



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:10 AM UTC

PDB ID : 5O9Z / pdb_00005o9z
EMDB ID : EMD-3766
Title : Cryo-EM structure of a pre-catalytic human spliceosome primed for activation (B complex)
Authors : Bertram, K.; Kastner, B.
Deposited on : 2017-06-20
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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:

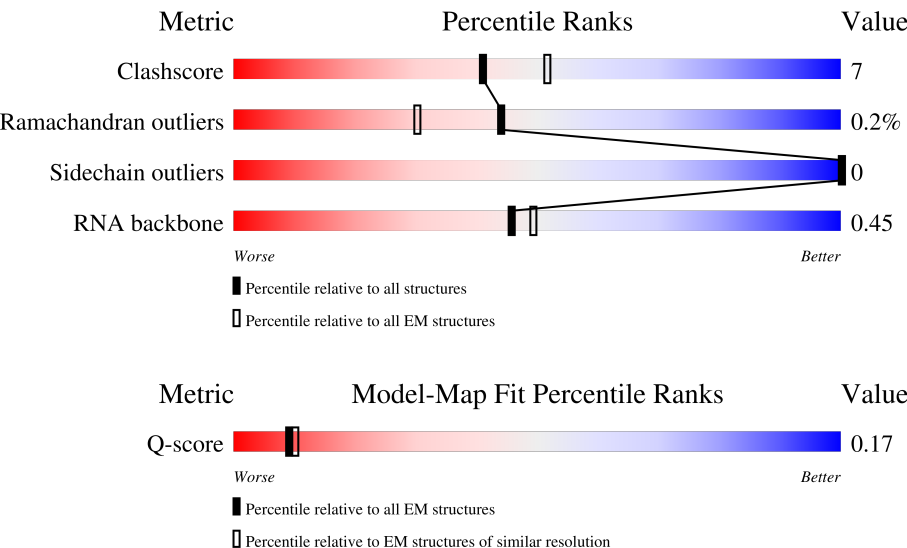
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	7% 89% 5% 6%
2	B	972	81% 6% 13%
3	C	2136	43% 75% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	357	
5	E	683	
6	F	521	
7	G	941	
8	H	499	
9	I	312	
10	J	142	
11	K	439	
12	L	513	
13	M	177	
14	N	199	
15	O	128	
16	P	800	
17	Q	376	
18	R	557	
19	S	118	
19	a	118	
19	h	118	
20	T	86	
20	b	86	
20	i	86	
21	U	92	
21	c	92	
21	j	92	
22	V	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
22	d	76	
22	k	76	
23	W	126	
23	e	126	
23	l	126	
24	X	240	
24	f	240	
24	m	240	
25	Z	119	
25	g	119	
25	n	119	
26	o	95	
27	p	102	
28	q	139	
29	r	91	
30	s	80	
31	t	103	
32	u	96	
33	v	1304	
34	w	1217	
35	x	86	
36	y	110	
37	z	256	
38	l	225	
39	Y	324	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2	188	53% 16% 15% 19% 47%
41	4	145	37% 47% 40% 8% 6%
42	5	116	15% 40% 45% 14%
43	6	106	37% 48% 30% 7% 15%

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 59243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2190	Total	C	N	O	0	0
			11100	6725	2190	2185		

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	844	Total	C	N	O	0	0
			4264	2577	844	843		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	1693	Total	C	N	O	0	0
			8538	5154	1693	1691		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	D	302	Total	C	0	302
			302	302		

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	219	Total	C	N	O	0	0
			1101	663	219	219		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	420	Total	C	N	O	0	0
			2100	1260	420	420		

- Molecule 7 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	804	Total	C	N	O	0	0
			4057	2449	804	804		

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	413	Total	C	N	O	0	0
			2068	1243	413	412		

- Molecule 9 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 10 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	135	Total	C	N	O	0	0
			677	408	135	134		

- Molecule 11 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	45	Total	C	N	O	0	0
			225	135	45	45		

- Molecule 12 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	459	Total	C	N	O	0	0
			2288	1370	459	459		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 14 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 15 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	126	Total	C	N	O	0	0
			636	385	126	125		

- Molecule 16 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	91	Total	C	N	O	0	0
			458	276	91	91		

- Molecule 17 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	75	Total	C	N	O	0	0
			378	228	75	75		

- Molecule 18 is a protein called Protein Red.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	16	Total	C	N	O	0	0
			79	47	16	16		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	a	78	Total	C	N	O	0	0
			393	237	78	78		
19	h	74	Total	C	N	O	0	0
			371	223	74	74		
19	S	87	Total	C			0	87
			87	87				

- Molecule 20 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	b	73	Total	C	N	O	0	0
			364	218	73	73		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
20	i	71	Total	C	N	O	0	0
			354	212	71	71		
20	T	74	Total	C			0	74
			74	74				

- Molecule 21 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	78	Total	C	N	O	0	0
			388	232	78	78		
21	j	78	Total	C	N	O	0	0
			388	232	78	78		
21	U	79	Total	C			0	79
			79	79				

- Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	d	69	Total	C	N	O	0	0
			344	206	69	69		
22	k	73	Total	C	N	O	0	0
			364	218	73	73		
22	V	74	Total	C			0	74
			74	74				

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	e	78	Total	C	N	O	0	0
			390	234	78	78		
23	l	71	Total	C	N	O	0	0
			353	211	71	71		
23	W	80	Total	C			0	80
			80	80				

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	f	64	Total	C	N	O	0	0
			319	191	64	64		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
24	m	64	Total	C	N	O	0	0
			316	188	64	64		
24	X	71	Total	C			0	71
			71	71				

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	g	93	Total	C	N	O	0	0
			469	283	93	93		
25	n	82	Total	C	N	O	0	0
			412	248	82	82		
25	Z	82	Total	C			0	82
			82	82				

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	o	90	Total	C	0	90
			90	90		

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms		AltConf	Trace
27	p	73	Total	C	0	73
			73	73		

- Molecule 28 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	q	80	Total	C	0	80
			80	80		

- Molecule 29 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	r	76	Total	C	0	76
			76	76		

- Molecule 30 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	s	69	Total	C	0	69
			69	69		

- Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	t	79	Total	C	0	79
			79	79		

- Molecule 32 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms		AltConf	Trace
32	u	62	Total	C	0	62
			62	62		

- Molecule 33 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	v	806	Total	C	0	806
			806	806		

- Molecule 34 is a protein called Splicing factor 3B subunit 3 (SF3B3).

Mol	Chain	Residues	Atoms		AltConf	Trace
34	w	1140	Total	C	0	1140
			1140	1140		

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

Mol	Chain	Residues	Atoms		AltConf	Trace
35	x	54	Total	C	0	54
			54	54		

- Molecule 36 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	y	89	Total	C	0	89
			89	89		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms		AltConf	Trace
37	z	162	Total	C	0	162
			162	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	89	ASP	CYS	conflict	UNP P09661
z	119	CYS	SER	conflict	UNP P09661
z	151A	PHE	-	insertion	UNP P09661

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms		AltConf	Trace
38	1	94	Total	C	0	94
			94	94		

- Molecule 39 is a RNA chain called MINX pre-mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Y	46	Total	C	N	O	P	
			972	435	167	324	46	0
								0

- Molecule 40 is a RNA chain called Human gene for small nuclear RNA U2 (snRNA U2).

Mol	Chain	Residues	Atoms				AltConf	Trace
40	2	100	Total	C	N	O	P	
			2123	947	367	709	100	0
								0

- Molecule 41 is a RNA chain called Homo sapiens U4A snRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	4	137	Total	C	N	O	P	
			2904	1298	501	968	137	0
								0

- Molecule 42 is a RNA chain called Homo sapiens U5 A small nuclear RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	5	114	Total	C	N	O	P	
			2397	1074	399	810	114	0
								0

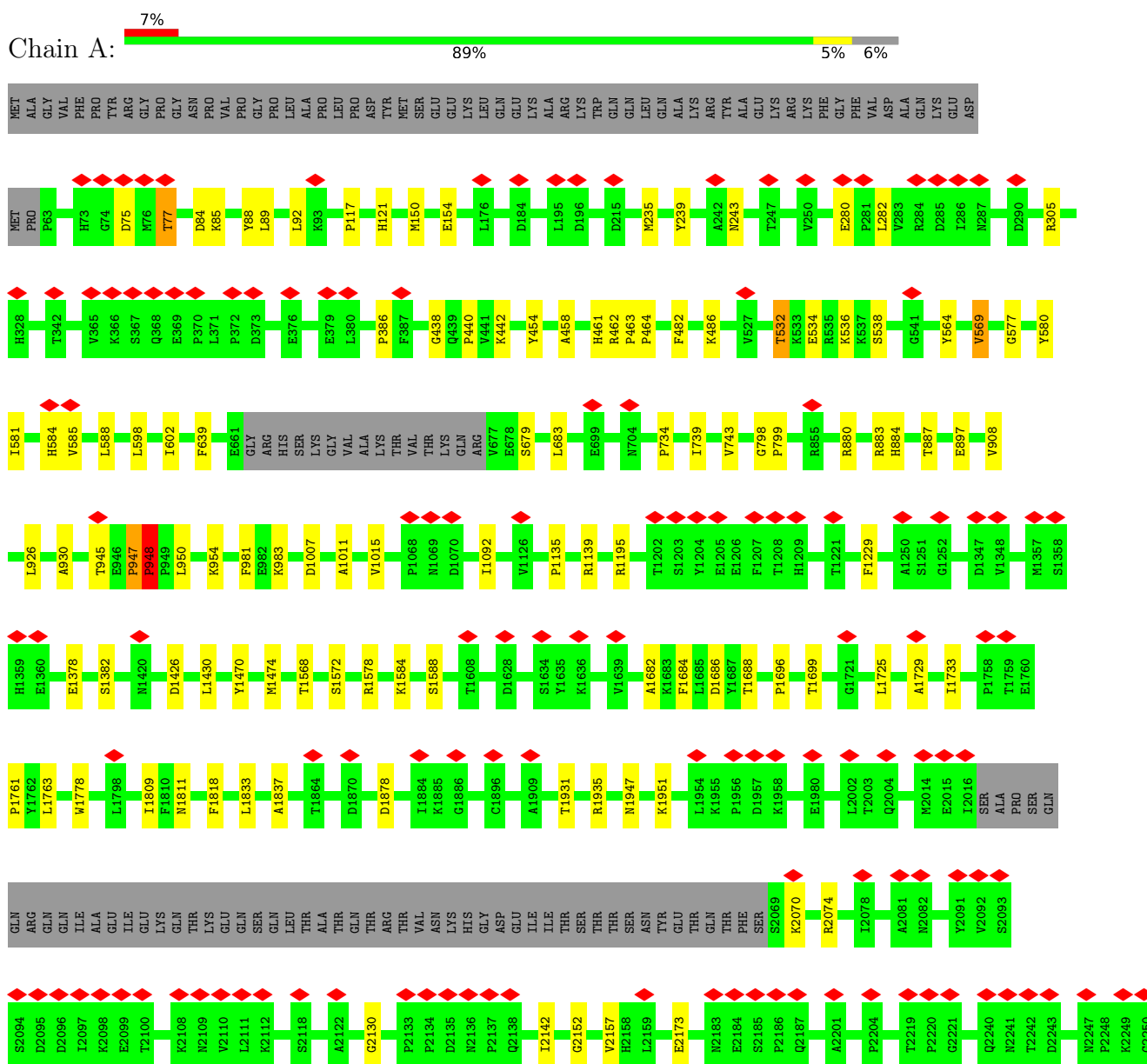
- Molecule 43 is a RNA chain called Homo sapiens RNA, U6 small nuclear 1 (RNU6-1), small nuclear RNA.

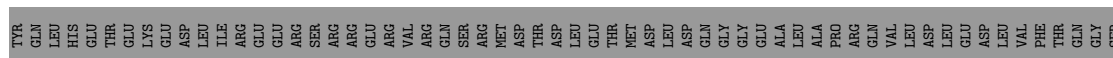
Mol	Chain	Residues	Atoms					AltConf	Trace
43	6	90	Total	C	N	O	P	0	0
			1926	861	353	622	90		

3 Residue-property plots

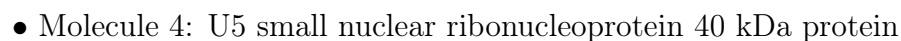
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

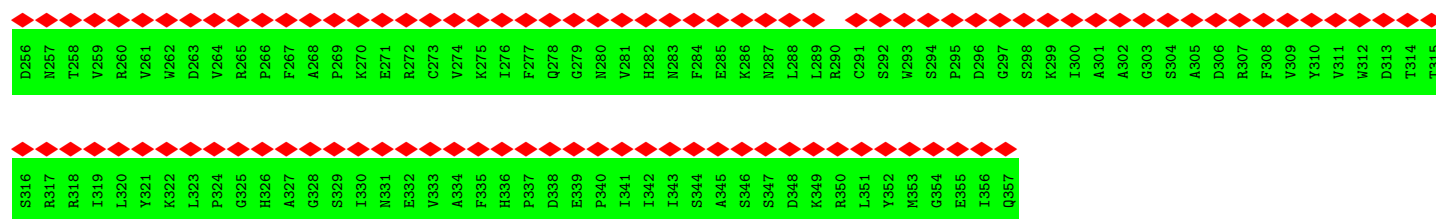




HIS	PHE	MET	ALA	ASN	LYS	ARG	CYS	GLN	LEU	PRO	ASP	G433	S434	F435	R436	R437	Q438	Y442	E443	E444	V445	H446	V447	P448	A449	L450	K451	P452	K453	P454	F455	G456	S457	E458	E459	Q460	L461	L462	P463	V464	E465	K466	Y470	A471	Q472	A473	G474	F475	E476	G477	F478	K479	T480	L481	M482	Q485
S486	K487	L488	Y489	R490	A491	A492	L493	E494	L501	T505	G506	A507	G508	K509	T510	N511	V512	A513	L514	M515	L518	R519	E520	I525	N526	M527	D528	G529	T530	I531	N532	V533	D534	D535	A542	P543	V548	Q549	V552	G553	G556	K557	R558	L559	A560	T561	Y562	I564	T565	V566						
A567	E568	L569	T570	G571	D572	H573	Q574	L575	C576	K577	E578	E579	I580	S581	A582	K599	G600	G601	E602	T606	Q607	I612	I613	L614	D615	H621	D622	G623	R624	V627	L628	E629	A630	A635	T642	Q643	E644	D645	V646	R647	G650	L651	P656	N657	D668	P669	A670	G671	G672							
L673	H678	S679	P682	V690	G691	I692	T693	E694	K695	K696	E714	H715	A716	G717	V725	R728	K729	A737	D740	M741	E744	L748	G749	L750	F751	E754	G755	S756	A757	S758	T759	E760	V761	L762	R763	T764	E767	Q768	G769	K770	L774	K775	L778	F782	N8002											
A783	I784	H785	H789	D799	K804	H805	L809	V810	S811	G818	V819	N820	A823	H824	K829	E837	K838	G839	R840	E843	L844	G845	A846	G854	G857	R858	P859	Q860	T863	K864	G865	E866	G867	I868	L869	I870	T871	S872	H873	G874	E875	L876	S881	L882	L883	M884										
Q885	Q886	L887	P888	I889	E890	S891	V894	S895	N912	R931	T934	L935	Y936	G937	I938	S939	H940	D941	D942	L943	K944	G945	D946	P947	Q951	D955	L956	V957	H958	T959	A960	A961	L962	K966	N967	N968	L969	V970	D973	K974	K975	T976	G977	N978	F979	Q980	V981	T982	E983	N1002						
Q1003	L1004	L1005	K1006	P1007	T1008	L1009	S1010	E1011	I1012	E1013	R1016	S1019	L1020	S1021	S1022	E1023	F1024	K1025	N1026	I1027	T1028	V1029	E1030	E1031	E1032	E1033	K1034	L1035	E1036	L1037	Q1038	K1039	L1040	L1041	E1042	R1043	V1044	P1045	I1046	P1047	V1048	L1049	E1050	S1051	I1052	E1053	E1054	P1055	S1056	A1057	K1058	I1059	N1060	V1061	L1062	I1067
S1068	Q1069	L1070	K1071	L1072	E1073	G1074	F1075	E1076	L1077	M1078	D1080	M1081	Y1082	Y1083	V1084	T1085	Q1086	S1087	A1088	M1092	N1101	R1102	G1103	W1104	A1105	D1119	K1120	R1121	M1122	W1123	M1126	L1129	K1134	L1135	P1136	V1139	V1140	I1143	E1144	K1145	E1151	L1152	L1153	Y1154	D1155	N1159	E1160	I1161								
L1164	I1165	K1169	M1170	E1171	K1172	T1173	I1174	H1179	K1183	L1184	E1185	L1186	V1188	H1189	L1190	S1196	I1204	T1205	P1206	W1210	K1213	V1214	H1215	G1216	S1217	S1218	F1221	L1224	V1228	D1229	S1230	E1231	V1232	I1233	L1234	H1235	H1236	K1242	A1243	K1244	F1255	V1256	P1257	P1261												
P1264	S1272	W1275	L1276	S1277	C1278	E1279	T1280	Q1281	S1285	F1286	R1287	H1288	L1289	I1290	L1291	P1292	E1293	K1294	Y1295	P1296	T1299	E1300	L1301	L1302	L1303	L1304	Q1305	P1306	L1307	P1308	V1309	S1310	A1311	L1312	R1313	N1314	S1315	A1316	S1319	L1320	Y1321	Q1322	D1323	K1324	P1325	F1327	F1328	N1329	P1330	I1331	Q1332					
F1336	N1337	T1338	N1341	S1342	D1343	D1344	N1345	V1346	F1347	V1348	G1353	S1354	G1355	K1356	T1357	A1360	L1369	Q1370	S1371	S1372	E1373	G1374	T1380	P1381	M1382	E1383	A1384	L1385	A1386	E1387	Q1388	V1389	Y1390	M1391	D1392	W1393	Y1394	E1395	K1396	F1397	Q1398	D1399	R1400	L1401	N1402	K1403	K1404	V1405	L1406	L1407	T1408	L1409	E1411			
T1412	S1413	T1414	D1415	L1416	L1417	L1418	K1421	L1425	P1429	E1430	K1431	Y1432	L1435	S1436	K1440	Q1441	R1442	L1443	V1453	D1454	E1455	V1456	H1457	G1461	E1462	P1465	V1466	L1467	Y1476	I1477	S1478	S1479	Q1480	I1481	E1482	R1483	P1484	L1490	A1501	G1505	A1508	T1509	S1510	T1511	H1515											
P1516	N1517	V1518	R1519	P1520	V1521	P1522	L1523	E1524	L1525	H1526	I1527	Q1528	G1529	F1530	N1531	I1532	S1533	H1534	T1535	Q1536	L1539	L1540	S1541	M1542	A1543	K1544	P1545	V1546	I1550	T1551	K1552	H1553	S1554	P1555	K1556	V1563	K1567	Q1568	T1569	R1570	L1571	T1572	A1573	I1574	D1575	I1576	L1577	T1578	T1579	C1580	A1581	A1582	D1583	I1584	Q1585	

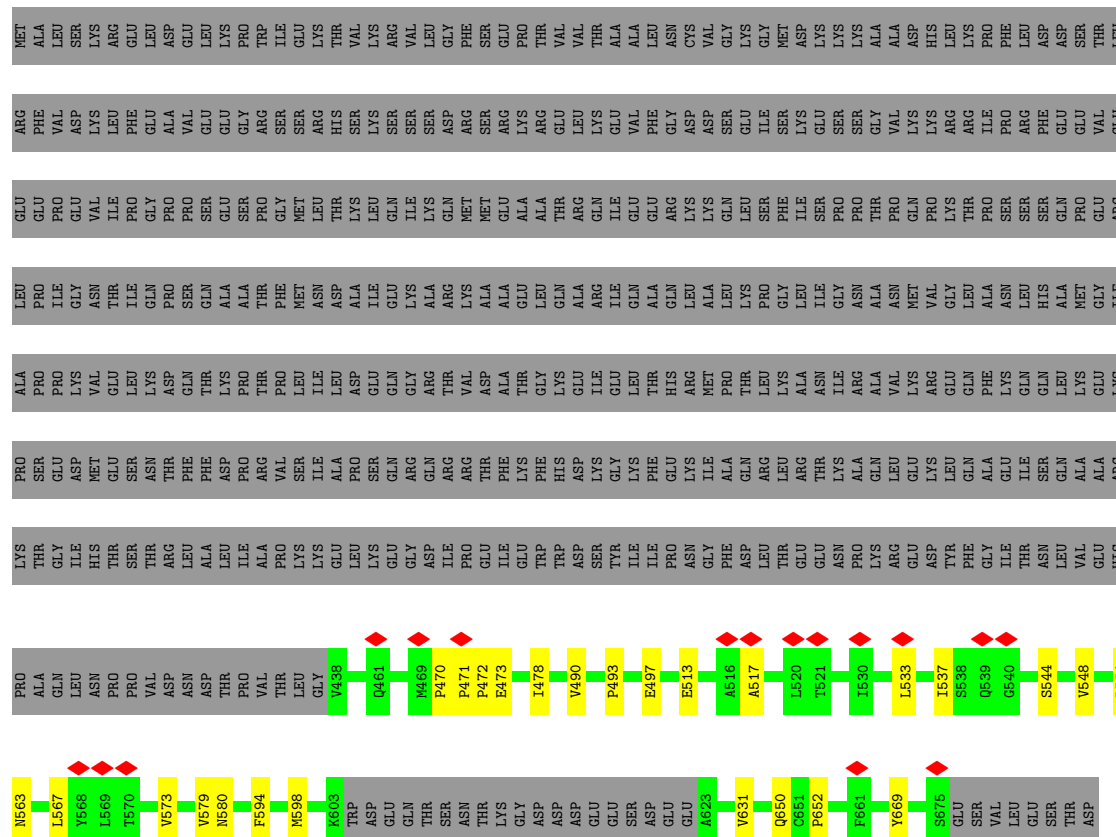


V196	L61	F125	L62	F126	L64	H65	E66	G67	E68	V69	Y70	C71	C72	C73	F74	H75	P76	N77	G78	S79	T80	L81	A82	S83	F86	D87	R88	L89	L92	W93	N94	V95	Y96	G97	D98	C99	D100	N101	Y102	A103	T104	L105	K106	G107	H108	V112	M113	E114	L115	H116	Y117	N118	T119	D120	G121	S122	M123	L124
L197	A198	V199	T200	F201	N202	D203	T204	S205	D206	Q207	I208	I209	S210	G211	G212	I213	D214	N215	D216	I217	K218	V219	W220	D221	L222	R223	Q224	N225	K226	L227	T228	Y229	T230	M231	R232	G233	H234	A235	D236	S237	V238	T239	G240	L241	S242	L243	S244	S245	E246	G247	S248	Y249	L250	L251	S252	M253	A254	Q195
F125	S126	A127	S128	W136	D137	S138	E139	T140	G141	E142	R143	V144	G149	H150	T151	S152	F153	V154	N155	S156	C157	Y158	P159	A160	R161	R162	G163	P164	Q165	L166	V167	C168	T169	G170	S171	D172	D173	G174	T175	V176	K177	L178	W179	D180	L181	R182	A186	L187	Q188	T189	F190	Q191	N192	T193	V194	Q195		



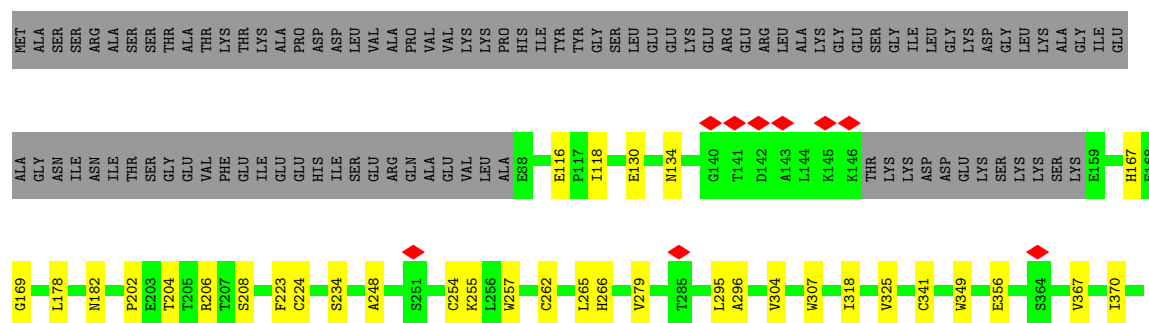
• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp3

Chain E: 28% 68%



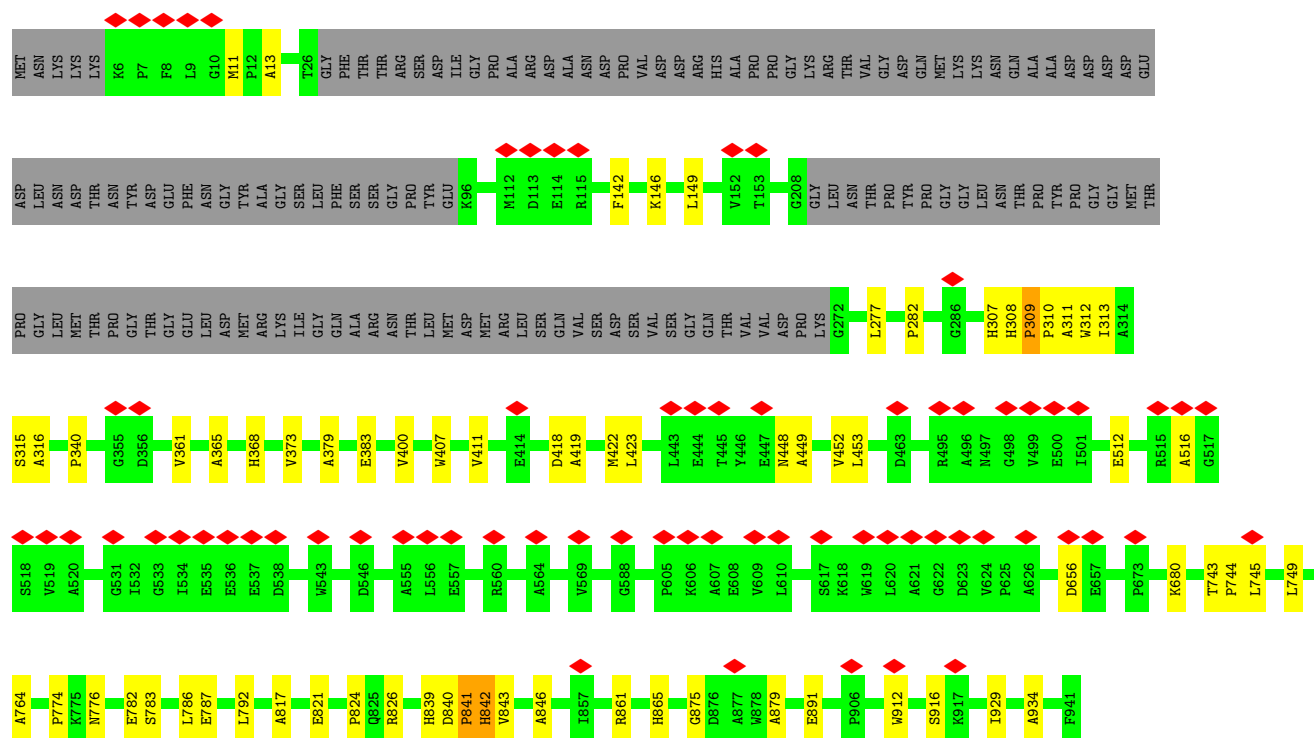
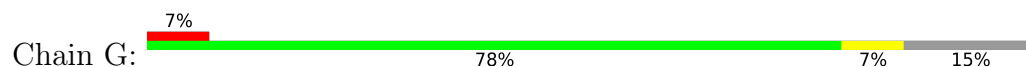
• Molecule 6: U4/U6 small nuclear ribonucleoprotein Prp4

Chain F: 71% 9% 19%

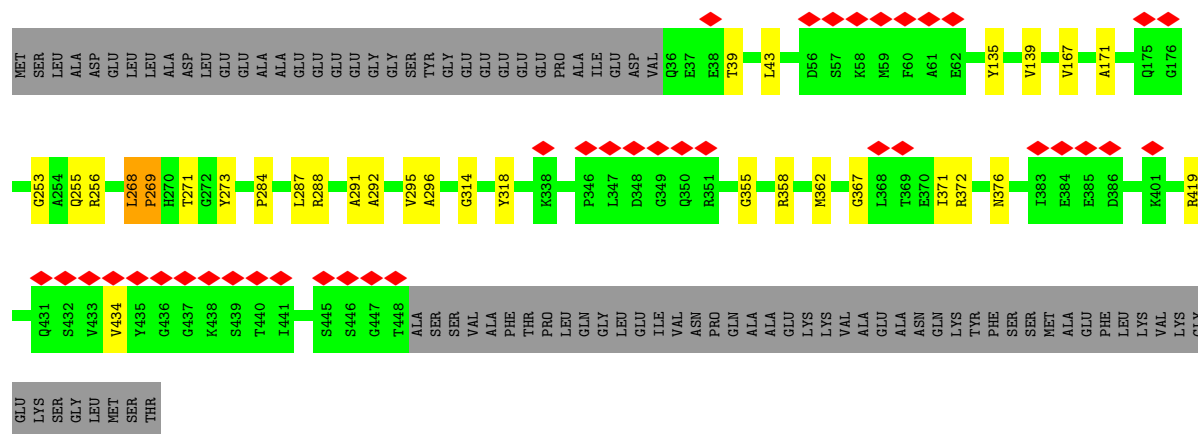
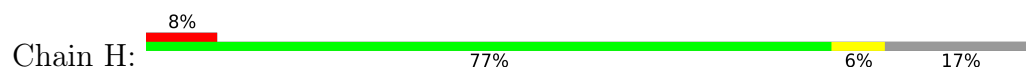




• Molecule 7: Pre-mRNA-processing factor 6



• Molecule 8: U4/U6 small nuclear ribonucleoprotein Prp31



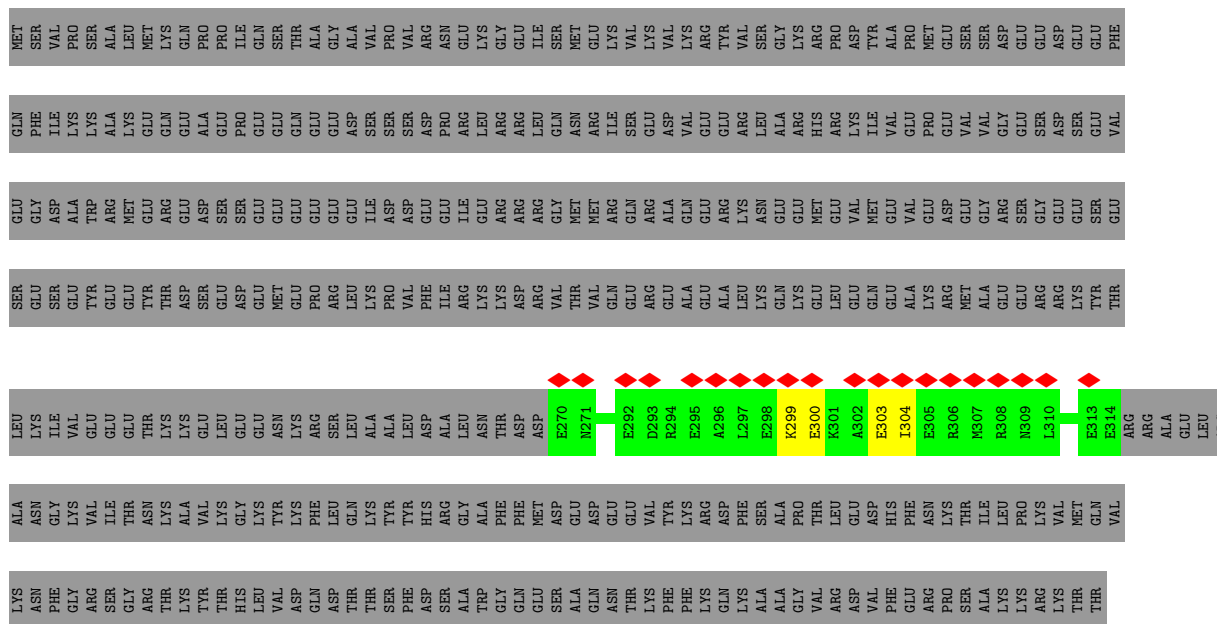
• Molecule 9: Pre-mRNA-splicing factor 38A



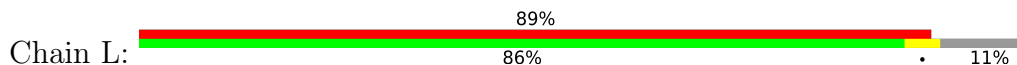
- Molecule 10: Thioredoxin-like protein 4A

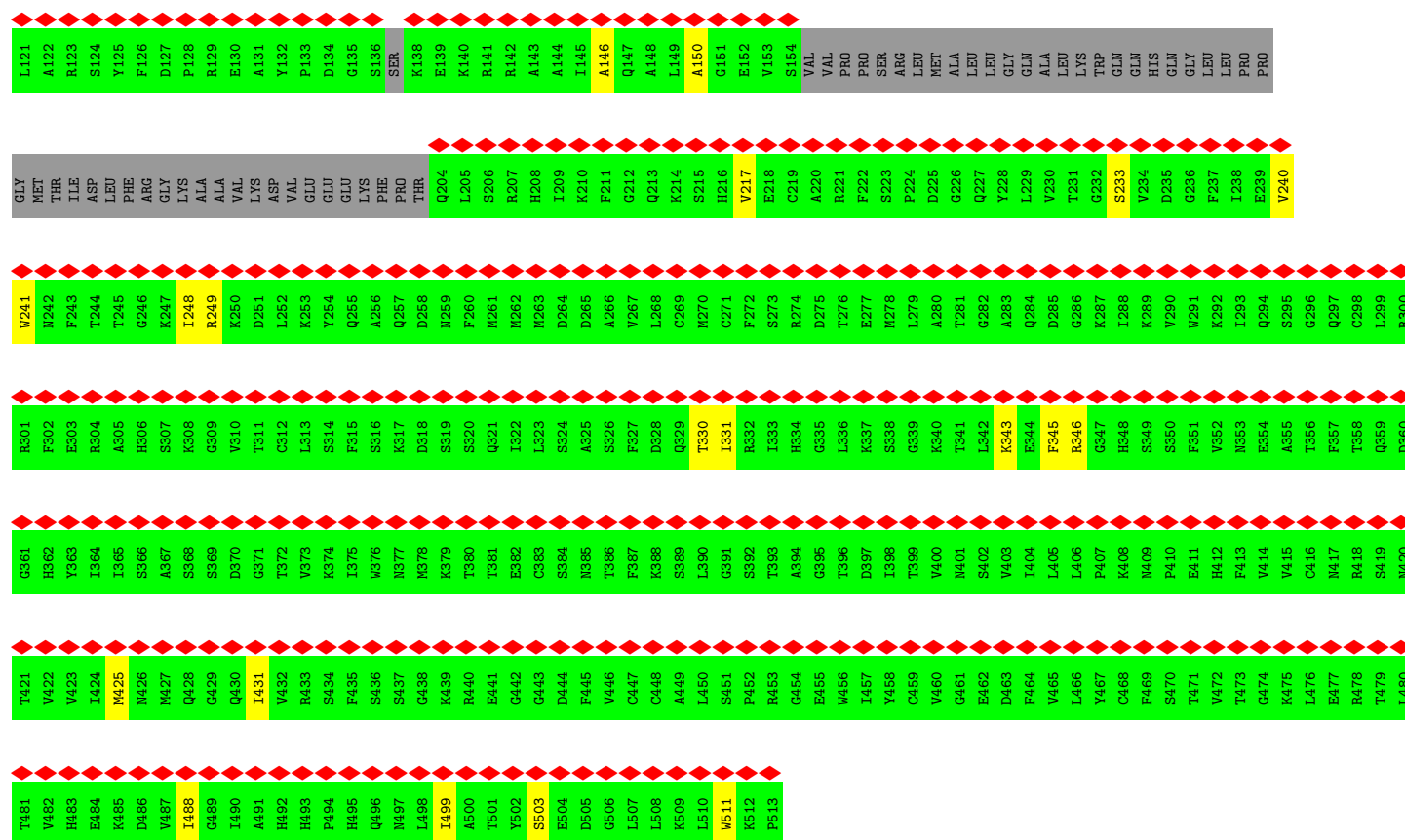


- Molecule 11: Microfibrillar-associated protein 1

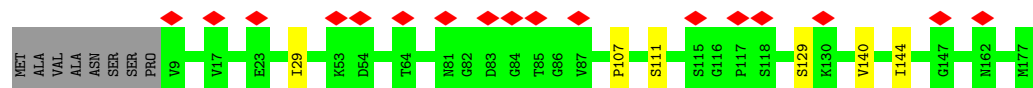


- Molecule 12: WD40 repeat-containing protein SMU1

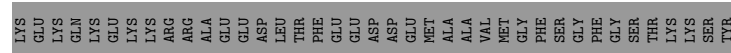
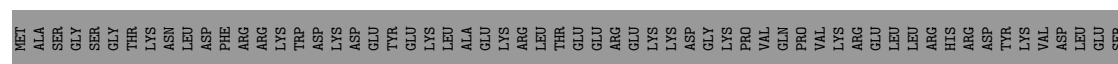




• Molecule 13: Peptidyl-prolyl cis-trans isomerase H



• Molecule 14: Zinc finger matrin-type protein 2

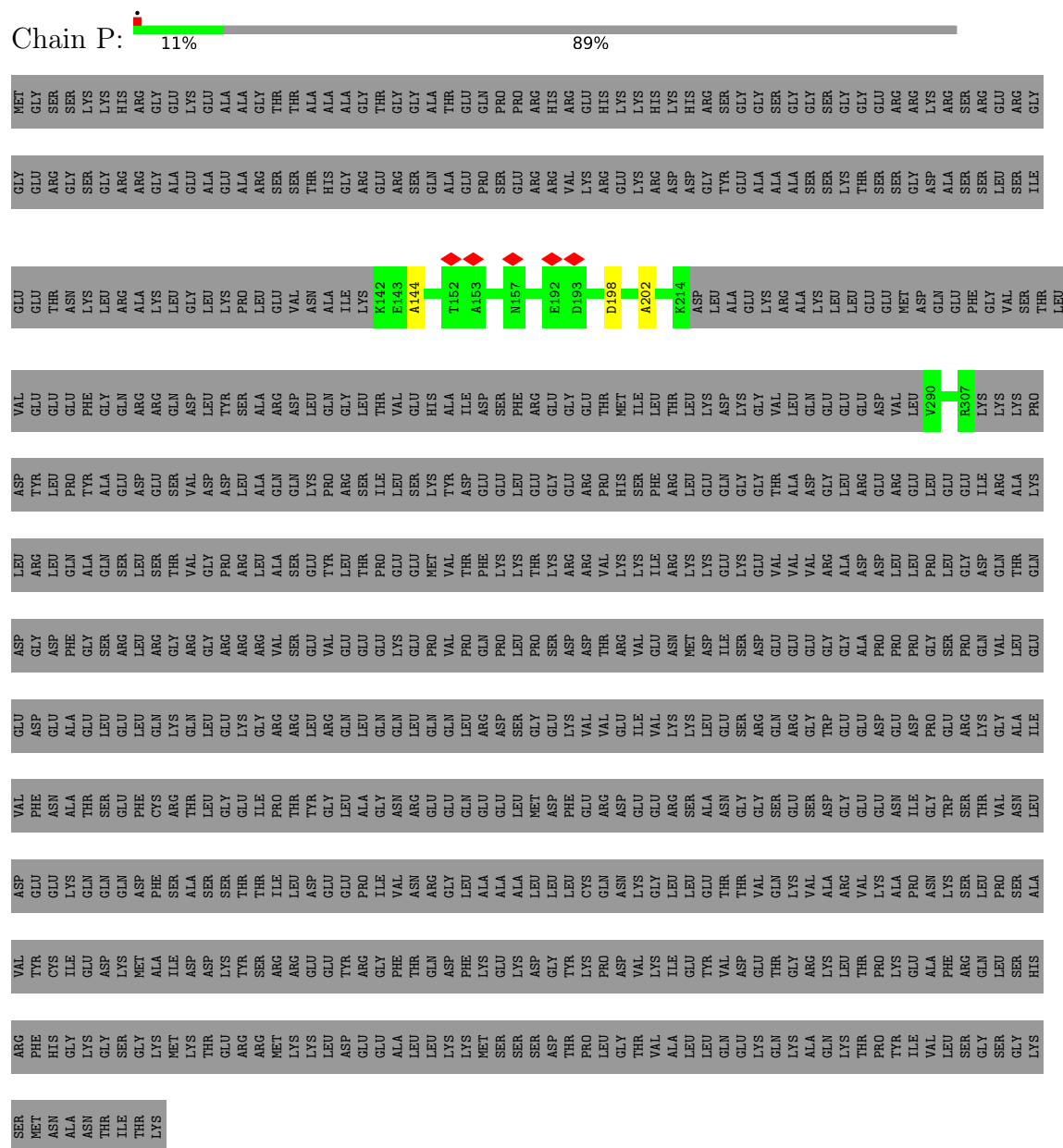


• Molecule 15: NHP2-like protein 1

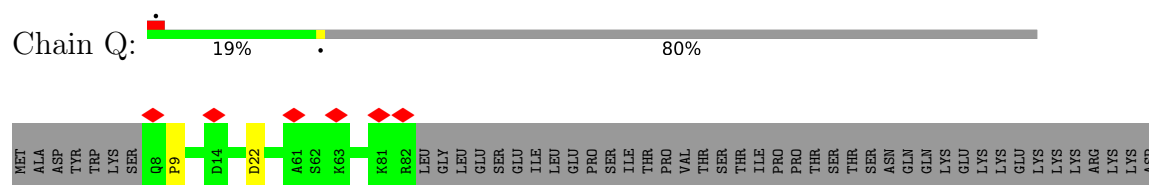




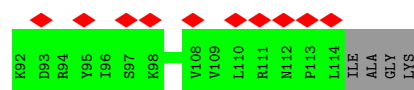
- Molecule 16: U4/U6.U5 tri-snRNP-associated protein 1



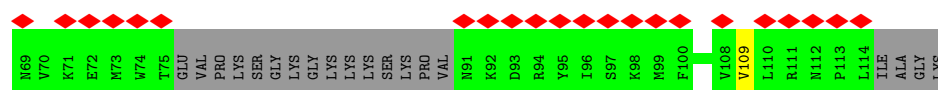
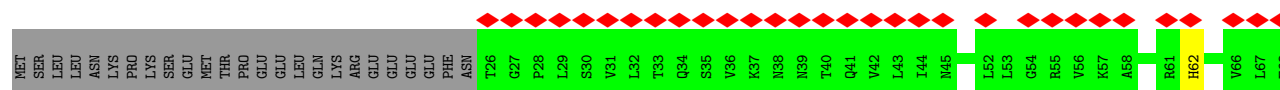
- Molecule 17: WW domain-binding protein 4



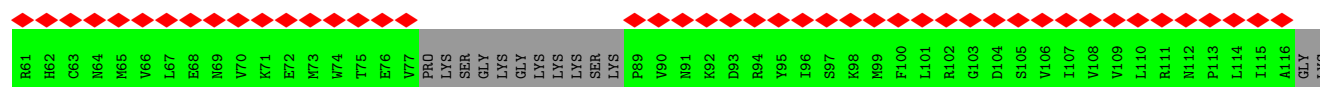
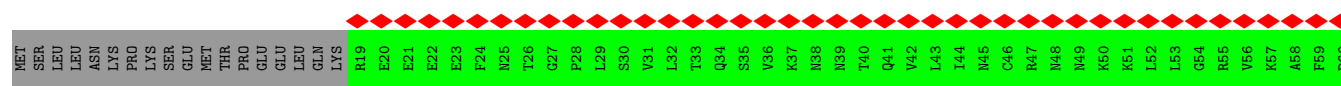




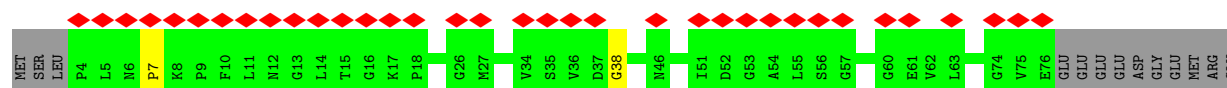
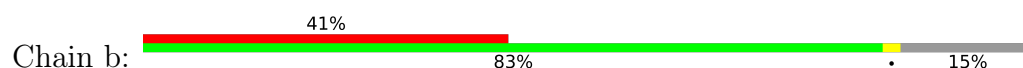
- Molecule 19: Small nuclear ribonucleoprotein Sm D2



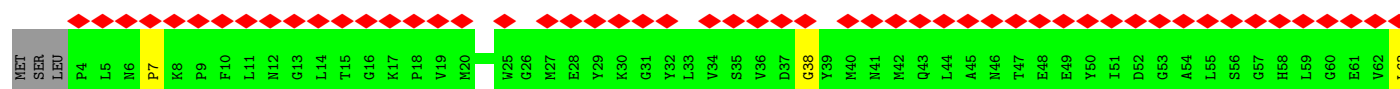
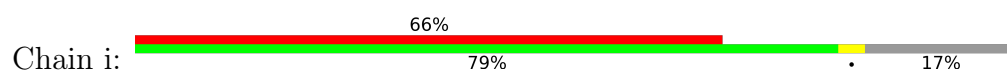
- Molecule 19: Small nuclear ribonucleoprotein Sm D2



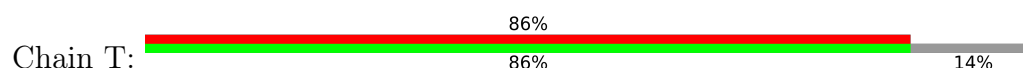
- Molecule 20: Small nuclear ribonucleoprotein F

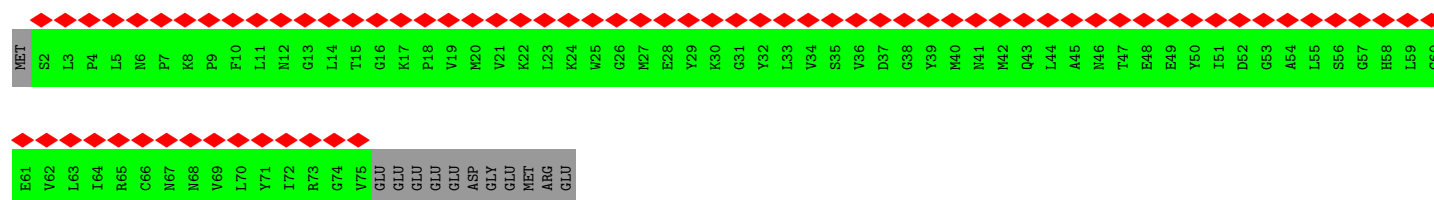


- Molecule 20: Small nuclear ribonucleoprotein F

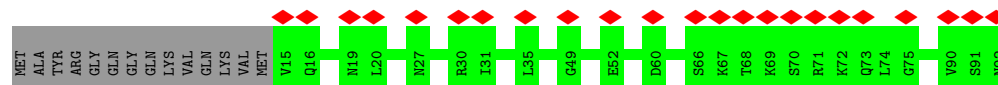
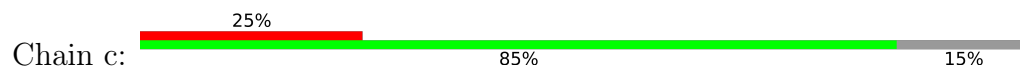


- Molecule 20: Small nuclear ribonucleoprotein F

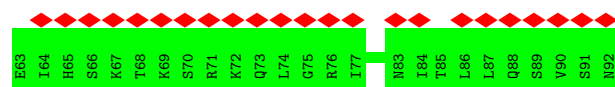
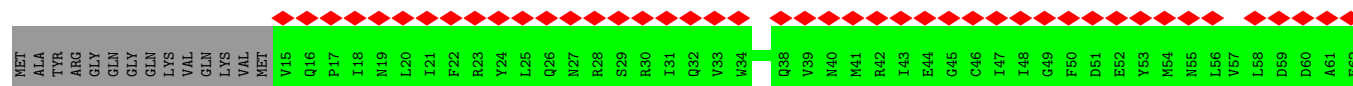
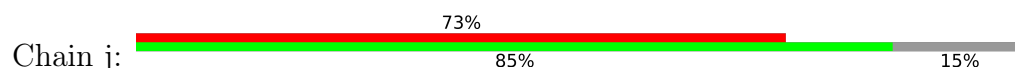




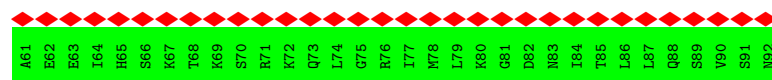
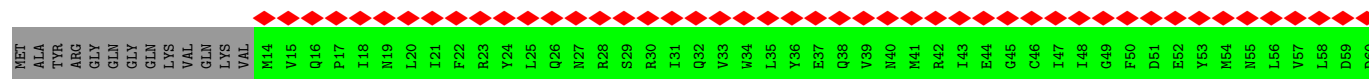
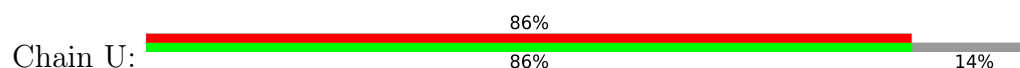
• Molecule 21: Small nuclear ribonucleoprotein E



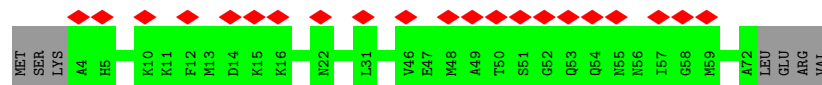
• Molecule 21: Small nuclear ribonucleoprotein E



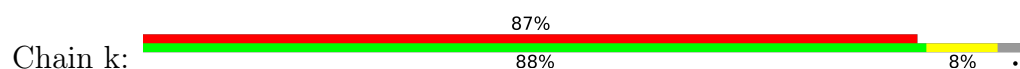
• Molecule 21: Small nuclear ribonucleoprotein E

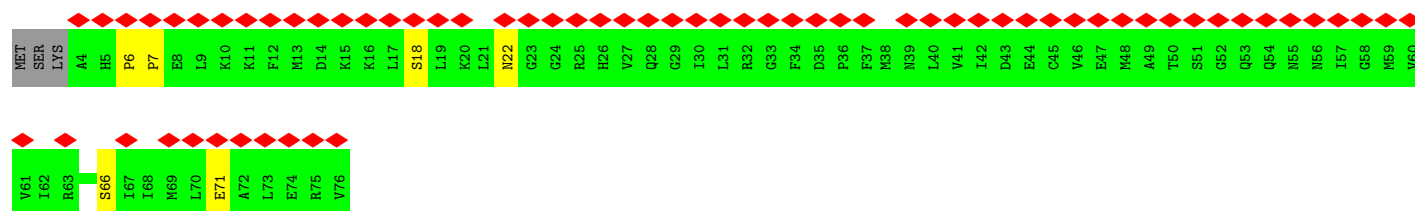


• Molecule 22: Small nuclear ribonucleoprotein G

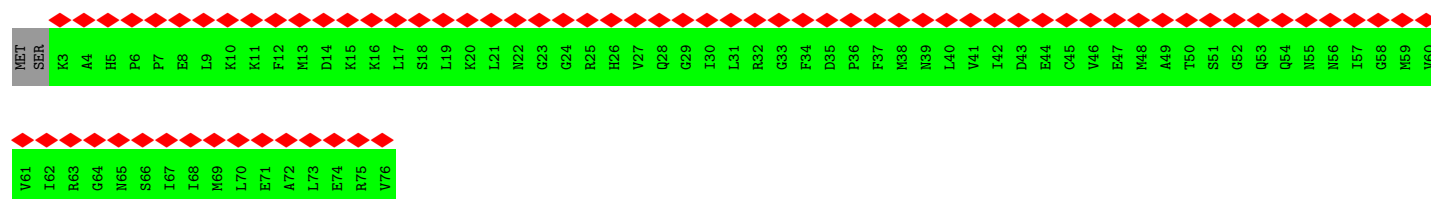


• Molecule 22: Small nuclear ribonucleoprotein G

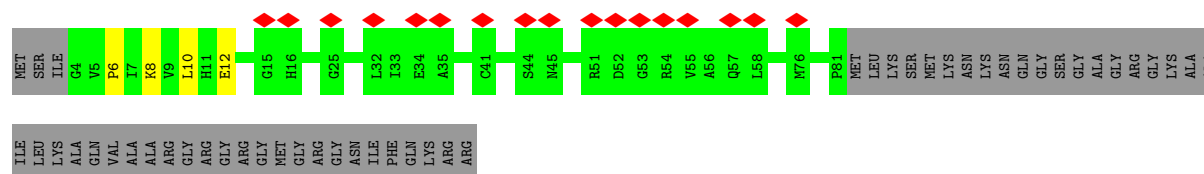




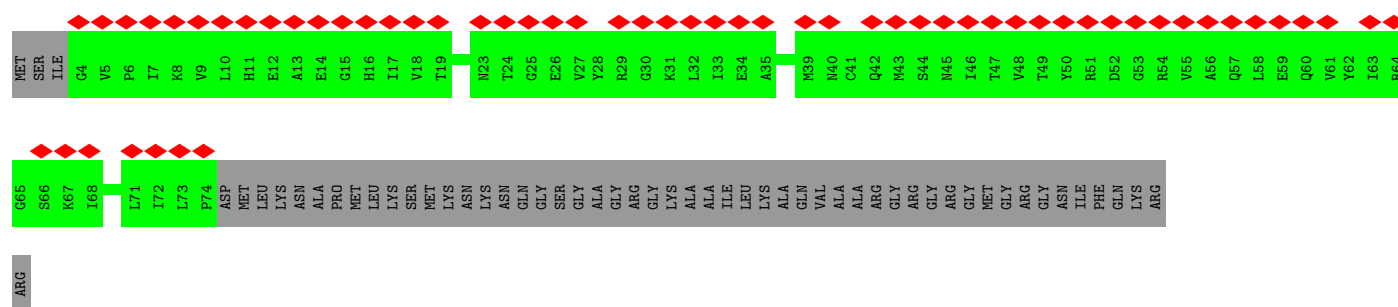
• Molecule 22: Small nuclear ribonucleoprotein G



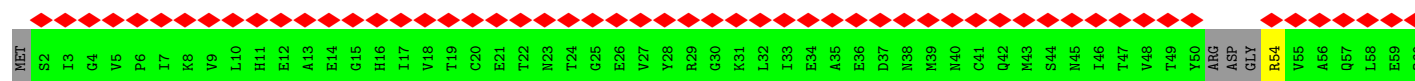
• Molecule 23: Small nuclear ribonucleoprotein Sm D3

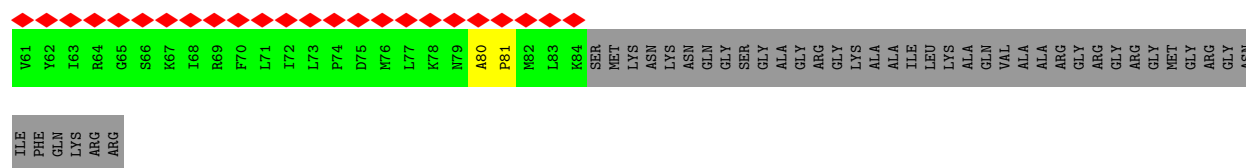


• Molecule 23: Small nuclear ribonucleoprotein Sm D3

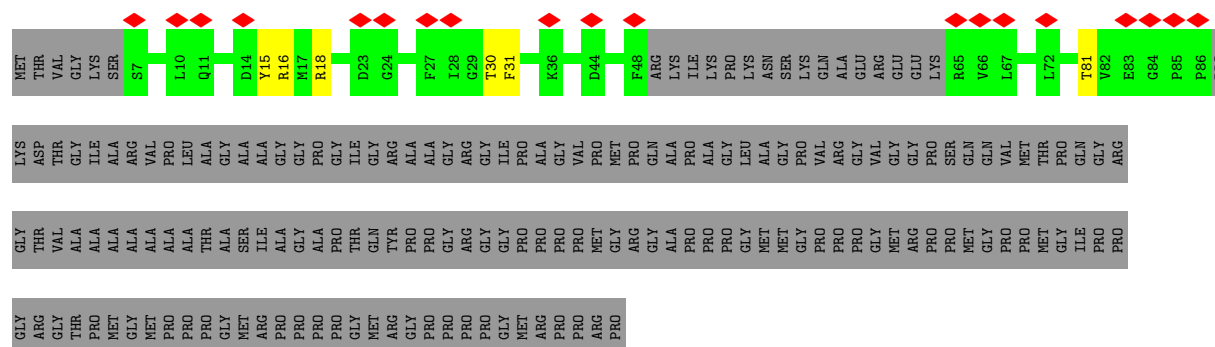


• Molecule 23: Small nuclear ribonucleoprotein Sm D3

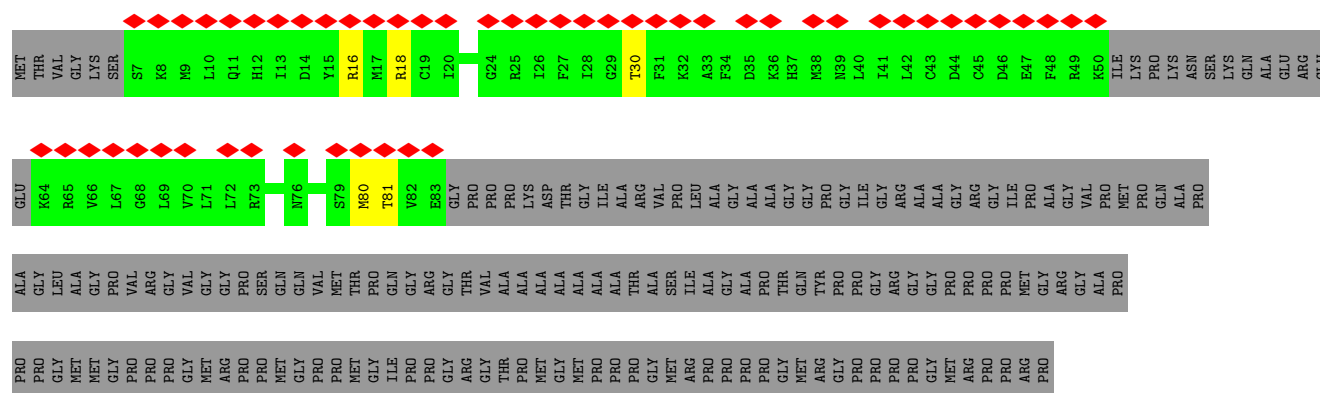




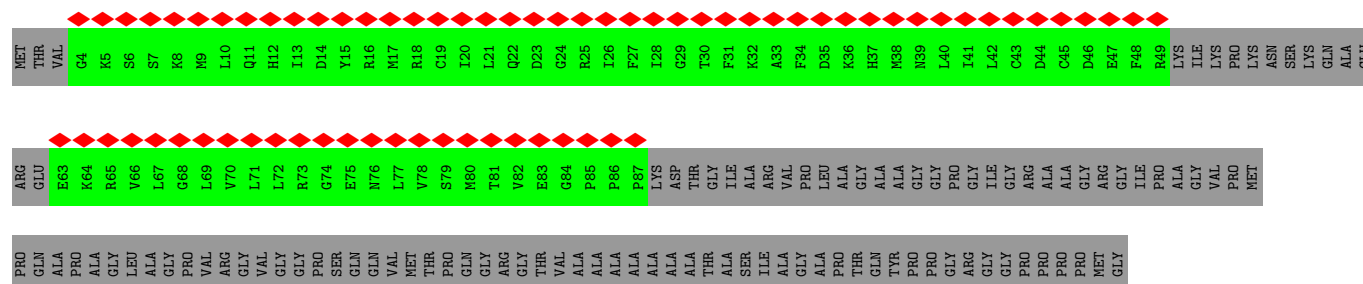
- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'



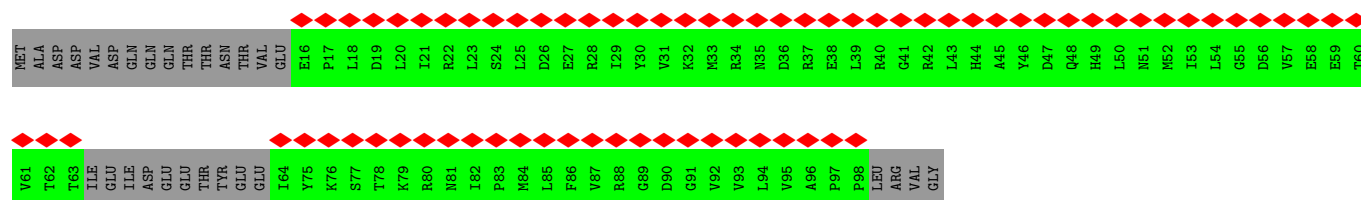
- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'



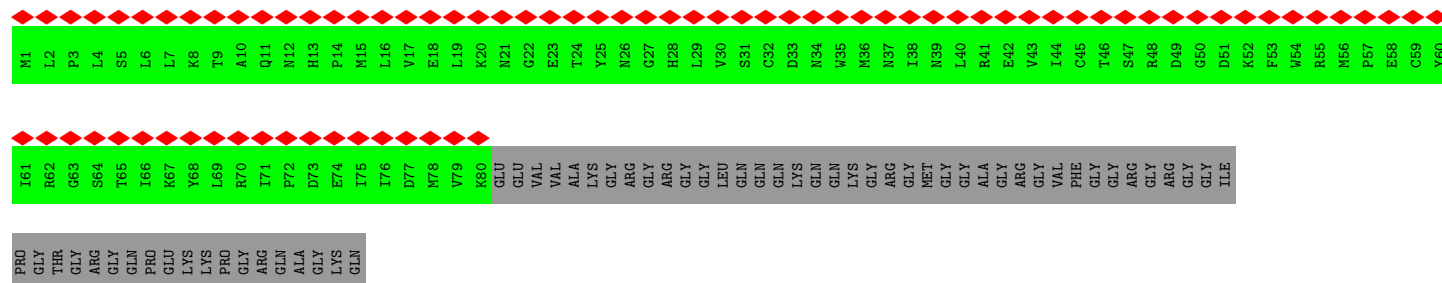
- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'



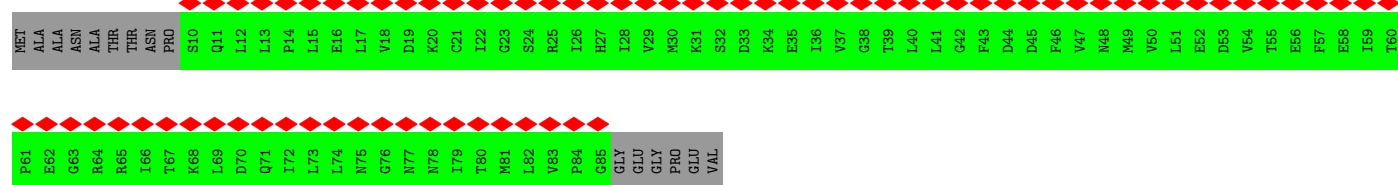
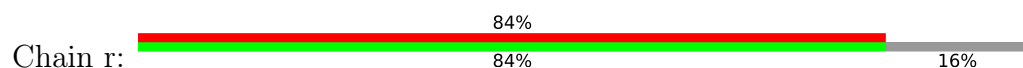




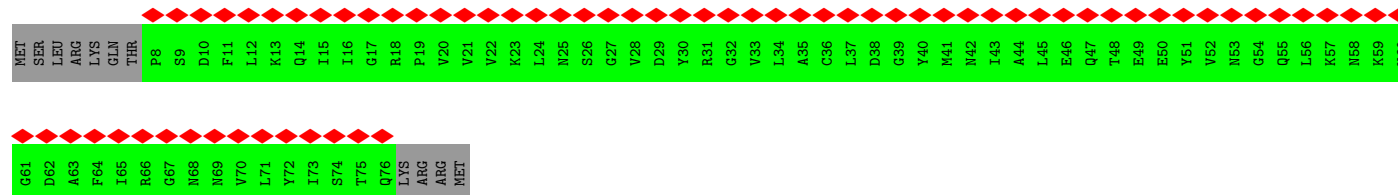
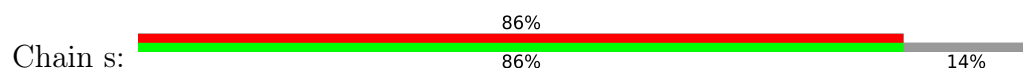
• Molecule 28: U6 snRNA-associated Sm-like protein LSm4



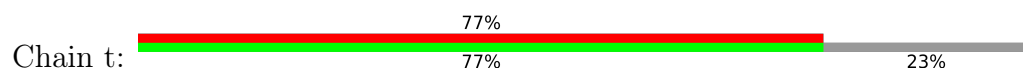
• Molecule 29: U6 snRNA-associated Sm-like protein LSm5

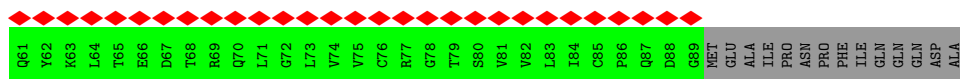


• Molecule 30: U6 snRNA-associated Sm-like protein LSm6



• Molecule 31: U6 snRNA-associated Sm-like protein LSm7

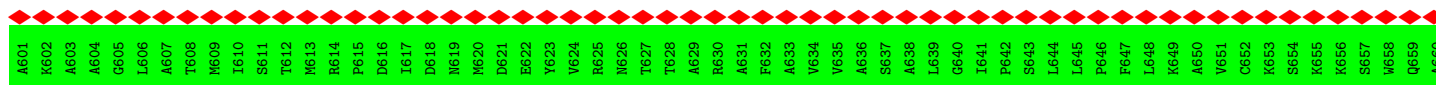
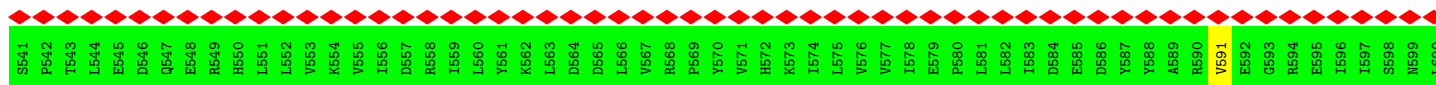
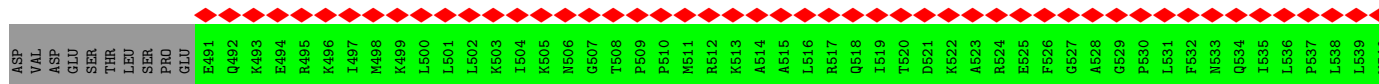
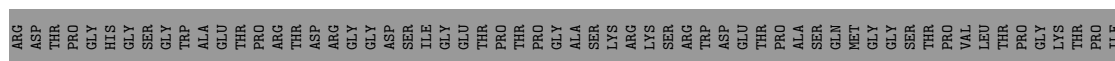
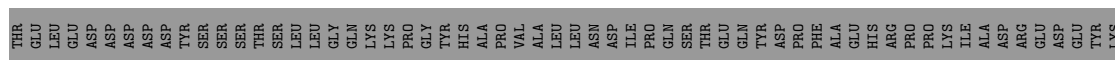
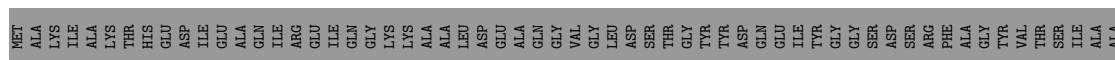




• Molecule 32: U6 snRNA-associated Sm-like protein LSm8



• Molecule 33: Splicing factor 3B subunit 1



- Molecule 34: Splicing factor 3B subunit 3 (SF3B3)

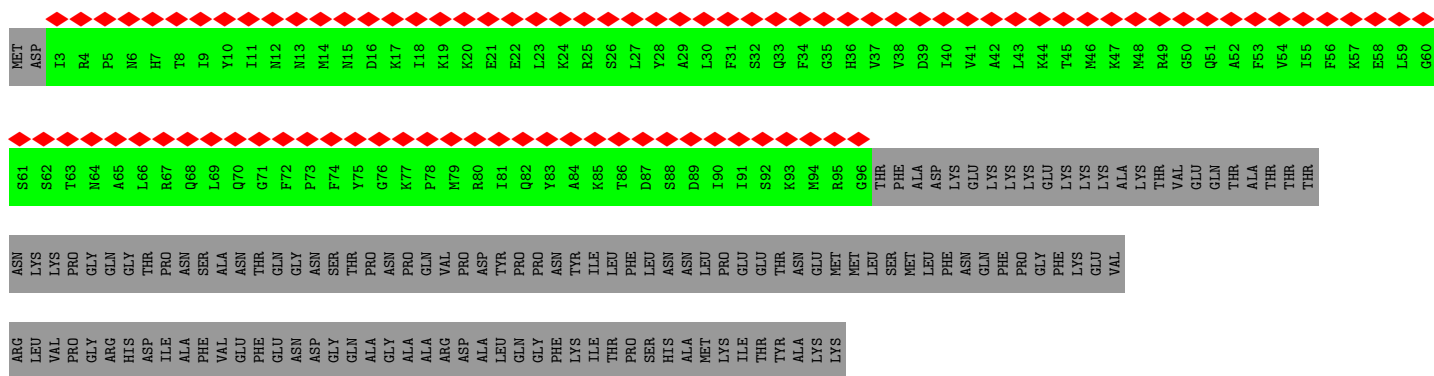
Response	Percentage
Yes	94%
No	6%

M1	F2	L3	Y4	N5	L6	T7	L8	Q9	R10	A11	T12	G13	I14	S15	F16	A17	I18	H19	G20	N21	F22	S23	G24	T25	K26	Q27	Q28	E29	I30	V31	V32	S33	R34	G35	K36	I37	L38	E39	L40	L41	R42	P43	D44	P45	N46	T47	G48	K49	V50	H51	T52	L53	L54	T55	V56	E57	V58	F59	G60
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

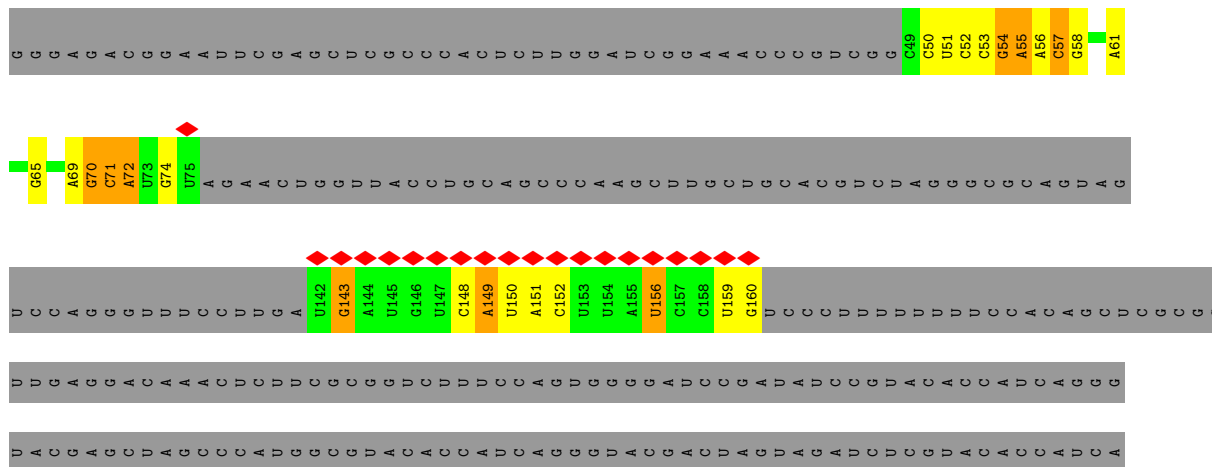
ALA	V61	L121	M181	G241	F301	I361	F421	A481	K541	R601	GLY	L781	ALA
PHE	I62	A122	F182	S242	L302	A362	Q422	T482	K542	S602	F662	Q782	PHE
LEU	R63	V123	A183	D243	A363	H563	L423	L483	T543	R603	L663	Q783	LEU
ASN	S64	D124	C184	G244	Q304	L364	Y424	V484	I544	F604	Y664	T784	ASN
GLU	L65	P125	E185	P245	T305	G365	V425	L485	V545	L605	L665	F785	GLU
ASN	M66	K126	E186	S246	E306	D366	A426	S486	K546	A606	M666	F786	ASN
LEU	A67	G127	M187	G247	Q307	D367	C427	I487	C547	V607	L667	Q787	LEU
	F68	R128	D188	V248	G308	D368	G428	G488	A548	G608	G668	R788	
	R69	A129	L189	L249	D309	E369	A429	E489	V549	L609	L669	F789	
	L70	V130	E190	L250	I310	E370	G430	T490	N550	V610	Q670	H790	
	T71	M131	E191	C251	F311	P371	P431	V491	Q551	D611	M671	L791	
	G72	I132	A192	S252	K312	E372	R432	E492	R552	N612	G672	F792	
	G73	I133	D193	E253	I313	F373	S433	E493	Q553	T613	V673	F793	
	T74	A134	N194	N254	T314	S374	S434	V494	V554	V614	L674	L794	
	K75	I135	D195	Y255	L315	S375	L435	T495	V555	R615	L675	S795	
	D76	E136	P196	I256	E316	A376	R436	D496	I556	T616	R676	Y796	
	Y77	K137	T197	T257	T317	M377	V437	S497	A557	L617	T677	E797	
	I78	Q138	G198	Y258	D318	P378	L438	G498	L558	S618	V678	T798	
	V79	K139	E199	K259	E319	L379	R439	F499	T559	L619	L679	L799	
	V80	L140	A200	N260	D320	E380	H440	G500	G560	D620	D680	E740	
	G81	V141	A201	F261	M321	E381	G441	L501	G561	P621	P681	F741	
	S82	Y142	A202	G262	V322	G382	L442	T502	E562	S622	V682	A742	
	D83	I143	N203	D263	T323	D383	GLU	T503	L563	D623	T683	S743	
	S84	L144	T204	Q264	E324	T384	V444	P504	V564	C624	G684	G744	
	G85	N145	Q205	P265	I325	F385	S445	T505	Y565	L625	D685	F745	
	R86	R146	Q206	D266	R326	F386	E446	L506	F566	Q626	L686	A746	
	I87	D147	T207	I267	L327	F387	M447	S507	E567	P627	S687	S747	
	V88	A148	L208	R268	K328	Q388	A448	C508	M568	L628	D688	E748	
	I89	A149	T209	C269	Y329	P389	V449	S509	D569	S629	T689	Q749	
	L90	A150	F210	P270	F330	R390	S450	L510	P570	M630	R690	C750	
	E91	R151	Y211	I271	D331	P391	E451	L511	S571	Q631	T691	F751	
	Y92	L152	E212	P272	T332	L392	L452	G512	G572	A632	R692	E752	
	Q93	T153	D213	R273	V333	K393	P453	D513	Q573	L633	TYR	G753	
	P94	I154	D214	R274	P334	N394	G454	D514	L574	P634	LEU	I754	
	S95	S155	L215	R275	V335	L395	M455	A515	N575	A635	G695	V755	
	K96	S156	G216	N276	A336	V396	P456	L516	E576	Q636	S696	A756	
	N97	P157	D217	D277	A337	L397	M457	V517	Y577	P637	R697	I757	
	M98	L158	N218	L278	A338	V398	A458	Q518	T578	E638	V698	S758	
	F99	E159	H219	D279	M339	D399	V459	V519	E579	S639	K700	T759	
	E100	A160	V220	D280	C340	E400	M460	V520	R580	L640	L701	M760	
	K101	H161	V221	P281	V341	L401	T461	P521	K581	C641	F702	N761	
	I102	K162	R222	E282	L342	D402	V462	D522	E582	T642	R703	L762	
	H103	A163	K223	R283	K343	S403	R463	G523	M583	V643	ALA	R763	
	Q104	N164	Y224	G284	T344	L404	A464	I524	S584	E644	GLY	V764	
	E105	T165	S225	M285	G345	S405	H465	R525	A585	L645	R705	I764	
	T106	L166	E226	I286	F346	P406	L466	H526	D586	M645	M706	L765	
	F107	V167	P227	F287	L347	I407	E467	H527	V587	GLY	Q707	A766	
	G108	Y168	L228	V288	F348	L408	D468	R528	V588	THR	G708	L767	
	K109	H169	E229	C289	V349	F409	E469	A529	C589	GLU	Q709	L767	
	S110	V170	E230	S290	A350	C410	F470	D530	M590	LYS	E710	LEU	
	G111	V171	H231	A291	S351	Q411	D471	K531	S591	ASP	A711	ALA	
	C112	G172	G232	T292	E352	T412	A472	R532	L592	GLU	V712	L713	
	R113	V173	N233	H293	F353	A413	Y473	V533	A593	GLY	L713	F774	
	D114	D174	F234	K294	G354	D414	I474	N534	N594	ARG	A714	M775	
	I115	V175	L235	T295	N355	L415	I475	E535	V595	GLY	H715	Q776	
	V116	G176	I236	K296	H356	A416	V476	M536	P596	SER	S716	V777	
	P117	F177	T237	S297	Y357	M417	S477	K537	P597	ILE	S717	A778	
	G118	E178	M298	M298	L358	E418	F478	T538	G598		R718	F779	
	Q119	N179	P239	F299	Y359	D419	V479	P539	E599		S719	P780	
	F120	P180	G240	F300	Q360	T420	M480	G540	Q600		W720		

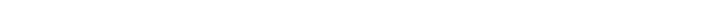


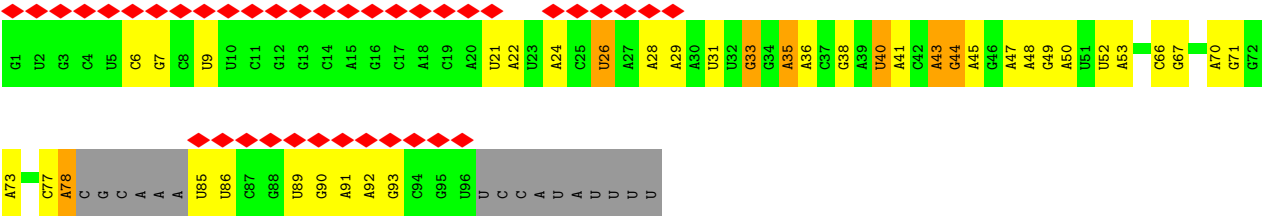
- Molecule 38: U2 small nuclear ribonucleoprotein B''



- Molecule 39: MINX pre-mRNA



Chain 6: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	501.12, 501.12, 501.12	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.14	0/11222	0.46	8/15747 (0.1%)
2	B	0.12	0/4312	0.38	1/6043 (0.0%)
3	C	0.10	0/8613	0.31	0/12069
5	E	0.18	0/1107	0.59	0/1547
6	F	0.14	0/2115	0.49	1/2951 (0.0%)
7	G	0.20	1/4089 (0.0%)	0.66	8/5728 (0.1%)
8	H	0.40	1/2082 (0.0%)	0.62	3/2910 (0.1%)
9	I	0.16	0/888	0.52	0/1241
10	J	0.12	0/681	0.45	0/952
11	K	0.07	0/224	0.35	0/312
12	L	0.14	0/2295	0.44	0/3198
13	M	0.17	0/853	0.47	0/1188
14	N	0.15	0/276	0.55	0/383
15	O	0.15	0/641	0.44	0/898
16	P	0.16	0/459	0.56	1/640 (0.2%)
17	Q	0.14	0/379	0.44	0/530
18	R	0.08	0/78	0.41	0/107
19	a	0.12	0/394	0.43	0/548
19	h	0.13	0/371	0.45	0/516
20	b	0.19	0/367	0.44	0/509
20	i	0.19	0/357	0.45	0/495
21	c	0.14	0/388	0.42	0/540
21	j	0.14	0/388	0.43	0/540
22	d	0.21	0/346	0.54	0/481
22	k	0.22	0/366	0.55	0/509
23	e	0.12	0/392	0.55	0/546
23	l	0.11	0/354	0.34	0/492
24	f	0.13	0/319	0.39	0/442
24	m	0.12	0/314	0.37	0/434
25	g	0.12	0/471	0.42	0/657
25	n	0.14	0/414	0.43	0/578
39	Y	0.42	5/1083 (0.5%)	0.20	0/1681
40	2	0.75	17/2366 (0.7%)	1.22	35/3677 (1.0%)
41	4	0.14	0/3240	0.27	0/5039

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	5	0.08	0/2672	0.20	0/4154
43	6	0.08	0/2155	0.19	0/3355
All	All	0.22	24/57071 (0.0%)	0.49	57/81637 (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	2
7	G	0	3
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	268	LEU	C-N	16.25	1.71	1.33
40	2	150	U	C1'-N1	7.13	1.59	1.48
40	2	182	U	C1'-N1	7.06	1.59	1.48
40	2	142	U	C1'-N1	6.97	1.58	1.48
40	2	137	U	C1'-N1	6.96	1.58	1.48
40	2	148	C	C1'-N1	6.69	1.58	1.48
40	2	97	G	C1'-N9	-6.62	1.38	1.48
39	Y	143	G	C1'-N9	-6.61	1.38	1.48
40	2	143	C	C1'-N1	6.55	1.58	1.48
40	2	141	C	C1'-N1	6.51	1.58	1.48
40	2	139	C	C1'-N1	6.51	1.58	1.48
40	2	111	G	C1'-N9	-6.50	1.37	1.47
40	2	179	C	C1'-N1	6.49	1.58	1.48
40	2	151	C	C1'-N1	6.43	1.58	1.48
40	2	144	C	C1'-N1	6.43	1.58	1.48
40	2	138	C	C1'-N1	6.41	1.58	1.48
40	2	184	C	C1'-N1	6.41	1.58	1.48
39	Y	156	U	C1'-N1	6.12	1.56	1.47
40	2	110	A	C1'-N9	-6.05	1.38	1.48
39	Y	148	C	C1'-N1	5.68	1.56	1.48
39	Y	152	C	C1'-N1	5.58	1.56	1.48
7	G	400	VAL	C-N	5.33	1.46	1.33
39	Y	149	A	C1'-N9	-5.21	1.40	1.48
40	2	107	A	C1'-N9	-5.16	1.40	1.48

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	307	HIS	CA-C-N	-10.93	111.13	122.28
7	G	307	HIS	C-N-CA	-10.93	111.13	122.28
7	G	839	HIS	CA-C-N	-8.94	113.16	122.28
7	G	839	HIS	C-N-CA	-8.94	113.16	122.28
40	2	119	G	O3'-P-O5'	-8.62	91.08	104.00
40	2	151	C	O3'-P-O5'	-8.61	91.08	104.00
40	2	181	G	O3'-P-O5'	-8.61	91.09	104.00
40	2	183	G	O3'-P-O5'	-8.60	91.10	104.00
40	2	142	U	O3'-P-O5'	-8.60	91.10	104.00
40	2	141	C	O3'-P-O5'	-8.59	91.11	104.00
40	2	150	U	O3'-P-O5'	-8.59	91.11	104.00
40	2	182	U	O3'-P-O5'	-8.59	91.12	104.00
40	2	180	G	O3'-P-O5'	-8.57	91.14	104.00
40	2	137	U	O3'-P-O5'	-8.57	91.14	104.00
40	2	139	C	O3'-P-O5'	-8.57	91.15	104.00
40	2	140	A	O3'-P-O5'	-8.56	91.16	104.00
40	2	179	C	O3'-P-O5'	-8.56	91.16	104.00
40	2	149	A	O3'-P-O5'	-8.55	91.17	104.00
40	2	138	C	O3'-P-O5'	-8.52	91.22	104.00
40	2	143	C	O3'-P-O5'	-8.52	91.22	104.00
40	2	148	C	O3'-P-O5'	-8.51	91.24	104.00
40	2	168	A	P-O5'-C5'	-7.61	109.48	120.90
40	2	167	U	O3'-P-O5'	-7.33	93.01	104.00
40	2	170	C	C3'-C2'-O2'	-6.99	104.12	114.60
40	2	164	C	C5'-C4'-O4'	-6.71	99.04	109.10
1	A	461	HIS	CA-C-N	-6.69	115.39	122.89
1	A	461	HIS	C-N-CA	-6.69	115.39	122.89
40	2	169	C	P-O3'-C3'	6.22	129.53	120.20
40	2	168	A	C5'-C4'-C3'	-6.17	106.75	116.00
1	A	77	THR	CB-CA-C	-6.12	108.51	115.79
40	2	163	G	O3'-P-O5'	-5.83	95.26	104.00
40	2	164	C	P-O3'-C3'	5.71	128.76	120.20
40	2	168	A	O4'-C1'-C2'	-5.60	102.00	107.60
40	2	157	G	P-O5'-C5'	-5.57	112.55	120.90
40	2	165	A	N9-C1'-C2'	5.56	120.34	112.00
1	A	532	THR	CB-CA-C	-5.52	110.19	116.54
40	2	160	A	P-O5'-C5'	-5.49	112.66	120.90
7	G	656	ASP	CB-CA-C	-5.43	110.33	116.63
16	P	144	ALA	CB-CA-C	-5.39	110.37	116.63
1	A	2316	ASN	CB-CA-C	-5.36	110.42	116.63
8	H	419	ARG	CB-CA-C	-5.35	110.43	116.63
8	H	256	ARG	CB-CA-C	-5.22	110.58	116.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	160	A	C4'-C3'-C2'	-5.21	97.39	102.60
7	G	891	GLU	CB-CA-C	-5.20	110.15	117.23
40	2	171	U	C2'-C3'-O3'	-5.19	105.91	113.70
7	G	277	LEU	CB-CA-C	-5.19	110.18	117.23
7	G	792	LEU	CB-CA-C	-5.18	109.63	115.79
1	A	1578	ARG	CB-CA-C	-5.17	110.20	117.23
6	F	456	PHE	CB-CA-C	-5.17	110.64	116.63
8	H	255	GLN	CB-CA-C	-5.14	110.23	117.23
2	B	161	TYR	CB-CA-C	-5.13	110.25	117.23
40	2	156	U	C4'-C3'-C2'	5.12	107.72	102.60
40	2	170	C	O4'-C1'-C2'	-5.12	100.68	105.80
40	2	160	A	N9-C1'-C2'	5.09	119.63	112.00
1	A	438	GLY	CA-C-N	-5.05	117.23	122.89
1	A	438	GLY	C-N-CA	-5.05	117.23	122.89
40	2	155	C	P-O3'-C3'	5.02	127.72	120.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	ARG	Peptide
1	A	948	PRO	Peptide
7	G	308	HIS	Peptide
7	G	840	ASP	Peptide
7	G	841	PRO	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	11100	0	5431	74	0
2	B	4264	0	2120	33	0
3	C	8538	0	4146	60	0
4	D	302	0	0	0	0
5	E	1101	0	543	15	0
6	F	2100	0	1038	24	0
7	G	4057	0	2089	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2068	0	1019	20	0
9	I	883	0	414	4	0
10	J	677	0	316	1	0
11	K	225	0	98	2	0
12	L	2288	0	1076	10	0
13	M	844	0	426	3	0
14	N	277	0	114	2	0
15	O	636	0	322	2	0
16	P	458	0	225	1	0
17	Q	378	0	190	1	0
18	R	79	0	32	1	0
19	S	87	0	0	0	0
19	a	393	0	176	0	0
19	h	371	0	162	2	0
20	T	74	0	0	0	0
20	b	364	0	181	1	0
20	i	354	0	177	2	0
21	U	79	0	0	0	0
21	c	388	0	167	0	0
21	j	388	0	167	0	0
22	V	74	0	0	0	0
22	d	344	0	168	0	0
22	k	364	0	176	3	0
23	W	80	0	0	2	0
23	e	390	0	188	2	0
23	l	353	0	166	0	0
24	X	71	0	0	0	0
24	f	319	0	144	3	0
24	m	316	0	133	3	0
25	Z	82	0	0	0	0
25	g	469	0	214	5	0
25	n	412	0	185	5	0
26	o	90	0	0	0	0
27	p	73	0	0	0	0
28	q	80	0	0	0	0
29	r	76	0	0	0	0
30	s	69	0	0	0	0
31	t	79	0	0	0	0
32	u	62	0	0	0	0
33	v	806	0	0	3	0
34	w	1140	0	0	3	0
35	x	54	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	89	0	0	2	0
37	z	162	0	0	0	0
38	1	94	0	0	0	0
39	Y	972	0	495	31	0
40	2	2123	0	1076	177	0
41	4	2904	0	1470	44	0
42	5	2397	0	1216	42	0
43	6	1926	0	973	33	0
All	All	59243	0	27233	588	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 7.

All (588) 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)
8:H:268:LEU:C	8:H:269:PRO:N	1.71	1.46
40:2:153:A:H2	40:2:178:A:N1	1.00	1.46
1:A:2313:HIS:CB	3:C:1045:PRO:HB3	1.47	1.44
40:2:153:A:C2'	40:2:154:C:H5'	1.46	1.42
33:v:591:VAL:CA	36:y:94:SER:CA	1.99	1.40
40:2:153:A:N1	40:2:178:A:N6	1.73	1.37
40:2:153:A:C2	40:2:178:A:N1	1.91	1.36
40:2:106:G:H21	40:2:107:A:N6	1.23	1.35
40:2:106:G:N2	40:2:107:A:C6	1.97	1.29
39:Y:149:A:N1	40:2:40:C:N4	1.78	1.29
40:2:153:A:O2'	40:2:154:C:C5'	1.79	1.29
40:2:108:G:H2'	40:2:109:C:C6	1.68	1.27
39:Y:143:G:O6	40:2:45:C:N4	1.71	1.21
40:2:153:A:C2	40:2:178:A:C6	2.31	1.18
40:2:153:A:O2'	40:2:154:C:H5'	1.01	1.17
40:2:153:A:C2'	40:2:154:C:C5'	2.22	1.16
40:2:106:G:N2	40:2:107:A:N6	1.94	1.13
40:2:156:U:H6	40:2:156:U:H5''	1.10	1.10
40:2:154:C:O2	40:2:178:A:N6	1.85	1.09
1:A:2268:LEU:O	3:C:1264:PRO:HG2	1.53	1.08
39:Y:149:A:H61	40:2:40:C:N4	1.50	1.07
39:Y:149:A:N6	40:2:40:C:N4	2.03	1.07
1:A:2268:LEU:O	3:C:1264:PRO:CG	2.04	1.06
39:Y:149:A:C6	40:2:40:C:N4	2.19	1.06
40:2:105:G:H2'	40:2:106:G:H5''	1.37	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:153:A:H2'	40:2:154:C:C5'	1.81	1.05
1:A:2074:ARG:CB	3:C:1047:PRO:HG2	1.86	1.03
39:Y:72:A:N6	43:6:33:G:H1	1.53	1.03
1:A:2313:HIS:CB	3:C:1045:PRO:CB	2.37	1.01
40:2:153:A:H2	40:2:178:A:C6	1.74	1.01
40:2:153:A:C2	40:2:178:A:N6	2.28	1.00
40:2:168:A:C8	40:2:168:A:H5''	1.99	0.98
40:2:112:G:C2	40:2:113:G:C5	2.51	0.97
42:5:12:U:H3	42:5:65:G:H1	1.12	0.97
41:4:91:A:H2	41:4:110:G:N2	1.61	0.97
40:2:153:A:H2'	40:2:154:C:H5'	1.34	0.96
40:2:112:G:H2'	40:2:113:G:H8	1.29	0.96
41:4:4:U:H3	43:6:71:G:H1	0.98	0.94
40:2:156:U:H5''	40:2:156:U:C6	2.02	0.93
39:Y:149:A:N1	40:2:40:C:C4	2.37	0.93
39:Y:149:A:N6	40:2:40:C:H42	1.62	0.93
39:Y:65:G:H1	43:6:40:U:H3	0.99	0.92
40:2:118:G:H2'	40:2:119:G:H8	1.33	0.92
40:2:153:A:N1	40:2:178:A:C6	2.34	0.91
40:2:112:G:O2'	40:2:113:G:H5'	1.69	0.91
40:2:168:A:H5''	40:2:168:A:H8	1.37	0.90
39:Y:149:A:H61	40:2:40:C:H41	1.14	0.90
40:2:112:G:N3	40:2:113:G:C8	2.40	0.89
40:2:144:C:H2'	40:2:145:A:H5''	1.54	0.89
39:Y:58:G:H1	42:5:41:U:H3	0.92	0.89
40:2:112:G:C2	40:2:113:G:N7	2.42	0.87
40:2:144:C:H3'	40:2:145:A:H5'	1.56	0.86
7:G:312:TRP:O	7:G:316:ALA:HB3	1.75	0.86
39:Y:143:G:O6	40:2:45:C:C4	2.29	0.86
40:2:108:G:H2'	40:2:109:C:H6	1.35	0.86
40:2:106:G:N2	40:2:107:A:N1	2.22	0.86
40:2:156:U:H6	40:2:156:U:C5'	1.89	0.86
39:Y:74:G:H1	43:6:31:U:H3	0.86	0.85
19:h:62:HIS:HA	41:4:118:A:H3'	1.60	0.82
40:2:105:G:C2'	40:2:106:G:H5''	2.09	0.81
40:2:108:G:H2'	40:2:109:C:C5	2.14	0.81
41:4:91:A:H2	41:4:110:G:H22	0.83	0.81
41:4:108:C:O2'	41:4:109:G:H5'	1.81	0.81
40:2:112:G:C4	40:2:113:G:N7	2.49	0.80
40:2:112:G:N3	40:2:113:G:N7	2.30	0.80
42:5:17:U:H3	42:5:60:G:H1	0.83	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:842:HIS:O	7:G:846:ALA:HB2	1.83	0.80
33:v:675:MET:CA	33:v:676:GLY:CA	2.59	0.80
40:2:101:U:H5''	40:2:102:U:H5'	1.64	0.80
40:2:154:C:C2	40:2:178:A:N6	2.47	0.79
40:2:178:A:O2'	40:2:179:C:H5'	1.85	0.77
39:Y:72:A:H61	43:6:33:G:H1	0.78	0.77
1:A:2070:LYS:O	3:C:1047:PRO:HG3	1.84	0.76
40:2:112:G:H2'	40:2:113:G:C8	2.18	0.76
39:Y:149:A:N1	40:2:40:C:N3	2.33	0.76
40:2:106:G:H4'	40:2:107:A:O4'	1.85	0.76
40:2:178:A:H2'	40:2:179:C:H6	1.49	0.75
1:A:464:PRO:HG2	42:5:20:G:H4'	1.69	0.75
40:2:144:C:H3'	40:2:145:A:C5'	2.17	0.75
18:R:211:ARG:CB	34:w:579:GLU:CA	2.66	0.74
1:A:75:ASP:HA	9:I:14:GLY:HA2	1.70	0.73
40:2:118:G:H2'	40:2:119:G:C8	2.23	0.72
2:B:441:PRO:O	2:B:445:ALA:HB2	1.88	0.72
7:G:361:VAL:O	7:G:365:ALA:HB2	1.89	0.72
40:2:109:C:H6	40:2:109:C:O5'	1.73	0.71
39:Y:143:G:O6	40:2:45:C:N3	2.23	0.71
8:H:288:ARG:O	8:H:292:ALA:HB2	1.91	0.70
40:2:153:A:H2'	40:2:154:C:O5'	1.91	0.70
40:2:154:C:H1'	40:2:178:A:N1	2.05	0.70
7:G:842:HIS:O	7:G:846:ALA:CB	2.39	0.70
1:A:2313:HIS:CA	3:C:1045:PRO:HB3	2.19	0.70
40:2:12:G:H1	43:6:86:U:H3	1.39	0.69
40:2:177:A:H2	40:2:178:A:H62	1.39	0.68
40:2:150:U:H3	40:2:181:G:H1	1.41	0.68
7:G:312:TRP:O	7:G:316:ALA:CB	2.42	0.68
8:H:292:ALA:O	8:H:296:ALA:HB2	1.93	0.68
15:O:113:LYS:O	15:O:117:GLN:CB	2.41	0.67
40:2:112:G:N1	40:2:113:G:C6	2.62	0.67
13:M:111:SER:HA	13:M:140:VAL:HA	1.76	0.67
7:G:841:PRO:O	7:G:843:VAL:N	2.27	0.67
41:4:24:U:H3	41:4:48:G:H1	1.42	0.67
41:4:2:G:O6	43:6:73:A:N1	2.27	0.67
11:K:299:LYS:O	11:K:303:GLU:CB	2.43	0.67
39:Y:150:U:H6	39:Y:150:U:O5'	1.77	0.67
41:4:111:C:O5'	41:4:111:C:H6	1.78	0.67
40:2:168:A:C8	40:2:168:A:C5'	2.75	0.66
42:5:78:U:O2'	42:5:80:U:OP1	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:e:8:LYS:O	23:e:12:GLU:CB	2.44	0.66
40:2:154:C:O2	40:2:178:A:C6	2.49	0.66
41:4:6:U:H2'	41:4:7:G:H8	1.61	0.65
42:5:58:U:H2'	42:5:59:G:H8	1.62	0.65
1:A:2152:GLY:HA3	1:A:2157:VAL:HA	1.79	0.65
41:4:117:C:O5'	41:4:117:C:H6	1.80	0.65
9:I:35:TRP:O	9:I:39:CYS:CB	2.45	0.65
6:F:349:TRP:HA	6:F:356:GLU:HA	1.78	0.65
23:e:6:PRO:O	23:e:10:LEU:CB	2.46	0.65
40:2:144:C:C3'	40:2:145:A:C5'	2.75	0.65
40:2:153:A:C2'	40:2:154:C:O5'	2.43	0.65
40:2:156:U:C6	40:2:156:U:C5'	2.72	0.64
25:g:86:LYS:O	25:g:90:LYS:CB	2.46	0.64
3:C:1084:VAL:O	3:C:1088:ALA:HB2	1.97	0.64
39:Y:149:A:C2	40:2:40:C:N3	2.65	0.64
3:C:1077:LEU:O	3:C:1081:MET:N	2.27	0.63
40:2:112:G:N1	40:2:113:G:C5	2.66	0.63
40:2:164:C:H6	40:2:164:C:H5'	1.63	0.63
2:B:371:GLU:O	2:B:375:GLU:CB	2.46	0.63
41:4:89:U:C2'	41:4:90:G:H5'	2.29	0.63
40:2:112:G:C2	40:2:113:G:C8	2.85	0.63
41:4:108:C:H2'	41:4:109:G:H8	1.63	0.62
1:A:2074:ARG:CB	3:C:1047:PRO:CG	2.73	0.62
7:G:311:ALA:O	7:G:315:SER:CB	2.47	0.62
41:4:89:U:O2'	41:4:90:G:H5'	1.99	0.62
3:C:1081:MET:O	3:C:1085:THR:CB	2.48	0.62
7:G:407:TRP:O	7:G:411:VAL:CB	2.48	0.62
41:4:91:A:O5'	41:4:91:A:H8	1.82	0.62
1:A:534:GLU:O	1:A:538:SER:CB	2.48	0.62
1:A:2317:PHE:CB	3:C:1043:ARG:CB	2.78	0.62
5:E:513:GLU:O	5:E:517:ALA:HB2	2.00	0.62
7:G:875:GLY:O	7:G:879:ALA:HB2	2.00	0.61
20:b:7:PRO:HB3	20:b:38:GLY:HA2	1.80	0.61
3:C:488:LEU:O	3:C:492:ALA:HB3	2.01	0.61
13:M:107:PRO:HG3	13:M:129:SER:HA	1.81	0.61
2:B:328:ALA:HA	2:B:332:GLY:HA3	1.83	0.61
7:G:745:LEU:O	7:G:749:LEU:CB	2.47	0.61
35:x:75:PRO:CA	35:x:76:CYS:CA	2.78	0.61
1:A:239:TYR:O	1:A:243:ASN:CB	2.49	0.61
40:2:147:G:H2'	40:2:148:C:H6	1.66	0.61
42:5:12:U:O4	42:5:65:G:O6	2.19	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:146:C:O5'	40:2:147:G:H4'	2.01	0.61
23:W:54:ARG:CA	40:2:151:C:O2	2.50	0.60
39:Y:151:A:O5'	39:Y:151:A:H8	1.84	0.60
40:2:146:C:OP2	40:2:147:G:H4'	2.01	0.60
40:2:157:G:H8	40:2:157:G:H5''	1.65	0.60
3:C:1393:TRP:O	3:C:1397:PHE:CB	2.49	0.60
3:C:1080:ASP:O	3:C:1084:VAL:CB	2.50	0.60
7:G:861:ARG:O	7:G:865:HIS:CB	2.50	0.59
3:C:774:LEU:O	3:C:778:LEU:N	2.31	0.59
1:A:1007:ASP:O	1:A:1011:ALA:HB2	2.02	0.59
7:G:379:ALA:O	7:G:383:GLU:CB	2.50	0.59
36:y:27:ASP:CA	36:y:28:GLY:CA	2.80	0.59
25:g:19:LEU:HA	25:g:65:ILE:HA	1.84	0.59
40:2:176:G:H2'	40:2:177:A:O4'	2.02	0.59
13:M:29:ILE:HA	13:M:144:ILE:HA	1.83	0.59
16:P:198:ASP:HA	16:P:202:ALA:HB3	1.84	0.59
3:C:482:ASN:O	3:C:486:SER:N	2.36	0.58
3:C:1084:VAL:O	3:C:1088:ALA:CB	2.52	0.58
41:4:110:G:O5'	41:4:110:G:H8	1.86	0.58
40:2:118:G:O2'	40:2:119:G:H5'	2.04	0.58
39:Y:143:G:C6	40:2:45:C:N3	2.71	0.58
40:2:114:A:O5'	40:2:114:A:H8	1.86	0.58
41:4:33:A:H62	41:4:43:G:H21	1.49	0.58
1:A:77:THR:HA	9:I:17:PRO:HD3	1.84	0.58
2:B:441:PRO:O	2:B:445:ALA:CB	2.51	0.58
6:F:130:GLU:O	6:F:134:ASN:CB	2.52	0.58
7:G:783:SER:O	7:G:787:GLU:CB	2.52	0.58
40:2:146:C:H2'	40:2:148:C:OP1	2.03	0.58
2:B:208:HIS:O	2:B:212:SER:N	2.37	0.57
2:B:474:LEU:HA	2:B:499:GLY:HA3	1.85	0.57
40:2:112:G:C2'	40:2:113:G:H5'	2.33	0.57
40:2:108:G:C5	40:2:109:C:C4	2.91	0.57
40:2:152:G:H2'	40:2:153:A:H8	1.68	0.57
40:2:144:C:C2'	40:2:145:A:H5''	2.30	0.57
8:H:372:ARG:O	8:H:376:ASN:CB	2.52	0.57
1:A:85:LYS:O	1:A:89:LEU:CB	2.53	0.57
1:A:305:ARG:HA	2:B:923:PRO:HG3	1.85	0.57
39:Y:74:G:O6	43:6:31:U:O4	2.22	0.57
41:4:108:C:C2'	41:4:109:G:H5'	2.34	0.57
2:B:428:THR:O	2:B:432:ASP:CB	2.53	0.56
42:5:61:A:H2'	42:5:62:G:H8	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1682:ALA:O	1:A:1686:ASP:CB	2.53	0.56
39:Y:57:C:N4	42:5:42:U:O4	2.36	0.56
40:2:146:C:P	40:2:147:G:H4'	2.45	0.56
40:2:183:G:H2'	40:2:184:C:H6	1.70	0.56
5:E:548:VAL:O	5:E:579:VAL:N	2.26	0.56
6:F:295:LEU:O	6:F:307:TRP:N	2.33	0.56
9:I:116:CYS:O	9:I:120:LEU:CB	2.53	0.56
11:K:300:GLU:O	11:K:304:ILE:CB	2.54	0.56
24:m:16:ARG:HA	24:m:30:THR:HA	1.86	0.56
40:2:143:C:C2	40:2:144:C:C5	2.93	0.56
34:w:624:CYS:CA	34:w:625:LEU:CA	2.83	0.56
40:2:109:C:C6	40:2:109:C:O5'	2.57	0.56
40:2:137:U:H2'	40:2:138:C:H6	1.71	0.56
40:2:138:C:C2	40:2:139:C:C5	2.93	0.56
1:A:950:LEU:O	1:A:954:LYS:CB	2.52	0.56
40:2:106:G:C2	40:2:107:A:C6	2.89	0.56
42:5:69:A:O2'	42:5:70:A:N3	2.39	0.56
42:5:109:C:H2'	42:5:110:A:H8	1.70	0.56
40:2:105:G:N2	40:2:107:A:H5'	2.20	0.56
40:2:141:C:H2'	40:2:142:U:H6	1.71	0.56
40:2:141:C:C2	40:2:142:U:C5	2.94	0.56
41:4:111:C:H2'	41:4:112:A:H8	1.69	0.56
3:C:485:GLN:O	3:C:489:TYR:CB	2.53	0.56
40:2:137:U:C2	40:2:138:C:C5	2.94	0.56
40:2:149:A:H2'	40:2:150:U:H6	1.70	0.56
3:C:1395:GLU:O	3:C:1399:ASP:CB	2.54	0.56
39:Y:65:G:O6	43:6:40:U:O4	2.24	0.56
40:2:142:U:C2	40:2:143:C:C5	2.94	0.56
41:4:108:C:H2'	41:4:109:G:C8	2.41	0.56
6:F:202:PRO:O	6:F:206:ARG:CB	2.55	0.55
7:G:11:MET:O	7:G:13:ALA:N	2.38	0.55
40:2:140:A:C4	40:2:141:C:C5	2.95	0.55
40:2:150:U:C2	40:2:151:C:C5	2.94	0.55
1:A:532:THR:O	1:A:536:LYS:CB	2.54	0.55
5:E:544:SER:HA	5:E:631:VAL:HA	1.87	0.55
40:2:147:G:H2'	40:2:148:C:C6	2.40	0.55
3:C:1332:GLN:O	3:C:1336:PHE:CB	2.54	0.55
40:2:143:C:H2'	40:2:144:C:H6	1.71	0.55
42:5:109:C:H2'	42:5:110:A:C8	2.41	0.55
7:G:419:ALA:O	7:G:423:LEU:CB	2.54	0.55
33:v:717:THR:CA	33:v:718:PRO:CA	2.84	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:106:G:N2	40:2:107:A:H61	1.98	0.55
40:2:142:U:H2'	40:2:143:C:H6	1.71	0.55
40:2:178:A:O2'	40:2:179:C:C5'	2.53	0.55
43:6:78:A:N1	43:6:85:U:OP1	2.39	0.55
1:A:584:HIS:O	1:A:588:LEU:CB	2.55	0.55
40:2:118:G:O2'	40:2:119:G:C5'	2.55	0.55
40:2:140:A:H2'	40:2:141:C:H6	1.71	0.55
40:2:181:G:C4	40:2:182:U:C5	2.95	0.55
41:4:113:U:H6	41:4:113:U:O5'	1.90	0.55
1:A:1725:LEU:O	1:A:1729:ALA:CB	2.55	0.55
2:B:588:ILE:HA	2:B:660:VAL:HA	1.89	0.55
40:2:138:C:H2'	40:2:139:C:H6	1.71	0.55
40:2:183:G:C4	40:2:184:C:C5	2.94	0.55
1:A:2268:LEU:O	3:C:1264:PRO:HG3	2.04	0.54
1:A:947:PRO:HG2	1:A:948:PRO:HD2	1.90	0.54
12:L:330:THR:HA	12:L:346:ARG:HA	1.88	0.54
42:5:17:U:O2	42:5:60:G:N2	2.28	0.54
2:B:448:LYS:O	2:B:452:THR:CB	2.55	0.54
5:E:650:GLN:H	5:E:652:PRO:HD2	1.72	0.54
39:Y:159:U:H3	40:2:31:G:H22	1.55	0.54
40:2:150:U:H2'	40:2:151:C:H6	1.71	0.54
40:2:153:A:O2'	40:2:154:C:H5''	1.95	0.54
41:4:2:G:N1	43:6:73:A:C2	2.75	0.54
42:5:107:G:H3'	42:5:108:G:H8	1.73	0.54
1:A:1729:ALA:O	1:A:1733:ILE:CB	2.56	0.54
3:C:489:TYR:O	3:C:493:LEU:CB	2.55	0.54
6:F:223:PHE:N	6:F:517:LEU:O	2.40	0.54
40:2:181:G:H2'	40:2:182:U:H6	1.70	0.54
2:B:324:ALA:O	2:B:328:ALA:CB	2.56	0.54
40:2:146:C:OP2	40:2:147:G:C4'	2.56	0.54
40:2:149:A:C4	40:2:150:U:C5	2.95	0.54
39:Y:58:G:N2	42:5:41:U:O2	2.28	0.53
40:2:164:C:H5'	40:2:164:C:C6	2.44	0.53
1:A:734:PRO:HB3	7:G:149:LEU:HA	1.89	0.53
40:2:178:A:H2'	40:2:179:C:C6	2.37	0.53
2:B:482:TYR:O	2:B:491:HIS:N	2.40	0.53
1:A:235:MET:O	1:A:239:TYR:CB	2.56	0.53
1:A:1426:ASP:O	1:A:1430:LEU:CB	2.57	0.53
7:G:841:PRO:C	7:G:843:VAL:H	2.17	0.53
3:C:1563:VAL:O	3:C:1648:ARG:N	2.41	0.53
40:2:112:G:N2	40:2:113:G:C4	2.77	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:4:4:U:O2	43:6:71:G:N2	2.33	0.53
2:B:118:PHE:O	2:B:122:LEU:CB	2.56	0.53
3:C:490:ARG:O	3:C:494:GLU:CB	2.57	0.53
42:5:98:C:H2'	42:5:99:C:C6	2.43	0.53
1:A:84:ASP:O	1:A:88:TYR:CB	2.57	0.53
2:B:643:ASP:O	2:B:647:MET:CB	2.57	0.53
8:H:287:LEU:O	8:H:291:ALA:HB3	2.09	0.53
41:4:118:A:OP2	41:4:118:A:H8	1.92	0.53
3:C:1412:THR:O	3:C:1416:LEU:CB	2.57	0.53
1:A:1135:PRO:O	1:A:1139:ARG:N	2.41	0.52
2:B:742:PRO:HG2	2:B:785:ARG:HA	1.90	0.52
8:H:288:ARG:O	8:H:292:ALA:CB	2.56	0.52
7:G:361:VAL:O	7:G:365:ALA:CB	2.55	0.52
1:A:1725:LEU:O	1:A:1729:ALA:HB3	2.09	0.52
5:E:554:PRO:O	5:E:557:LYS:N	2.42	0.52
12:L:425:MET:HA	12:L:431:ILE:HA	1.92	0.52
8:H:268:LEU:C	8:H:269:PRO:CA	2.75	0.52
41:4:2:G:H1	43:6:73:A:H2	1.56	0.52
43:6:52:U:O4	43:6:53:A:N6	2.42	0.52
7:G:875:GLY:O	7:G:879:ALA:CB	2.58	0.52
3:C:1224:LEU:HA	3:C:1236:HIS:HA	1.92	0.52
3:C:1033:GLU:O	3:C:1037:LEU:CB	2.58	0.51
8:H:167:VAL:O	8:H:171:ALA:CB	2.58	0.51
3:C:1389:VAL:O	3:C:1393:TRP:CB	2.57	0.51
24:f:16:ARG:HA	24:f:30:THR:HA	1.92	0.51
39:Y:69:A:O2'	43:6:35:A:N6	2.42	0.51
41:4:143:U:H2'	41:4:144:G:H5''	1.92	0.51
40:2:152:G:H2'	40:2:153:A:C8	2.45	0.51
1:A:1931:THR:O	1:A:1935:ARG:CB	2.59	0.51
5:E:493:PRO:O	5:E:497:GLU:CB	2.59	0.51
7:G:418:ASP:O	7:G:422:MET:CB	2.58	0.51
8:H:355:GLY:H	41:4:58:C:H41	1.56	0.51
1:A:1684:PHE:O	1:A:1688:THR:CB	2.59	0.51
2:B:430:PHE:O	2:B:434:CYS:CB	2.59	0.51
6:F:204:THR:O	6:F:208:SER:CB	2.59	0.51
8:H:292:ALA:O	8:H:296:ALA:CB	2.59	0.51
42:5:99:C:H2'	42:5:100:U:C6	2.46	0.51
6:F:167:HIS:C	6:F:169:GLY:H	2.19	0.51
40:2:108:G:C2'	40:2:109:C:C6	2.65	0.51
42:5:48:A:H2'	42:5:49:A:H8	1.76	0.51
3:C:1221:PHE:HA	3:C:1272:SER:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1432:TRP:O	3:C:1436:SER:CB	2.59	0.51
25:n:19:LEU:HA	25:n:65:ILE:HA	1.93	0.51
6:F:224:CYS:HA	7:G:764:ALA:HB2	1.91	0.50
6:F:304:VAL:N	6:F:318:ILE:O	2.39	0.50
2:B:393:PRO:O	2:B:397:ASP:CB	2.58	0.50
3:C:1665:ASP:HA	3:C:1706:CYS:HA	1.93	0.50
5:E:573:VAL:N	5:E:580:ASN:O	2.41	0.50
15:O:56:MET:O	15:O:83:VAL:N	2.43	0.50
42:5:97:G:H2'	42:5:98:C:H6	1.77	0.50
6:F:370:ILE:HA	6:F:381:THR:HA	1.92	0.50
40:2:112:G:C4	40:2:113:G:C8	2.96	0.50
40:2:177:A:N3	40:2:178:A:N7	2.58	0.50
1:A:564:TYR:O	1:A:569:VAL:N	2.45	0.50
1:A:1584:LYS:O	1:A:1588:SER:CB	2.59	0.50
7:G:142:PHE:O	7:G:146:LYS:CB	2.59	0.50
8:H:367:GLY:O	8:H:371:ILE:N	2.41	0.50
41:4:52:U:O2'	41:4:56:U:OP2	2.22	0.50
1:A:1378:GLU:O	1:A:1382:SER:CB	2.60	0.50
1:A:1833:LEU:O	1:A:1837:ALA:CB	2.60	0.50
10:J:25:VAL:N	10:J:55:PHE:O	2.40	0.50
1:A:880:ARG:O	1:A:884:HIS:CB	2.60	0.50
1:A:150:MET:O	1:A:154:GLU:CB	2.60	0.49
7:G:782:GLU:O	7:G:786:LEU:CB	2.59	0.49
40:2:117:U:H2'	40:2:118:G:C8	2.47	0.49
40:2:113:G:H2'	40:2:114:A:C8	2.47	0.49
41:4:111:C:H2'	41:4:112:A:C8	2.46	0.49
42:5:97:G:H2'	42:5:98:C:C6	2.47	0.49
42:5:17:U:O4	42:5:60:G:O6	2.31	0.49
42:5:25:C:H2'	42:5:26:A:C8	2.47	0.49
2:B:369:PHE:O	2:B:373:ILE:CB	2.60	0.49
2:B:777:GLY:N	2:B:782:GLU:O	2.46	0.49
25:n:39:HIS:HA	25:n:59:SER:HA	1.94	0.49
5:E:554:PRO:HG3	43:6:78:A:H8	1.78	0.49
6:F:254:CYS:HA	6:F:266:HIS:HA	1.95	0.49
6:F:506:ILE:N	6:F:518:TRP:O	2.41	0.49
3:C:778:LEU:HA	3:C:782:PHE:O	2.13	0.49
3:C:872:SER:O	3:C:876:LEU:N	2.45	0.49
1:A:581:ILE:O	1:A:585:VAL:CB	2.61	0.49
43:6:24:A:H4'	43:6:26:U:H1'	1.94	0.49
1:A:2268:LEU:O	3:C:1264:PRO:CD	2.59	0.49
39:Y:69:A:H62	43:6:35:A:H2'	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5:58:U:H2'	42:5:59:G:C8	2.46	0.48
1:A:280:GLU:O	1:A:282:LEU:N	2.46	0.48
40:2:116:A:O5'	40:2:116:A:H8	1.95	0.48
1:A:1007:ASP:O	1:A:1011:ALA:CB	2.60	0.48
2:B:508:LYS:N	2:B:566:THR:O	2.39	0.48
7:G:512:GLU:O	7:G:516:ALA:HB3	2.12	0.48
6:F:431:LYS:HA	6:F:443:THR:HA	1.94	0.48
7:G:449:ALA:O	7:G:453:LEU:CB	2.61	0.48
1:A:2070:LYS:O	3:C:1047:PRO:CG	2.59	0.48
7:G:817:ALA:O	7:G:821:GLU:CB	2.61	0.48
42:5:72:U:H2'	42:5:73:C:H6	1.78	0.48
1:A:883:ARG:O	1:A:887:THR:CB	2.62	0.48
19:h:109:VAL:N	20:i:63:LEU:O	2.42	0.48
41:4:110:G:H2'	41:4:111:C:C6	2.49	0.48
1:A:121:HIS:HA	1:A:482:PHE:HA	1.96	0.48
6:F:178:LEU:O	6:F:182:ASN:CB	2.62	0.48
40:2:108:G:C2'	40:2:109:C:C5	2.92	0.48
41:4:2:G:C6	43:6:73:A:N1	2.82	0.48
1:A:1947:ASN:O	1:A:1951:LYS:CB	2.62	0.47
3:C:612:ILE:N	3:C:647:ARG:O	2.47	0.47
3:C:1037:LEU:O	3:C:1041:LEU:CB	2.62	0.47
39:Y:151:A:H2	40:2:38:A:N1	2.12	0.47
40:2:143:C:H2'	40:2:144:C:C6	2.49	0.47
42:5:23:C:H3'	42:5:24:G:H4'	1.96	0.47
3:C:725:VAL:N	3:C:811:SER:O	2.46	0.47
3:C:1761:TYR:O	3:C:1765:THR:CB	2.62	0.47
1:A:1778:TRP:HA	1:A:1811:ASN:HA	1.96	0.47
2:B:816:VAL:O	2:B:820:PHE:CB	2.63	0.47
3:C:1088:ALA:O	3:C:1092:MET:CB	2.63	0.47
40:2:142:U:H2'	40:2:143:C:C6	2.49	0.47
42:5:98:C:H2'	42:5:99:C:H6	1.80	0.47
42:5:110:A:H2'	42:5:111:A:C8	2.49	0.47
1:A:1568:THR:O	1:A:1572:SER:CB	2.62	0.47
3:C:1964:PRO:HA	3:C:2054:PRO:HG3	1.96	0.47
8:H:135:TYR:O	8:H:139:VAL:CB	2.62	0.47
3:C:1831:LEU:O	3:C:1835:SER:CB	2.62	0.47
7:G:680:LYS:HA	7:G:934:ALA:HB1	1.97	0.47
25:n:17:ILE:HA	25:n:68:PHE:HA	1.97	0.47
41:4:109:G:H2'	41:4:110:G:C8	2.50	0.47
1:A:117:PRO:HA	1:A:486:LYS:HA	1.96	0.47
2:B:261:ASP:O	2:B:265:LEU:CB	2.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:291:ALA:O	8:H:295:VAL:CB	2.63	0.47
7:G:841:PRO:C	7:G:843:VAL:N	2.73	0.47
40:2:117:U:H2'	40:2:118:G:H8	1.79	0.47
1:A:981:PHE:C	1:A:983:LYS:H	2.23	0.46
24:f:18:ARG:N	24:f:81:THR:O	2.39	0.46
24:m:80:MET:O	25:n:59:SER:N	2.44	0.46
1:A:1470:TYR:O	1:A:1474:MET:CB	2.63	0.46
3:C:525:ILE:HA	3:C:531:ILE:HA	1.98	0.46
5:E:554:PRO:HG3	43:6:78:A:C8	2.50	0.46
34:w:916:ASN:CA	34:w:917:PRO:CA	2.93	0.46
40:2:138:C:H2'	40:2:139:C:C6	2.50	0.46
41:4:11:A:H2'	41:4:12:G:C8	2.50	0.46
3:C:1620:LEU:N	3:C:1645:VAL:O	2.48	0.46
7:G:309:PRO:HB2	7:G:310:PRO:HD3	1.97	0.46
40:2:154:C:O5'	40:2:154:C:H6	1.97	0.46
6:F:325:VAL:HA	6:F:341:CYS:HA	1.97	0.46
7:G:309:PRO:O	7:G:313:ILE:CB	2.63	0.46
40:2:137:U:H2'	40:2:138:C:C6	2.50	0.46
40:2:149:A:H2'	40:2:150:U:C6	2.50	0.46
1:A:1833:LEU:O	1:A:1837:ALA:HB3	2.14	0.46
8:H:253:GLY:HA3	8:H:273:TYR:H	1.81	0.46
40:2:140:A:H2'	40:2:141:C:C6	2.50	0.46
40:2:150:U:H2'	40:2:151:C:C6	2.50	0.46
40:2:181:G:H2'	40:2:182:U:C6	2.50	0.46
1:A:88:TYR:O	1:A:92:LEU:CB	2.64	0.46
2:B:833:PHE:N	2:B:900:VAL:O	2.41	0.46
40:2:180:G:H2'	40:2:181:G:H8	1.81	0.46
1:A:2130:GLY:HA3	1:A:2142:ILE:HA	1.98	0.46
7:G:824:PRO:C	7:G:826:ARG:H	2.24	0.46
14:N:105:GLN:O	14:N:110:MET:N	2.34	0.46
43:6:40:U:H2'	43:6:41:A:C8	2.51	0.46
2:B:508:LYS:HA	2:B:524:ILE:HA	1.98	0.46
5:E:563:ASN:O	5:E:567:LEU:N	2.48	0.46
8:H:167:VAL:O	8:H:171:ALA:HB3	2.16	0.46
43:6:66:C:H2'	43:6:67:G:C8	2.50	0.46
7:G:512:GLU:O	7:G:516:ALA:CB	2.63	0.46
25:g:16:THR:HA	25:g:26:HIS:HA	1.98	0.46
40:2:112:G:N2	40:2:113:G:C5	2.82	0.46
40:2:112:G:C6	40:2:113:G:O6	2.69	0.46
6:F:421:ILE:N	6:F:433:TRP:O	2.49	0.45
8:H:39:THR:O	8:H:43:LEU:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:i:7:PRO:HB3	20:i:38:GLY:HA2	1.98	0.45
25:n:16:THR:HA	25:n:26:HIS:HA	1.98	0.45
40:2:183:G:H2'	40:2:184:C:C6	2.50	0.45
42:5:61:A:H2'	42:5:62:G:C8	2.50	0.45
6:F:255:LYS:N	6:F:265:LEU:O	2.49	0.45
40:2:178:A:C2'	40:2:179:C:O5'	2.64	0.45
1:A:463:PRO:O	42:5:24:G:N2	2.47	0.45
1:A:798:GLY:N	1:A:799:PRO:HD3	2.32	0.45
40:2:3:C:H2'	40:2:4:G:C8	2.51	0.45
40:2:177:A:H2	40:2:178:A:N6	2.09	0.45
7:G:912:TRP:O	7:G:916:SER:CB	2.64	0.45
40:2:148:C:H2'	40:2:149:A:H8	1.82	0.45
40:2:151:C:H2'	40:2:152:G:H8	1.81	0.45
3:C:912:ASN:HA	3:C:978:ASN:HA	1.98	0.45
40:2:153:A:HO2'	40:2:154:C:C5'	2.15	0.45
40:2:179:C:H2'	40:2:180:G:H8	1.81	0.45
1:A:598:LEU:O	1:A:602:ILE:CB	2.64	0.45
17:Q:9:PRO:HB2	17:Q:22:ASP:HA	1.98	0.45
2:B:324:ALA:O	2:B:328:ALA:HB2	2.17	0.45
40:2:112:G:C2	40:2:113:G:C4	3.04	0.45
40:2:182:U:H2'	40:2:183:G:H8	1.81	0.45
42:5:10:U:H2'	42:5:11:U:C6	2.52	0.45
6:F:234:SER:N	6:F:248:ALA:O	2.49	0.45
40:2:119:G:H2'	40:2:120:A:H8	1.82	0.45
2:B:715:GLY:O	2:B:719:GLN:CB	2.64	0.44
40:2:116:A:O5'	40:2:116:A:C8	2.70	0.44
43:6:91:A:H2'	43:6:92:A:H8	1.82	0.44
3:C:2067:VAL:HA	3:C:2079:ILE:HA	2.00	0.44
40:2:141:C:H2'	40:2:142:U:C6	2.50	0.44
1:A:1809:ILE:O	1:A:1818:PHE:N	2.49	0.44
3:C:1522:PRO:HG2	12:L:343:LYS:HA	1.99	0.44
6:F:367:VAL:HA	6:F:383:GLY:HA2	2.00	0.44
7:G:340:PRO:HB2	7:G:368:HIS:O	2.18	0.44
1:A:897:GLU:O	1:A:908:VAL:N	2.48	0.44
3:C:785:HIS:N	3:C:810:VAL:O	2.51	0.44
41:4:115:G:H2'	41:4:116:G:C8	2.52	0.44
40:2:139:C:H2'	40:2:140:A:H8	1.81	0.44
43:6:89:U:H2'	43:6:90:G:C8	2.53	0.44
43:6:90:G:H2'	43:6:91:A:H8	1.82	0.44
5:E:594:PHE:O	5:E:598:MET:CB	2.66	0.44
43:6:91:A:H2'	43:6:92:A:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:118:G:O6	40:2:140:A:N6	2.51	0.44
41:4:91:A:H2'	41:4:92:C:C6	2.53	0.44
1:A:1878:ASP:HA	7:G:282:PRO:HA	1.99	0.43
41:4:118:A:OP2	41:4:118:A:C8	2.70	0.43
2:B:215:VAL:O	2:B:219:LEU:CB	2.66	0.43
8:H:284:PRO:O	8:H:288:ARG:N	2.48	0.43
40:2:117:U:C2'	40:2:118:G:H5'	2.48	0.43
42:5:72:U:H2'	42:5:73:C:C6	2.53	0.43
8:H:355:GLY:N	41:4:58:C:H41	2.16	0.43
24:f:15:TYR:O	24:f:31:PHE:N	2.40	0.43
39:Y:71:C:H2'	39:Y:72:A:H8	1.83	0.43
43:6:40:U:H2'	43:6:41:A:H8	1.83	0.43
3:C:1186:LEU:HA	3:C:1204:ILE:HA	2.00	0.43
40:2:108:G:C4	40:2:109:C:C4	3.07	0.43
42:5:74:U:H2'	42:5:75:G:C8	2.52	0.43
5:E:513:GLU:O	5:E:517:ALA:CB	2.64	0.43
8:H:358:ARG:O	8:H:362:MET:CB	2.66	0.43
12:L:499:ILE:N	12:L:511:TRP:O	2.43	0.43
39:Y:70:G:H22	43:6:36:A:H2	1.66	0.43
6:F:279:VAL:N	6:F:296:ALA:O	2.51	0.43
8:H:314:GLY:O	8:H:318:TYR:CB	2.67	0.43
42:5:31:U:H2'	42:5:32:C:C6	2.54	0.43
1:A:440:PRO:HB2	1:A:442:LYS:H	1.83	0.43
1:A:1195:ARG:O	1:A:1229:PHE:N	2.46	0.43
2:B:642:HIS:O	2:B:646:LYS:CB	2.67	0.43
40:2:144:C:C4	40:2:146:C:OP1	2.72	0.43
40:2:153:A:H2'	40:2:154:C:H6	1.84	0.43
40:2:157:G:H5''	40:2:157:G:C8	2.50	0.43
1:A:679:SER:O	1:A:683:LEU:CB	2.67	0.43
1:A:1761:PRO:C	1:A:1763:LEU:H	2.27	0.43
3:C:548:VAL:O	3:C:552:VAL:CB	2.67	0.43
40:2:178:A:H2'	40:2:179:C:O5'	2.18	0.43
43:6:89:U:H2'	43:6:90:G:H8	1.84	0.43
3:C:783:ALA:HB3	3:C:809:LEU:HA	2.01	0.42
6:F:380:GLY:HA2	6:F:390:VAL:HA	2.00	0.42
12:L:488:ILE:H	12:L:503:SER:HA	1.84	0.42
2:B:396:LEU:O	2:B:400:GLY:N	2.51	0.42
40:2:108:G:C5	40:2:109:C:N4	2.87	0.42
40:2:114:A:O5'	40:2:114:A:C8	2.70	0.42
40:2:118:G:C2'	40:2:119:G:O5'	2.67	0.42
12:L:146:ALA:O	12:L:150:ALA:CB	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:TYR:O	1:A:584:HIS:CB	2.67	0.42
3:C:488:LEU:O	3:C:492:ALA:CB	2.66	0.42
3:C:1390:TYR:O	3:C:1394:TYR:CB	2.67	0.42
43:6:92:A:H2'	43:6:93:G:H8	1.83	0.42
7:G:448:ASN:O	7:G:452:VAL:CB	2.68	0.42
12:L:331:ILE:N	12:L:345:PHE:O	2.44	0.42
23:W:80:ALA:CA	23:W:81:PRO:CA	2.98	0.42
40:2:98:G:H5'	40:2:104:U:OP2	2.19	0.42
1:A:926:LEU:O	1:A:930:ALA:CB	2.67	0.42
40:2:155:C:H2'	40:2:156:U:H5''	2.02	0.42
3:C:1386:ALA:O	3:C:1390:TYR:CB	2.68	0.42
41:4:90:G:H2'	41:4:91:A:C8	2.55	0.42
2:B:227:LEU:O	2:B:256:CYS:N	2.46	0.42
40:2:157:G:H2'	40:2:158:G:O4'	2.19	0.42
41:4:107:U:H2'	41:4:108:C:H6	1.85	0.42
12:L:241:TRP:HA	12:L:248:ILE:HA	2.01	0.42
40:2:3:C:H2'	40:2:4:G:H8	1.84	0.42
2:B:828:MET:HA	2:B:906:ILE:HA	2.01	0.42
41:4:14:G:H2'	41:4:15:G:C8	2.55	0.42
43:6:92:A:H2'	43:6:93:G:C8	2.54	0.42
1:A:2130:GLY:O	1:A:2173:GLU:N	2.53	0.41
42:5:75:G:H2'	42:5:76:A:C8	2.55	0.41
1:A:577:GLY:O	1:A:581:ILE:CB	2.68	0.41
3:C:1609:LEU:O	3:C:1613:LEU:CB	2.68	0.41
22:k:22:ASN:N	22:k:66:SER:O	2.49	0.41
42:5:31:U:H2'	42:5:32:C:H6	1.85	0.41
42:5:59:G:C2	42:5:60:G:C8	3.08	0.41
2:B:166:CYS:C	2:B:168:THR:H	2.29	0.41
3:C:823:ALA:O	3:C:857:GLY:N	2.50	0.41
6:F:257:TRP:N	6:F:262:CYS:O	2.43	0.41
1:A:639:PHE:O	42:5:28:A:O2'	2.35	0.41
40:2:171:U:H2'	40:2:172:C:O4'	2.21	0.41
1:A:1696:PRO:HB2	1:A:1699:THR:O	2.21	0.41
3:C:1915:ILE:O	3:C:1919:ALA:CB	2.69	0.41
41:4:22:C:H2'	41:4:23:G:C8	2.56	0.41
42:5:71:C:H2'	42:5:72:U:C6	2.56	0.41
14:N:80:TYR:O	14:N:89:VAL:N	2.47	0.41
41:4:55:U:H2'	41:4:56:U:C6	2.56	0.41
42:5:9:G:O2'	42:5:10:U:O5'	2.37	0.41
3:C:1058:LYS:O	3:C:1062:LEU:CB	2.69	0.41
39:Y:54:G:O2'	39:Y:55:A:H5''	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:117:U:H6	40:2:117:U:H5'	1.85	0.41
42:5:5:U:H2'	42:5:6:C:C6	2.56	0.41
42:5:38:C:N4	42:5:39:C:N3	2.68	0.41
2:B:121:ASP:O	2:B:125:ASN:CB	2.69	0.41
3:C:1431:LYS:O	3:C:1435:LEU:CB	2.69	0.41
7:G:774:PRO:C	7:G:776:ASN:H	2.29	0.41
40:2:103:U:C3'	40:2:104:U:H5'	2.51	0.41
40:2:107:A:H2'	40:2:108:G:C8	2.56	0.41
41:4:72:U:O2'	41:4:73:U:H5''	2.21	0.41
42:5:100:U:H2'	42:5:101:U:C6	2.57	0.41
43:6:43:A:H3'	43:6:44:G:H8	1.86	0.41
6:F:116:GLU:O	6:F:118:ILE:N	2.52	0.40
7:G:743:THR:N	7:G:744:PRO:HD3	2.36	0.40
12:L:240:VAL:O	12:L:249:ARG:N	2.52	0.40
25:g:87:VAL:O	25:g:91:LYS:CB	2.69	0.40
5:E:470:PRO:O	5:E:472:PRO:HD3	2.21	0.40
12:L:217:VAL:HA	12:L:233:SER:HA	2.04	0.40
22:k:18:SER:N	22:k:71:GLU:O	2.51	0.40
40:2:149:A:C6	40:2:150:U:C4	3.09	0.40
43:6:66:C:H2'	43:6:67:G:H8	1.85	0.40
1:A:454:TYR:O	1:A:458:ALA:HB2	2.22	0.40
1:A:739:ILE:O	1:A:743:VAL:CB	2.69	0.40
5:E:471:PRO:O	5:E:473:GLU:N	2.54	0.40
25:g:89:SER:O	25:g:93:GLU:CB	2.69	0.40
40:2:183:G:C6	40:2:184:C:N4	2.89	0.40
41:4:14:G:H2'	41:4:15:G:H8	1.87	0.40
5:E:669:TYR:HA	6:F:483:PRO:HG3	2.04	0.40
22:k:6:PRO:HB2	22:k:7:PRO:HD3	2.02	0.40
24:m:18:ARG:N	24:m:81:THR:O	2.40	0.40
41:4:110:G:O5'	41:4:110:G:C8	2.70	0.40

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	2184/2335 (94%)	1969 (90%)	208 (10%)	7 (0%)	36	71
2	B	842/972 (87%)	772 (92%)	70 (8%)	0	100	100
3	C	1689/2136 (79%)	1624 (96%)	63 (4%)	2 (0%)	48	83
5	E	215/683 (32%)	174 (81%)	37 (17%)	4 (2%)	6	32
6	F	416/521 (80%)	376 (90%)	39 (9%)	1 (0%)	43	77
7	G	798/941 (85%)	700 (88%)	94 (12%)	4 (0%)	24	63
8	H	411/499 (82%)	359 (87%)	49 (12%)	3 (1%)	18	55
9	I	174/312 (56%)	158 (91%)	15 (9%)	1 (1%)	21	58
10	J	133/142 (94%)	126 (95%)	7 (5%)	0	100	100
11	K	43/439 (10%)	42 (98%)	1 (2%)	0	100	100
12	L	451/513 (88%)	437 (97%)	14 (3%)	0	100	100
13	M	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
14	N	54/199 (27%)	47 (87%)	7 (13%)	0	100	100
15	O	124/128 (97%)	119 (96%)	5 (4%)	0	100	100
16	P	87/800 (11%)	79 (91%)	8 (9%)	0	100	100
17	Q	73/376 (19%)	70 (96%)	3 (4%)	0	100	100
18	R	14/557 (2%)	13 (93%)	1 (7%)	0	100	100
19	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
19	h	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
20	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
20	i	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
21	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
21	j	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
22	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100
22	k	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
23	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
23	l	69/126 (55%)	69 (100%)	0	0	100	100
24	f	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
24	m	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
25	g	89/119 (75%)	84 (94%)	5 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	n	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
All	All	8883/13444 (66%)	8186 (92%)	675 (8%)	22 (0%)	44	77

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	957	VAL
7	G	842	HIS
7	G	373	VAL
8	H	434	VAL
1	A	1015	VAL
3	C	531	ILE
9	I	157	VAL
1	A	1092	ILE
5	E	478	ILE
5	E	490	VAL
1	A	569	VAL
1	A	945	THR
5	E	533	LEU
7	G	309	PRO
7	G	929	ILE
1	A	948	PRO
8	H	271	THR
1	A	947	PRO
5	E	537	ILE
1	A	386	PRO
8	H	269	PRO
6	F	459	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/2108 (6%)	125 (100%)	0	100	100
2	B	49/866 (6%)	49 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	77/1908 (4%)	77 (100%)	0	100	100
5	E	8/599 (1%)	8 (100%)	0	100	100
6	F	17/441 (4%)	17 (100%)	0	100	100
7	G	35/792 (4%)	35 (100%)	0	100	100
8	H	15/424 (4%)	15 (100%)	0	100	100
9	I	6/293 (2%)	6 (100%)	0	100	100
10	J	5/130 (4%)	5 (100%)	0	100	100
12	L	11/450 (2%)	11 (100%)	0	100	100
13	M	10/148 (7%)	10 (100%)	0	100	100
15	O	6/111 (5%)	6 (100%)	0	100	100
16	P	3/681 (0%)	3 (100%)	0	100	100
17	Q	2/333 (1%)	2 (100%)	0	100	100
19	a	3/110 (3%)	3 (100%)	0	100	100
19	h	2/110 (2%)	2 (100%)	0	100	100
20	b	4/74 (5%)	4 (100%)	0	100	100
20	i	4/74 (5%)	4 (100%)	0	100	100
21	c	1/84 (1%)	1 (100%)	0	100	100
21	j	1/84 (1%)	1 (100%)	0	100	100
22	d	3/66 (4%)	3 (100%)	0	100	100
22	k	3/66 (4%)	3 (100%)	0	100	100
23	e	3/101 (3%)	3 (100%)	0	100	100
23	l	2/101 (2%)	2 (100%)	0	100	100
24	f	2/177 (1%)	2 (100%)	0	100	100
25	g	4/101 (4%)	4 (100%)	0	100	100
25	n	3/101 (3%)	3 (100%)	0	100	100
All	All	404/10533 (4%)	404 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	Y	44/324 (13%)	14 (31%)	0
40	2	96/188 (51%)	18 (18%)	3 (3%)
41	4	134/145 (92%)	41 (30%)	4 (2%)
42	5	113/116 (97%)	36 (31%)	2 (1%)
43	6	88/106 (83%)	22 (25%)	3 (3%)
All	All	475/879 (54%)	131 (27%)	12 (2%)

All (131) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
39	Y	50	C
39	Y	51	U
39	Y	52	C
39	Y	53	C
39	Y	54	G
39	Y	55	A
39	Y	56	A
39	Y	57	C
39	Y	61	A
39	Y	70	G
39	Y	71	C
39	Y	72	A
39	Y	156	U
39	Y	160	G
40	2	111	G
40	2	112	G
40	2	113	G
40	2	116	A
40	2	117	U
40	2	118	G
40	2	145	A
40	2	146	C
40	2	147	G
40	2	154	C
40	2	156	U
40	2	157	G
40	2	164	C
40	2	165	A
40	2	168	A
40	2	169	C
40	2	177	A
40	2	178	A
41	4	19	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	4	20	A
41	4	25	A
41	4	26	G
41	4	36	U
41	4	41	C
41	4	44	A
41	4	45	G
41	4	52	U
41	4	53	U
41	4	54	A
41	4	55	U
41	4	56	U
41	4	58	C
41	4	69	C
41	4	71	U
41	4	73	U
41	4	76	C
41	4	78	A
41	4	80	A
41	4	81	C
41	4	82	C
41	4	84	C
41	4	85	G
41	4	90	G
41	4	100	A
41	4	103	A
41	4	109	G
41	4	114	U
41	4	115	G
41	4	118	A
41	4	119	A
41	4	120	U
41	4	121	U
41	4	122	U
41	4	124	U
41	4	125	G
41	4	126	A
41	4	127	C
41	4	144	G
41	4	145	G
42	5	8	G
42	5	10	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	5	20	G
42	5	21	A
42	5	22	U
42	5	23	C
42	5	24	G
42	5	25	C
42	5	26	A
42	5	27	U
42	5	34	U
42	5	36	C
42	5	38	C
42	5	39	C
42	5	41	U
42	5	42	U
42	5	45	C
42	5	48	A
42	5	52	U
42	5	53	U
42	5	54	U
42	5	57	G
42	5	68	C
42	5	69	A
42	5	70	A
42	5	79	C
42	5	80	U
42	5	83	A
42	5	88	A
42	5	90	U
42	5	92	U
42	5	93	U
42	5	94	U
42	5	95	G
42	5	96	A
42	5	108	G
43	6	6	C
43	6	7	G
43	6	9	U
43	6	21	U
43	6	22	A
43	6	26	U
43	6	28	A
43	6	29	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	6	33	G
43	6	35	A
43	6	38	G
43	6	40	U
43	6	43	A
43	6	44	G
43	6	45	A
43	6	47	A
43	6	48	A
43	6	49	G
43	6	50	A
43	6	70	A
43	6	77	C
43	6	78	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	2	156	U
40	2	164	C
40	2	168	A
41	4	43	G
41	4	55	U
41	4	99	C
41	4	114	U
42	5	78	U
42	5	94	U
43	6	28	A
43	6	49	G
43	6	77	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	L	1
3	C	1
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	39:ASN	C	40:THR	N	8.39
1	C	1296:PRO	C	1297:PRO	N	3.45
1	H	268:LEU	C	269:PRO	N	1.71

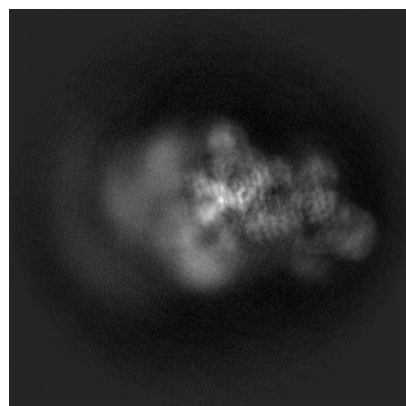
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3766. These allow visual inspection of the internal detail of the map and identification of artifacts.

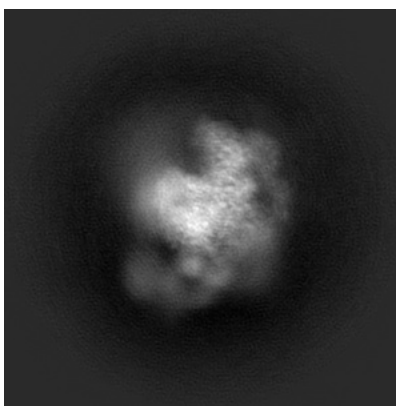
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

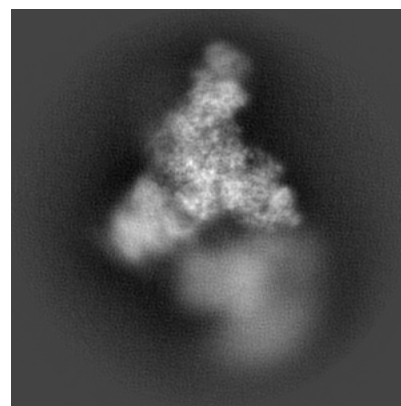
6.1.1 Primary map



X

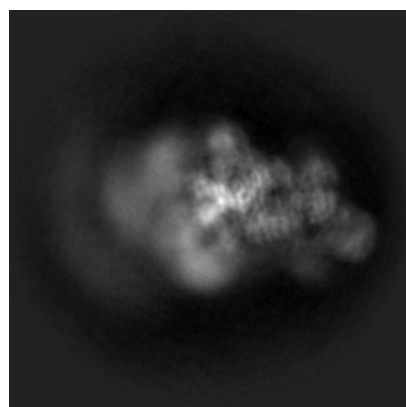


Y

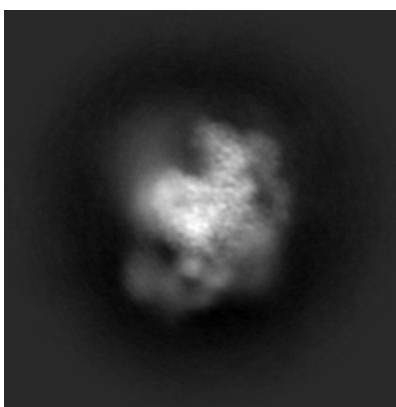


Z

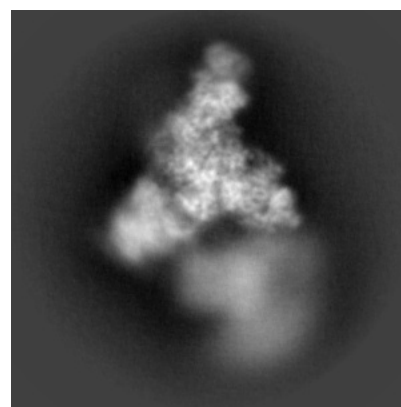
6.1.2 Raw map



X



Y

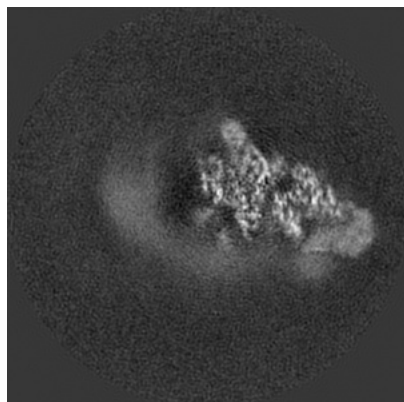


Z

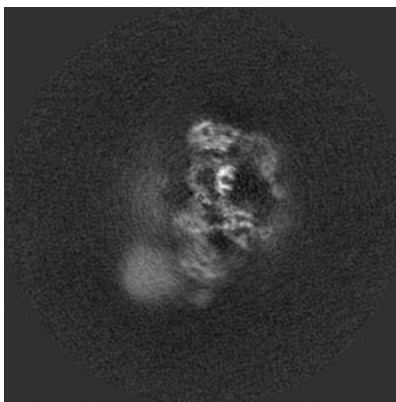
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

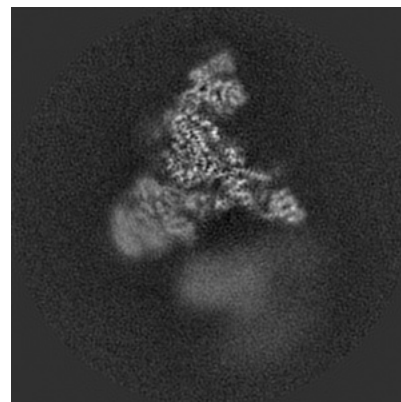
6.2.1 Primary map



X Index: 216

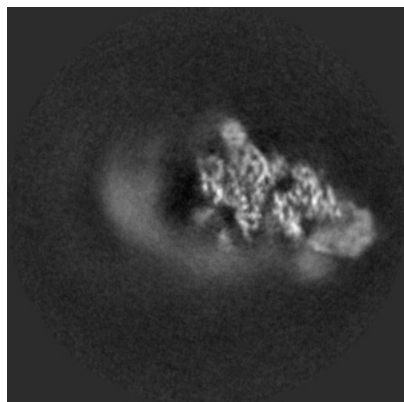


Y Index: 216

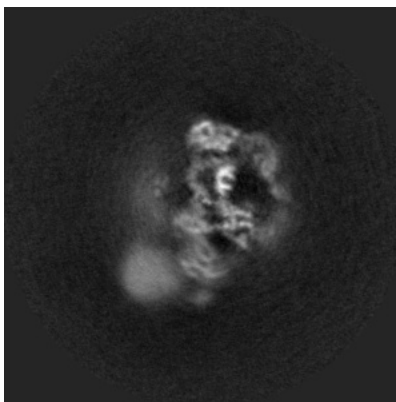


Z Index: 216

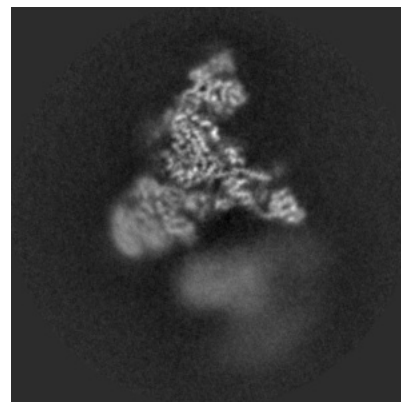
6.2.2 Raw map



X Index: 216



Y Index: 216

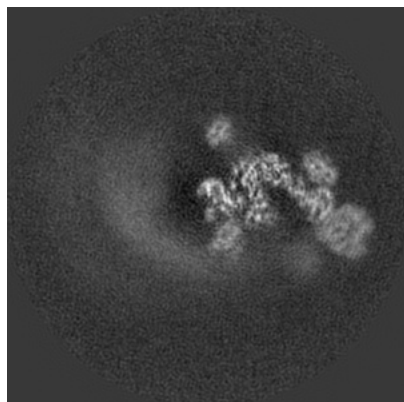


Z Index: 216

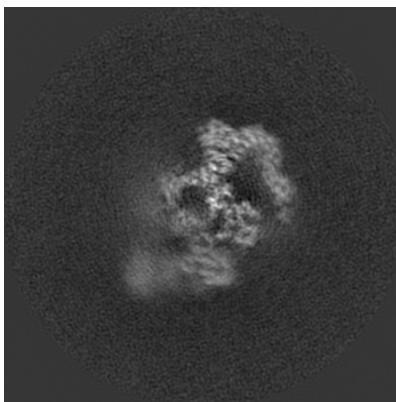
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

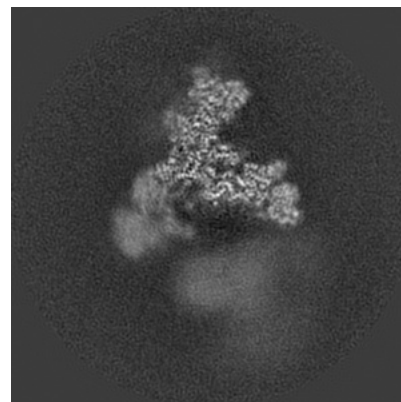
6.3.1 Primary map



X Index: 237

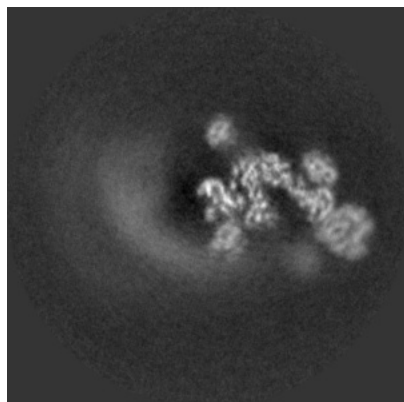


Y Index: 229

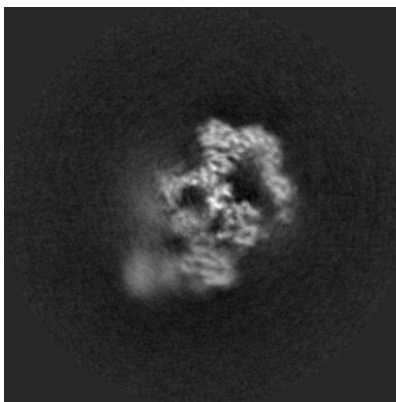


Z Index: 225

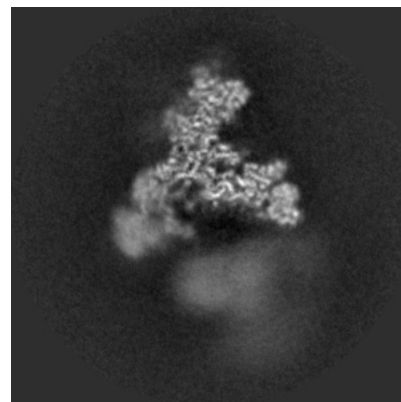
6.3.2 Raw map



X Index: 237



Y Index: 229

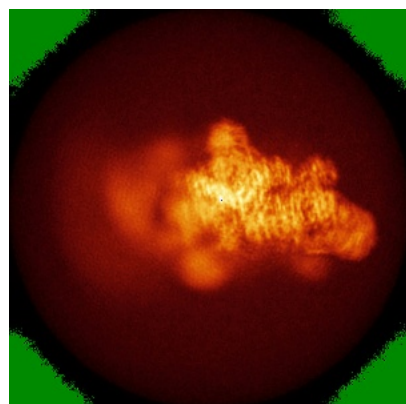


Z Index: 225

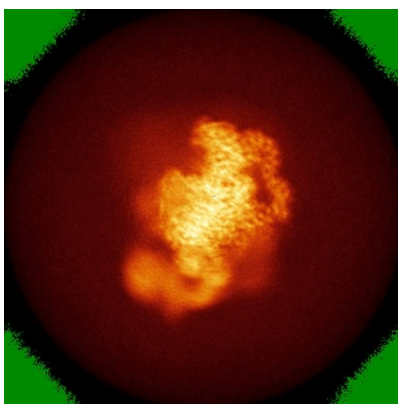
The images above show the largest variance slices of the map in three orthogonal directions.

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

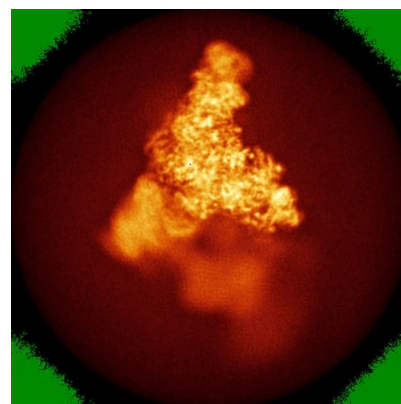
6.4.1 Primary map



X

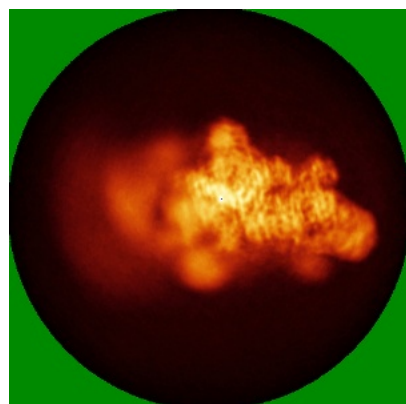


Y

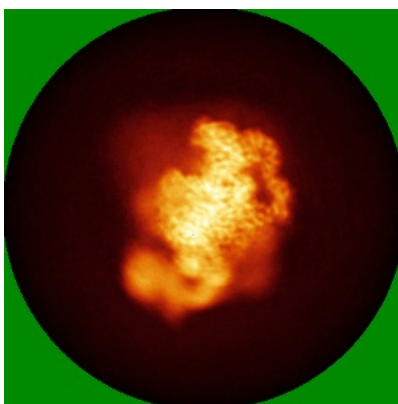


Z

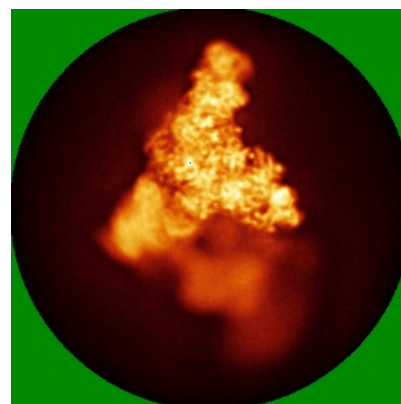
6.4.2 Raw map



X



Y

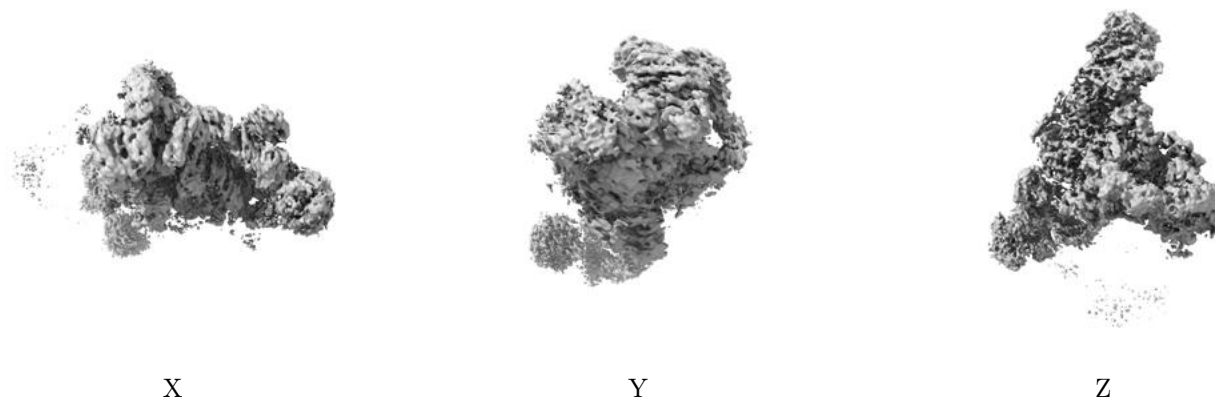


Z

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.

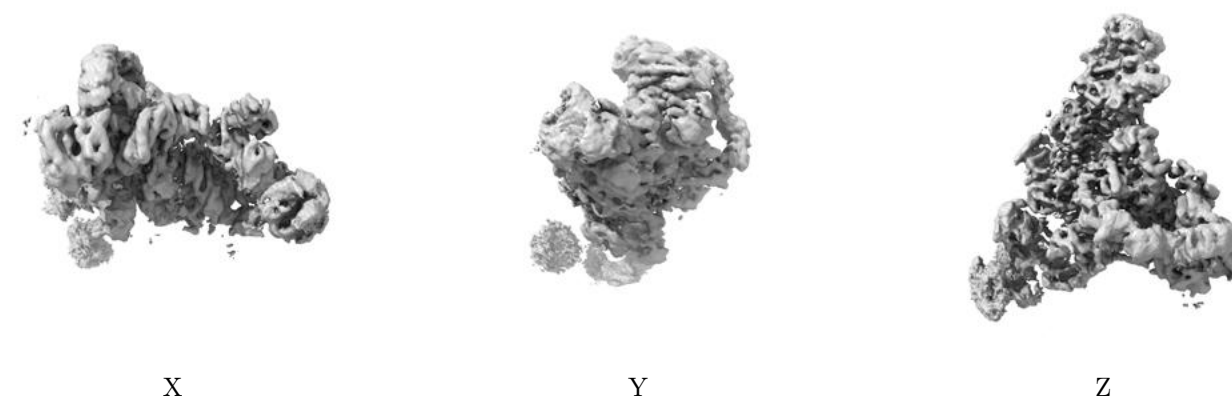
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

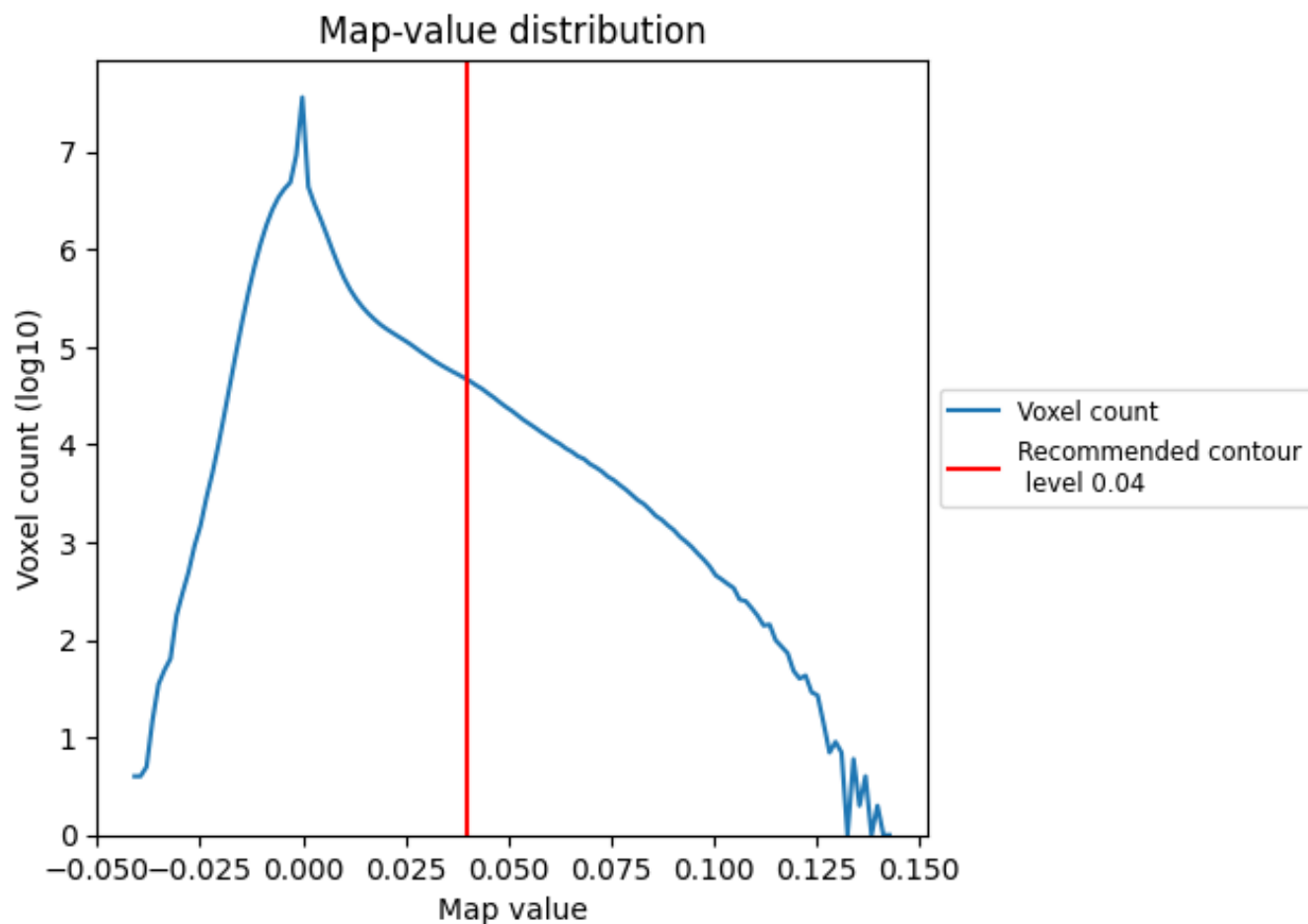
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

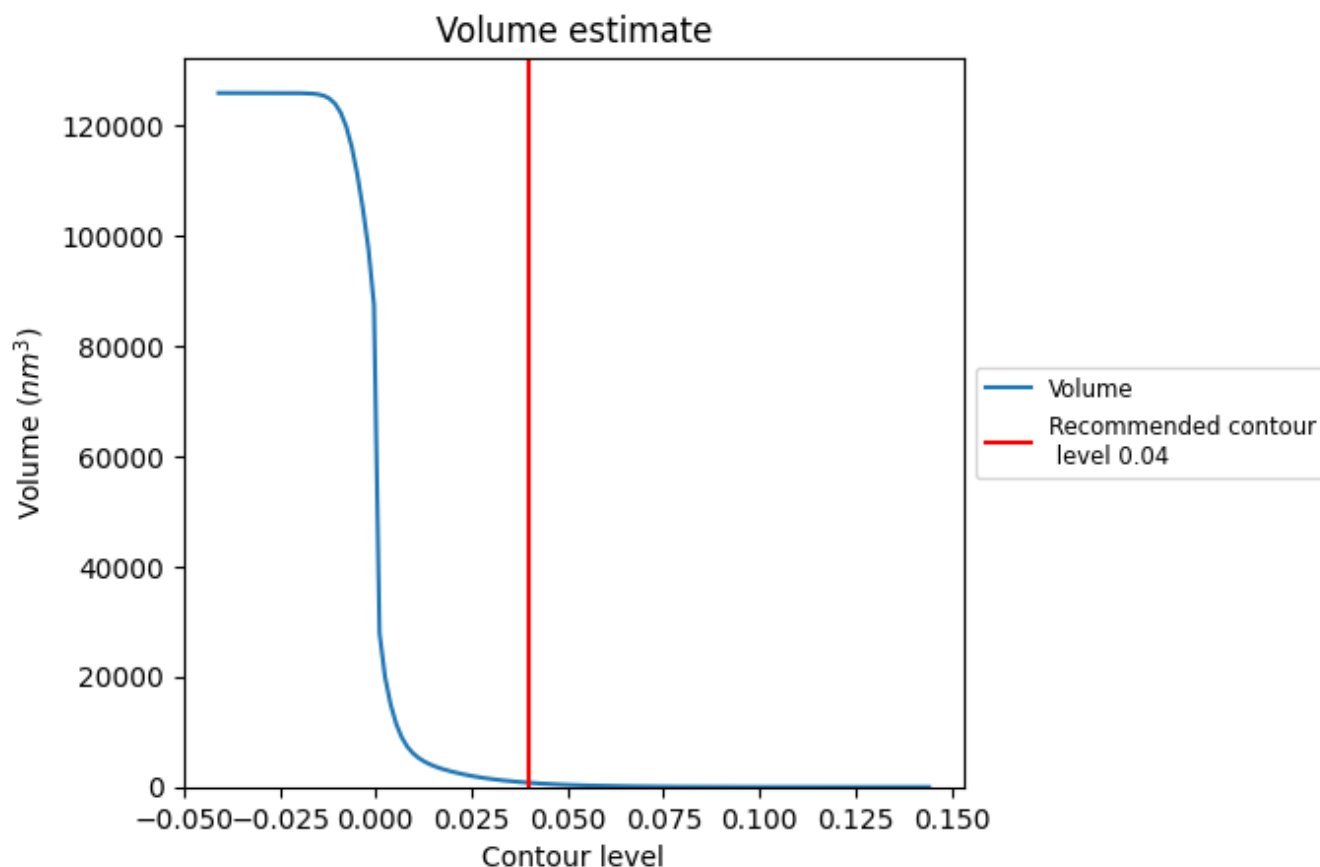
This section contains the results of statistical analysis of the map.

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.

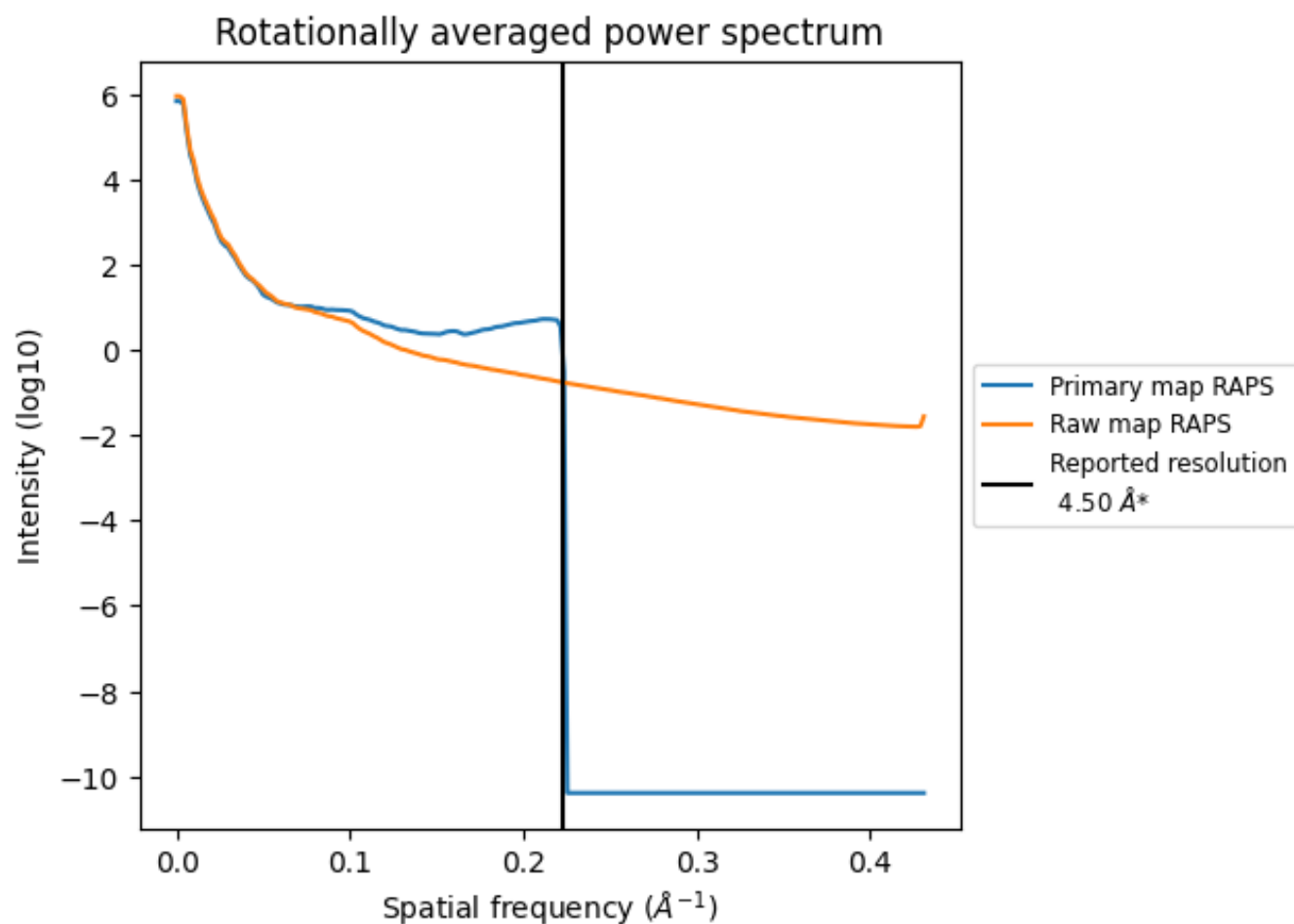
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 761 nm^3 ; this corresponds to an approximate mass of 688 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

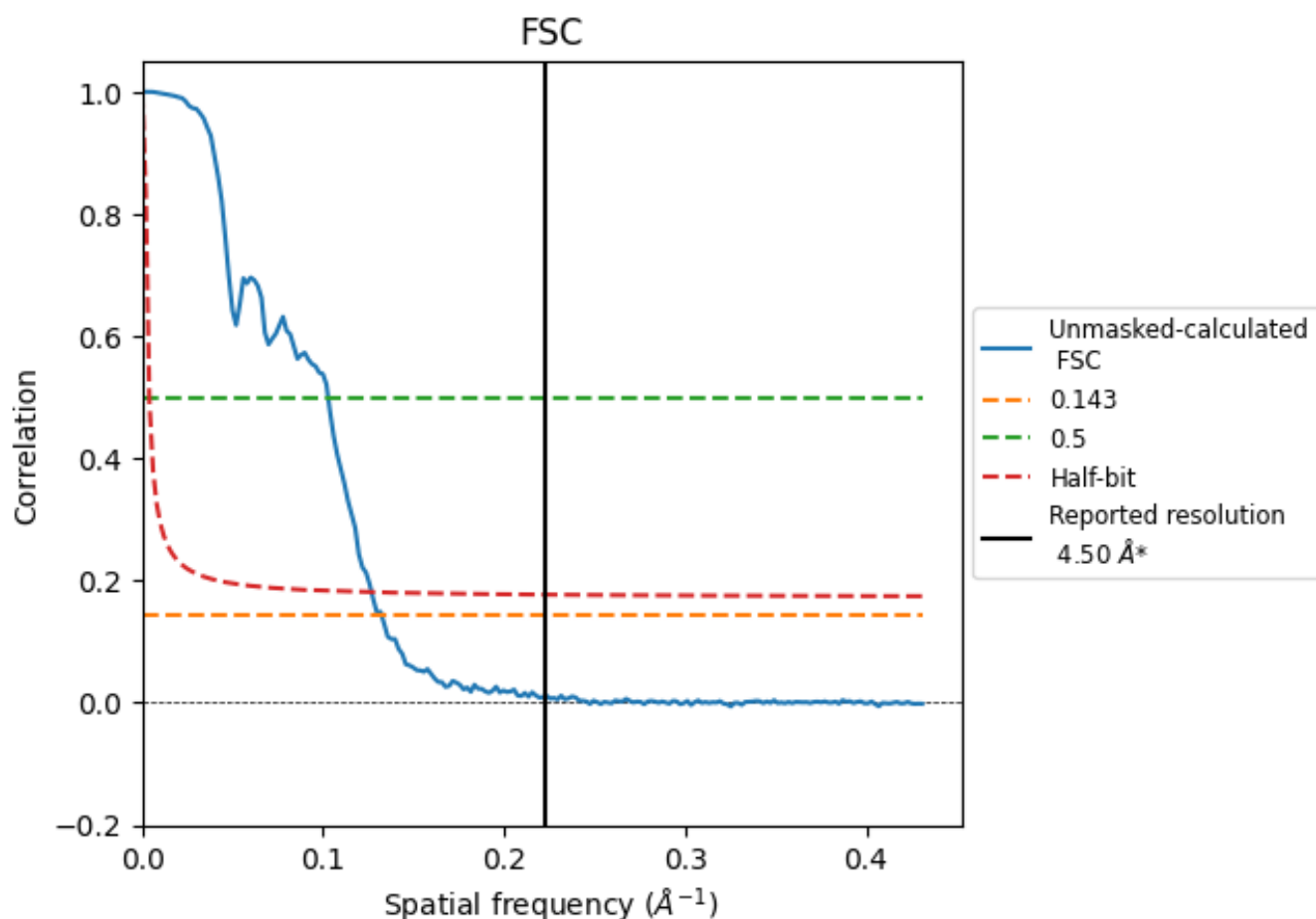


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

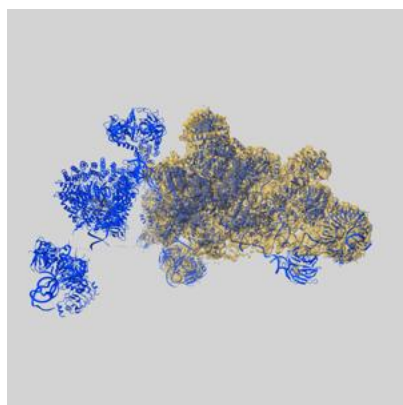
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.56	9.74	7.89

*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 7.56 differs from the reported value 4.5 by more than 10 %

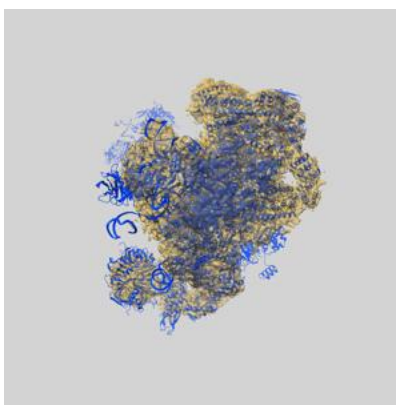
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3766 and PDB model 5O9Z. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

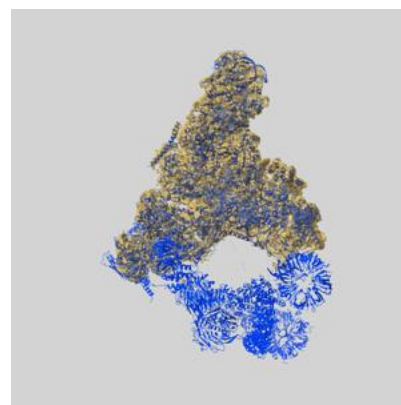
9.1 Map-model overlay [i](#)



X



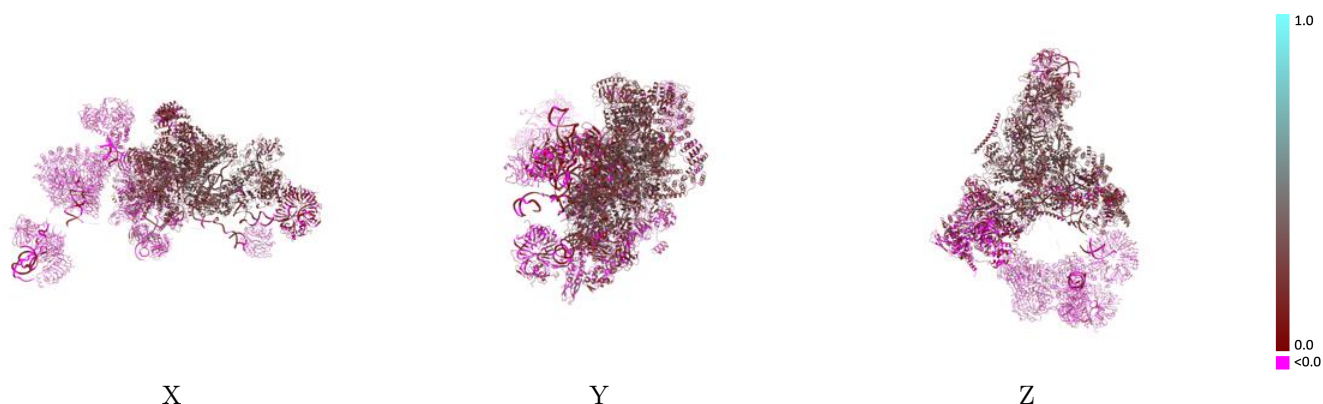
Y



Z

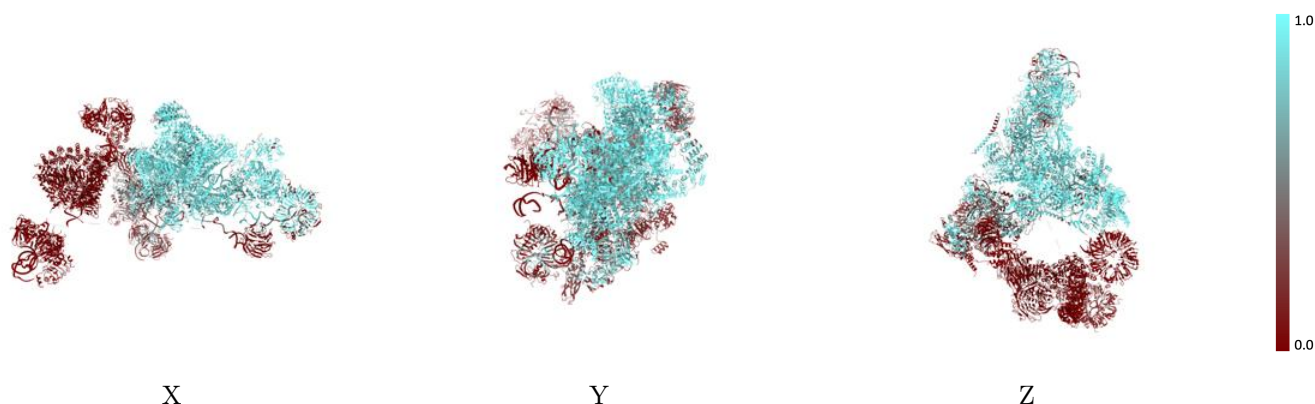
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



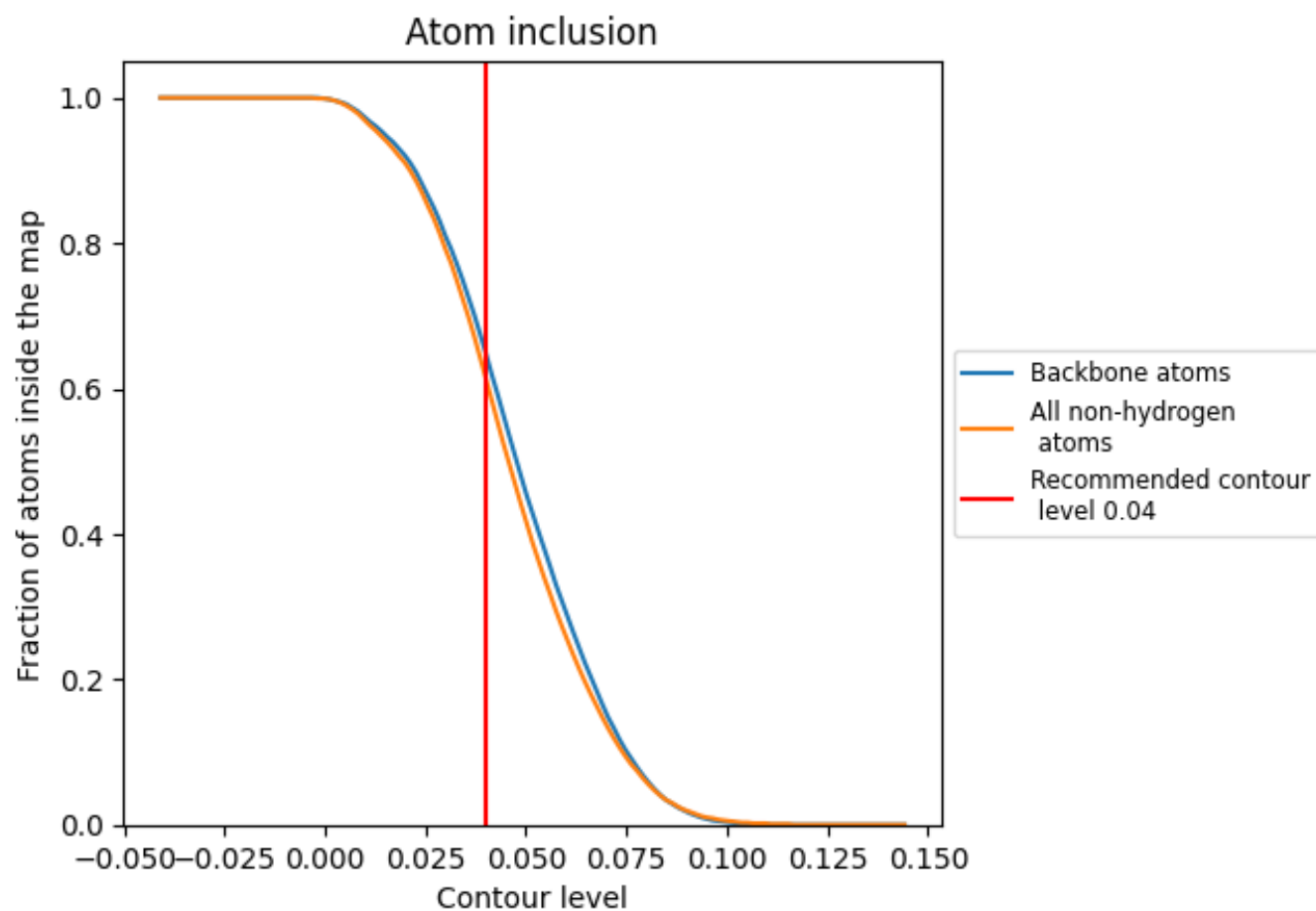
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6150	 0.1700
1	 0.0000	 -0.0190
2	 0.0030	 0.0020
4	 0.5470	 0.1530
5	 0.7510	 0.1460
6	 0.5120	 0.1590
A	 0.8730	 0.2930
B	 0.9020	 0.2720
C	 0.4550	 0.1010
D	 0.0800	 0.0160
E	 0.8720	 0.2380
F	 0.9360	 0.2270
G	 0.8540	 0.2100
H	 0.8560	 0.2640
I	 0.8640	 0.2710
J	 0.9080	 0.3400
K	 0.5330	 0.1580
L	 0.0020	 0.0000
M	 0.8450	 0.1800
N	 0.8880	 0.2410
O	 0.9100	 0.3320
P	 0.8670	 0.2450
Q	 0.8440	 0.2290
R	 0.0000	 -0.0450
S	 0.0000	 -0.0040
T	 0.0000	 0.0150
U	 0.0000	 0.0170
V	 0.0000	 -0.0160
W	 0.0000	 0.0150
X	 0.0000	 -0.0380
Y	 0.4810	 0.1140
Z	 0.0000	 0.0200
a	 0.6460	 0.0580
b	 0.5220	 0.0720
c	 0.6750	 0.1070



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.6980	 0.1330
e	 0.7260	 0.1590
f	 0.6740	 0.1190
g	 0.4970	 0.0860
h	 0.3130	 0.0490
i	 0.1810	 0.0130
j	 0.1780	 -0.0180
k	 0.1130	 -0.0050
l	 0.2010	 -0.0270
m	 0.1990	 0.0790
n	 0.2380	 -0.0190
o	 0.0000	 0.0070
p	 0.0000	 -0.0560
q	 0.0000	 0.0160
r	 0.0000	 0.0060
s	 0.0000	 0.0340
t	 0.0000	 0.0120
u	 0.0000	 0.0350
v	 0.0000	 0.0080
w	 0.0010	 0.0070
x	 0.0000	 0.0850
y	 0.0000	 -0.0320
z	 0.0000	 0.0070