



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:18 PM UTC

PDB ID : 5GAN / pdb_00005gan
EMDB ID : EMD-8012
Title : The overall structure of the yeast spliceosomal U4/U6.U5 tri-snRNP at 3.7 Angstrom
Authors : Nguyen, T.H.D.; Galej, W.P.; Bai, X.C.; Oubridge, C.; Scheres, S.H.W.; Newman, A.J.; Nagai, K.
Deposited on : 2015-12-15
Resolution : 3.70 Å(reported)

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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:

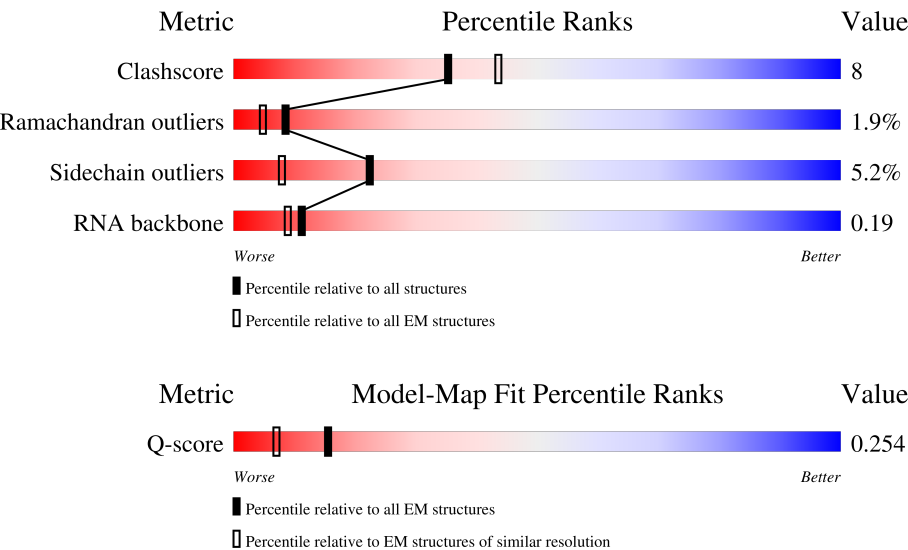
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 Å.

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



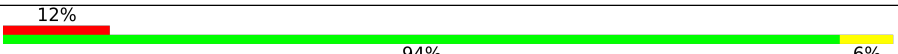
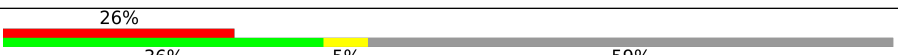
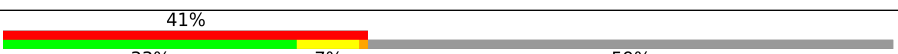
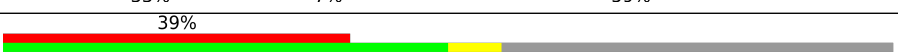
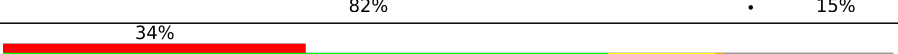
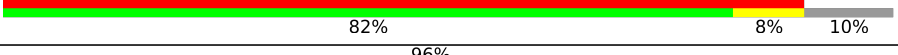
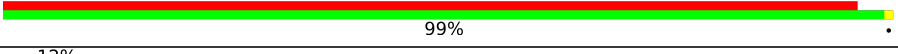
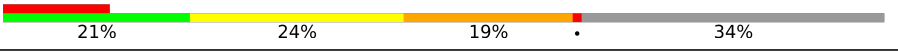
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	V	160	
2	W	112	
3	A	2413	

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Mol	Chain	Length	Quality of chain
4	H	465	
5	J	899	
6	D	143	
7	F	494	
8	G	469	
9	B	2163	
10	x	100	
11	b	196	
11	k	196	
12	h	146	
12	l	146	
13	j	110	
13	m	110	
14	d	101	
14	n	101	
15	e	94	
15	p	94	
16	f	86	
16	q	86	
17	g	77	
17	r	77	
18	E	328	
19	U	214	
20	K	126	
21	2	95	

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Mol	Chain	Length	Quality of chain
22	3	89	87% 79% 7% 13%
23	4	187	40% 37% 60%
24	5	93	81% 76% 19%
25	6	86	86% 81% 5% 14%
26	7	115	57% 55% 43%
27	8	109	59% 58% 41%
28	C	1008	7% 59% 23% 15%

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 77370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	124	Total	C	N	O	P	0	0
			2635	1179	459	873	124		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	80	Total	C	N	O	P	0	0
			1697	759	293	565	80		

- Molecule 3 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2196	Total	C	N	O	S	0	0
			17778	11444	3045	3226	63		

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	357	Total	C	N	O	S	0	0
			2789	1743	501	532	13		

- Molecule 5 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	729	Total	C	N	O	S	0	0
			5822	3726	992	1079	25		

- Molecule 6 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	140	Total	C	N	O	S	0	0
			1151	728	200	212	11		

- Molecule 7 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	415	Total	C	N	O	S	0	0
			3218	2052	575	580	11		

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	318	Total	C	N	O	S	0	0
			2632	1659	469	488	16		

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1781	Total	C	N	O	S	1	0
			14212	9098	2372	2685	57		

- Molecule 10 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	x	100	Total	C	N	O	0	0
			500	300	100	100		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
11	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	91	Total	C	N	O	S	0	0
			720	455	129	134	2		
12	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	94	Total	C	N	O	S	0	0
			737	474	140	119	4		
13	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
14	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
15	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
16	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		
17	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 18 is a protein called Snu66.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	328	Total	C	N	O		0	0
			1713	1033	342	338			

- Molecule 19 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 20 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	124	Total	C	N	O	S	0	0
			936	597	161	174	4		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	90	Total	C	N	O	S	0	0
			735	469	124	139	3		

- Molecule 22 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	77	Total	C	N	O	S	0	0
			611	382	105	121	3		

- Molecule 23 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	74	Total	C	N	O	S	0	0
			588	381	96	108	3		

- Molecule 24 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	75	Total	C	N	O	S	0	0
			588	378	98	110	2		

- Molecule 25 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	74	Total	C	N	O	S	0	0
			577	364	95	116	2		

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	66	Total	C	N	O	S	0	0
			504	325	85	91	3		

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	8	64	Total	C	N	O	S	0	0
			498	320	86	90	2		

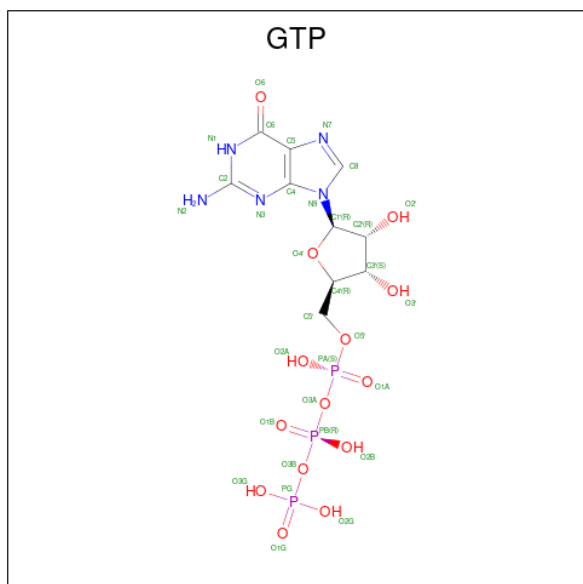
- Molecule 28 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	855	Total	C	N	O	S	0	0
			6450	4195	1089	1143	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	530	SER	GLU	conflict	UNP P36048
C	531	LYS	ASP	conflict	UNP P36048
C	532	THR	ASP	conflict	UNP P36048

- Molecule 29 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

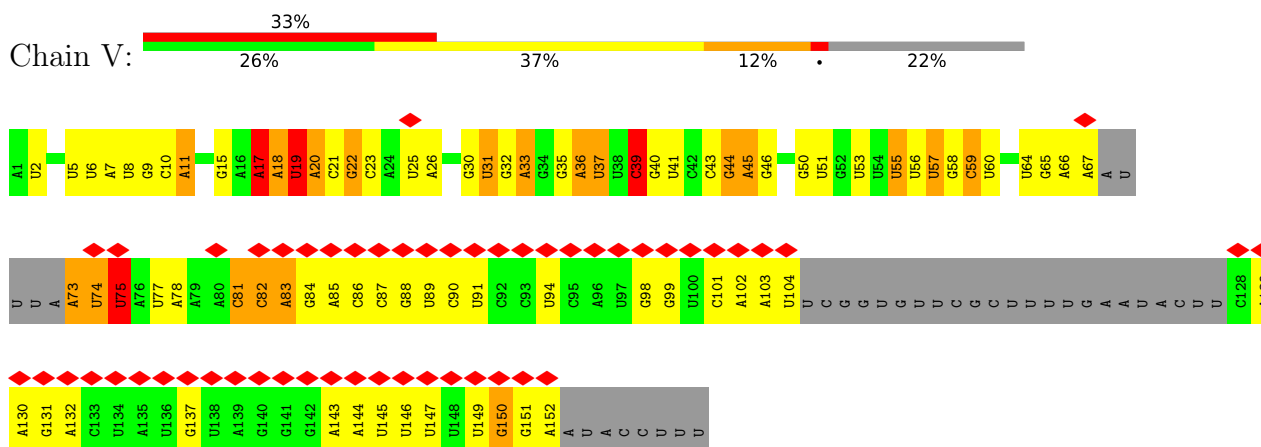


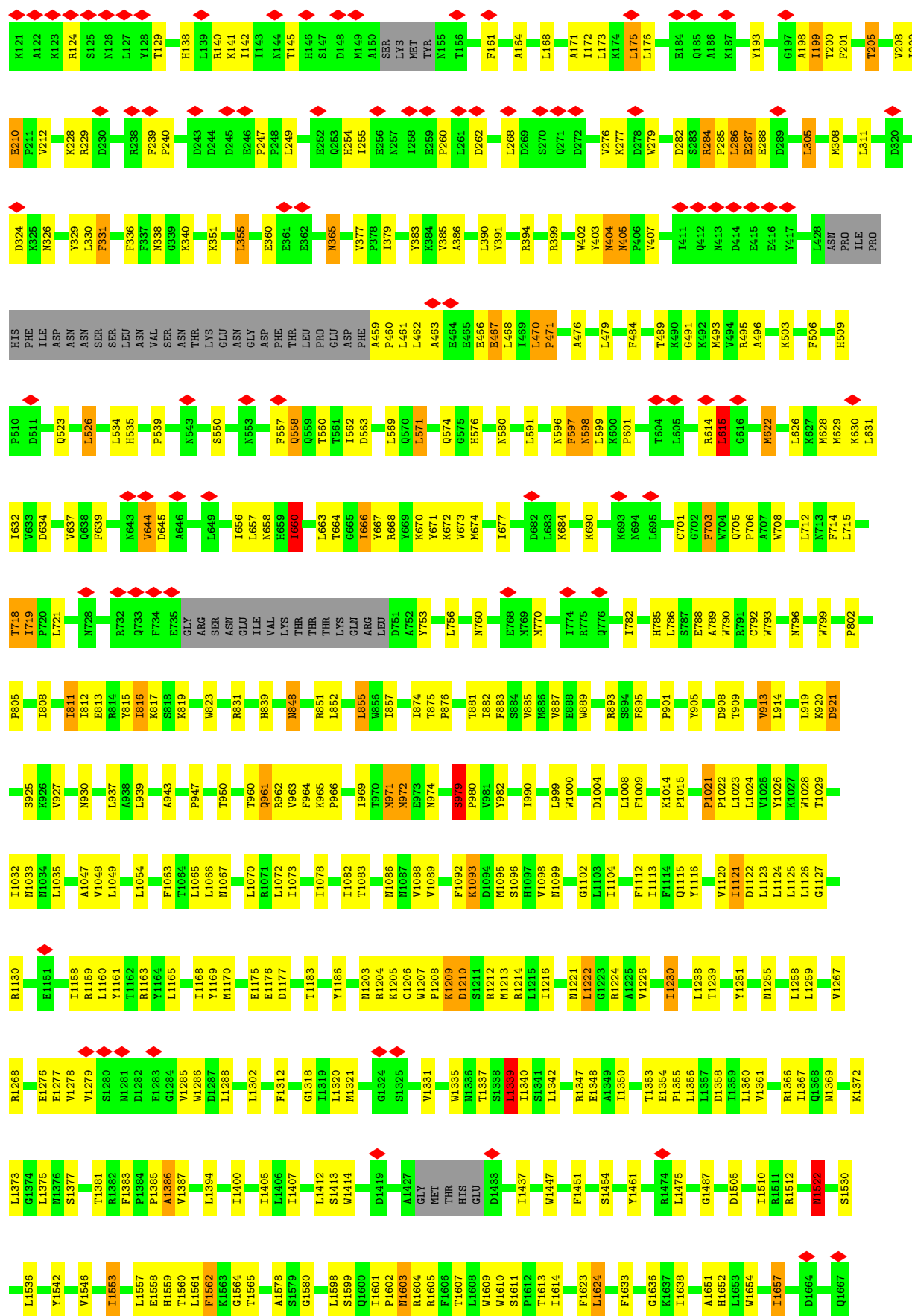
Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

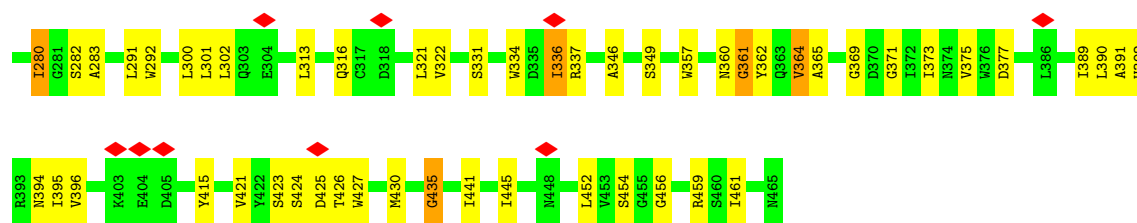
3 Residue-property plots

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.

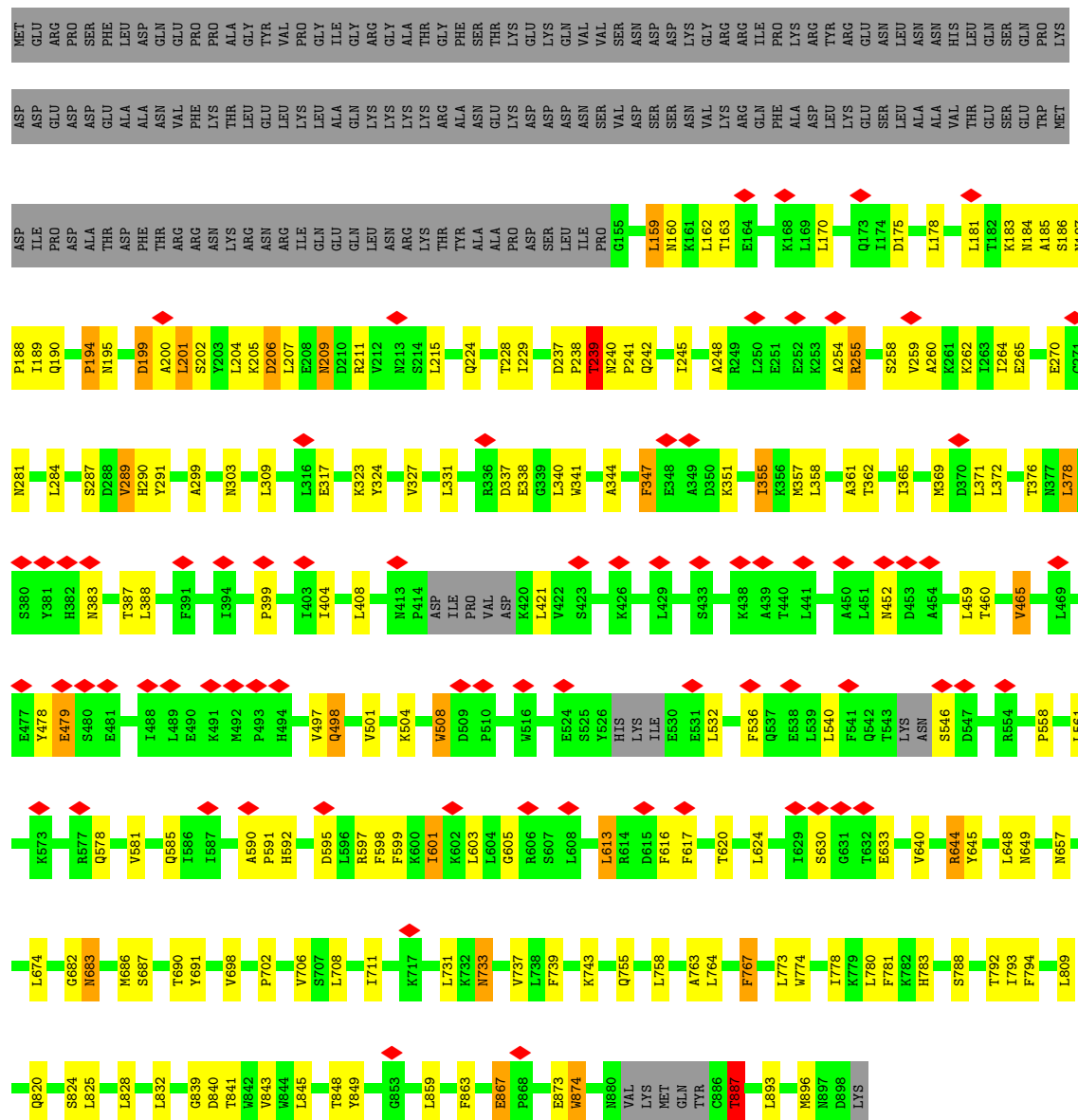
• Molecule 1: U4 snRNA





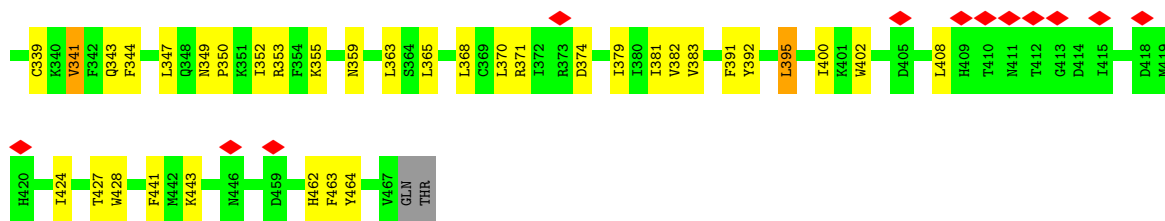


• Molecule 5: Pre-mRNA-splicing factor 6

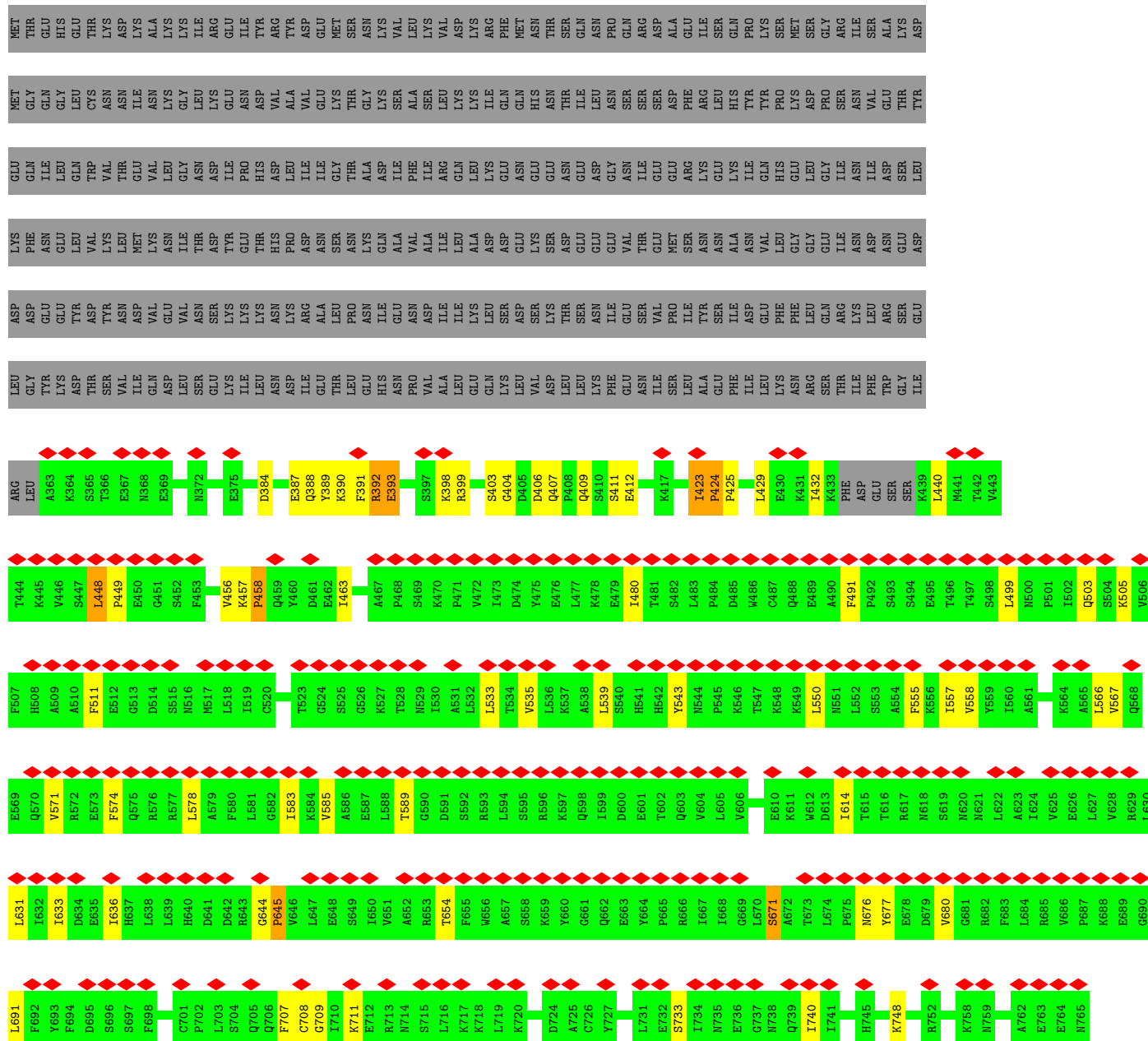


• Molecule 6: Spliceosomal protein DIB1

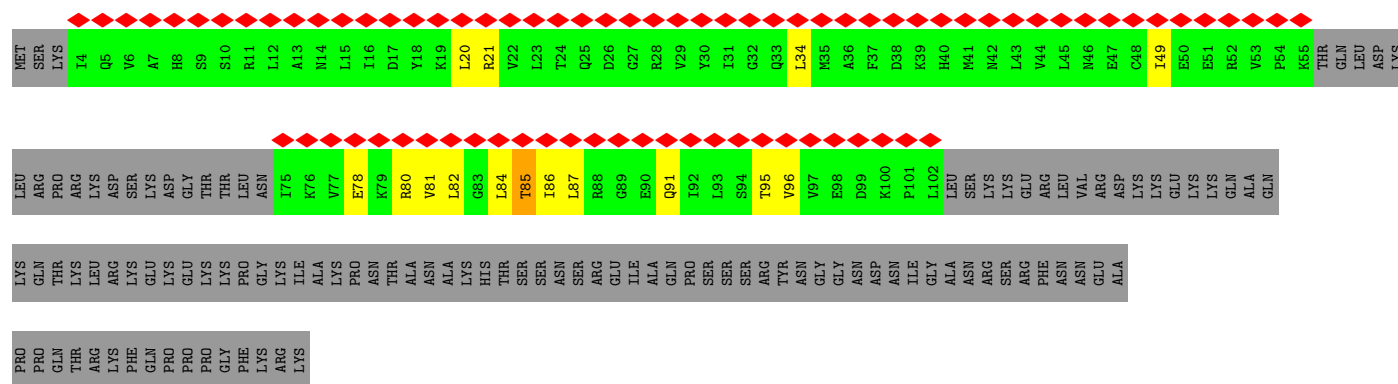




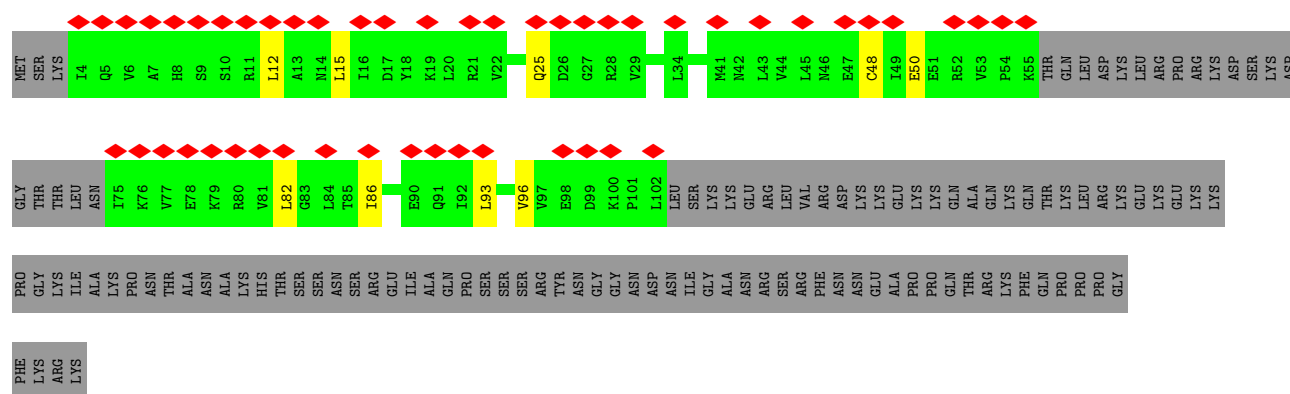
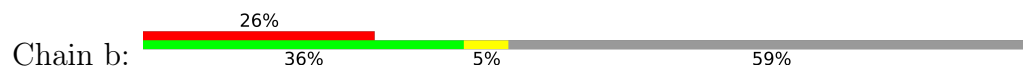
• Molecule 9: Pre-mRNA-splicing helicase BRR2



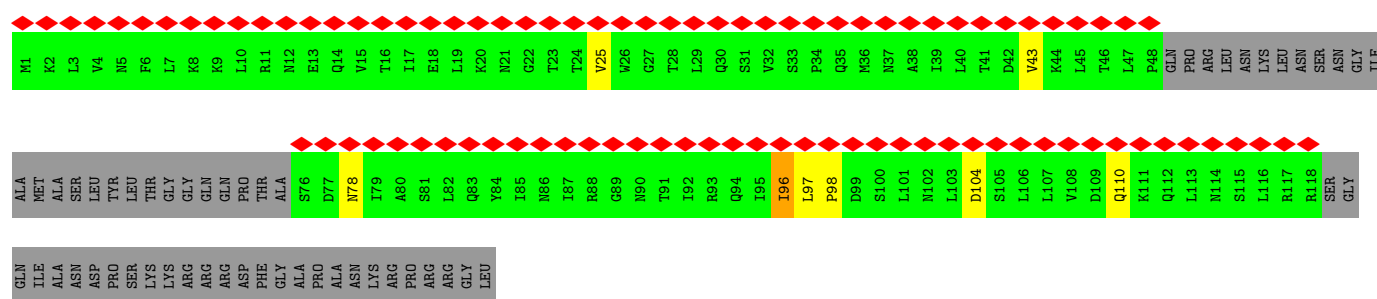
P1543	P1544	L1544	E1545	I1546	N1547	I1548	E1489	T1490	L1491	S1492	R1493	R1494	M1495	I1496	F1497	I1498	A1499	T1500	Q1501	L1502	S1562	M1563	L1564	Q1565	L1566	A1567	F1568	E1569	A1570	S1571	A1572	A1573	A1574	A1575	G1576	N1577	R1578	N1579	S1580	S1581	S1582	V1583	F1584	L1585	P1586	S1587	R1588	K1589	D1590	C1591	M1592	E1593	V1594	F1595	S1596	A1597	F1598	K1599	L1600	F1601	S1602
V1483	Y1484	G1485	A1486	V1487	Y1488	E1489	T1490	L1491	S1492	R1493	R1494	M1495	I1496	F1497	I1498	A1499	T1500	Q1501	L1502	S1562	M1563	L1564	Q1565	L1566	A1567	F1568	E1569	A1570	S1571	A1572	A1573	A1574	A1575	G1576	N1577	R1578	N1579	S1580	S1581	S1582	V1583	F1584	L1585	P1586	S1587	R1588	K1589	D1590	C1591	M1592	E1593	V1594	F1595	S1596	A1597	F1598	K1599	L1600	F1601	S1602	
K1423	I1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	P1432	S1433	L1434	L1435	L1436	K1437	L1438	L1439	A1440	K1441	S1442	H1443	V1444	L1445	L1446	A1447	T1448	P1449	V1450	Q1451	F1452	E1453	L1454	L1455	S1456	R1457	R1458	W1459	R1460	Q1461	L1462	K1463	N1464	I1465	Q1466	S1467	L1468	E1469	L1470	M1471	I1472	Y1473	N1474	D1475	A1476	H1477	E1478	I1479	Q1481	G1482			
N1363	D1364	S1365	V1366	F1367	L1368	G1369	S1370	G1371	K1372	G1373	T1374	G1375	K1376	T1377	P1378	M1379	A1380	E1381	L1382	A1383	L1384	L1385	N1386	H1387	L1388	R1389	Q1390	N1391	K1392	G1393	L1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	N1412	N1413	K1414	L1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422		
E1303	T1304	P1305	V1306	S1307	F1308	N1309	K1310	F1311	K1312	L1313	F1314	K1315	K1316	F1317	P1318	P1319	P1320	T1321	P1322	L1323	L1324	E1325	M1326	I1327	S1328	I1329	S1330	T1331	S1332	E1333	L1334	A1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	N1412	N1413	K1414	L1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422	
K1423	I1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	P1432	S1433	L1434	L1435	L1436	K1437	L1438	L1439	A1440	K1441	S1442	H1443	V1444	L1445	L1446	A1447	T1448	P1449	V1450	Q1451	F1452	E1453	L1454	L1455	S1456	R1457	R1458	W1459	R1460	Q1461	L1462	K1463	N1464	I1465	Q1466	S1467	L1468	E1469	L1470	M1471	I1472	Y1473	N1474	D1475	A1476	H1477	E1478	I1479	Q1481	G1482			
V1483	Y1484	G1485	A1486	V1487	Y1488	E1489	T1490	L1491	S1492	R1493	R1494	M1495	I1496	F1497	I1498	A1499	T1500	Q1501	L1502	S1562	M1563	L1564	Q1565	L1566	A1567	F1568	E1569	A1570	S1571	A1572	A1573	A1574	A1575	G1576	N1577	R1578	N1579	S1580	S1581	S1582	V1583	F1584	L1585	P1586	S1587	R1588	K1589	D1590	C1591	M1592	E1593	V1594	F1595	S1596	A1597	F1598	K1599	L1600	F1601	S1602	
L1916	V1917	D1918	N1919	N1920	N1921	A1922	E1923	V1924	V1925	A1926	G1927	N1928	I1929	K1930	C1931	R1932	N1933	D1934	A1935	V1936	N1937	W1938	L1939	A1940	Y1941	T1942	Y1943	L1944	R1947	E1948	L1949	A1950	S1951	P1952	M1953	L1954	Y1955	K1956	V1957	P1958	D1959	I1960	S1961	S1962	D1963	G1964	Q1965	L1966	K1967	S1970	E1971	S1972	L1973	V1974	H1975	S1976					
A1977	L1978	C1979	I1980	L1981	K1982	E1983	Q1984	E1985	L1986	V1987	L1988	Y1989	D1990	A1991	E1992	N1993	D1994	V1995	E1996	E1997	A1998	T1999	D1000	L1001	G1002	N1003	S1007	F1008	Y1009	I1010	N1011	H1012	A1013	M1015	D1016	V1017	R1020	E1021	L1022	D1023	E1024	H1025	F1032	R1033	I1034	F1035	S1036	M1037	S1038	E1039	E1040	F1041	K1042	Y1043							
E1049	R1052	L1053	L1054	E1059	K1060	A1061	P1062	I1065	D1070	L1073	A1074	N1077	V1078	L1079	L1080	Q1081	F1084	S1085	Q1086	L1087	K1088	F1089	E1090	G1091	F1092	A1093	L1094	N1095	I1098	F1099	I1101	H1102	Q1103	N1104	A1105	L1108	L1109	R1110	A1111	M1112	F1113	E1114	I1115	C1116	L1117	K1118	R1119	G1120	W1121												
G1122	H1123	R1126	M1127	L1128	N1129	N1130	L1131	C1132	K1133	S1134	A1135	T1136	T1137	K1138	M1139	W1140	P1141	T1142	N1143	C1144	P1145	L1146	R1147	Q1148	F1149	K1150	T1151	C1152	P1153	V1154	E1155	W1156	I1157	K1158	R1159	L1160	E1161	A1162	S1163	T1164	V1165	P1166	W1167	G1168	D1169	Y1170	L1171	Q1172	L1173	E1174	T1175	P1176	A1177	E1178	V1179	G1180	R1181	A1182			
I1183	R1184	S1185	E1186	K1187	Y1188	G1189	K1190	Q1191	V1192	Y1193	D1194	L1195	L1196	K1197	R1198	F1199	P1200	K1201	M1202	S1203	V1204	T1205	C1206	N1207	A1208	Q1209	P1210	I1211	T1212	R1213	S1214	V1215	M1216	F1217	R1218	N1219	I1220	E1221	L1222	L1223	A1224	D1225	W1226	L1227	W1228	D1229	M1230	N1231	V1232	H1233	G1234	S1235	L1236	E1237	P1238	F1239	L1240	L1241	M1242		
L1243	E1244	D1245	T1246	D1247	G1248	D1249	S1250	I1251	V1252	Y1253	Y1254	D1255	V1256	L1257	F1258	I1259	T1260	K1261	D1262	L1263	V1264	G1265	H1266	E1267	F1268	T1269	L1270	S1271	F1272	T1273	Y1274	E1275	L1276	K1277	Q1278	N1280	Q1281	N1282	N1283	L1284	P1285	P1286	N1287	F1288	F1289	L1290	T1291	L1292	L1293	S1294	E1295	N1296	W1297	H1298	H1299	S1300	E1301	F1302			
E1303	T1304	P1305	V1306	S1307	F1308	N1309	K1310	F1311	K1312	L1313	F1314	K1315	K1316	F1317	P1318	P1319	P1320	T1321	P1322	L1323	L1324	E1325	M1326	I1327	S1328	I1329	S1330	T1331	S1332	E1333	L1334	A1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	N1412	N1413	K1414	L1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422	
K1423	I1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	P1432	S1433	L1434	L1435	L1436	K1437	L1438	L1439	A1440	K1441	S1442	H1443	V1444	L1445	L1446	A1447	T1448	P1449	V1450	Q1451	F1452	E1453	L1454	L1455	S1456	R1457	R1458	W1459	R1460	Q1461	L1462	K1463	N1464	I1465	Q1466	S1467	L1468	E1469	L1470	M1471	I1472	Y1473	N1474	D1475	A1476	H1477	E1478	I1479	Q1481	G1482			
V1483	Y1484	G1485	A1486	V1487	Y1488	E1489	T1490	L1491	S1492	R1493	R1494	M1495	I1496	F1497	I1498	A1499	T1500	Q1501	L1502	S1562	M1563	L1564	Q1565	L1566	A1567	F1568	E1569	A1570	S1571	A1572	A1573	A1574	A1575	G1576	N1577	R1578	N1579	S1580	S1581	S1582	V1583	F1584	L1585	P1586	S1587	R1588	K1589	D1590	C1591	M1592	E1593	V1594	F1595	S1596	A1597	F1598	K1599	L1600	F1601	S1602	



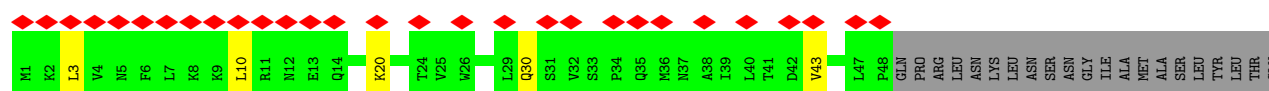
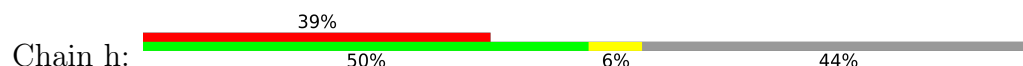
• Molecule 11: Small nuclear ribonucleoprotein-associated protein B

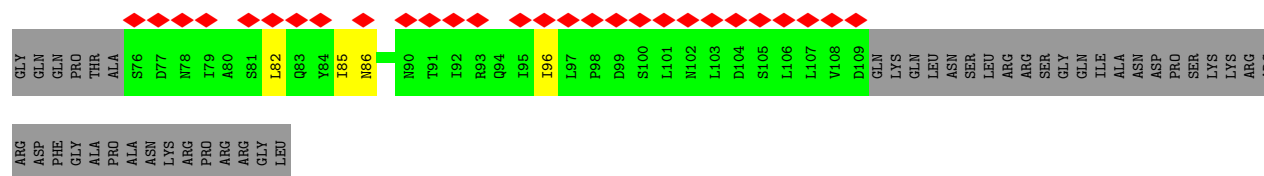


• Molecule 12: Small nuclear ribonucleoprotein Sm D1

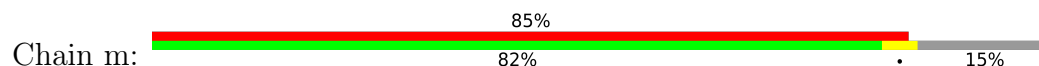


• Molecule 12: Small nuclear ribonucleoprotein Sm D1

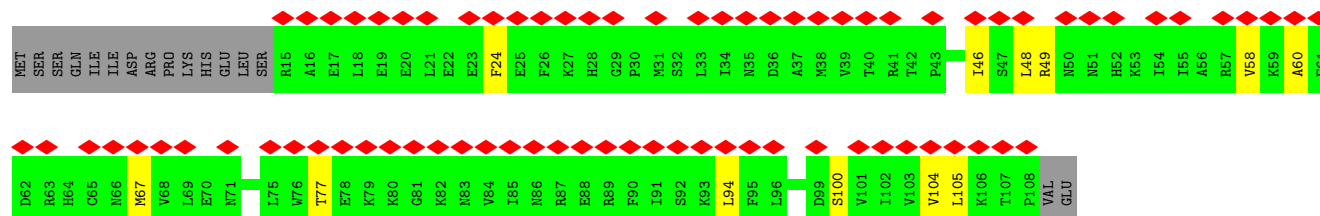
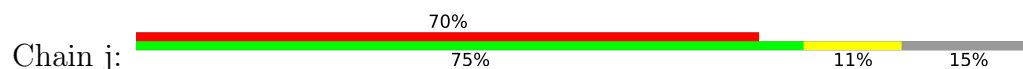




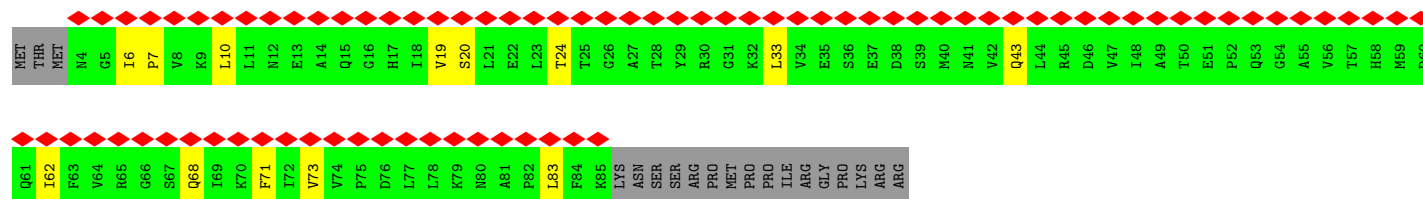
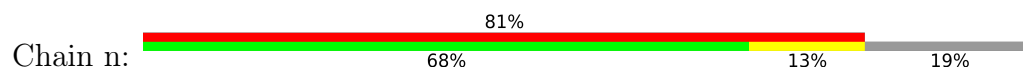
- Molecule 13: Small nuclear ribonucleoprotein Sm D2



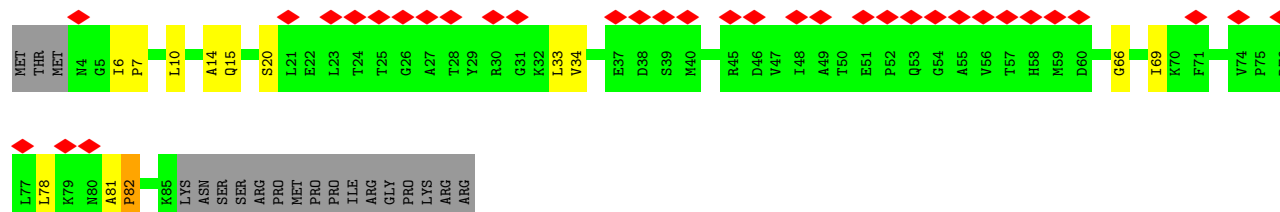
- Molecule 13: Small nuclear ribonucleoprotein Sm D2



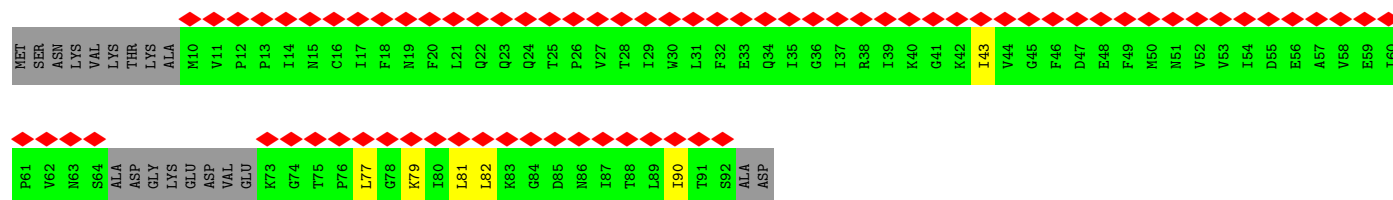
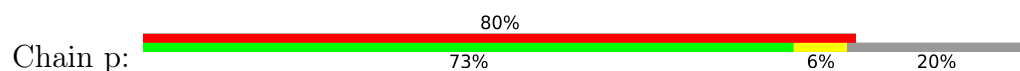
- Molecule 14: Small nuclear ribonucleoprotein Sm D3



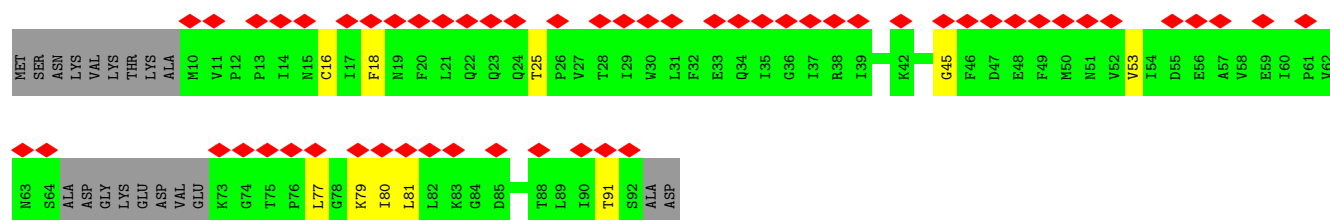
- Molecule 14: Small nuclear ribonucleoprotein Sm D3



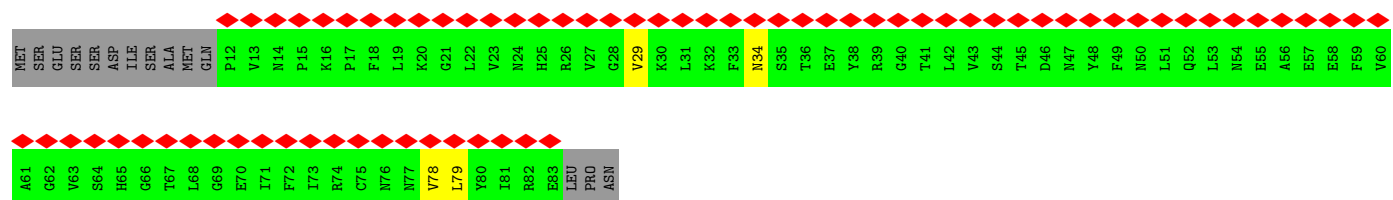
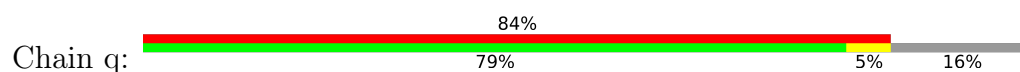
- Molecule 15: Small nuclear ribonucleoprotein E



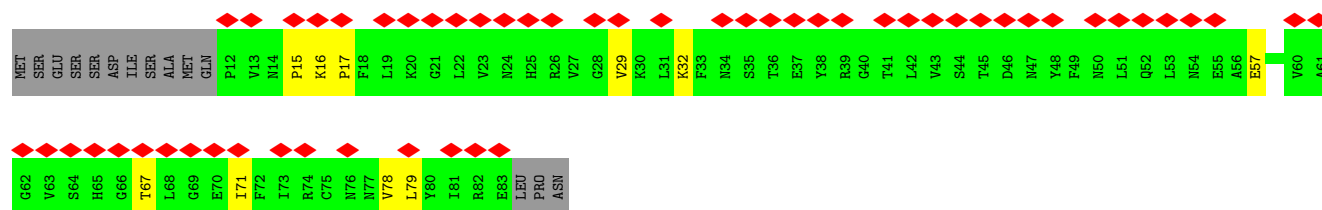
- Molecule 15: Small nuclear ribonucleoprotein E



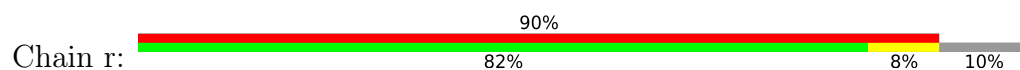
- Molecule 16: Small nuclear ribonucleoprotein F



- Molecule 16: Small nuclear ribonucleoprotein F

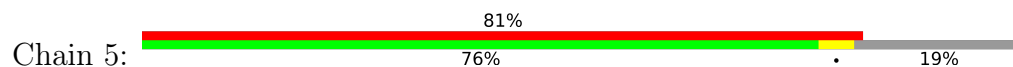


- Molecule 17: Small nuclear ribonucleoprotein G



SER
PRO
GLN
LYS
VAL
GLU
PHE

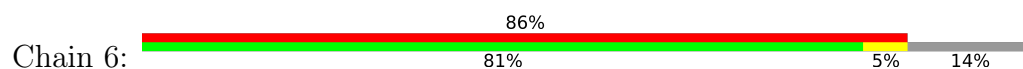
- Molecule 24: U6 snRNA-associated Sm-like protein LSm5



MET SER LEU P4 E5 T6 L7 P8 L9 E10 E11 V11 I12 D13 K14 T15 I16 I17 Q18 K19 V20 L21 L22 V23 L24 Q25 S26 S27 R28 E29 F30 E31 G32 T33 L34 V35 G36 F37 D38 D39 F40 V41 M42 V43 I44 L45 E46 D47 A48 V49 E50 W51 L52 I53 D54 PRO GLU ASP GLU SER ARG

N61 E62 K63 V64 M65 Q66 H67 H68 G69 M71 L72 L73 S74 G75 N76 M77 I78 A79 I80 V82 P83 G84 LYS LYS THR PRO THR ALA LEU

- Molecule 25: U6 snRNA-associated Sm-like protein LSm6



MET SER GLY LYS ALA SER THR GLY GLU SER V11 T12 T13 E14 F15 L16 S17 I18 I19 I20 Q21 K22 K23 V24 N25 V26 K27 L28 A29 G31 G32 L33 Y34 S35 G36 R37 L38 E39 S40 I41 D42 G43 F44 M45 N46 V47 A48 L49 S50 S51 A52 T53 E54 H55 Y56 E57 S58 N59 N60

N61 K62 L63 L64 M65 K66 F67 N68 D70 V71 F72 L73 R74 G75 T76 Q77 V78 M79 Y80 I81 S82 E83 Q84 LYS ILE

- Molecule 26: U6 snRNA-associated Sm-like protein LSm7



MET HIS GLN HIS SER LYS SER ASN PRO GLN GLN ARG LYS PHE GLU PRO LYS ARG GLU A26 I27 L28 D29 L30 A31 K32 Y33 K34 D35 S36 K37 I38 R39 V40 K41 L42 M43 G44 G45 K46 L47 V48 I49 G50 V51 A52 L52 K53 G54 Y55 D56 Q57 L58 M59 N60

L61 V62 L63 D64 D65 T66 V67 E68 G69 M70 SER ASN PRO ARG ASP ASP GLU ASN ASN THR GLU LEU ILE SER N85 A86 R87 K88 L89 G90 L91 T92 V93 I94 R95 G96 T97 I98 L99 V100 S101 L102 S103 S104 A105 GLU GLY SER ASP VAL LEU TYR MET GLN LYS

- Molecule 27: U6 snRNA-associated Sm-like protein LSm8

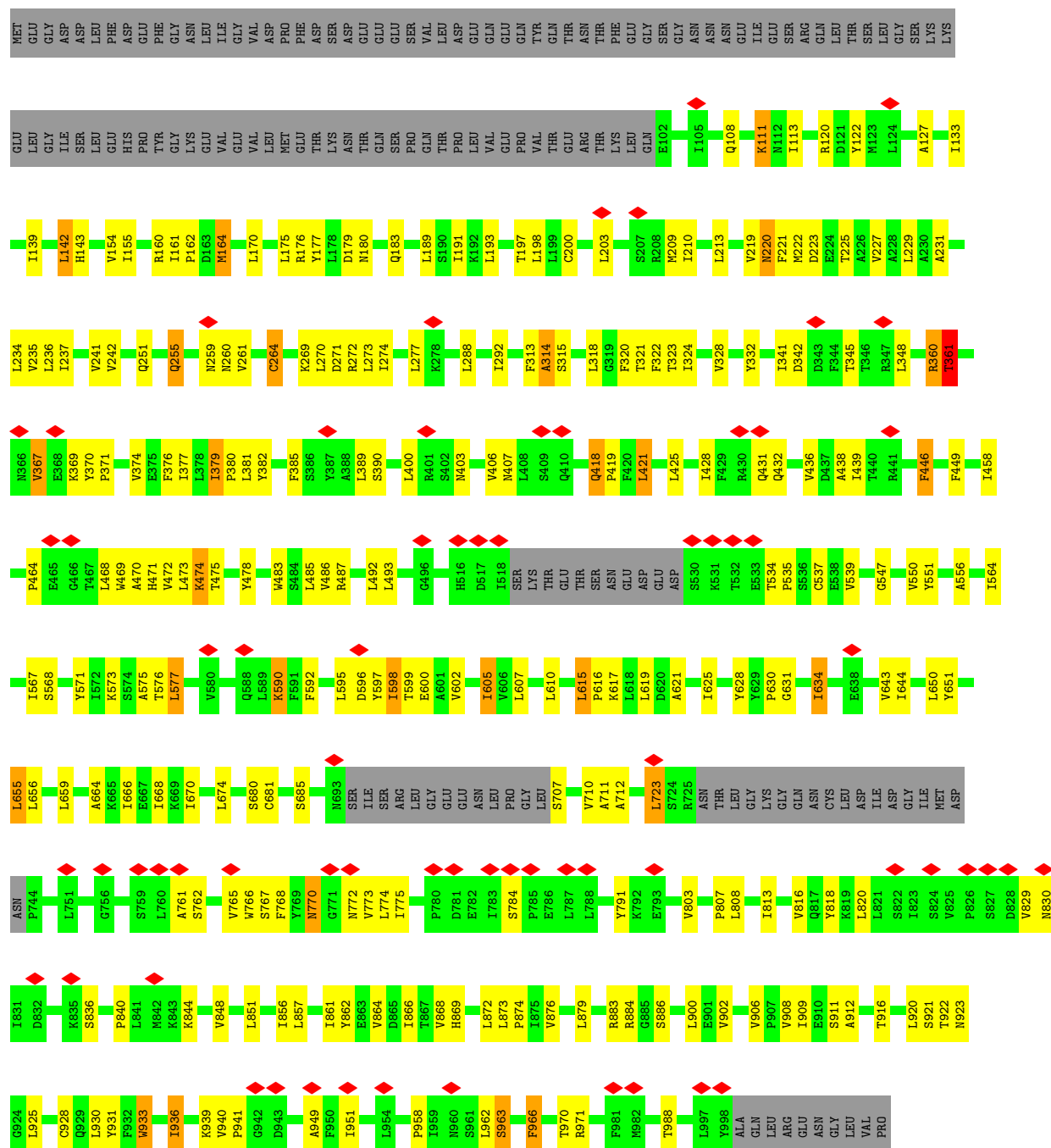


MET SER ALA T4 L5 K6 D7 Y8 L9 N10 N11 K12 V13 V14 I15 I16 K17 V18 D19 G20 E21 C22 L23 L24 A25 S26 L27 N28 G29 F30 D31 K32 N33 T34 N35 L36 F37 T38 T39 N40 V41 F42 N43 N44 I45 S46 K47 E48 F49 I50 C51 K52 A53 Q54 L55 L56 H57 Q58 S59 E60

I61 A62 L63 V64 G65 L66 I67 ASP ASP ALA GLU ASN ASP ASP SER LEU ALA PRO ILE ASP GLU LYS VAL PRO MET LEU LYS ASP THR LYS ASN ILE GLU ASN HIS VAL TRP LYS VAL TYR GLU SER LYS THR LYS

- Molecule 28: Pre-mRNA-splicing factor SNU114





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.036	Depositor
Map size ($\text{\AA}$)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.43, 1.43, 1.43	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	V	0.44	0/2943	0.88	12/4577 (0.3%)
2	W	0.42	0/1891	0.94	11/2933 (0.4%)
3	A	0.61	2/18226 (0.0%)	1.09	36/24737 (0.1%)
4	H	0.58	0/2845	0.96	2/3843 (0.1%)
5	J	0.61	0/5934	1.24	10/8039 (0.1%)
6	D	0.61	0/1172	1.13	0/1578
7	F	0.65	1/3273 (0.0%)	1.24	7/4413 (0.2%)
8	G	0.60	0/2687	1.03	3/3611 (0.1%)
9	B	0.60	0/14518	0.96	8/19682 (0.0%)
11	b	0.58	0/636	0.72	0/856
11	k	0.64	0/636	0.75	1/856 (0.1%)
12	h	0.56	0/649	0.79	0/880
12	l	0.64	0/725	0.82	0/980
13	j	0.58	0/753	0.90	0/1013
13	m	0.64	0/749	0.84	0/1009
14	d	0.55	0/634	0.85	0/859
14	n	0.62	0/634	0.78	0/859
15	e	0.65	0/585	0.87	0/795
15	p	0.70	0/585	0.86	0/795
16	f	0.62	0/585	0.87	0/791
16	q	0.63	0/585	0.82	0/791
17	g	0.57	0/532	0.80	0/715
17	r	0.61	0/529	0.74	0/711
18	E	0.54	0/184	1.04	0/238
19	U	0.45	0/3350	0.89	7/5209 (0.1%)
20	K	0.69	0/949	1.20	3/1292 (0.2%)
21	2	0.68	0/745	0.91	0/1005
22	3	0.63	0/617	0.76	0/836
23	4	0.62	0/594	0.78	0/802
24	5	0.63	0/595	0.77	0/806
25	6	0.62	0/584	0.82	0/787
26	7	0.61	0/505	0.65	0/675

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	8	0.64	0/501	0.75	0/673
28	C	0.61	0/6590	1.10	11/8975 (0.1%)
All	All	0.59	3/77520 (0.0%)	1.02	111/106621 (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
3	A	0	9
5	J	0	2
7	F	0	1
9	B	0	2
11	k	0	1
28	C	0	2
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	376	LYS	C-O	-6.12	1.16	1.24
3	A	1369	ASN	C-O	-5.35	1.17	1.24
3	A	719	ILE	CA-CB	5.35	1.56	1.54

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	719	ILE	O-C-N	8.92	126.13	120.42
1	V	17	A	C2'-C3'-O3'	8.89	127.03	113.70
5	J	199	ASP	N-CA-C	-8.69	97.16	110.10
1	V	19	U	C2'-C3'-O3'	8.39	122.09	109.50
3	A	404	ASN	N-CA-C	8.35	121.10	110.33

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	286	LEU	Peptide
3	A	467	GLU	Peptide
3	A	557	PHE	Peptide

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Mol	Chain	Res	Type	Group
3	A	974	ASN	Peptide
3	A	979	SER	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	V	2635	0	1328	40	0
2	W	1697	0	858	79	0
3	A	17778	0	17575	427	0
4	H	2789	0	2725	62	0
5	J	5822	0	5792	133	0
6	D	1151	0	1138	30	0
7	F	3218	0	3297	79	0
8	G	2632	0	2599	46	0
9	B	14212	0	14210	111	0
10	x	500	0	110	4	0
11	b	631	0	670	7	0
11	k	631	0	670	9	0
12	h	644	0	686	6	0
12	l	720	0	772	2	0
13	j	741	0	778	6	0
13	m	737	0	767	1	0
14	d	625	0	647	8	0
14	n	625	0	647	9	0
15	e	575	0	597	4	0
15	p	575	0	597	1	0
16	f	573	0	572	5	0
16	q	573	0	572	1	0
17	g	529	0	557	4	0
17	r	526	0	555	3	0
18	E	1713	0	567	1	0
19	U	2999	0	1516	56	0
20	K	936	0	987	44	0
21	2	735	0	744	11	0
22	3	611	0	620	4	0
23	4	588	0	602	2	0
24	5	588	0	594	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	6	577	0	572	2	0
26	7	504	0	557	1	0
27	8	498	0	533	1	0
28	C	6450	0	6419	174	0
29	C	32	0	12	0	0
All	All	77370	0	72442	1189	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 8.

The worst 5 of 1189 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)
3:A:462:LEU:CD2	28:C:403:ASN:HD22	1.12	1.53
3:A:459:ALA:C	28:C:376:PHE:HE1	1.22	1.47
2:W:26:A:C5	3:A:671:TYR:CD1	2.10	1.39
3:A:462:LEU:CD2	28:C:403:ASN:ND2	1.77	1.38
3:A:459:ALA:C	28:C:376:PHE:CE1	2.03	1.35

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	2182/2413 (90%)	1924 (88%)	217 (10%)	41 (2%)	6	33
4	H	355/465 (76%)	301 (85%)	43 (12%)	11 (3%)	3	26
5	J	719/899 (80%)	643 (89%)	59 (8%)	17 (2%)	4	29
6	D	138/143 (96%)	124 (90%)	9 (6%)	5 (4%)	2	23
7	F	413/494 (84%)	361 (87%)	35 (8%)	17 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	316/469 (67%)	274 (87%)	34 (11%)	8 (2%)	4	29
9	B	1776/2163 (82%)	1623 (91%)	132 (7%)	21 (1%)	10	40
11	b	76/196 (39%)	67 (88%)	9 (12%)	0	100	100
11	k	76/196 (39%)	70 (92%)	5 (7%)	1 (1%)	9	38
12	h	78/146 (53%)	73 (94%)	4 (5%)	1 (1%)	9	38
12	l	87/146 (60%)	76 (87%)	9 (10%)	2 (2%)	5	30
13	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
13	m	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
14	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	9	38
14	n	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
15	e	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
15	p	71/94 (76%)	64 (90%)	7 (10%)	0	100	100
16	f	70/86 (81%)	64 (91%)	4 (6%)	2 (3%)	3	26
16	q	70/86 (81%)	63 (90%)	7 (10%)	0	100	100
17	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
17	r	65/77 (84%)	58 (89%)	7 (11%)	0	100	100
18	E	21/328 (6%)	20 (95%)	1 (5%)	0	100	100
20	K	122/126 (97%)	113 (93%)	7 (6%)	2 (2%)	7	35
21	2	88/95 (93%)	76 (86%)	11 (12%)	1 (1%)	11	42
22	3	75/89 (84%)	71 (95%)	4 (5%)	0	100	100
23	4	70/187 (37%)	65 (93%)	5 (7%)	0	100	100
24	5	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
25	6	72/86 (84%)	67 (93%)	4 (6%)	1 (1%)	9	37
26	7	62/115 (54%)	57 (92%)	5 (8%)	0	100	100
27	8	62/109 (57%)	59 (95%)	3 (5%)	0	100	100
28	C	847/1008 (84%)	734 (87%)	82 (10%)	31 (4%)	2	22
All	All	8462/10902 (78%)	7560 (89%)	740 (9%)	162 (2%)	8	33

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	247	PRO
3	A	470	LEU

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Mol	Chain	Res	Type
3	A	471	PRO
3	A	597	PHE
3	A	796	ASN

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	
3	A	1918/2182 (88%)	1827 (95%)	91 (5%)	23	48
4	H	305/410 (74%)	287 (94%)	18 (6%)	18	44
5	J	627/813 (77%)	594 (95%)	33 (5%)	20	46
6	D	129/132 (98%)	118 (92%)	11 (8%)	10	35
7	F	346/445 (78%)	303 (88%)	43 (12%)	4	22
8	G	289/436 (66%)	277 (96%)	12 (4%)	26	51
9	B	1592/1955 (81%)	1531 (96%)	61 (4%)	29	53
11	b	70/176 (40%)	70 (100%)	0	100	100
11	k	70/176 (40%)	68 (97%)	2 (3%)	37	57
12	h	77/129 (60%)	75 (97%)	2 (3%)	40	60
12	l	85/129 (66%)	81 (95%)	4 (5%)	23	48
13	j	79/103 (77%)	74 (94%)	5 (6%)	16	43
13	m	78/103 (76%)	75 (96%)	3 (4%)	29	53
14	d	69/89 (78%)	67 (97%)	2 (3%)	37	57
14	n	69/89 (78%)	66 (96%)	3 (4%)	26	50
15	e	65/83 (78%)	60 (92%)	5 (8%)	12	38
15	p	65/83 (78%)	61 (94%)	4 (6%)	16	44
16	f	63/77 (82%)	62 (98%)	1 (2%)	55	68
16	q	63/77 (82%)	61 (97%)	2 (3%)	34	56
17	g	58/66 (88%)	57 (98%)	1 (2%)	53	67
17	r	57/66 (86%)	55 (96%)	2 (4%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	E	20/20 (100%)	19 (95%)	1 (5%)	22	48
20	K	102/104 (98%)	91 (89%)	11 (11%)	6	27
21	2	85/91 (93%)	76 (89%)	9 (11%)	6	27
22	3	71/81 (88%)	69 (97%)	2 (3%)	38	58
23	4	64/172 (37%)	64 (100%)	0	100	100
24	5	66/84 (79%)	66 (100%)	0	100	100
25	6	66/75 (88%)	66 (100%)	0	100	100
26	7	56/103 (54%)	54 (96%)	2 (4%)	31	54
27	8	56/99 (57%)	55 (98%)	1 (2%)	51	67
28	C	673/910 (74%)	617 (92%)	56 (8%)	10	35
All	All	7433/9558 (78%)	7046 (95%)	387 (5%)	22	47

5 of 387 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	B	956	LYS
16	q	79	LEU
9	B	1077	ASN
9	B	1689	ASP
12	h	30	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
15	e	15	ASN
28	C	290	HIS
16	f	77	ASN
22	3	53	ASN
4	H	465	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	122/160 (76%)	63 (51%)	13 (10%)
19	U	138/214 (64%)	77 (55%)	21 (15%)
2	W	77/112 (68%)	35 (45%)	12 (15%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	337/486 (69%)	175 (51%)	46 (13%)

5 of 175 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	15	G
1	V	17	A
1	V	18	A

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	U	32	G
19	U	82	A
19	U	40	C
19	U	75	A
19	U	95	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](#)

1 ligand 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
29	GTP	C	1101	-	33,34,34	1.12	4 (12%)	50,54,54	1.69	7 (14%)

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
29	GTP	C	1101	-	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	1101	GTP	C5-C4	3.00	1.47	1.38
29	C	1101	GTP	C5-N7	-2.49	1.34	1.39
29	C	1101	GTP	C6-N1	-2.21	1.34	1.38
29	C	1101	GTP	C4-N9	-2.09	1.32	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	1101	GTP	C5-C4-N3	-5.64	119.41	128.39
29	C	1101	GTP	C2-N3-C4	4.75	120.48	112.30
29	C	1101	GTP	N9-C4-N3	4.40	134.74	125.95
29	C	1101	GTP	C6-C5-N7	3.20	136.11	130.29
29	C	1101	GTP	O6-C6-C5	-2.64	119.57	126.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

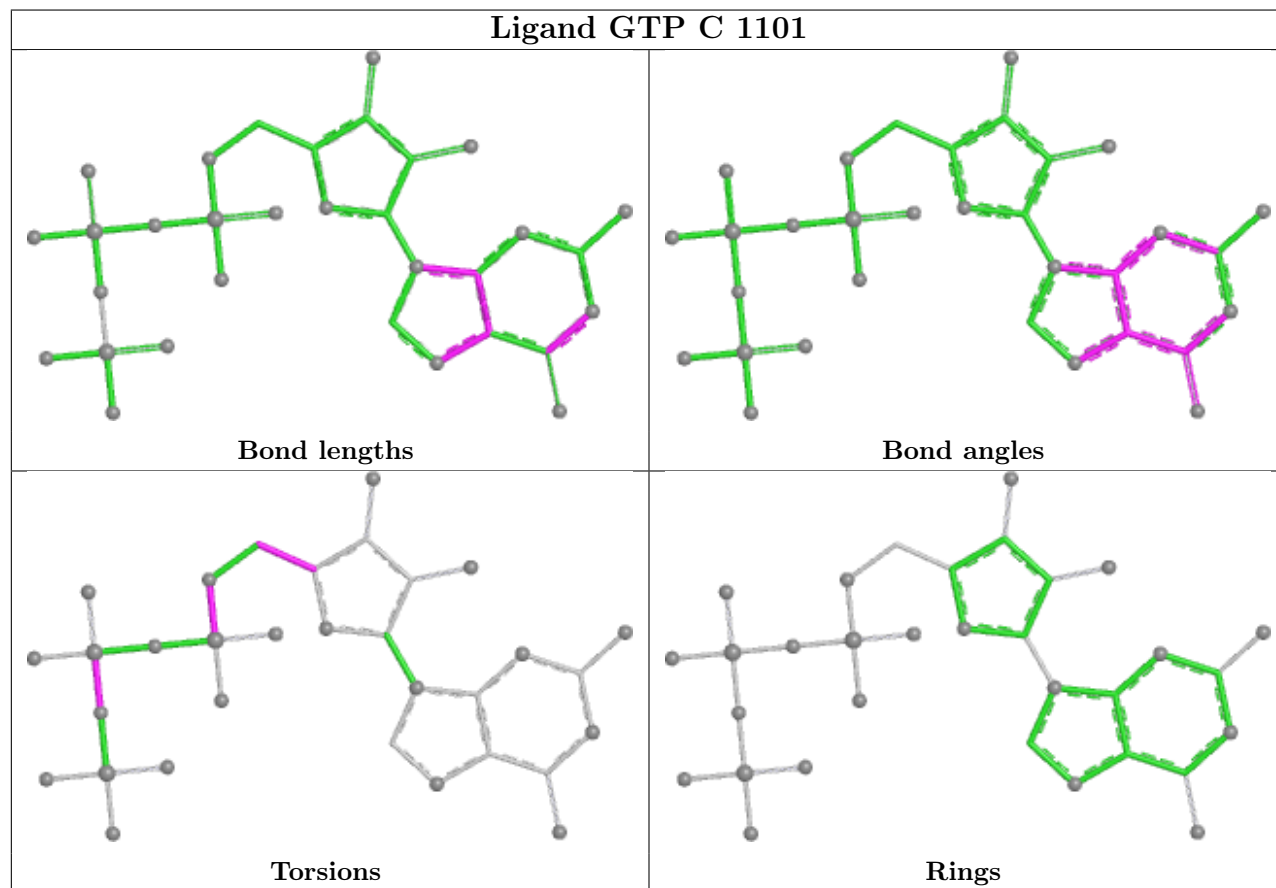
Mol	Chain	Res	Type	Atoms
29	C	1101	GTP	C5'-O5'-PA-O1A
29	C	1101	GTP	O4'-C4'-C5'-O5'
29	C	1101	GTP	C3'-C4'-C5'-O5'
29	C	1101	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	E	13

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Mol	Chain	Number of breaks
10	x	2
3	A	1
19	U	1

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	120:UNK	C	201:UNK	N	117.38
1	x	62:UNK	C	101:UNK	N	54.41
1	E	132:UNK	C	150:UNK	N	36.51
1	E	170:UNK	C	180:UNK	N	34.13
1	E	102:UNK	C	120:UNK	N	31.43

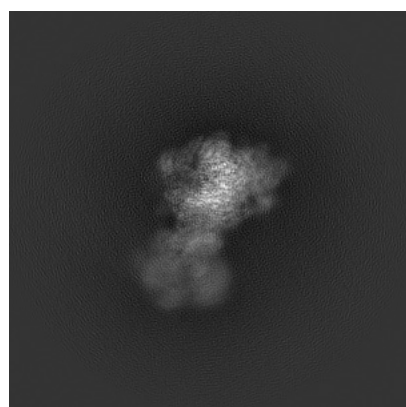
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8012. These allow visual inspection of the internal detail of the map and identification of artifacts.

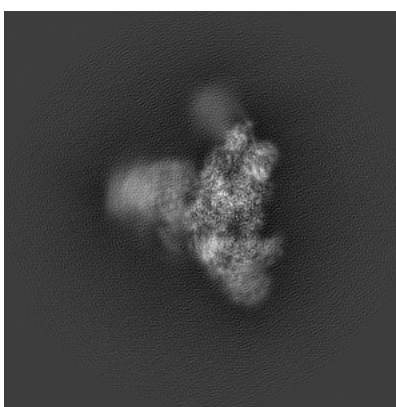
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

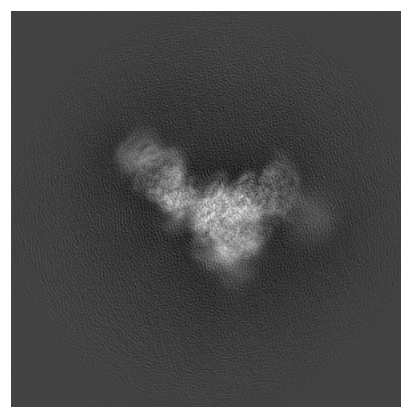
6.1.1 Primary map



X



Y

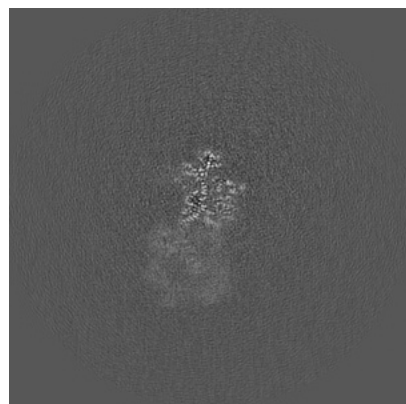


Z

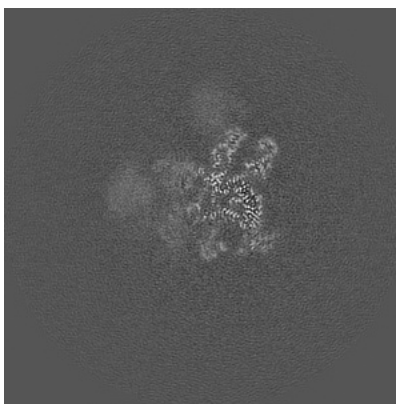
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

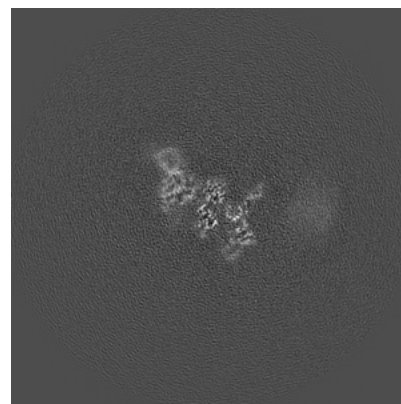
6.2.1 Primary map



X Index: 190



Y Index: 190

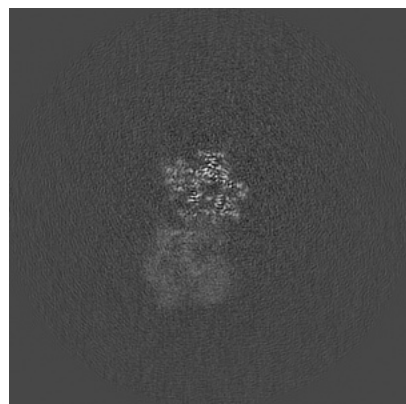


Z Index: 190

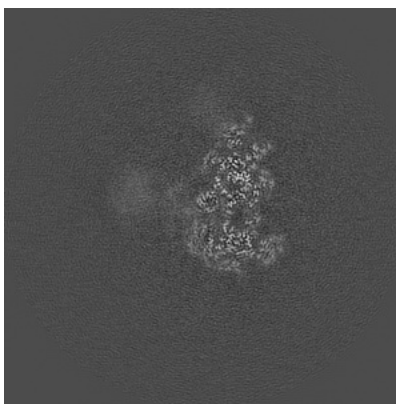
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

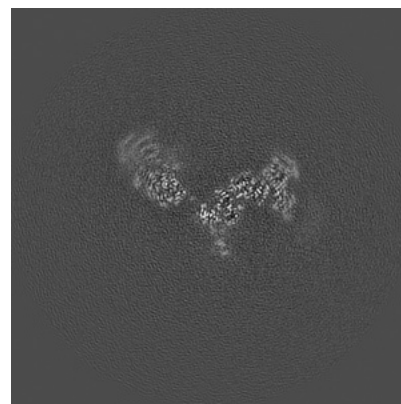
6.3.1 Primary map



X Index: 196



Y Index: 202

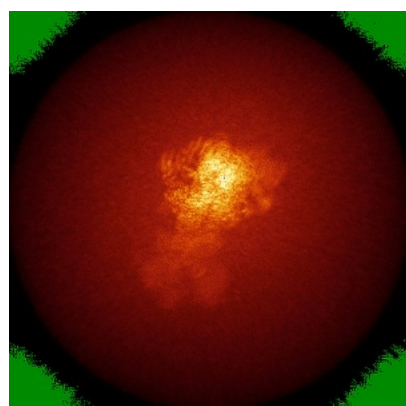


Z Index: 221

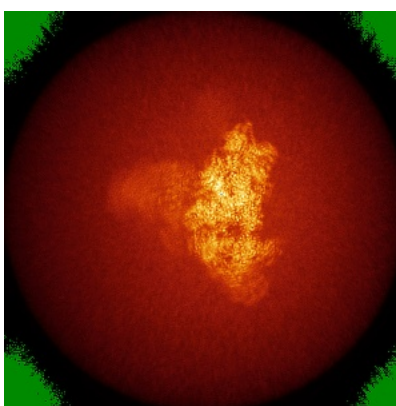
The images above show the largest variance slices of the map in three orthogonal directions.

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

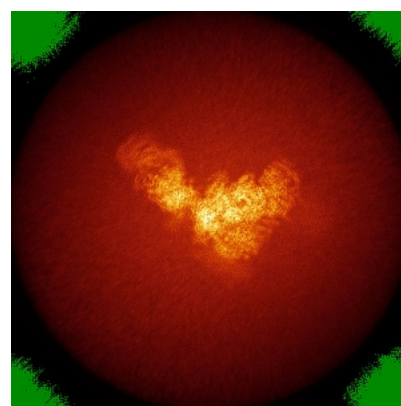
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

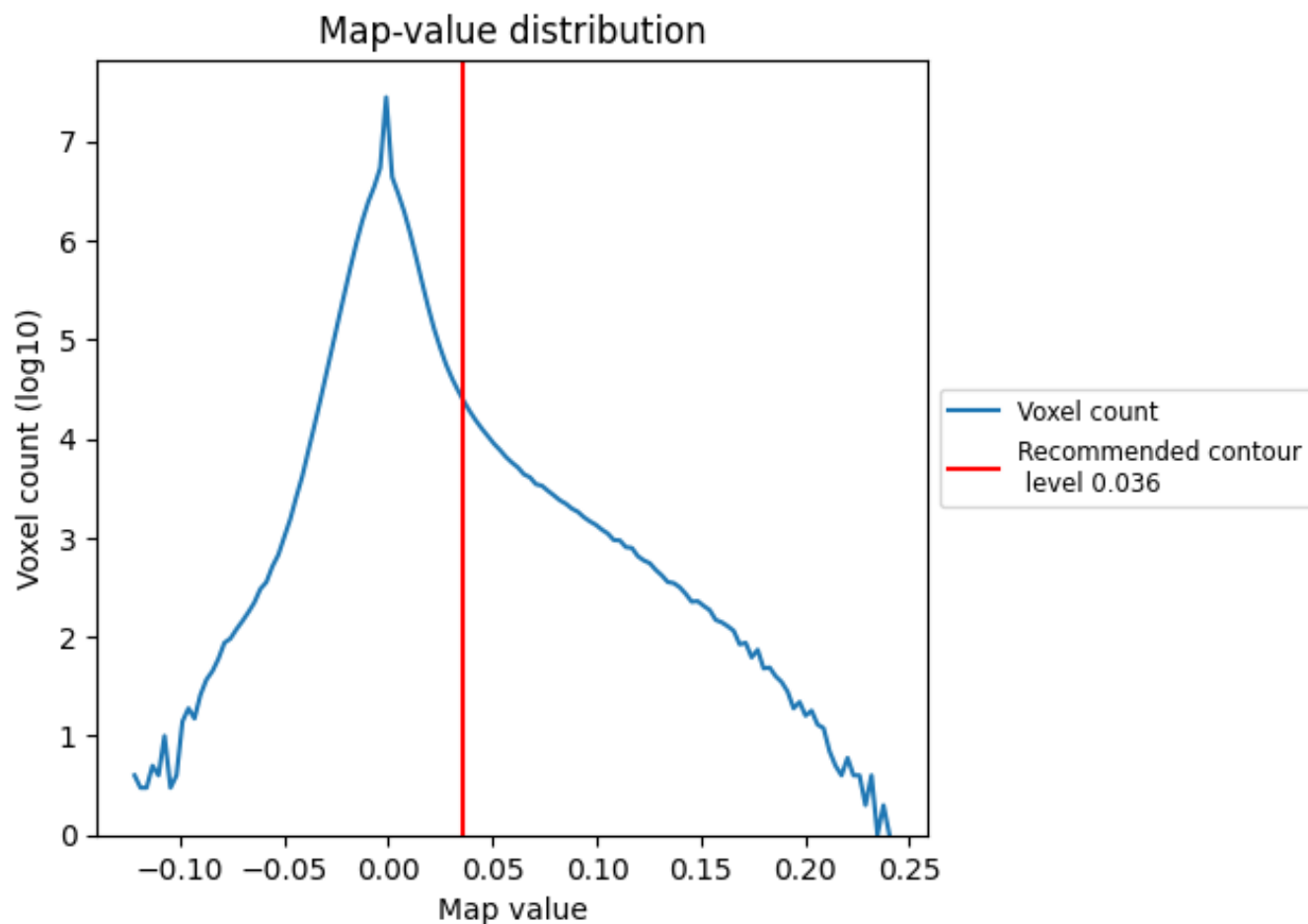
6.6 Mask visualisation

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

7 Map analysis [i](#)

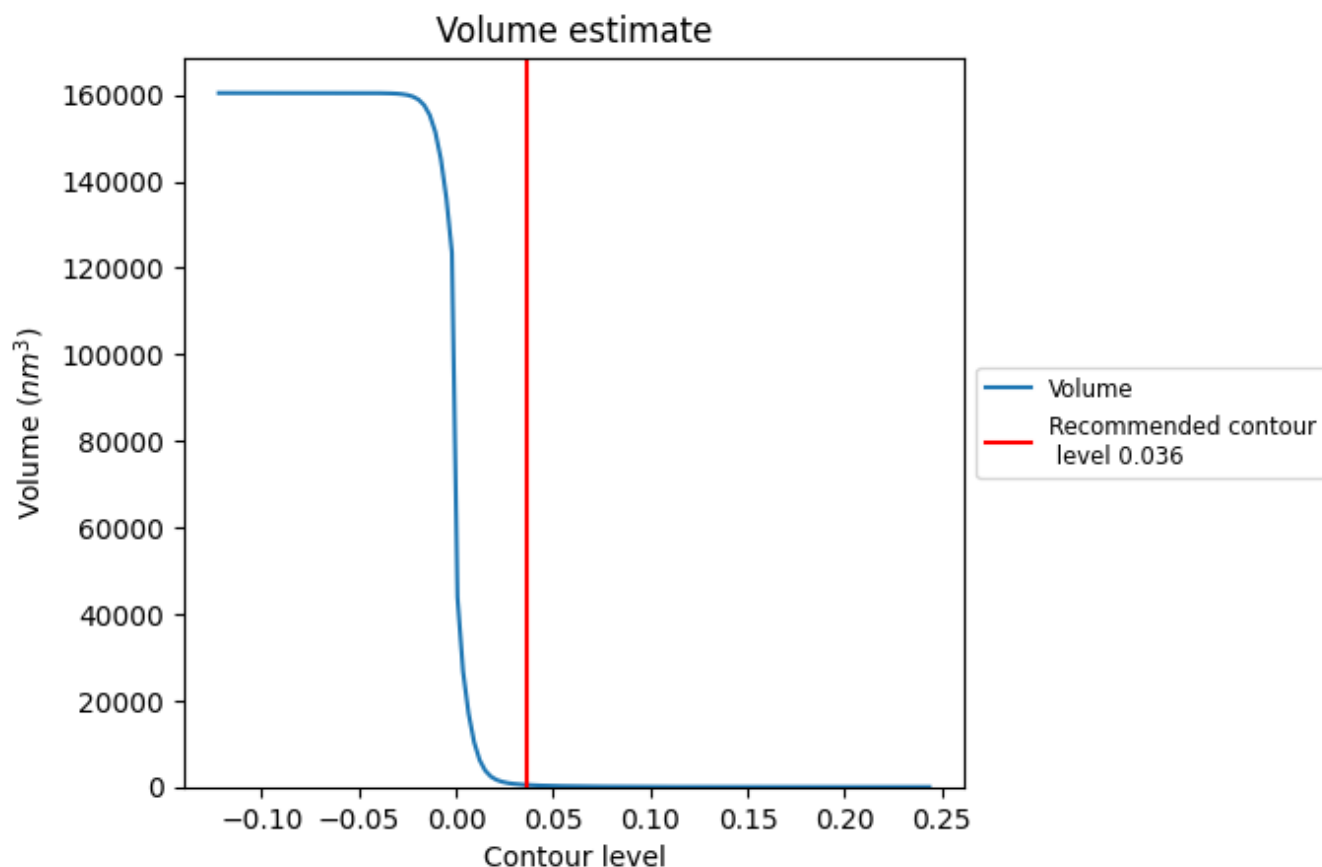
This section contains the results of statistical analysis of the map.

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.

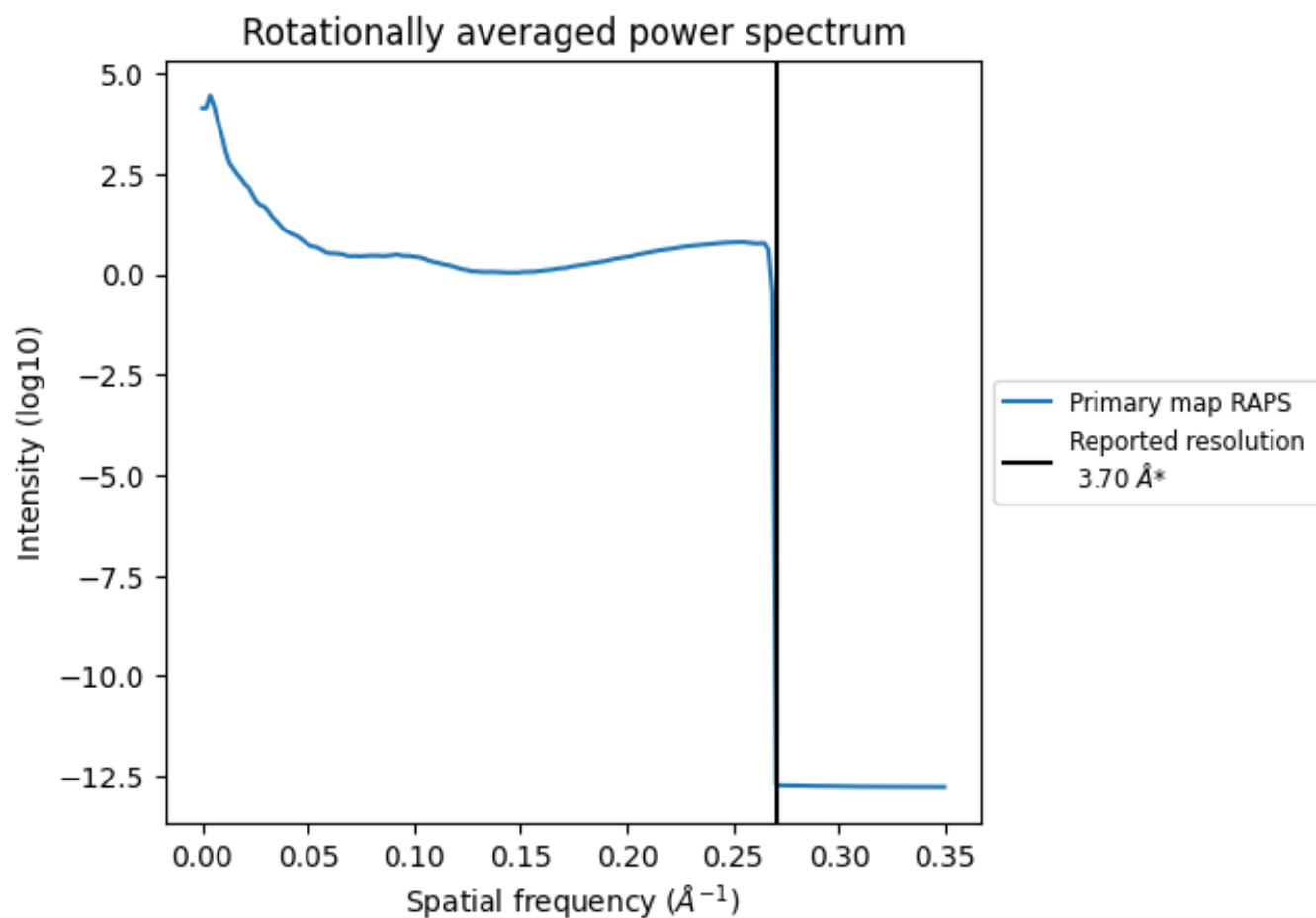
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478 nm^3 ; this corresponds to an approximate mass of 432 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 ⓘ

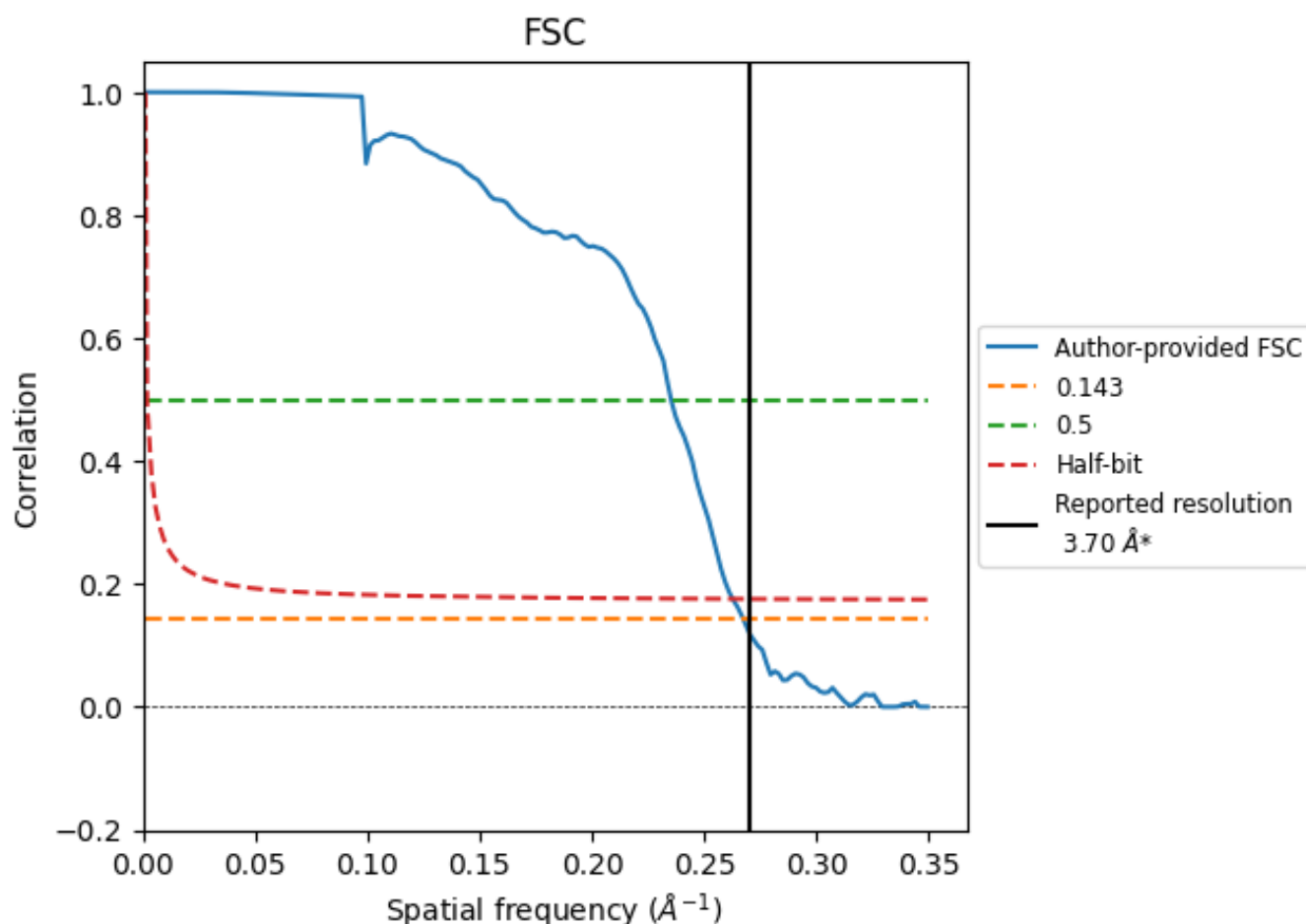


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

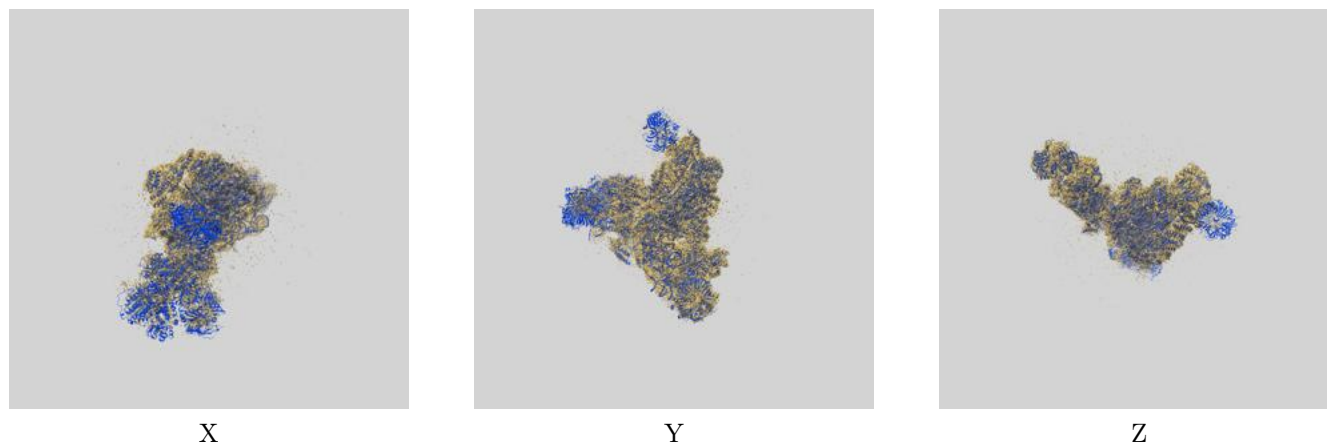
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.25	3.81
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

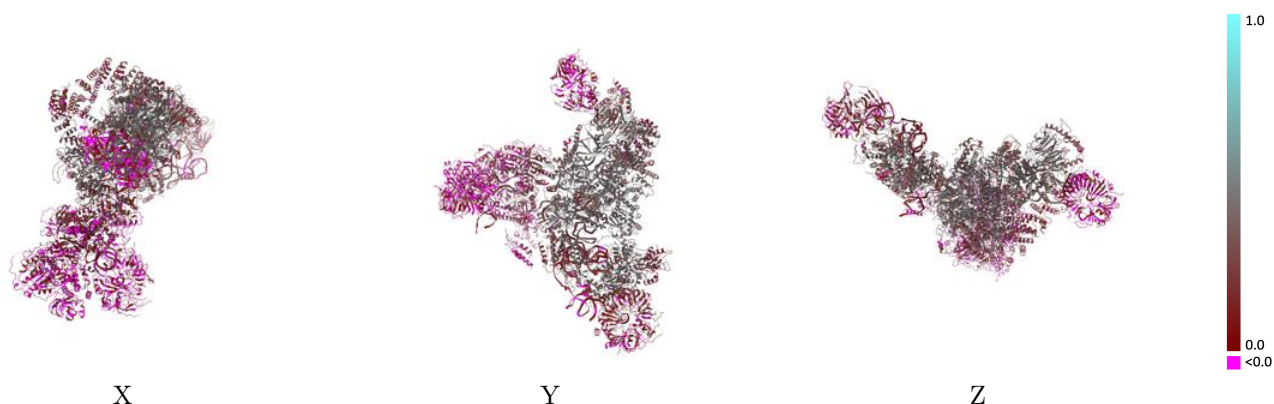
This section contains information regarding the fit between EMDB map EMD-8012 and PDB model 5GAN. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



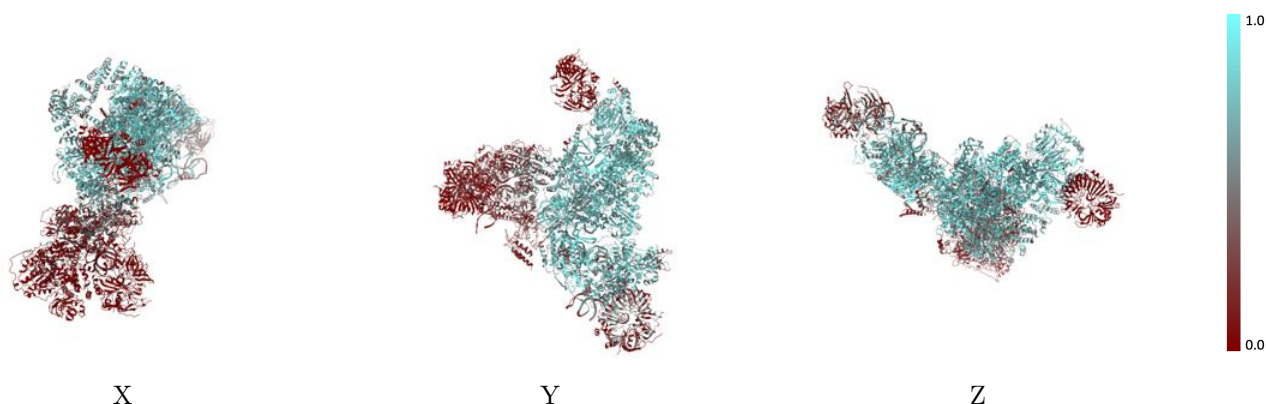
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



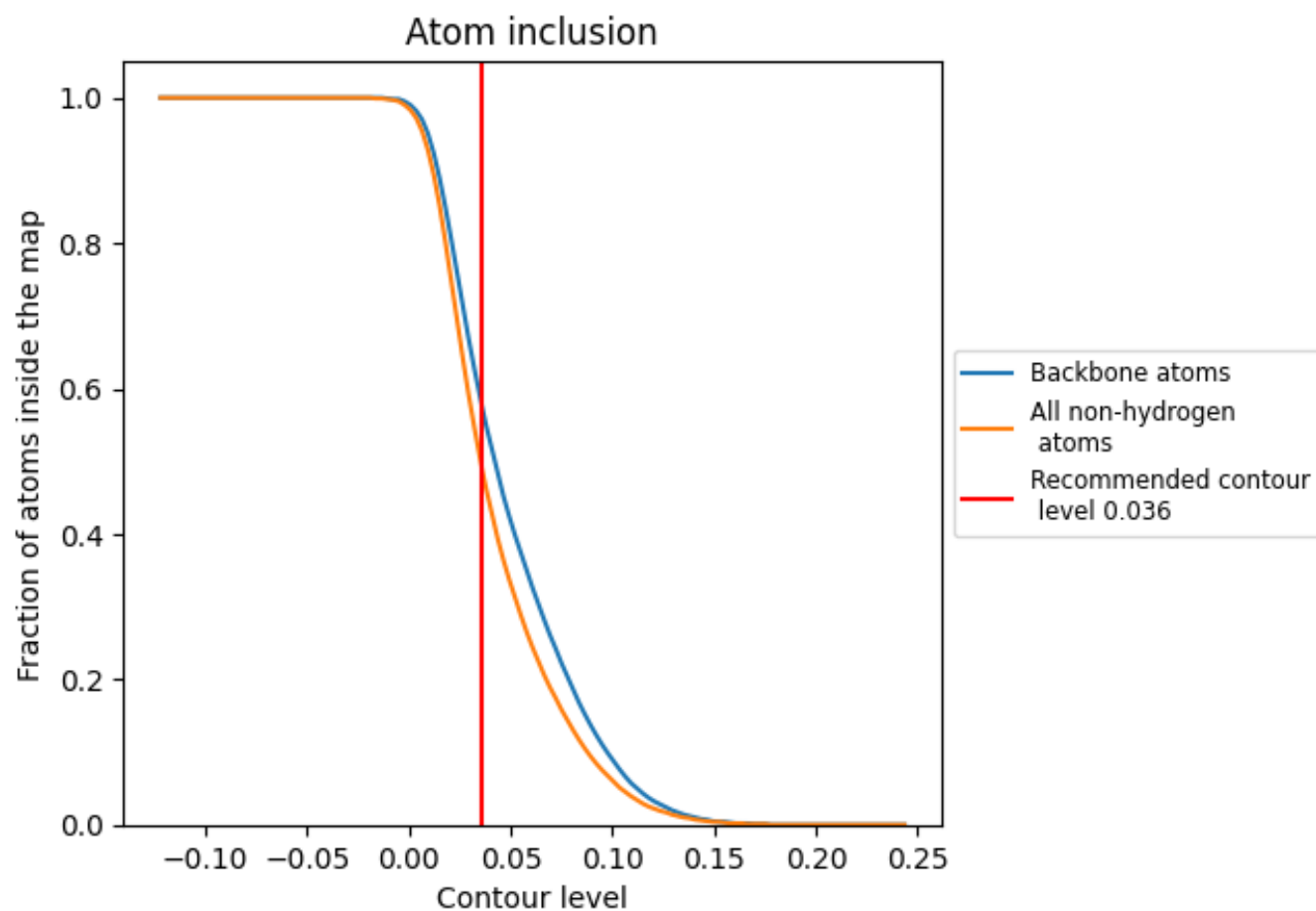
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 49% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.2540
2	 0.0220	 0.0760
3	 0.0080	 0.0640
4	 0.0190	 0.0770
5	 0.0000	 0.0550
6	 0.0040	 0.0430
7	 0.0100	 0.0630
8	 0.0100	 0.0410
A	 0.6810	 0.3630
B	 0.1810	 0.1170
C	 0.7240	 0.3730
D	 0.7460	 0.4020
E	 0.0850	 0.0850
F	 0.7670	 0.4080
G	 0.6910	 0.3490
H	 0.7420	 0.3860
J	 0.6790	 0.3010
K	 0.8000	 0.4520
U	 0.6440	 0.2000
V	 0.5710	 0.2740
W	 0.7070	 0.2760
b	 0.3310	 0.1900
d	 0.4320	 0.2390
e	 0.2380	 0.1230
f	 0.2310	 0.0880
g	 0.3300	 0.1810
h	 0.2890	 0.1520
j	 0.2060	 0.1110
k	 0.0310	 0.0540
l	 0.0340	 0.0340
m	 0.0370	 0.0270
n	 0.0100	 0.0140
p	 0.0070	 0.0770
q	 0.0180	 0.0120
r	 0.0080	 0.0270
x	 0.7280	 0.3730

