Total	C	N	O	S	0	0
			906	582	157	163	4		

- Molecule 34 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	105	Total	C	N	O	S	0	0
			811	502	145	151	13		

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5	81	Total	C	N	O	S	0	0
			669	422	117	124	6		

- Molecule 36 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	379	Total	C	N	O	S	0	0
			2636	1633	479	516	8		

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	8	115	Total	C	N	O	S	0	0
			931	602	154	170	5		

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

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

- Molecule 39 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	v	173	Total	C	N	O	S	0	0
			1041	602	219	217	3		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

- Molecule 42 is a protein called Small nuclear ribonucleoprotein F.

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

- Molecule 43 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

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

- Molecule 44 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 45 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 46 is a protein called Small nuclear ribonucleoprotein E.

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

- Molecule 47 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	n	80	Total	C	N	O	0	0
			402	242	80	80		

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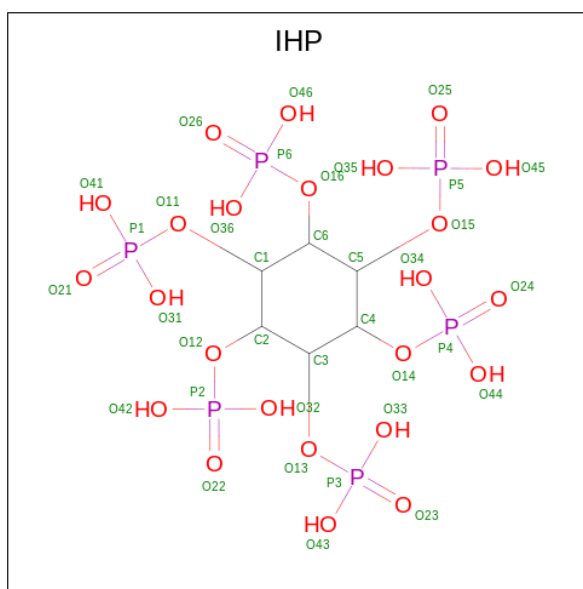
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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	b	82	328	164	82	82	0	0

- Molecule 48 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

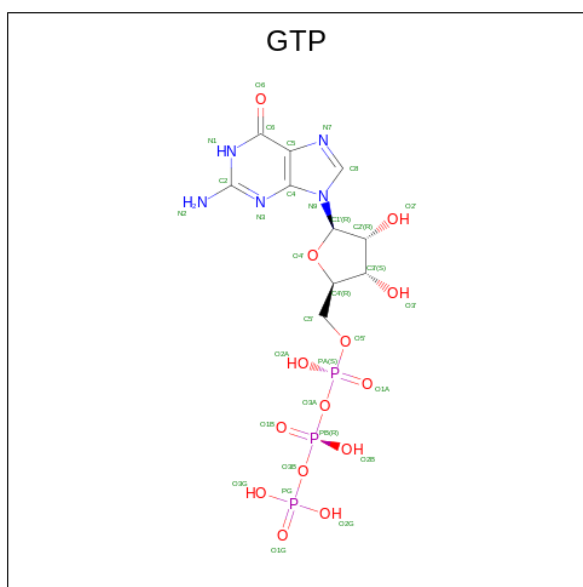
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	z	177	1402	884	243	270	5	1	0

- Molecule 49 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

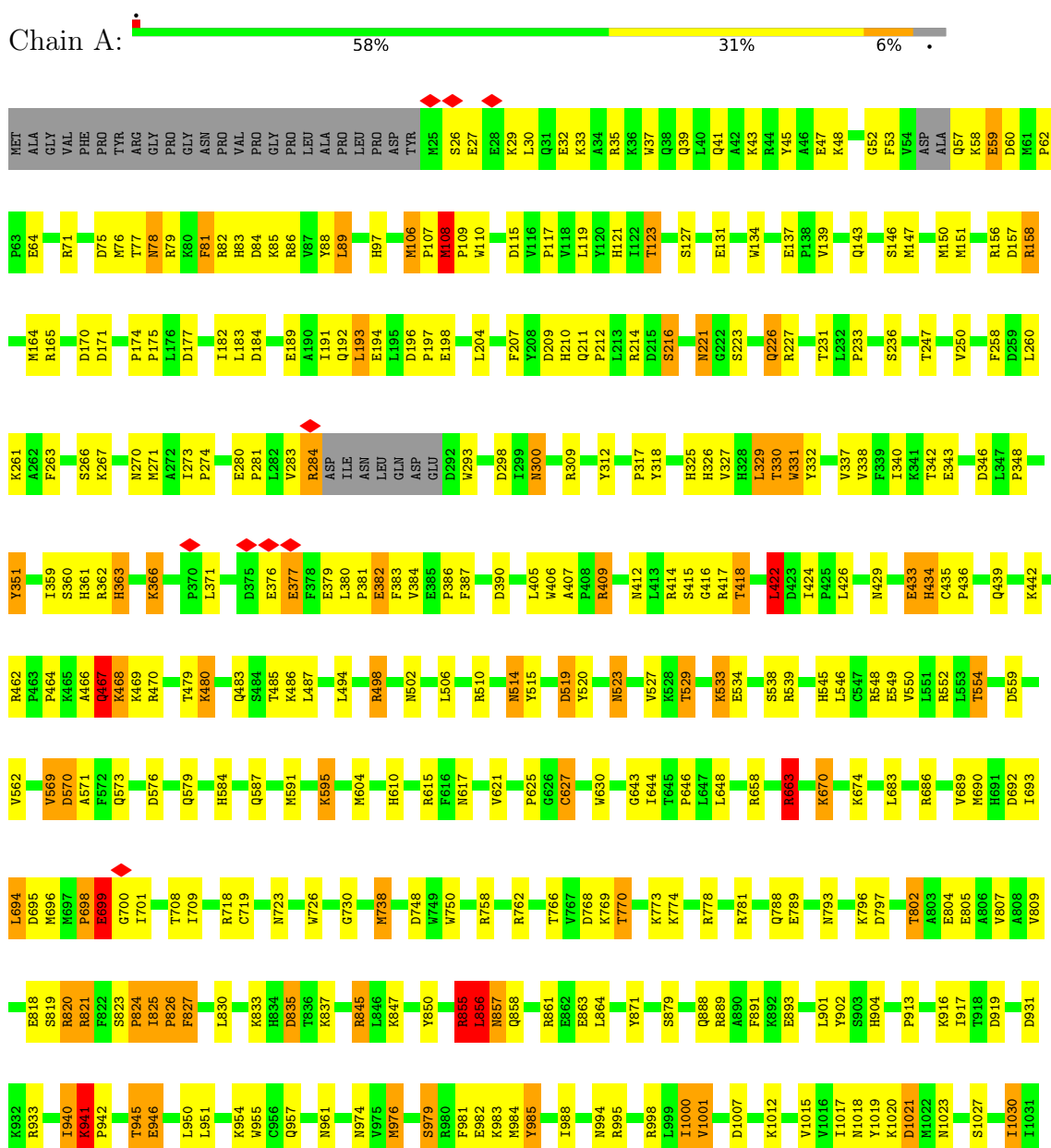
- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	K	1	Total	Zn	0
			1	1	
52	N	3	Total	Zn	0
			3	3	
52	7	3	Total	Zn	0
			3	3	

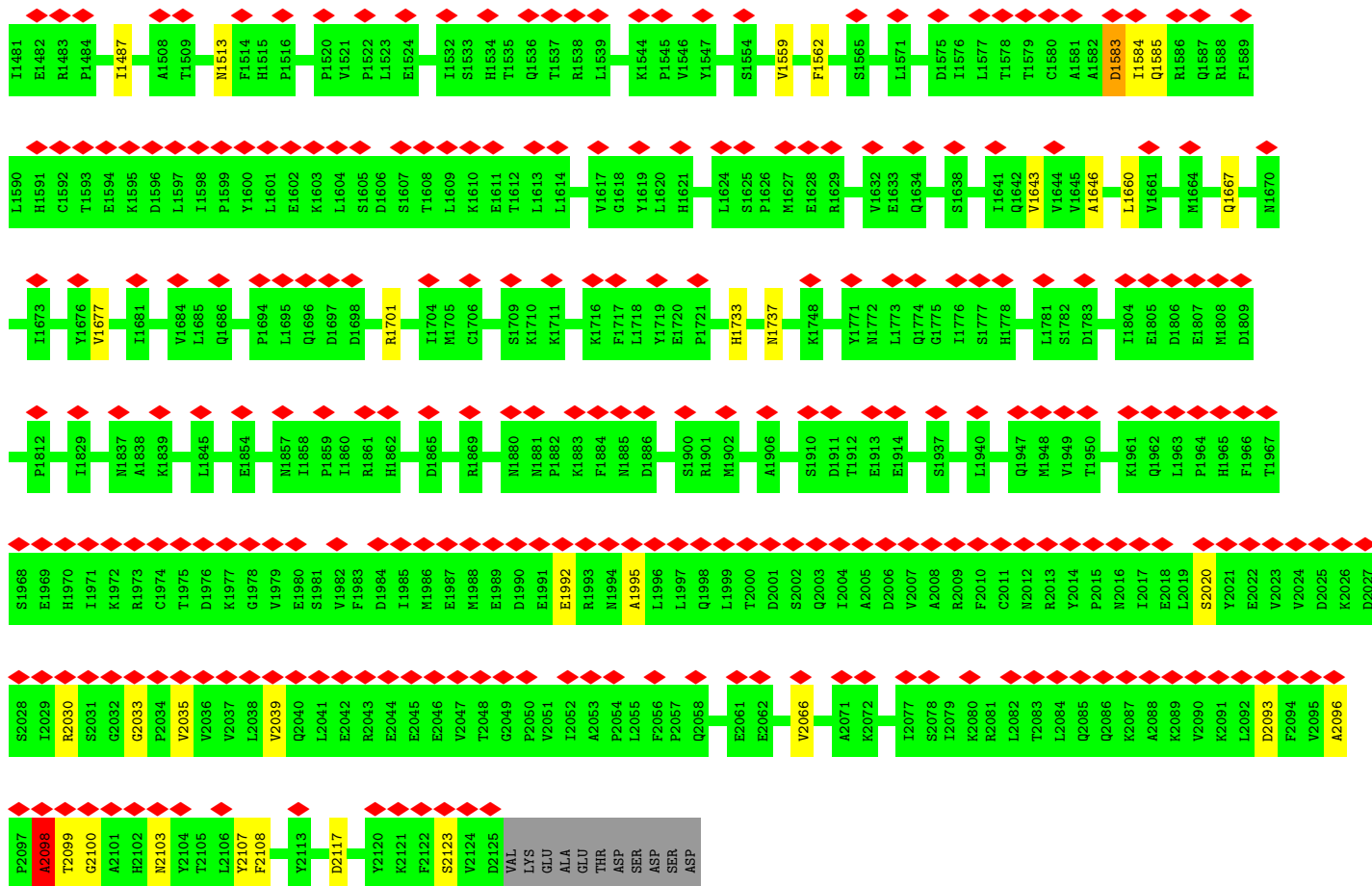
3 Residue-property plots

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.

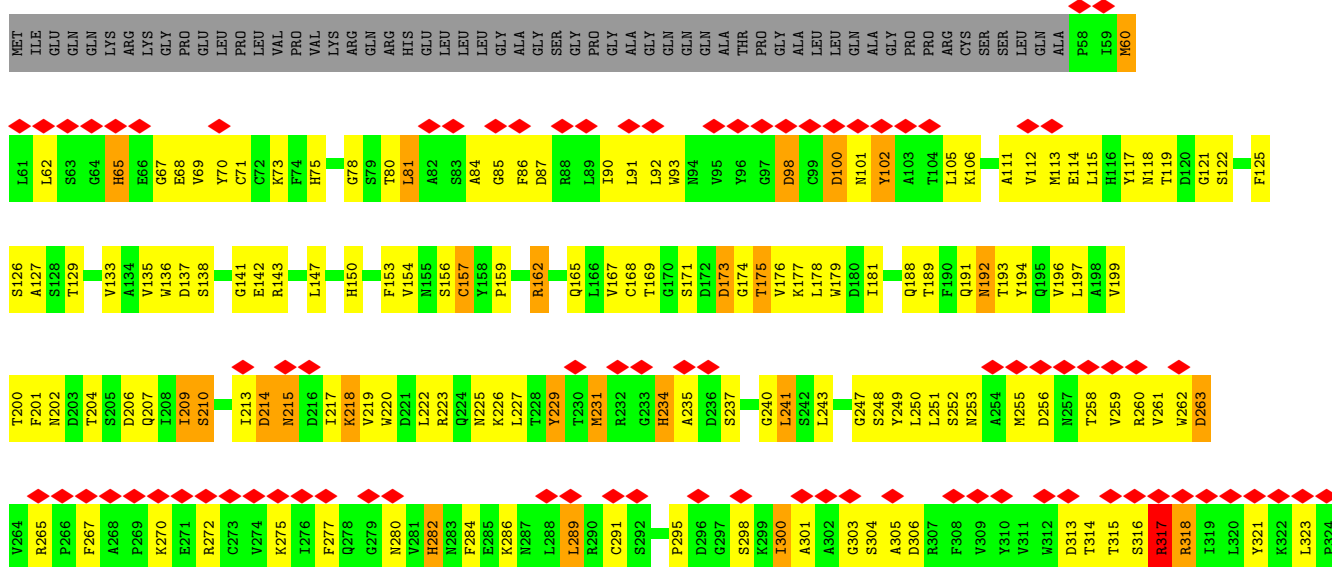
• Molecule 1: Pre-mRNA-processing-splicing factor 8

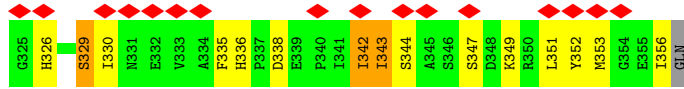


K2210	G2234	L2140	I2007	L1836	A1545	T1440	T1353	A1250	M1148	R1032
T2211	Y2235	E2141	R2008	A1837	M1546	D1441	H1352	S1251	M1151	F1036
I2212	E2236	I2142	D2009	K1838	V1547	K1449	H1359	G1252	R1151	A1037
I2213	E2237	W2069	I2010	W1839	Y1548	K1457	H1361	T1257	K1158	S1038
I2214	Y2228	K2070	W1922	K1840	V1549	H1457	E1360	K1258	T1167	H1048
T2215	E2229	L2011	W1923	L1841	L1550	Q1458	D1362	Q1363	T1167	L1055
C2216	K2230	L2012	K1925	L1842	F1551	H1460	D1362	K1262	V1168	L1055
S2217	E2231	G2013	T1926	A1843	Q1552	H1460	Q1363	K1262	V1168	L1055
F2218	R2232	M2014	I1927	E1844	V1553	H1460	Q1363	W1263	V1168	L1055
T2219	S2233	E2015	S1928	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
S2222	C2223	I2015	W1928	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
E2223	T2224	I2015	S1929	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
T2226	A2227	ALA	W1930	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
Y2228	E2228	ALA	Y1930	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
K2229	R2230	ALA	R1930	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
L2230	T2231	ALA	R1930	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
T2231	G2234	ALA	R1930	L1844	V1553	H1460	Q1363	W1263	V1168	L1055
G2234	Y2235	L2163	I1952	R1885	V1572	L1501	R1388	I1295	E1171	S1059
E2236	E2236	P2164	I1953	P1888	S1572	F1502	R1388	Q1296	E1171	S1059
W2237	W2237	Q2166	L1954	P1888	S1572	F1502	R1388	Q1296	E1171	S1059
G2238	R2239	E2167	R1955	P1888	S1572	F1502	R1388	Q1296	E1171	S1059
R2239	Q2240	E2168	K1956	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
Q2240	K2241	L2169	L1957	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
N2241	E2171	K2170	D1957	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
T2242	M2172	E2172	K1958	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
D2243	E2173	P2174	L1959	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
K2244	L2106	P2174	T1959	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
C2245	L2175	G2176	E1975	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
N2246	K2108	G2176	L1798	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
N2247	M2109	L2177	P1802	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
P2248	V2110	L2178	I1803	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
K2249	L2111	H2179	H1803	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
G2250	K2112	E2180	M1804	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
Y2251	K2113	Q2181	I1807	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
L2252	L2115	P2182	F1808	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
P2253	L2116	L2188	R1813	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
S2254	C2116	L2188	R1814	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
H2255	L2117	S2189	G1815	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
E2257	S2118	P2190	L1816	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
R2258	D2191	Q2191	L1817	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
V2259	Q2192	D2192	L1818	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
Q2260	V2193	T2194	F1818	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
M2261	T2194	T2194	F1818	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
L2262	T2195	H2196	L1819	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
L2263	Q2123	H2196	K1820	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
S2264	L2124	A2201	I1821	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
D2265	Y2127	D2202	I1822	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
R2266	L2128	D2202	H1823	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
F2267	Y2129	N2203	H1824	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
L2268	Y2129	N2203	E1745	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
G2269	Q2130	S2206	E1745	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
F2270	W2131	S2206	E1745	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
	S2206	S2206	E1745	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
	W2206	S2206	E1745	L1888	S1572	F1502	R1388	Q1296	E1171	S1059
	E2209	S2206	E1745	L1888	S1572	F1502	R1388	Q1296	E1171	S1059

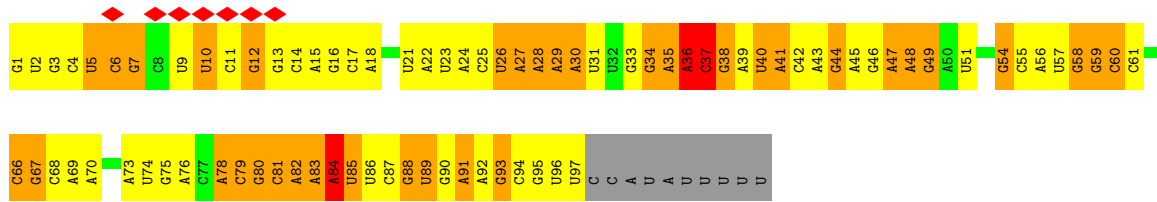


• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

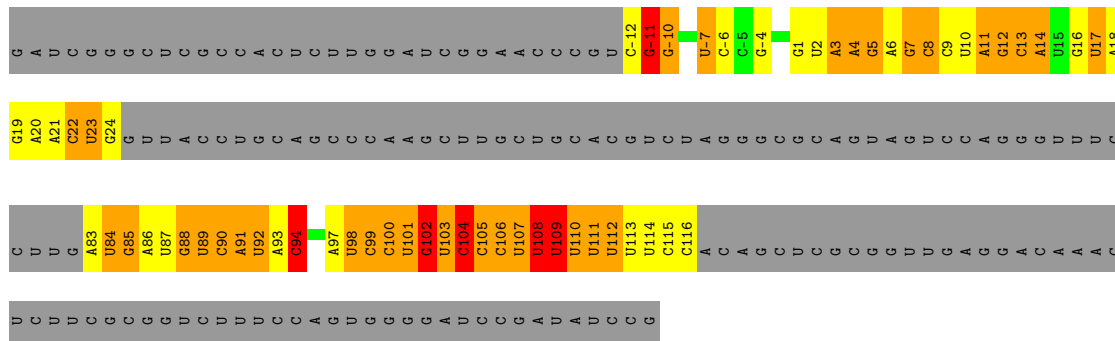




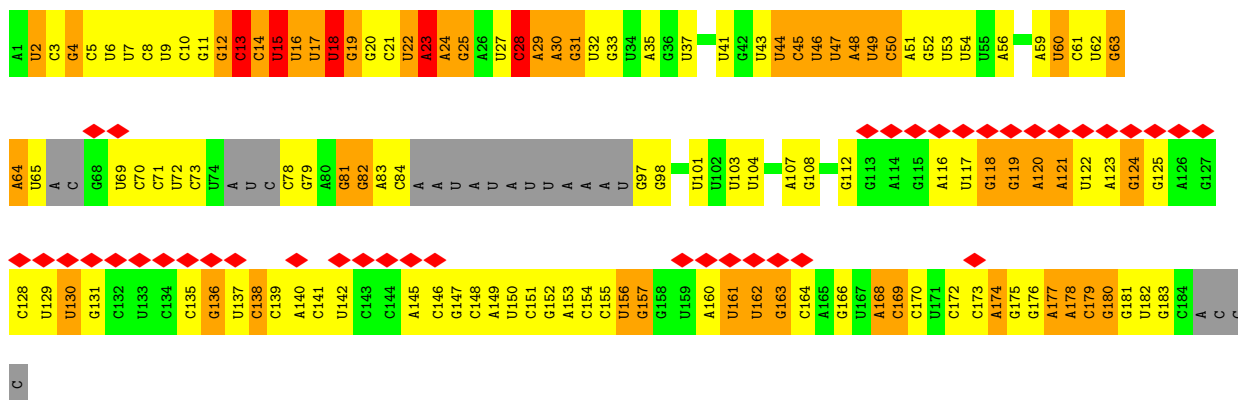
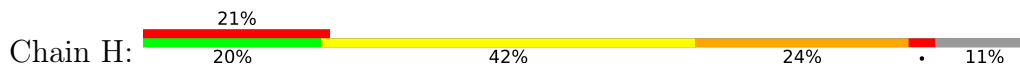
• Molecule 6: U6 snRNA



• Molecule 7: pre-mRNA

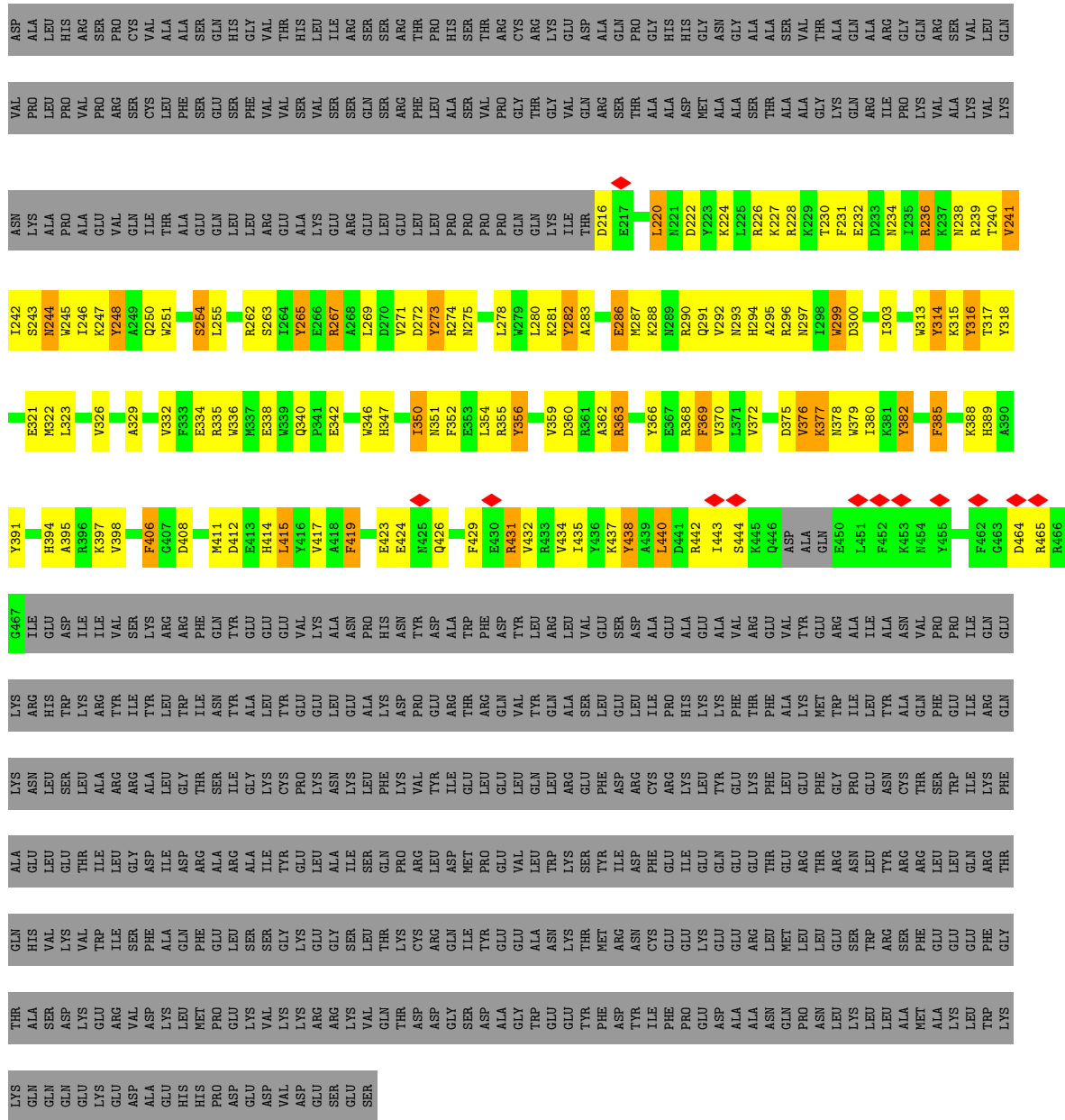


• Molecule 8: U2 snRNA

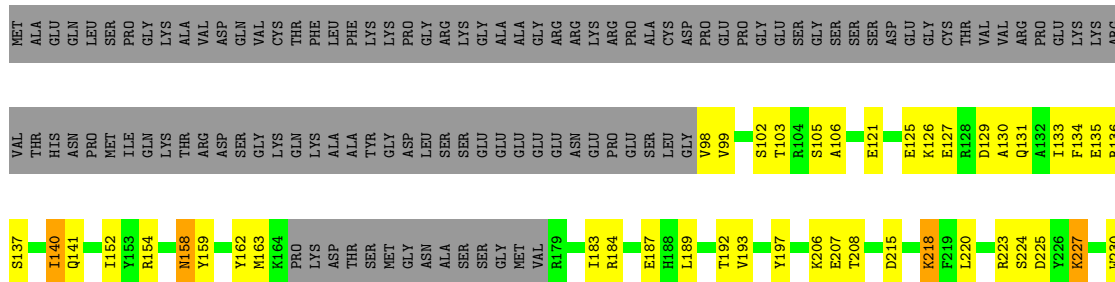


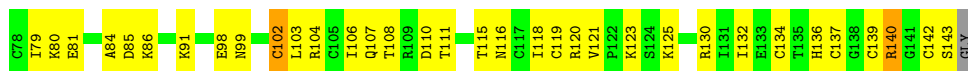
• Molecule 9: Pre-mRNA-splicing factor SYF1



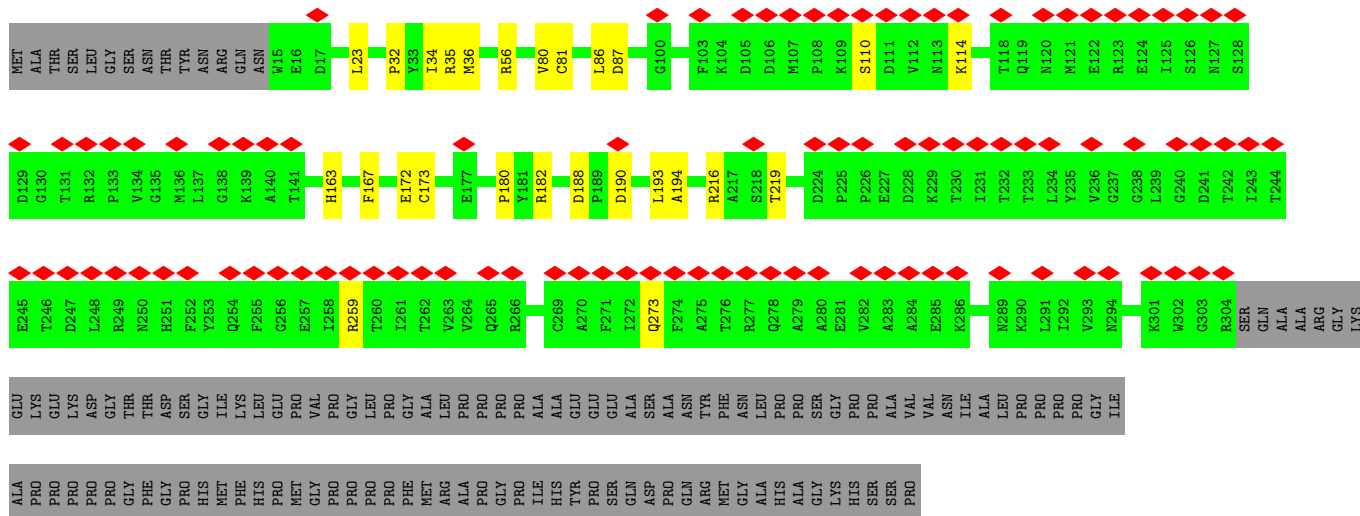


- Molecule 11: RING finger protein 113A

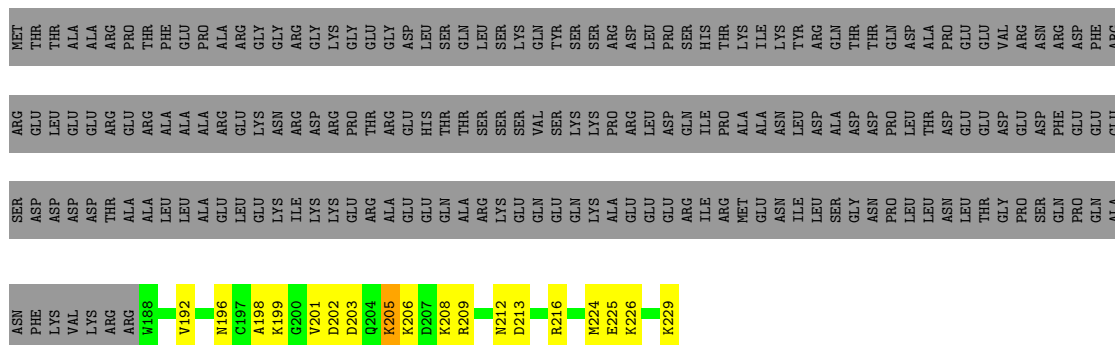




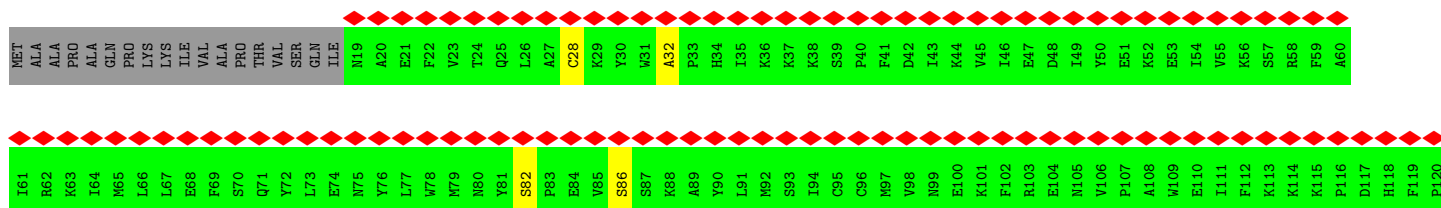
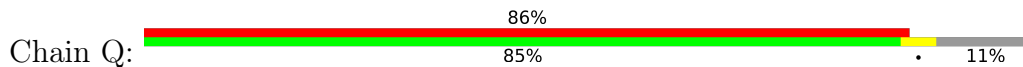
• Molecule 14: Pre-mRNA-splicing factor RBM22



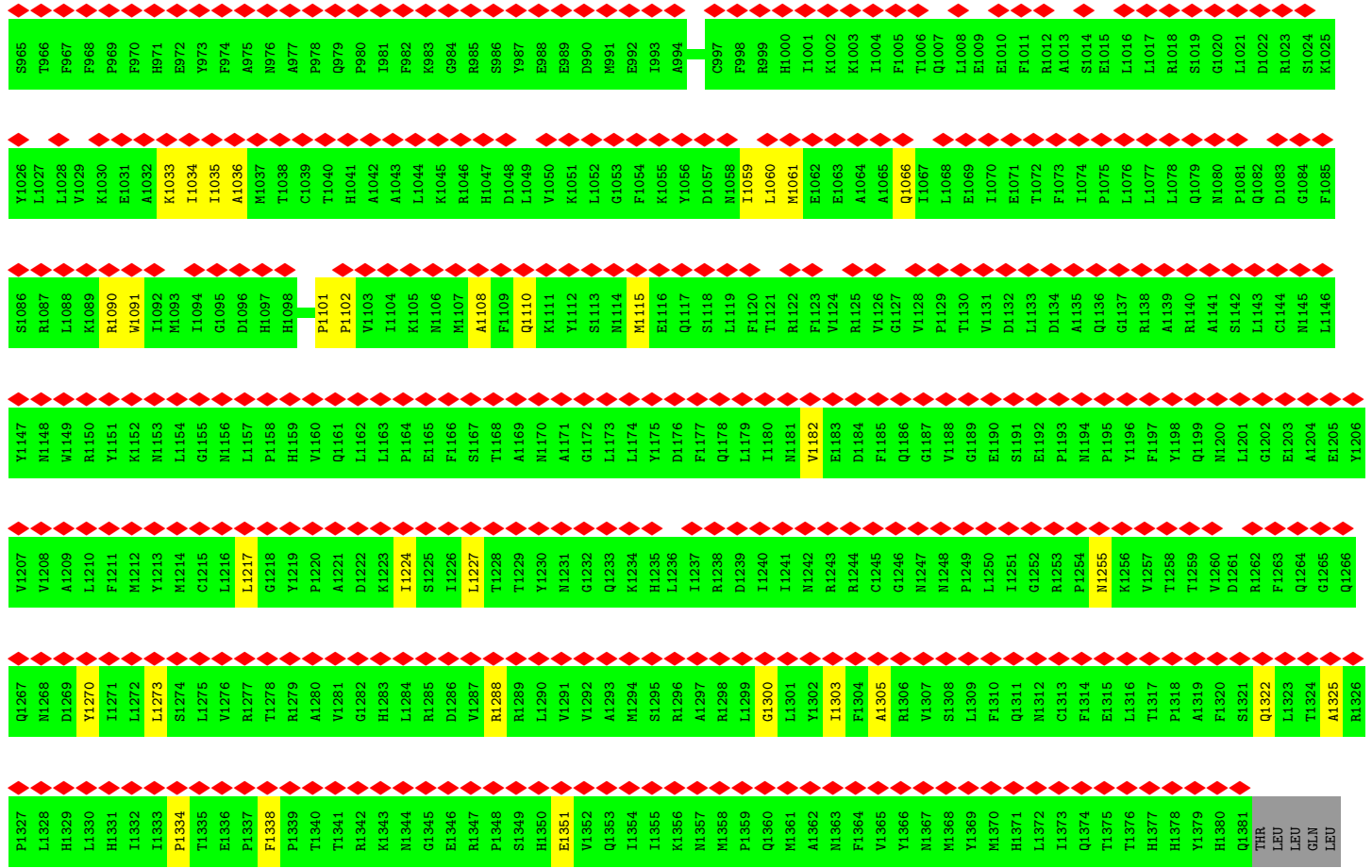
• Molecule 15: Spliceosome-associated protein CWC15 homolog



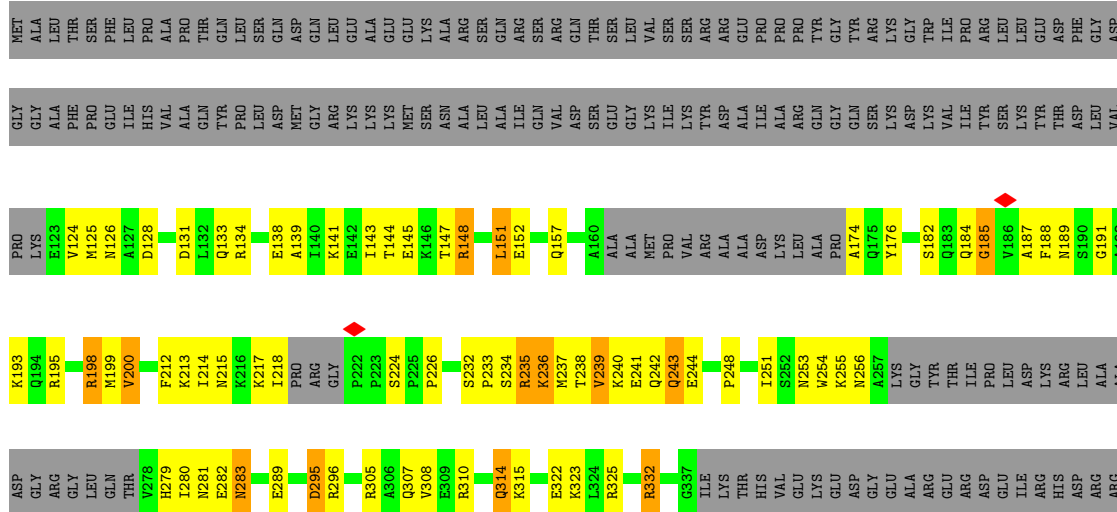
• Molecule 16: RNA helicase aquarius

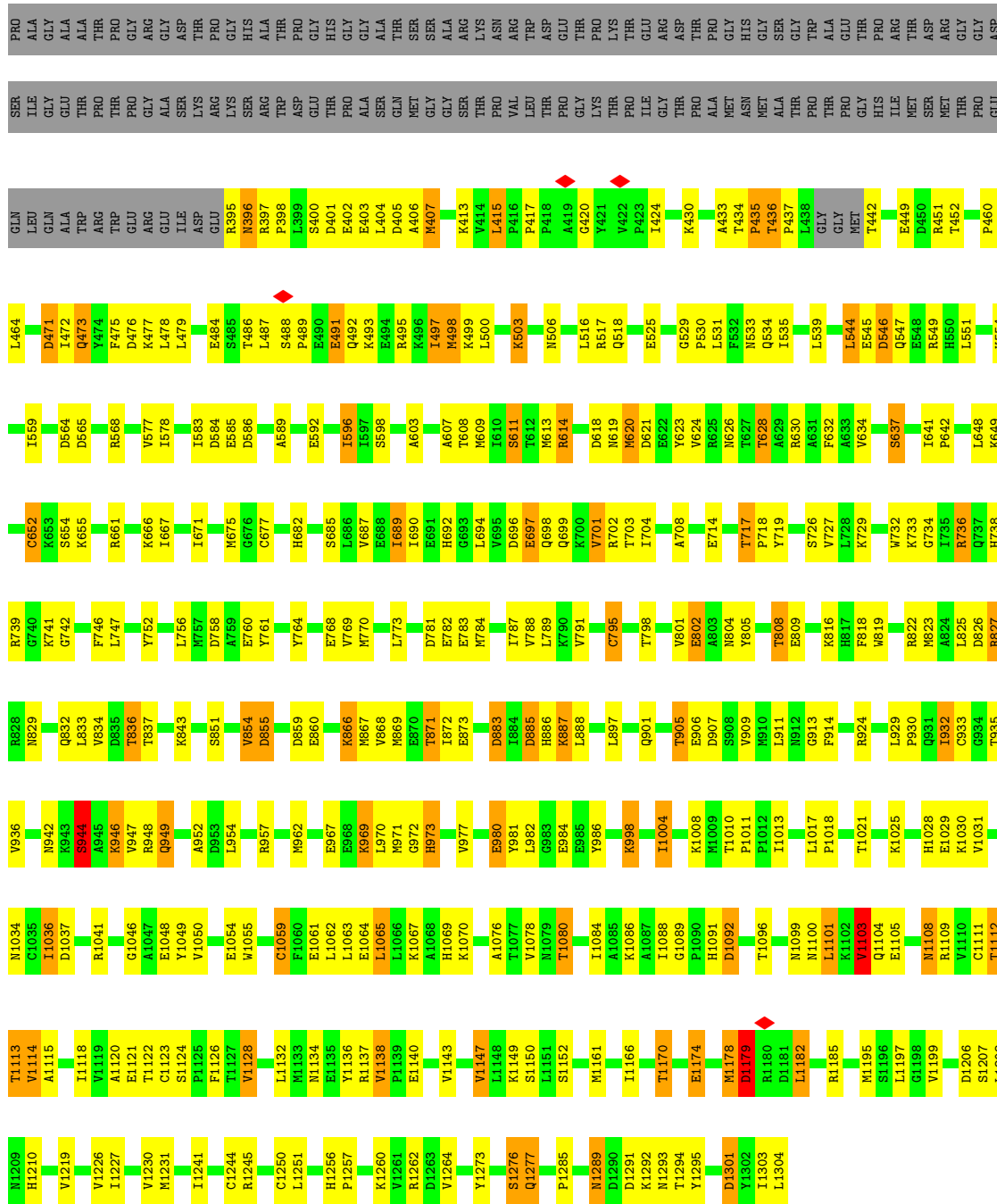


F121	A181	P241	L301	T361	L421	I481	L541	L601	L781	H723	V783	M843	R905
F122	R182	V242	L302	R362	M422	R482	N542	D602	LYS	H724	L784	P844	I906
F123	L183	T243	D303	E363	Q423	Q483	L543	D603	GLU	K725	T785	P845	E907
K124	E184	M244	M304	S364	M424	D484	N544	R604	ASN	A726	M786	P846	L908
H125	L185	K245	K305	L365	P425	I485	V545	R606	F666	S727	R787	Q847	R909
I126	E186	K246	K306	V366	L426	E486	R546	V607	R667	F728	G788	R848	E910
L127	E187	V247	F307	K367	Y427	D487	D547	L608	L668	F729	F789	T849	E911
K128	K188	H248	Y308	F368	P428	S488	H548	E609	L669	G730	V790	L850	V912
A129	K189	Y249	T309	F369	T429	V489	L649	ASP	E671	H731	F791	I851	K913
A130	T190	C250	G310	G370	E430	S490	K550	PRD	T672	N732	V792	H852	R914
L131	P191	E251	F311	P371	K431	R491	D551	GLU	I673	W733	M793	T853	L915
A132	K192	R252	E312	L372	I432	M492	E552	P614	R674	K734	Q794	H854	Q916
T133	L193	F253	I313	S373	I433	K493	M553	R615	N675	W735	F795	S855	K917
T134	R194	I254	N314	S374	I434	P494	E554	R616	L676	T736	K796	M856	S918
D135	K195	E255	D315	N375	D435	M495	G555	P617	M677	W737	R797	Q857	L919
G136	F196	L256	Q316	T376	E436	Q496	L556	M617	M678	E738	M798	A858	Q920
E137	M197	M257	T317	L377	M437	S497	R557	L618	M679	D739	T799	L859	V921
F138	M198	I258	G318	H378	I438	E498	K558	E621	D680	P740	V799	R860	T922
S139	L199	D259	N319	Q379	Y439	Y499	H559	S622	C681	A741	R801	Q861	G923
L140	T200	L260	A320	V380	P440	G500	D560	R623	V682	L742	F802	L862	D924
H141	K201	E261	L321	A381	T441	G501	V561	T624	W683	Q743	T803	F863	A925
E142	K202	A262	T322	S382	E442	V502	C562	F625	P684	I744	H804	E864	S926
Q143	N203	L263	E323	Y383	Y443	V503	F563	R626	M686	P745	T805	R865	Y927
T144	D204	L264	N324	L384	Y444	F504	L564	V627	L687	F747	Q806	M866	T928
V145	E205	P265	E325	C385	S445	G505	L565	W628	H688	R748	E807	R867	C929
L146	K206	T266	M326	L386	G446	G506	T566	L629	H689	I749	A808	L868	E930
L147	M207	R267	T327	L387	E447	M507	V567	L630	D690	T750	R809	R869	T931
L148	D208	R268	T328	P388	G448	A508	R568	P631	D691	F751	I810	A870	A932
F149	P209	F269	I329	T389	C449	M509	P569	N632	L692	W752	L811	L871	G933
L150	E210	W270	H330	L390	L450	A511	T570	O633	L693	F753	A812	D872	Y934
D151	A211	N271	Y331	F391	A451	Q512	K571	W634	L694	W754	G813	E873	F935
H152	R212	T272	D332	K392	L452	P513	F573	O635	O695	ARG	H814	M874	F936
C153	E213	I273	R333	N393	P453	P513	Y573	Q636	D696	SER	H815	H875	L937
F154	Q214	I274	I334	E394	K454	G574	G574	D637	P697	GLY	Q815	L876	Y938
M155	A215	D275	T335	D395	L455	A516	T575	M638	S698	GLY	Q817	L877	Q939
S156	Y216	D276	S336	T396	M456	A516	K576	T639	S699	LYS	L818	H881	V940
L157	Y217	S277	S337	T397	M457	F517	F577	N640	F699	LYS	T819	G882	N941
E158	E218	H278	Q338	F398	Q458	W519	D578	T641	H701	ARG	H820	E883	S942
V159	R219	L279	R339	D399	F459	V520	R579	R642	Y702	ASP	W821	E884	R943
D160	R220	L280	A340	K400	L460	E521	R580	O643	S703	ALA	V822	E885	E945
L161	F221	V281	A341	E401	T461	V522	F582	N644	K704	VAL	G823	L886	E946
I162	F222	H282	A342	F402	L462	A523	P582	R645	M705	GLU	P824	E887	Y947
R163	S223	C283	A343	L403	H463	A524	F583	A646	P706	ASP	P825	T888	I948
S164	Q224	Y284	H344	L404	D464	K524	L584	E647	W707	GLU	R826	E889	S949
Q165	L225	L285	F345	E405	Y465	N526	E585	D648	Q708	THR	T827	K890	K950
V166	L226	S286	P346	L406	L466	L527	Q586	V649	L709	GLU	G828	D891	V951
Q167	Q227	N287	E347	L407	L467	G528	V587	W650	A710	GLU	H829	F892	I952
Q168	K228	L288	E348	V408	R468	E529	G588	L589	T711	L712	T830	S893	K953
L169	F229	V289	Y349	S409	M469	N530	L590	V590	A711	A774	H831	R894	L953
I170	R230	R290	D350	R410	F470	W531	N531	W591	L716	K775	W832	Y895	LYS
S171	S231	R291	F351	H411	M471	P532	W532	Y591	D713	T776	W833	G896	SER
L172	V232	E292	A352	E412	L472	T533	E592	L655	F714	L777	W834	R897	THR
M173	L233	E293	L353	R413	R473	R534	R593	L656	M715	I778	Q835	V898	LEU
W175	K234	E294	S354	R414	R474	W535	G594	M657	D716	W779	I836	N899	P959
M176	S235	G295	N355	I415	L475	R536	C595	H658	F718	T717	I837	Y900	D960
G177	V236	H296	V356	S416	E476	A537	E596	R659	L719	F718	S838	Y901	T962
L178	P237	L297	E357	Q417	S477	D538	L597	H659	S720	L719	H839	I902	G963
Q179	L238	F298	V359	I418	T478	W539	Q598	L599	I721	E722	Y841	A903	V984
Q300	S239	S299	D360	Q420	Y479	T540	M600	N600	E722		H842	R904	

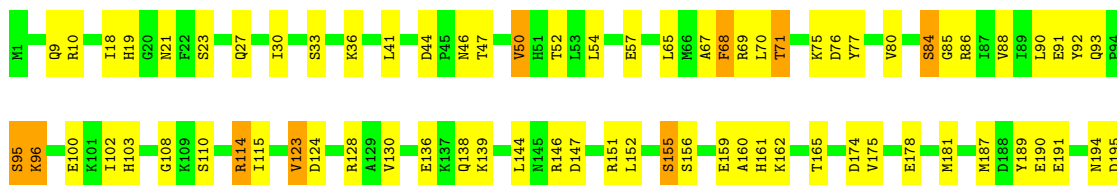


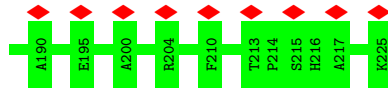
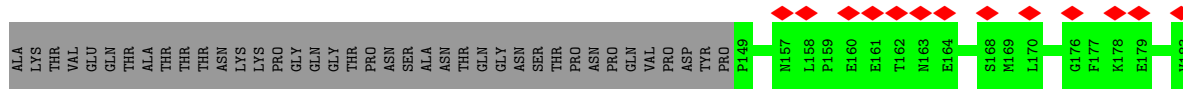
● Molecule 17: SNW domain-containing protein 1



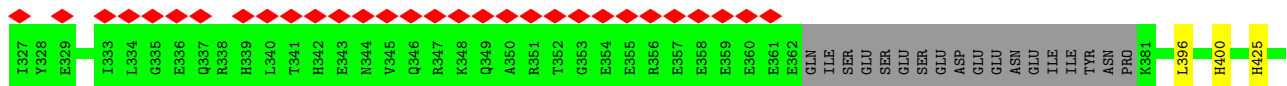
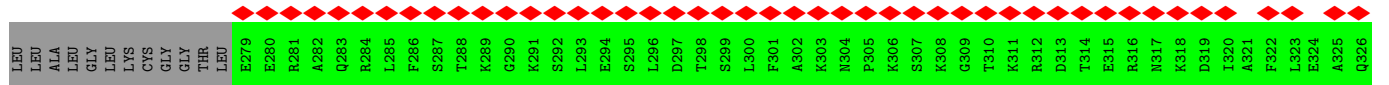
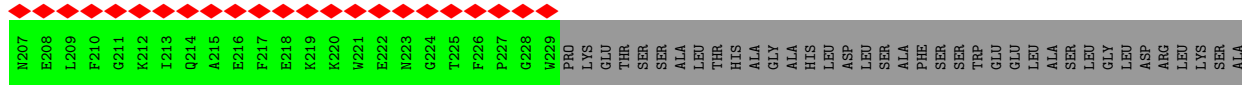
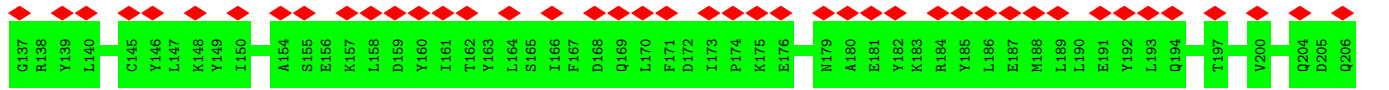
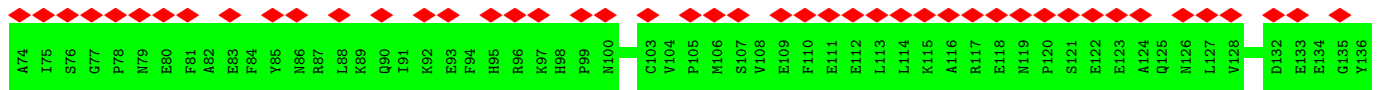
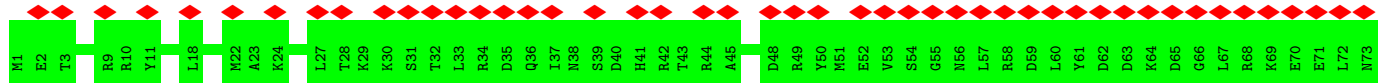
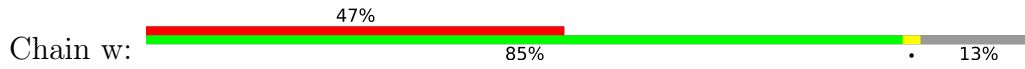


● Molecule 27: Splicing factor 3B subunit 3

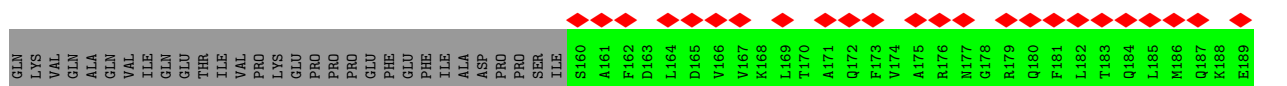
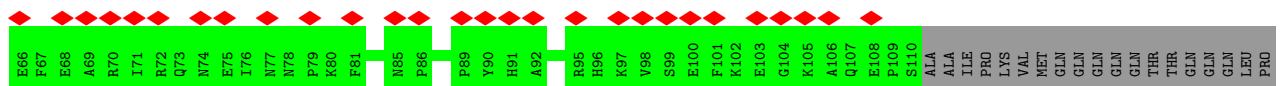
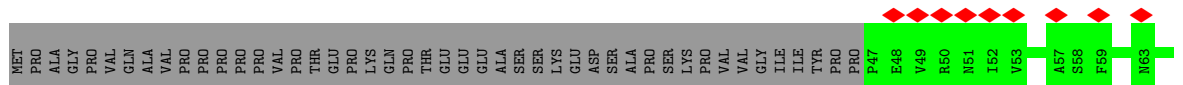


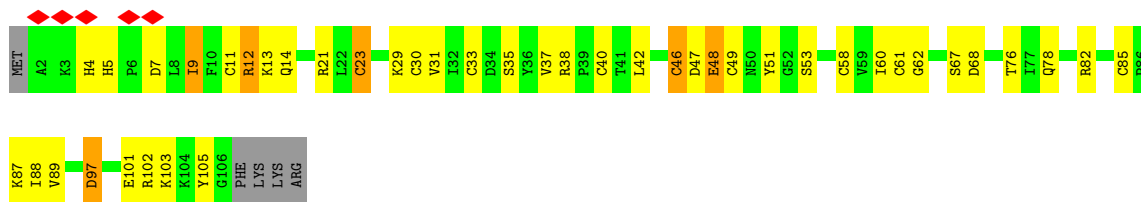


• Molecule 29: Splicing factor 3A subunit 3

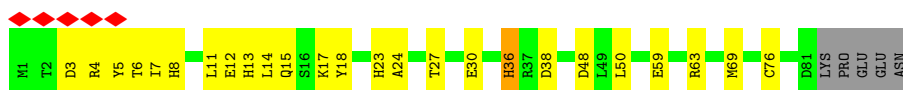


• Molecule 30: Splicing factor 3A subunit 1

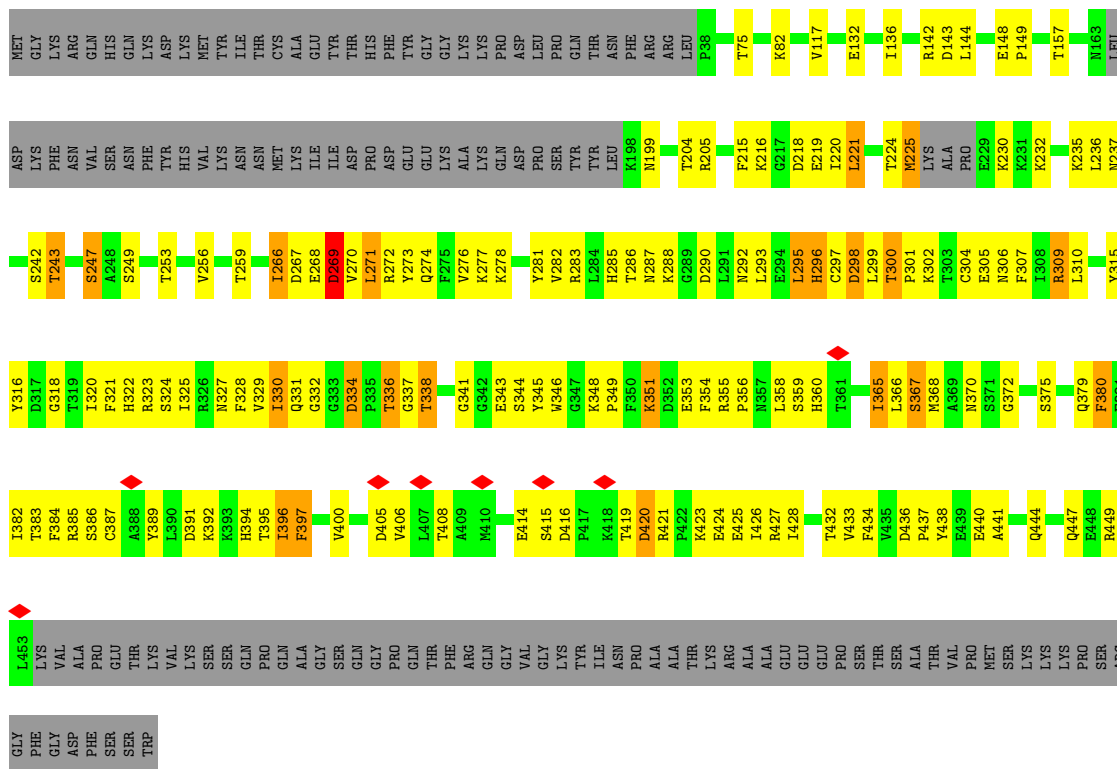




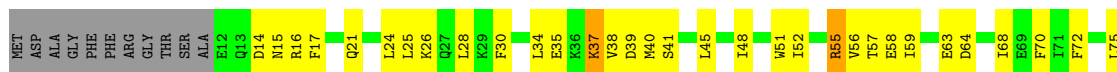
• Molecule 35: Splicing factor 3B subunit 5



• Molecule 36: RING-type E3 ubiquitin-protein ligase PPIL2



• Molecule 37: Serine/arginine repetitive matrix protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136665	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	3.781	Depositor
Minimum map value	-1.945	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.24	Depositor
Map size (\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 (\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: SEP, ZN, MG, IHP, 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	0.81	5/19056 (0.0%)	0.67	10/25857 (0.0%)
2	B	1.10	2/2303 (0.1%)	1.11	6/3579 (0.2%)
3	C	0.45	0/6873	0.59	1/9346 (0.0%)
4	D	0.25	0/8527	0.44	0/11887
5	E	0.29	0/2392	0.60	1/3242 (0.0%)
6	F	1.23	8/2323 (0.3%)	1.20	11/3619 (0.3%)
7	G	0.99	1/1648 (0.1%)	1.20	14/2558 (0.5%)
8	H	0.76	2/3947 (0.1%)	1.10	8/6138 (0.1%)
9	I	0.24	0/3013	0.45	0/4223
10	J	0.32	0/2171	0.54	0/2929
11	K	0.67	0/1081	0.60	0/1447
12	L	0.62	0/850	0.61	0/1146
13	N	0.34	0/1210	0.55	0/1622
14	O	0.25	0/1432	0.45	0/1993
15	P	0.83	0/369	0.68	0/489
16	Q	0.24	0/6796	0.43	0/9527
17	R	0.57	0/1920	0.59	1/2576 (0.0%)
18	S	0.25	0/3178	0.43	0/4425
19	T	0.91	4/2574 (0.2%)	0.72	2/3511 (0.1%)
20	U	0.36	0/424	0.53	0/582
21	V	0.38	0/3043	0.51	0/4156
22	W	0.63	0/33	0.78	0/42
23	X	0.42	0/1312	0.56	0/1769
24	Y	0.63	0/966	0.62	1/1303 (0.1%)
25	Z	0.46	0/1166	0.56	0/1559
26	1	0.74	7/8004 (0.1%)	0.69	10/10830 (0.1%)
27	3	0.61	0/9408	0.65	4/12767 (0.0%)
28	p	0.25	0/857	0.45	0/1196
29	w	0.30	0/2311	0.47	0/3008
30	u	0.23	0/842	0.41	0/1110
31	2	0.56	0/1837	0.64	1/2473 (0.0%)
32	4	0.26	0/790	0.46	0/1095

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.37	0/925	0.56	0/1247
34	7	0.54	0/825	0.54	0/1106
35	5	0.77	0/688	0.64	0/930
36	9	0.36	0/2675	0.56	0/3631
37	8	0.40	0/946	0.51	0/1270
38	y	0.25	0/389	0.44	0/540
39	v	0.47	0/1054	0.55	0/1385
40	o	0.24	0/821	0.48	0/1149
41	c	0.23	0/387	0.52	0/482
41	h	0.25	0/485	0.46	0/677
42	d	0.24	0/295	0.54	0/367
42	i	0.27	0/362	0.49	0/502
43	a	0.25	0/343	0.54	0/427
43	m	0.25	0/416	0.52	0/581
44	g	0.24	0/322	0.52	0/399
44	l	0.25	0/417	0.50	0/581
45	f	0.24	0/295	0.54	0/367
45	k	0.24	0/366	0.51	0/509
46	e	0.23	0/315	0.50	0/392
46	j	0.24	0/403	0.49	0/561
47	b	0.24	0/327	0.53	0/407
47	n	0.24	0/404	0.47	0/564
48	z	0.59	0/1436	0.58	0/1945
All	All	0.60	29/117552 (0.0%)	0.66	70/162023 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
3	C	0	7
4	D	0	2
9	I	0	1
13	N	0	1
15	P	0	2
16	Q	0	2
17	R	0	1
23	X	0	1
26	1	0	5
27	3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	2	0	1
48	z	0	1
All	All	0	42

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	827	PHE	C-N	8.64	1.50	1.34
19	T	307	SER	CA-CB	-8.22	1.40	1.52
19	T	349	SER	CA-CB	-7.69	1.41	1.52
1	A	826	PRO	C-O	-7.65	1.07	1.23
19	T	307	SER	C-O	-7.26	1.09	1.23

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1108	ASN	CB-CA-C	-9.45	91.49	110.40
8	H	15	U	C2-N1-C1'	-9.39	106.43	117.70
7	G	104	C	N1-C2-O2	8.48	123.99	118.90
8	H	15	U	C6-N1-C1'	8.47	133.06	121.20
26	1	942	ASN	CB-CA-C	-7.91	94.57	110.40

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	GLU	Peptide
1	A	467	GLN	Peptide
1	A	699	GLU	Peptide
1	A	700	GLY	Peptide
1	A	81	PHE	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	18543	0	18403	623	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2066	0	1047	54	0
3	C	6724	0	6696	310	0
4	D	8528	0	3745	42	0
5	E	2338	0	2275	125	0
6	F	2075	0	1048	104	0
7	G	1481	0	755	81	0
8	H	3539	0	1791	123	0
9	I	2991	0	1473	11	0
10	J	2116	0	1977	100	0
11	K	1059	0	1012	36	0
12	L	829	0	837	22	0
13	N	1184	0	1193	50	0
14	O	1433	0	621	18	0
15	P	362	0	356	13	0
16	Q	6730	0	3268	32	0
17	R	1889	0	1866	73	0
18	S	3180	0	1441	20	0
19	T	2507	0	2451	80	0
20	U	422	0	291	15	0
21	V	3008	0	2288	89	0
22	W	229	0	85	3	0
23	X	1279	0	1284	66	0
24	Y	948	0	954	34	0
25	Z	1142	0	1112	35	0
26	1	7866	0	7964	285	0
27	3	9220	0	9139	407	0
28	p	851	0	423	0	0
29	w	2275	0	1347	0	0
30	u	834	0	325	0	0
31	2	1807	0	1622	57	0
32	4	792	0	367	16	0
33	6	906	0	913	49	0
34	7	811	0	790	29	0
35	5	669	0	631	16	0
36	9	2636	0	2228	125	0
37	8	931	0	960	39	0
38	y	390	0	190	0	0
39	v	1041	0	800	0	0
40	o	816	0	386	0	0
41	c	388	0	102	0	0
41	h	482	0	220	0	0
42	d	296	0	87	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	i	359	0	179	0	0
43	a	344	0	93	0	0
43	m	413	0	194	0	0
44	g	324	0	89	0	0
44	l	415	0	198	0	0
45	f	296	0	84	0	0
45	k	364	0	176	0	0
46	e	316	0	85	0	0
46	j	403	0	173	0	0
47	b	328	0	89	0	0
47	n	402	0	184	0	0
48	z	1402	0	1336	0	0
49	A	36	0	6	2	0
50	C	32	0	12	3	0
51	C	1	0	0	0	0
51	F	5	0	0	0	0
52	7	3	0	0	0	0
52	K	1	0	0	0	0
52	N	3	0	0	0	0
All	All	115060	0	89661	2901	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 15.

The worst 5 of 2901 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)
26:1:933:CYS:SG	26:1:970:LEU:HD21	1.63	1.38
26:1:933:CYS:SG	26:1:970:LEU:HD11	1.74	1.27
26:1:933:CYS:SG	26:1:970:LEU:CD2	2.35	1.13
26:1:933:CYS:SG	26:1:970:LEU:CD1	2.43	1.06
21:V:580:ARG:HE	25:Z:545:MET:HB2	1.19	1.04

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2232/2335 (96%)	2012 (90%)	205 (9%)	15 (1%)	19	54
3	C	854/972 (88%)	748 (88%)	99 (12%)	7 (1%)	16	51
4	D	1720/2136 (80%)	1598 (93%)	118 (7%)	4 (0%)	44	77
5	E	297/357 (83%)	268 (90%)	28 (9%)	1 (0%)	37	70
9	I	591/855 (69%)	492 (83%)	98 (17%)	1 (0%)	44	77
10	J	245/848 (29%)	229 (94%)	15 (6%)	1 (0%)	30	66
11	K	124/343 (36%)	115 (93%)	9 (7%)	0	100	100
12	L	97/802 (12%)	89 (92%)	8 (8%)	0	100	100
13	N	141/144 (98%)	119 (84%)	20 (14%)	2 (1%)	9	37
14	O	288/420 (69%)	271 (94%)	17 (6%)	0	100	100
15	P	40/229 (18%)	30 (75%)	9 (22%)	1 (2%)	4	24
16	Q	1319/1485 (89%)	1237 (94%)	82 (6%)	0	100	100
17	R	227/536 (42%)	208 (92%)	18 (8%)	1 (0%)	30	66
18	S	639/1041 (61%)	600 (94%)	39 (6%)	0	100	100
19	T	318/514 (62%)	295 (93%)	23 (7%)	0	100	100
20	U	68/2752 (2%)	59 (87%)	9 (13%)	0	100	100
21	V	464/908 (51%)	438 (94%)	26 (6%)	0	100	100
22	W	4/122 (3%)	4 (100%)	0	0	100	100
23	X	152/396 (38%)	136 (90%)	16 (10%)	0	100	100
24	Y	116/322 (36%)	111 (96%)	5 (4%)	0	100	100
25	Z	135/619 (22%)	126 (93%)	8 (6%)	1 (1%)	19	54
26	1	984/1304 (76%)	910 (92%)	68 (7%)	6 (1%)	22	57
27	3	1165/1217 (96%)	1058 (91%)	104 (9%)	3 (0%)	37	70
28	p	165/225 (73%)	155 (94%)	10 (6%)	0	100	100
29	w	428/501 (85%)	393 (92%)	35 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	u	183/793 (23%)	175 (96%)	8 (4%)	0	100	100
31	2	246/895 (28%)	221 (90%)	25 (10%)	0	100	100
32	4	157/424 (37%)	143 (91%)	14 (9%)	0	100	100
33	6	107/125 (86%)	99 (92%)	8 (8%)	0	100	100
34	7	103/110 (94%)	95 (92%)	8 (8%)	0	100	100
35	5	79/86 (92%)	69 (87%)	10 (13%)	0	100	100
36	9	373/520 (72%)	336 (90%)	35 (9%)	2 (0%)	25	61
37	8	113/904 (12%)	106 (94%)	7 (6%)	0	100	100
38	y	77/301 (26%)	73 (95%)	4 (5%)	0	100	100
39	v	165/464 (36%)	156 (94%)	9 (6%)	0	100	100
40	o	160/255 (63%)	145 (91%)	15 (9%)	0	100	100
41	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
41	h	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
42	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
42	i	70/86 (81%)	66 (94%)	4 (6%)	0	100	100
43	a	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
43	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
44	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
44	l	81/126 (64%)	74 (91%)	7 (9%)	0	100	100
45	f	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
45	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
46	e	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
46	j	79/92 (86%)	71 (90%)	8 (10%)	0	100	100
47	b	80/119 (67%)	75 (94%)	5 (6%)	0	100	100
47	n	78/119 (66%)	70 (90%)	8 (10%)	0	100	100
48	z	176/472 (37%)	163 (93%)	13 (7%)	0	100	100
All	All	15859/28446 (56%)	14501 (91%)	1313 (8%)	45 (0%)	38	70

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	THR
1	A	856	LEU

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Mol	Chain	Res	Type
3	C	801	LEU
3	C	824	THR
13	N	40	LYS

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	2012/2108 (95%)	1706 (85%)	306 (15%)	2	11
3	C	747/866 (86%)	633 (85%)	114 (15%)	2	11
5	E	256/300 (85%)	212 (83%)	44 (17%)	1	8
9	I	23/749 (3%)	23 (100%)	0	100	100
10	J	205/751 (27%)	169 (82%)	36 (18%)	1	8
11	K	111/294 (38%)	95 (86%)	16 (14%)	2	13
12	L	86/709 (12%)	72 (84%)	14 (16%)	2	9
13	N	130/130 (100%)	111 (85%)	19 (15%)	2	12
15	P	40/203 (20%)	36 (90%)	4 (10%)	6	25
16	Q	71/1336 (5%)	70 (99%)	1 (1%)	62	83
17	R	200/459 (44%)	164 (82%)	36 (18%)	1	7
19	T	273/441 (62%)	234 (86%)	39 (14%)	2	13
20	U	21/2432 (1%)	19 (90%)	2 (10%)	7	28
21	V	194/838 (23%)	166 (86%)	28 (14%)	2	13
22	W	4/4 (100%)	4 (100%)	0	100	100
23	X	139/349 (40%)	119 (86%)	20 (14%)	2	13
24	Y	105/291 (36%)	88 (84%)	17 (16%)	2	10
25	Z	118/545 (22%)	100 (85%)	18 (15%)	2	11
26	1	840/1103 (76%)	709 (84%)	131 (16%)	2	11
27	3	1018/1051 (97%)	852 (84%)	166 (16%)	2	9
28	p	8/195 (4%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	w	112/446 (25%)	102 (91%)	10 (9%)	8	31
30	u	10/709 (1%)	10 (100%)	0	100	100
31	2	152/776 (20%)	126 (83%)	26 (17%)	1	8
33	6	97/109 (89%)	80 (82%)	17 (18%)	1	8
34	7	90/95 (95%)	72 (80%)	18 (20%)	1	5
35	5	72/77 (94%)	65 (90%)	7 (10%)	6	27
36	9	218/456 (48%)	179 (82%)	39 (18%)	1	8
37	8	104/831 (12%)	93 (89%)	11 (11%)	5	23
39	v	78/382 (20%)	68 (87%)	10 (13%)	3	16
40	o	6/218 (3%)	6 (100%)	0	100	100
41	h	5/110 (4%)	5 (100%)	0	100	100
42	i	4/74 (5%)	4 (100%)	0	100	100
43	m	4/177 (2%)	4 (100%)	0	100	100
44	l	3/101 (3%)	3 (100%)	0	100	100
45	k	3/66 (4%)	3 (100%)	0	100	100
46	j	1/84 (1%)	1 (100%)	0	100	100
47	n	3/101 (3%)	3 (100%)	0	100	100
48	z	152/416 (36%)	133 (88%)	19 (12%)	3	17
All	All	7715/20382 (38%)	6547 (85%)	1168 (15%)	4	12

5 of 1168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	3	574	LEU
39	v	59	CYS
27	3	707	GLN
27	3	568	MET
31	2	581	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
27	3	817	GLN
27	3	932	ASN
36	9	327	ASN

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Mol	Chain	Res	Type
3	C	154	HIS
3	C	140	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	27 (28%)	3 (3%)
6	F	96/107 (89%)	49 (51%)	6 (6%)
7	G	69/220 (31%)	43 (62%)	9 (13%)
8	H	163/188 (86%)	72 (44%)	7 (4%)
All	All	424/632 (67%)	191 (45%)	25 (5%)

5 of 191 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	G	101	U
7	G	108	U
8	H	47	U
7	G	106	C
8	H	12	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
26	SEP	1	129	26	8,9,10	1.46	1 (12%)	8,12,14	1.21	0

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
26	SEP	1	129	26	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	129	SEP	P-O1P	3.13	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	129	SEP	N-CA-CB-OG

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 15 ligands modelled in this entry, 13 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
50	GTP	C	1500	51	26,34,34	1.34	2 (7%)	32,54,54	1.82	8 (25%)
49	IHP	A	2401	-	36,36,36	1.41	6 (16%)	54,60,60	1.80	12 (22%)

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
50	GTP	C	1500	51	-	6/18/38/38	0/3/3/3
49	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	1500	GTP	C5-C6	-4.65	1.38	1.47
49	A	2401	IHP	P1-O31	-2.81	1.44	1.54
49	A	2401	IHP	P5-O35	-2.54	1.45	1.54
49	A	2401	IHP	P5-O45	-2.32	1.45	1.54
50	C	1500	GTP	C5-C4	-2.23	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	1500	GTP	PB-O3B-PG	-5.17	115.10	132.83
49	A	2401	IHP	O15-C5-C4	4.72	119.81	108.69
49	A	2401	IHP	C5-C4-C3	4.49	120.24	110.41
49	A	2401	IHP	O14-C4-C5	3.86	117.80	108.69
49	A	2401	IHP	C5-C6-C1	3.85	118.84	110.41

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

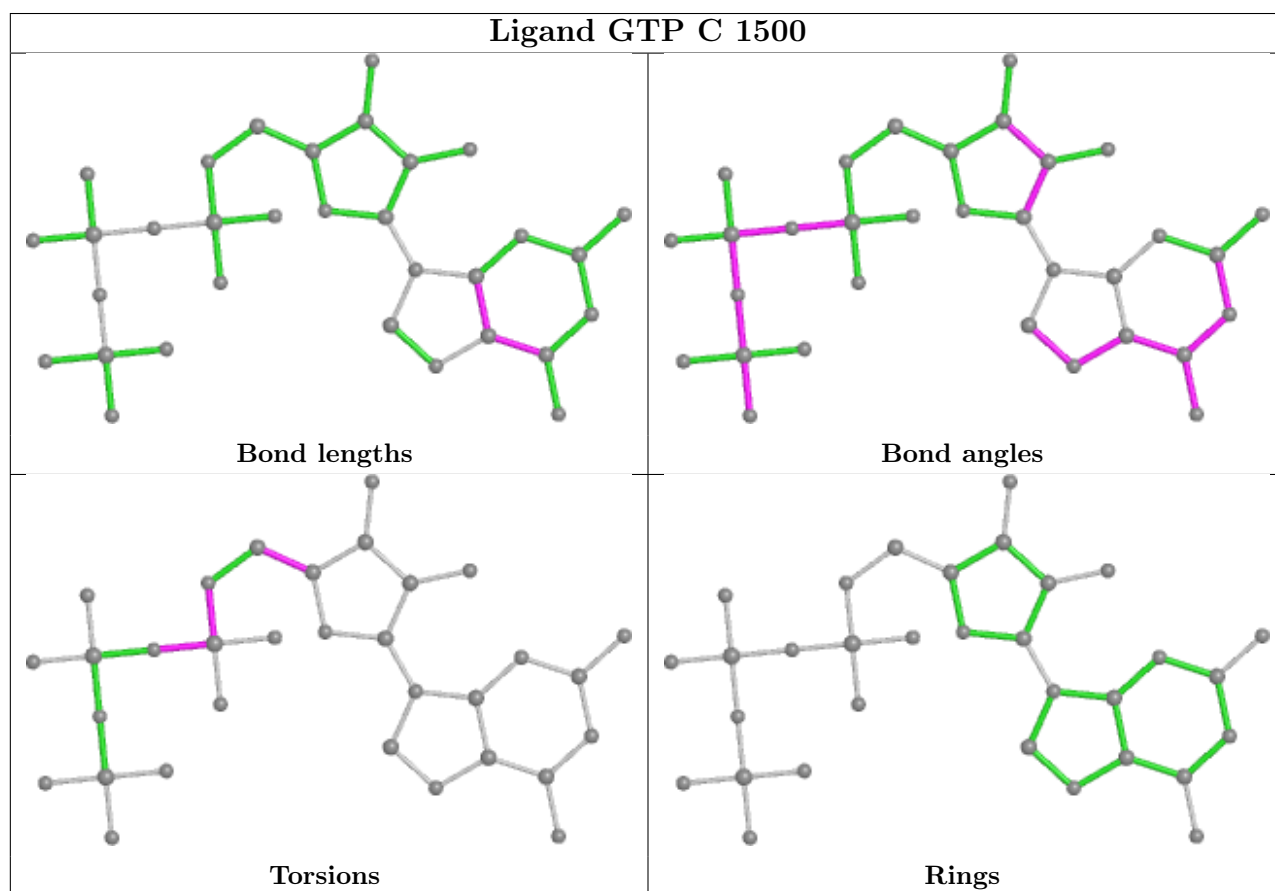
Mol	Chain	Res	Type	Atoms
49	A	2401	IHP	C2-O12-P2-O22
49	A	2401	IHP	C3-O13-P3-O43
50	C	1500	GTP	C5'-O5'-PA-O3A
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	O4'-C4'-C5'-O5'

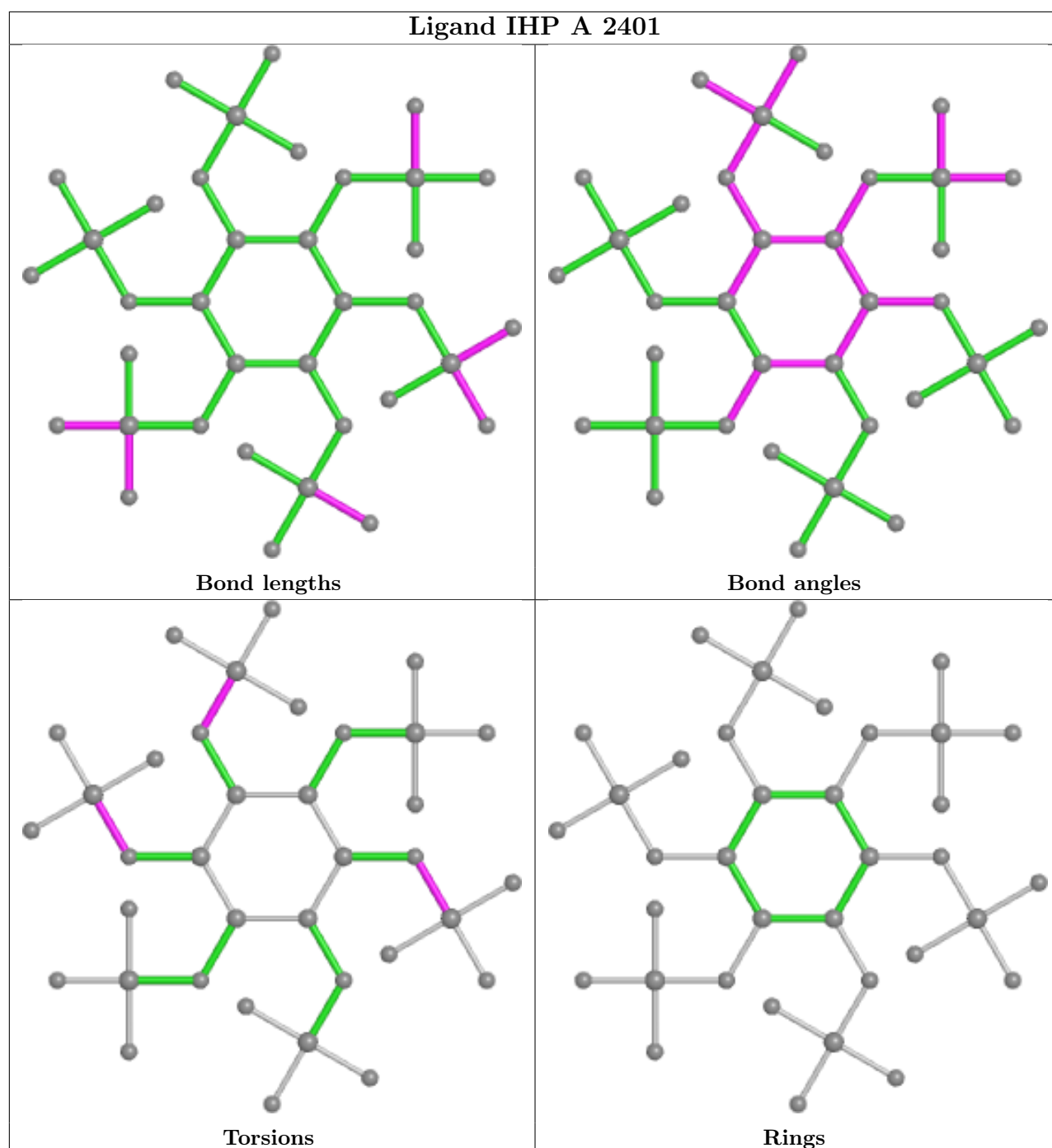
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C	1500	GTP	3	0
49	A	2401	IHP	2	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.

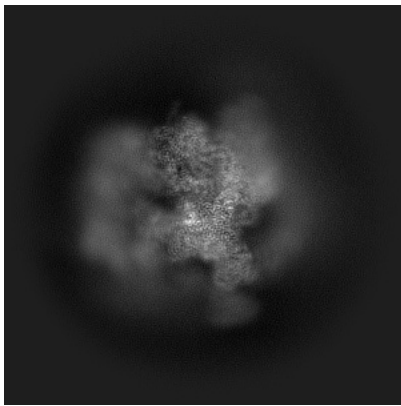
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35107. These allow visual inspection of the internal detail of the map and identification of artifacts.

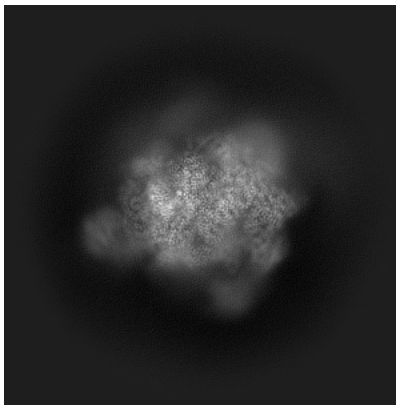
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

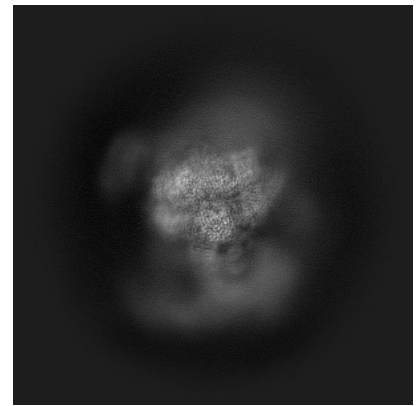
6.1.1 Primary map



X

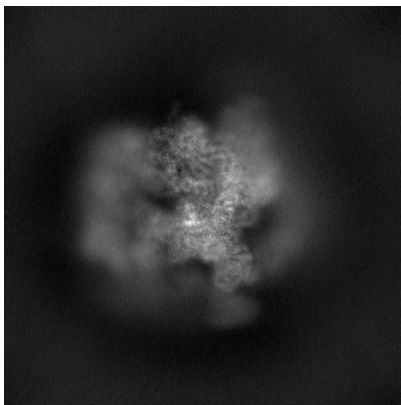


Y

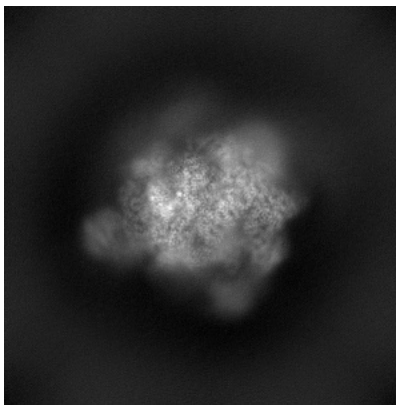


Z

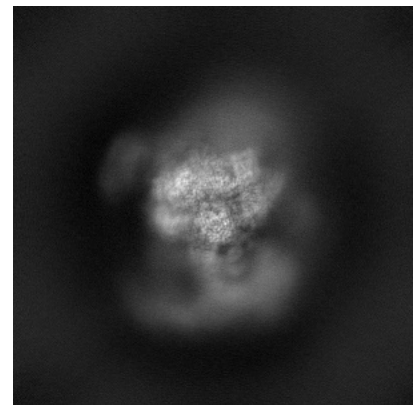
6.1.2 Raw map



X



Y

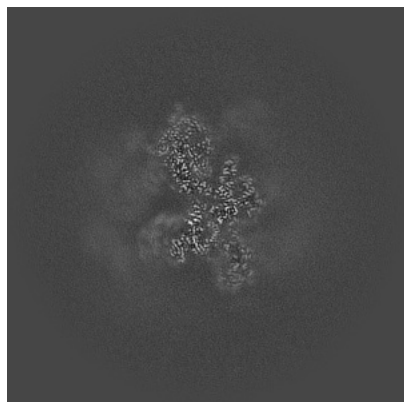


Z

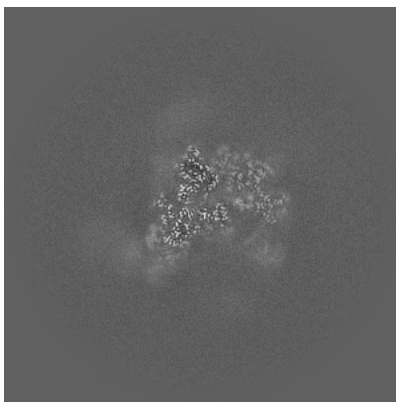
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

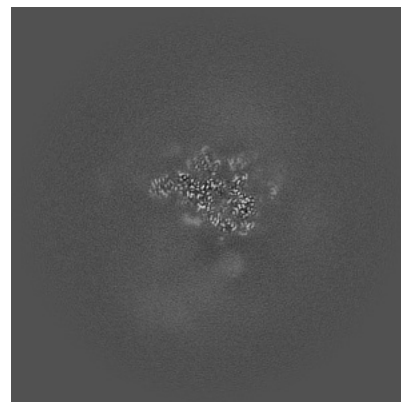
6.2.1 Primary map



X Index: 240

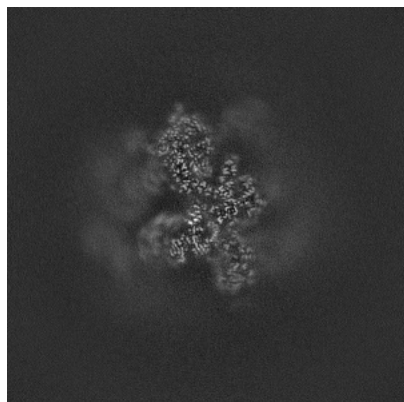


Y Index: 240

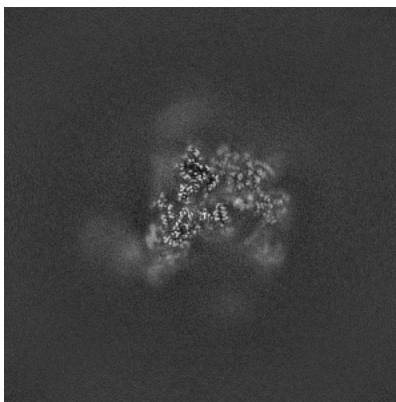


Z Index: 240

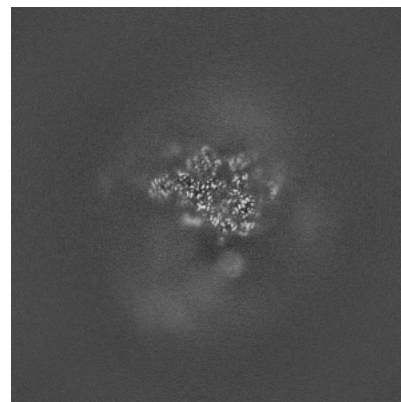
6.2.2 Raw map



X Index: 240



Y Index: 240

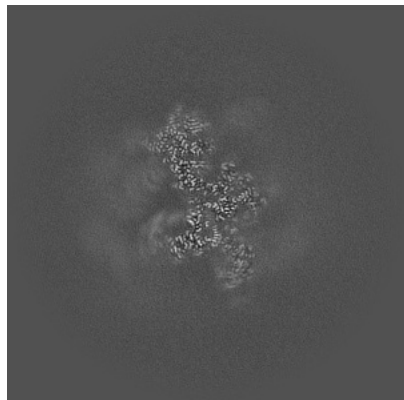


Z Index: 240

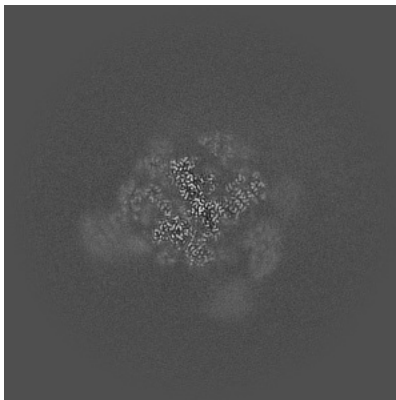
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

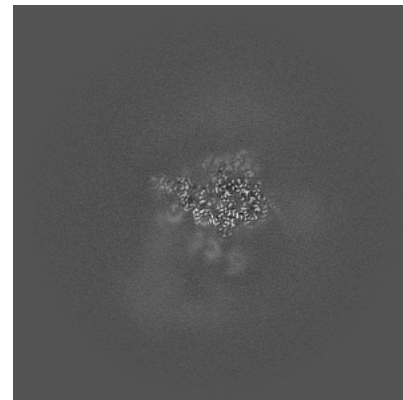
6.3.1 Primary map



X Index: 237

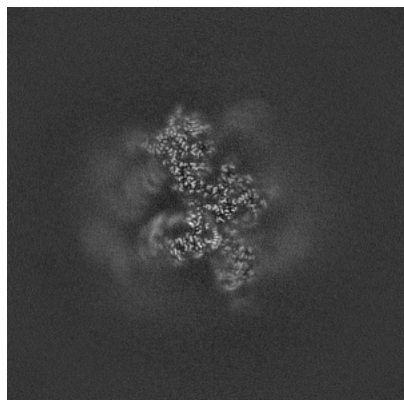


Y Index: 262

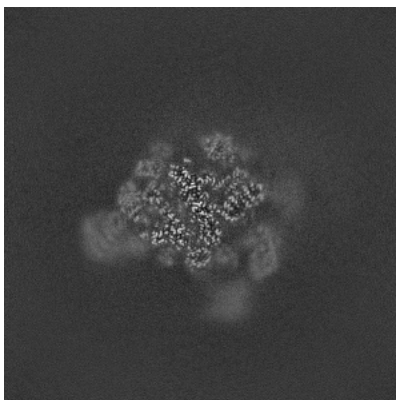


Z Index: 220

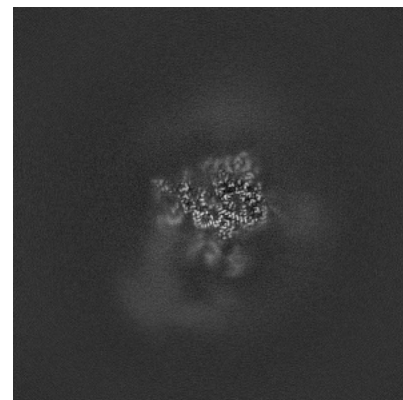
6.3.2 Raw map



X Index: 237



Y Index: 266

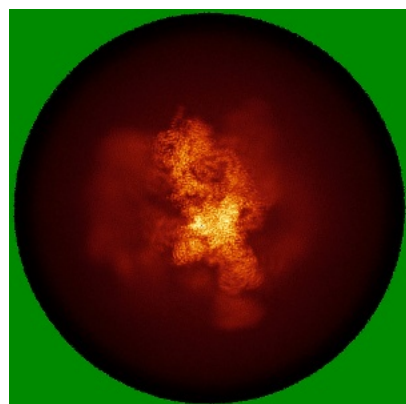


Z Index: 219

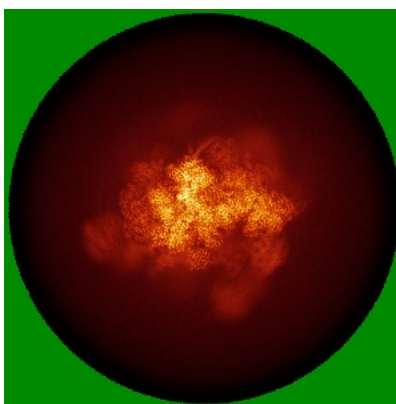
The images above show the largest variance slices of the map in three orthogonal directions.

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

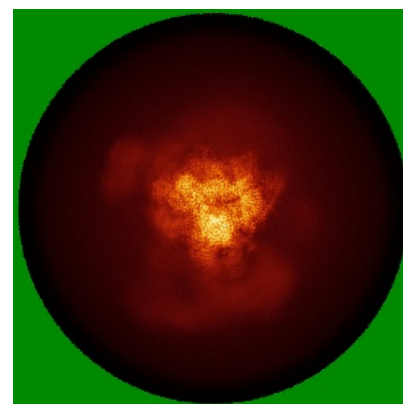
6.4.1 Primary map



X

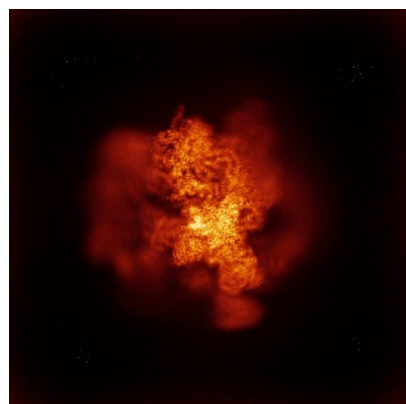


Y

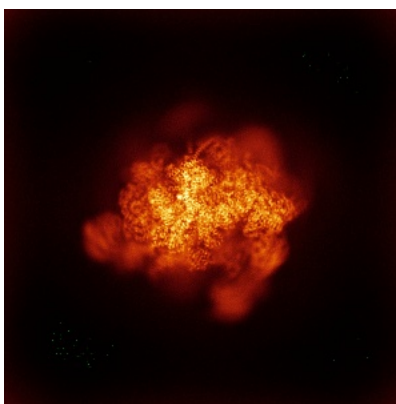


Z

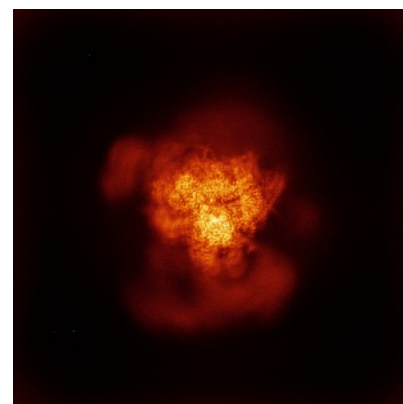
6.4.2 Raw map



X



Y

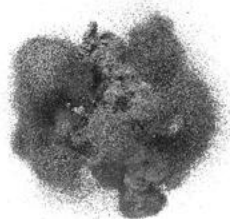


Z

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



X



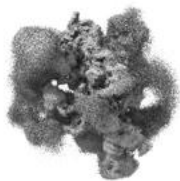
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

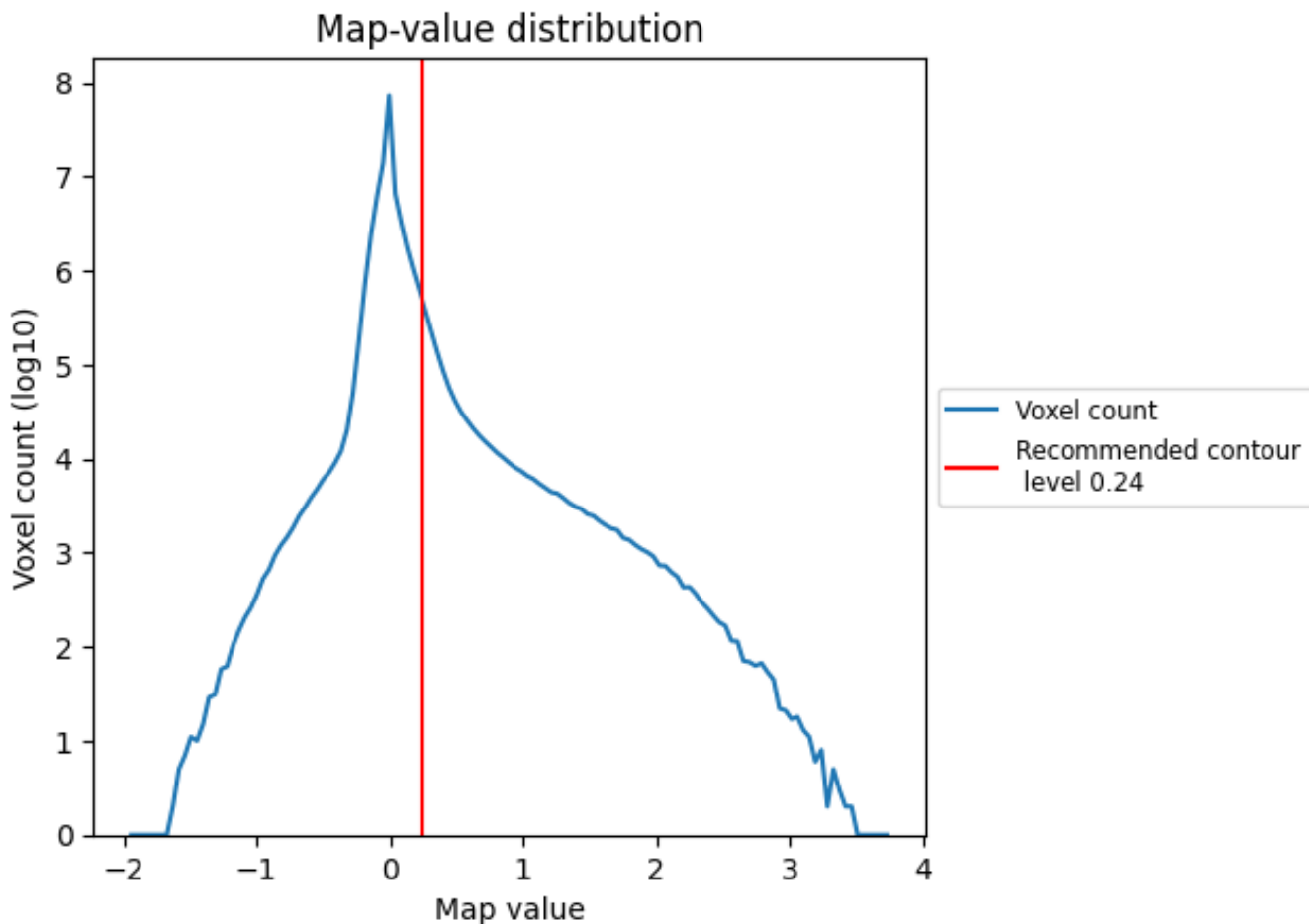
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

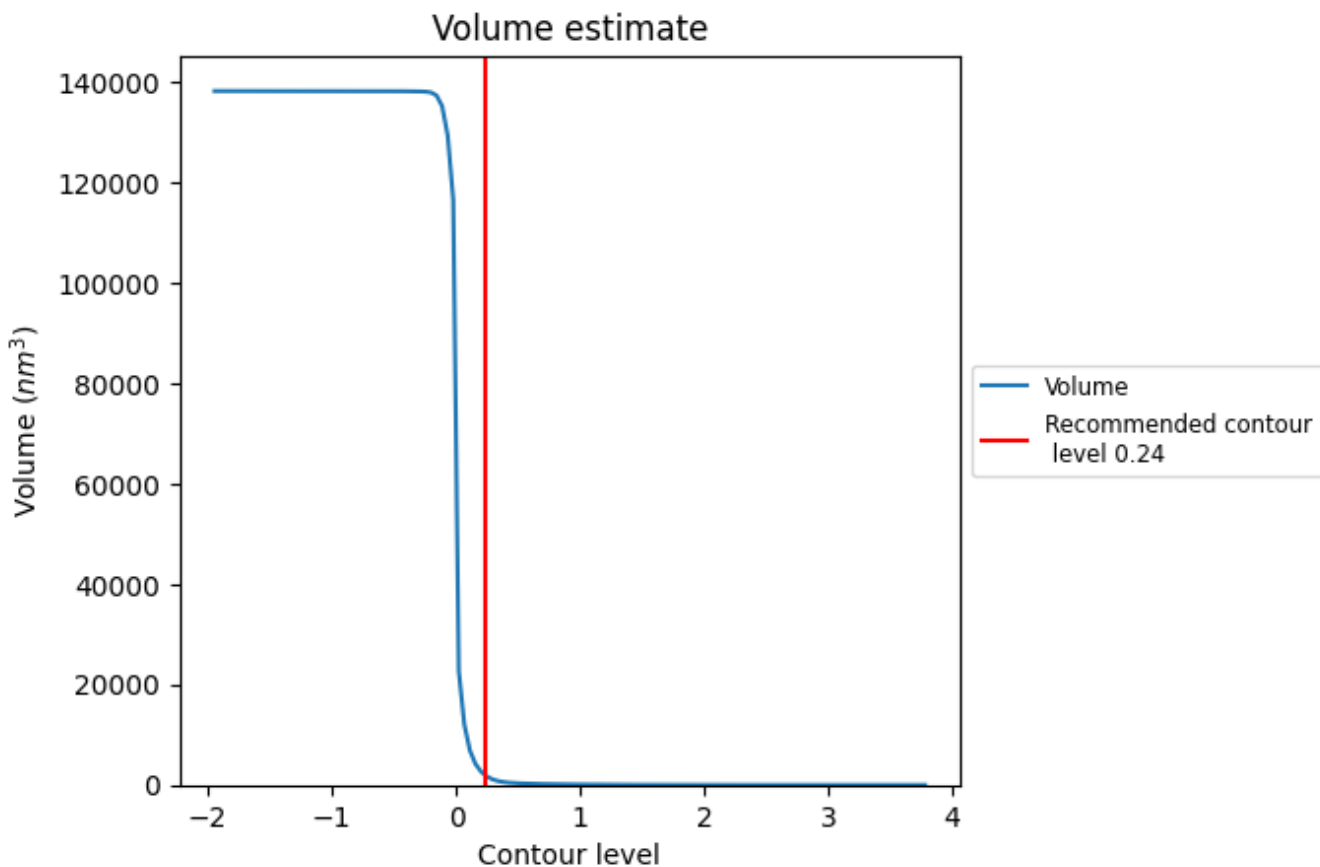
This section contains the results of statistical analysis of the map.

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.

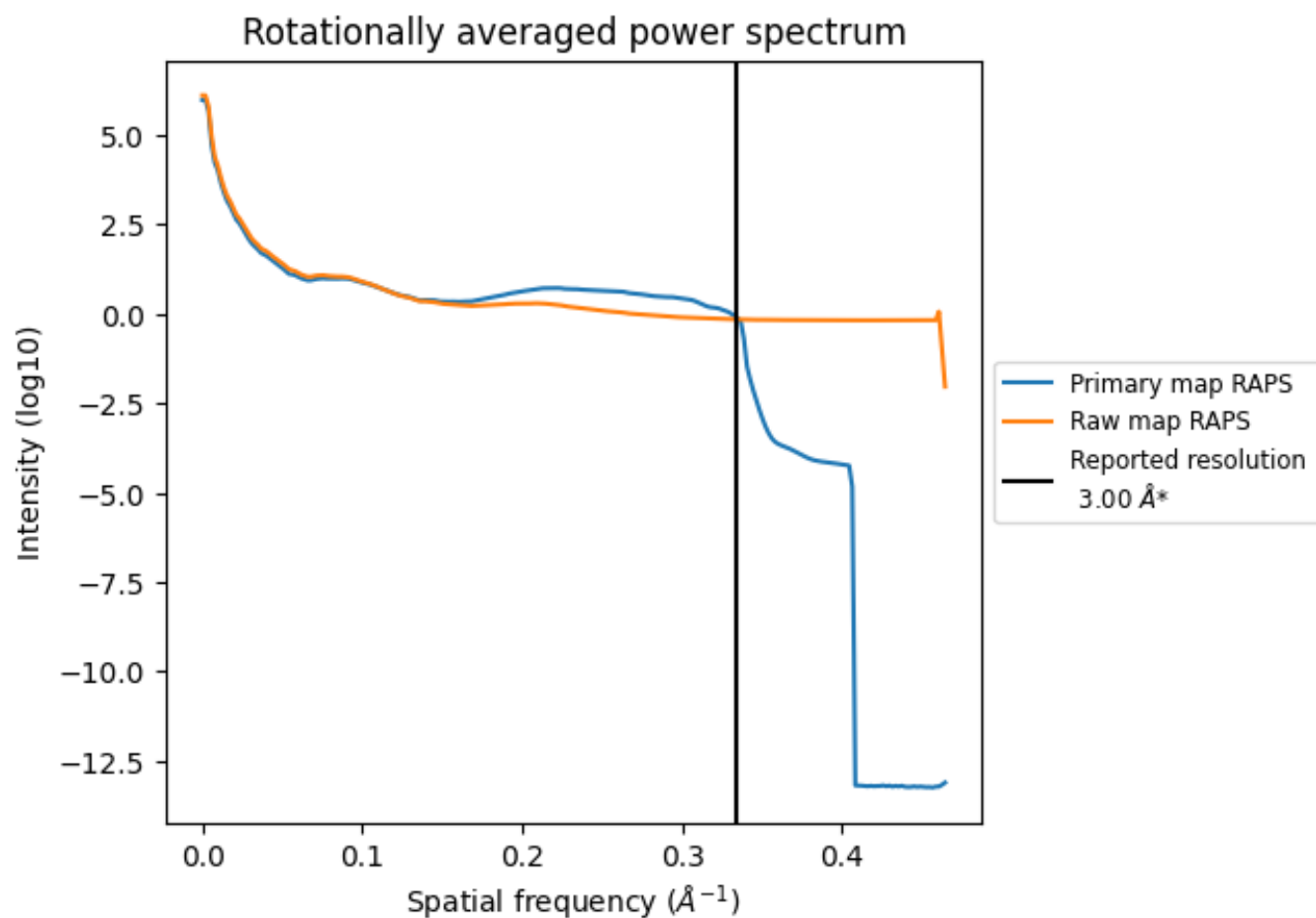
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1878 nm³; this corresponds to an approximate mass of 1697 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](#)

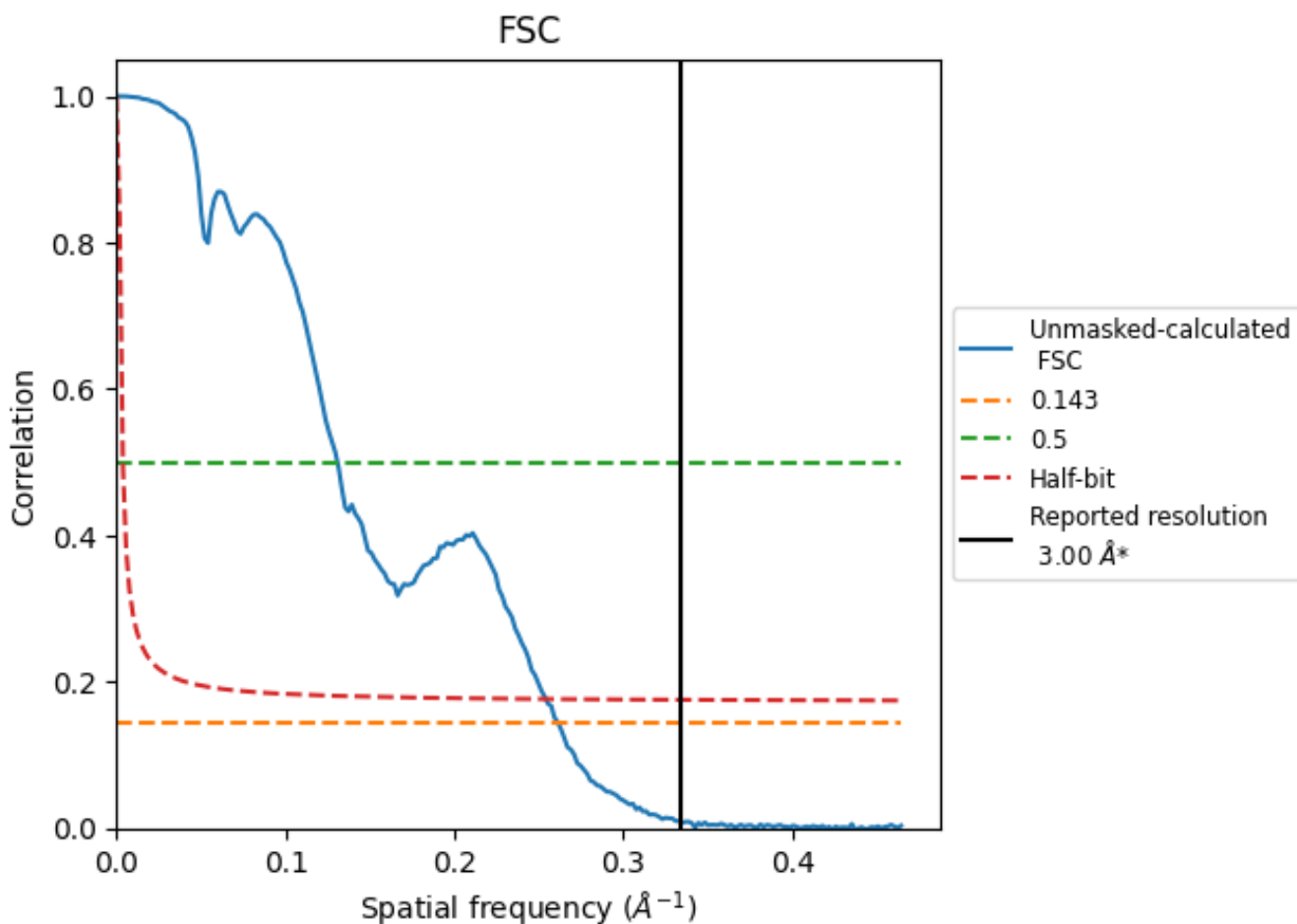


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

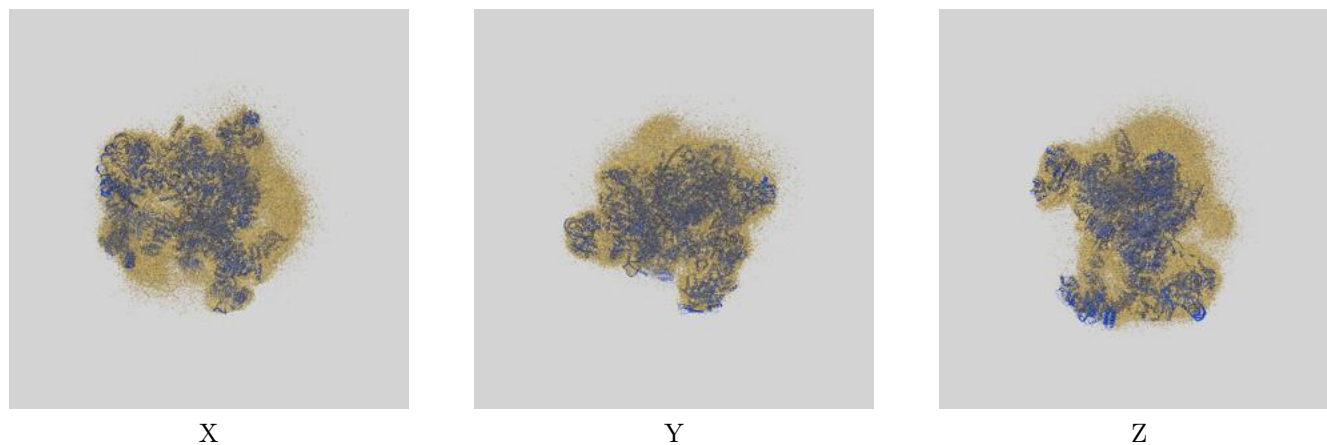
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.65	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

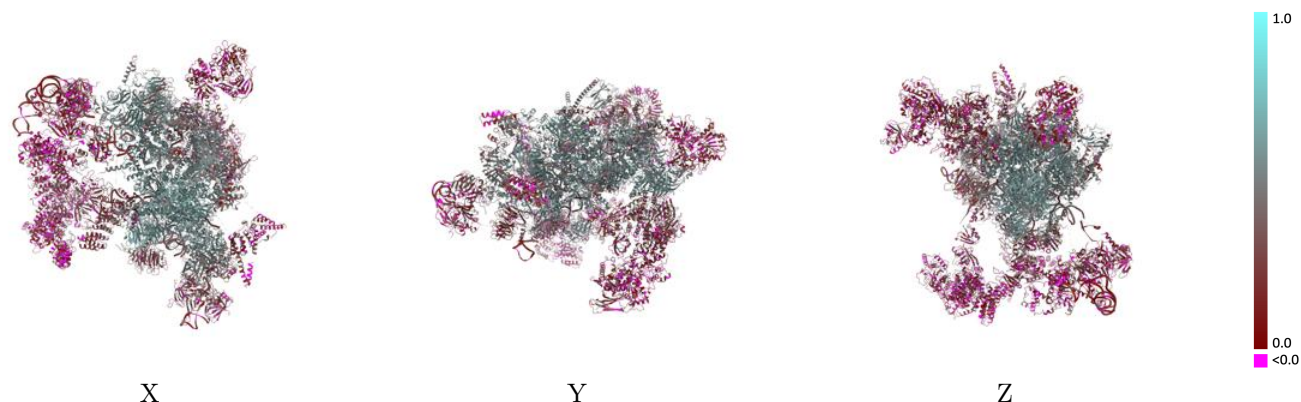
This section contains information regarding the fit between EMDB map EMD-35107 and PDB model 8I0R. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



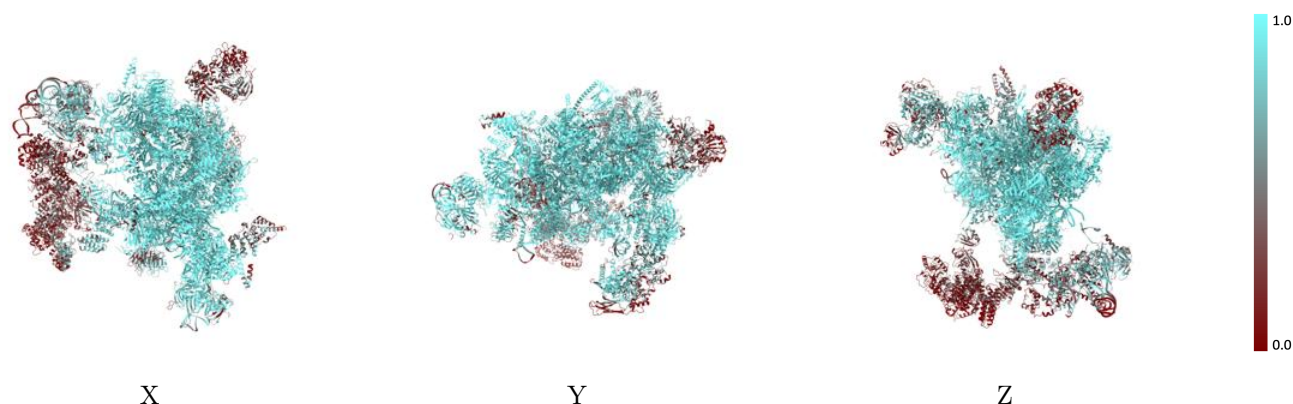
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



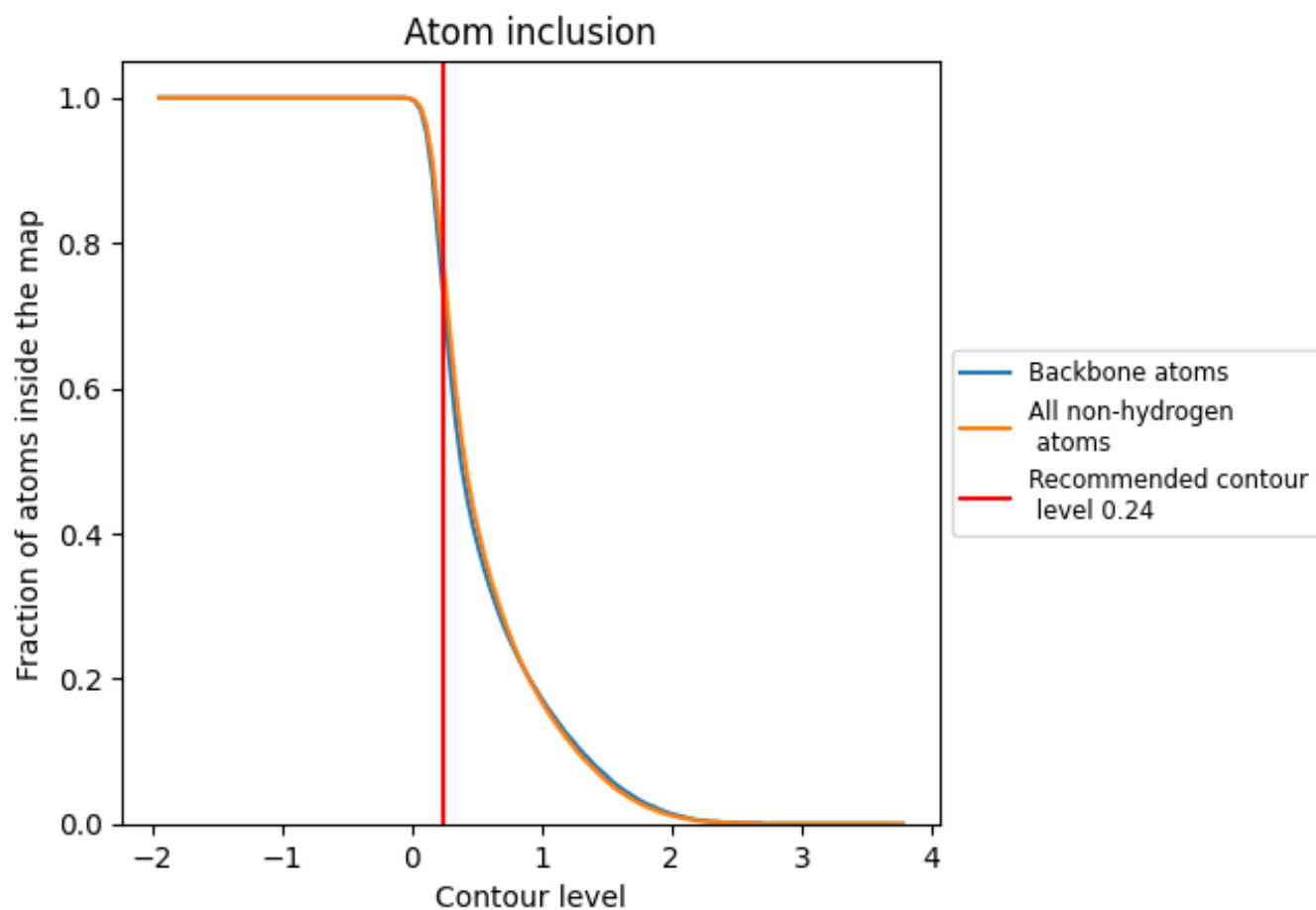
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 78% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.3880
1	 0.9580	 0.5450
2	 0.8750	 0.4670
3	 0.9680	 0.4970
4	 0.7370	 0.2210
5	 0.9130	 0.5330
6	 0.9390	 0.4230
7	 0.9170	 0.5070
8	 0.9470	 0.4500
9	 0.8880	 0.3600
A	 0.9370	 0.5370
B	 0.9000	 0.3820
C	 0.9660	 0.4770
D	 0.6980	 0.2090
E	 0.5950	 0.2590
F	 0.8920	 0.3750
G	 0.9370	 0.3900
H	 0.6720	 0.2550
I	 0.3100	 0.1380
J	 0.8480	 0.2900
K	 0.9090	 0.5550
L	 0.9780	 0.5670
N	 0.9300	 0.4500
O	 0.6680	 0.2620
P	 0.9550	 0.5210
Q	 0.1020	 0.1460
R	 0.9300	 0.4930
S	 0.2830	 0.1640
T	 0.9920	 0.6000
U	 0.6610	 0.2900
V	 0.7560	 0.3430
W	 0.8680	 0.4140
X	 0.9540	 0.4960
Y	 0.9690	 0.5740
Z	 0.8500	 0.4850



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Chain	Atom inclusion	Q-score
a	 0.7670	 0.2450
b	 0.8720	 0.2450
c	 0.7420	 0.2020
d	 0.8040	 0.2300
e	 0.8130	 0.2130
f	 0.7330	 0.3120
g	 0.8980	 0.3170
h	 0.6140	 0.1890
i	 0.6680	 0.1730
j	 0.6650	 0.2140
k	 0.5880	 0.1740
l	 0.5570	 0.1680
m	 0.6370	 0.2450
n	 0.5450	 0.1990
o	 0.4720	 0.1700
p	 0.6100	 0.1980
u	 0.2810	 0.1830
v	 0.7100	 0.4520
w	 0.5330	 0.2690
y	 0.2800	 0.1760
z	 0.9840	 0.5600