



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:08 AM UTC

PDB ID : 3JCM / pdb_00003jcm
EMDB ID : EMD-6561
Title : Cryo-EM structure of the spliceosomal U4/U6.U5 tri-snRNP
Authors : Wan, R.; Yan, C.; Bai, R.; Wang, L.; Huang, M.; Wong, C.C.; Shi, Y.
Deposited on : 2015-12-23
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

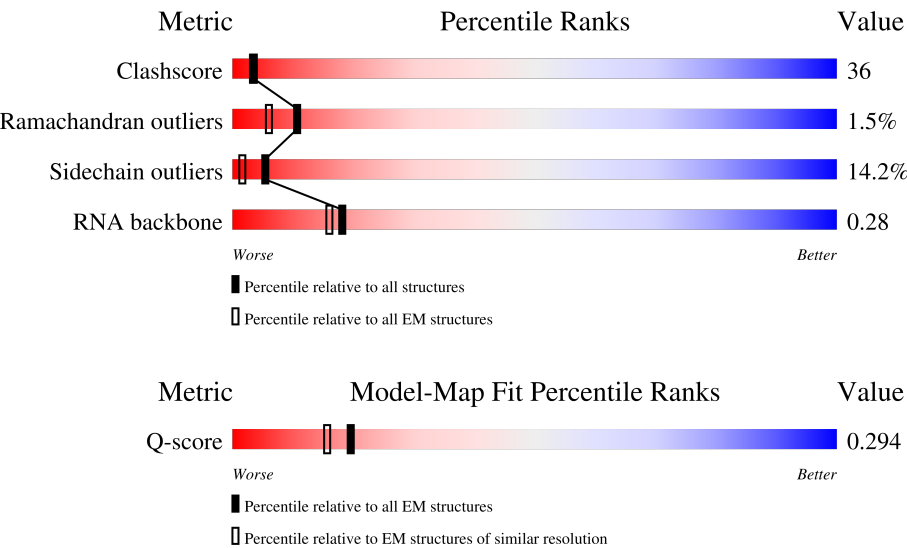
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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.



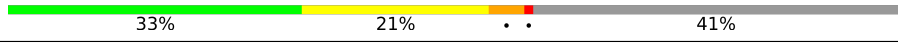
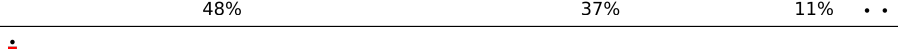
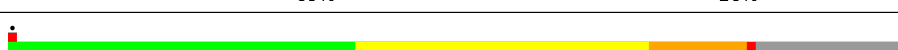
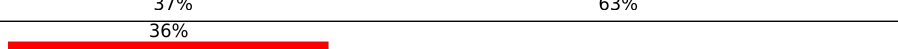
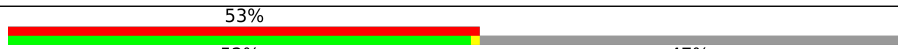
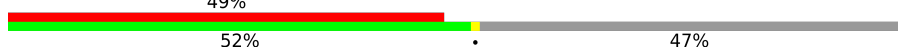
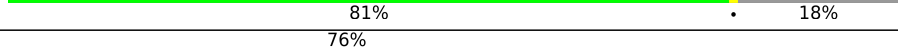
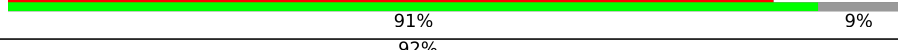
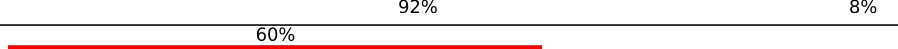
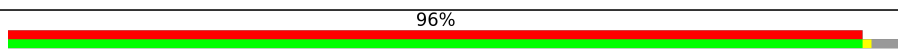
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9193 (3.31 - 4.31)

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	2413	11% 52% 30% 8% 10%
2	B	465	38% 43% 10% 8%
3	I	494	40% 33% 11% 16%

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Mol	Chain	Length	Quality of chain
4	G	899	
5	K	469	
6	L	143	
7	M	126	
8	H	1008	
9	N	2163	
10	J	101	
10	R	101	
11	O	196	
11	S	196	
12	P	146	
12	T	146	
13	Q	110	
13	U	110	
14	V	94	
14	Y	94	
15	W	86	
15	Z	86	
16	X	77	
16	a	77	
17	b	109	
18	c	95	
19	d	89	
20	e	86	
21	f	93	

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Mol	Chain	Length	Quality of chain
22	g	115	
23	h	187	
24	C	20	
25	D	112	
26	E	160	
27	F	214	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	GTP	H	1500	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 58253 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-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2174	Total	C	N	O	S	0	0
			16889	10715	2978	3138	58		

- Molecule 2 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3378	2102	610	652	14		

- Molecule 3 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	416	Total	C	N	O	S	0	0
			3171	2001	573	585	12		

- Molecule 4 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	734	Total	C	N	O	S	0	0
			4927	3063	911	939	14		

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	279	Total	C	N	O	S	0	0
			2328	1476	422	416	14		

- Molecule 6 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	139	Total	C	N	O	S	0	0
			1146	725	199	211	11		

- Molecule 7 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	126	Total	C	N	O	S	0	0
			950	605	163	177	5		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	843	Total	C	N	O	S	0	0
			6732	4350	1119	1235	28		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	1686	Total	C	N	O	0	0
			6744	3372	1686	1686		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	79	Total	C	N	O	0	0
			316	158	79	79		
10	J	79	Total	C	N	O	0	0
			316	158	79	79		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	S	73	Total	C	N	O	0	0
			292	146	73	73		
11	O	73	Total	C	N	O	0	0
			292	146	73	73		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	T	77	Total	C	N	O	0	0
			308	154	77	77		
12	P	77	Total	C	N	O	0	0
			308	154	77	77		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	90	Total	C	N	O	0	0
			360	180	90	90		
13	Q	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	72	Total	C	N	O	0	0
			288	144	72	72		
14	Y	72	Total	C	N	O	0	0
			288	144	72	72		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	W	70	Total	C	N	O	0	0
			280	140	70	70		
15	Z	70	Total	C	N	O	0	0
			280	140	70	70		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	70	Total	C	N	O	0	0
			280	140	70	70		
16	a	71	Total	C	N	O	0	0
			284	142	71	71		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	b	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	92	Total	C	N	O	0	0
			368	184	92	92		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	d	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	f	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 22 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	g	66	Total	C	N	O	0	0
			264	132	66	66		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	h	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 24 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	20	Total	C	N	O	P	0	0
			429	193	79	137	20		

- Molecule 25 is a RNA chain called SNR6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	45	Total	C	N	O	P	0	0
			945	422	170	308	45		

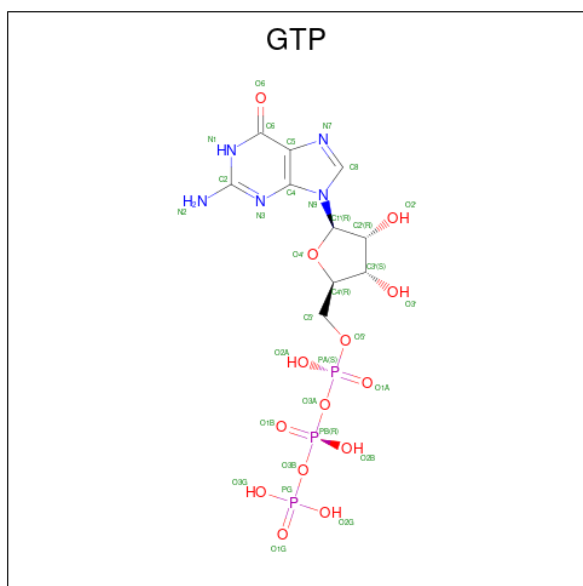
- Molecule 26 is a RNA chain called SNR14 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	85	Total	C	N	O	P	0	0
			1806	807	309	605	85		

- Molecule 27 is a RNA chain called SNR7-L snRNA.

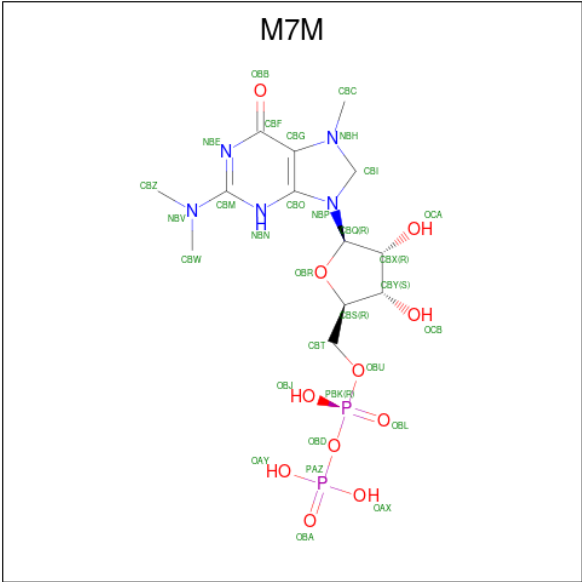
Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	113	Total	C	N	O	P	0	0
			2385	1068	405	799	113		

- Molecule 28 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 29 is N,N,7-trimethylguanosine 5'-(trihydrogen diphosphate) (CCD ID: M7M) (formula: $C_{13}H_{23}N_5O_{11}P_2$).

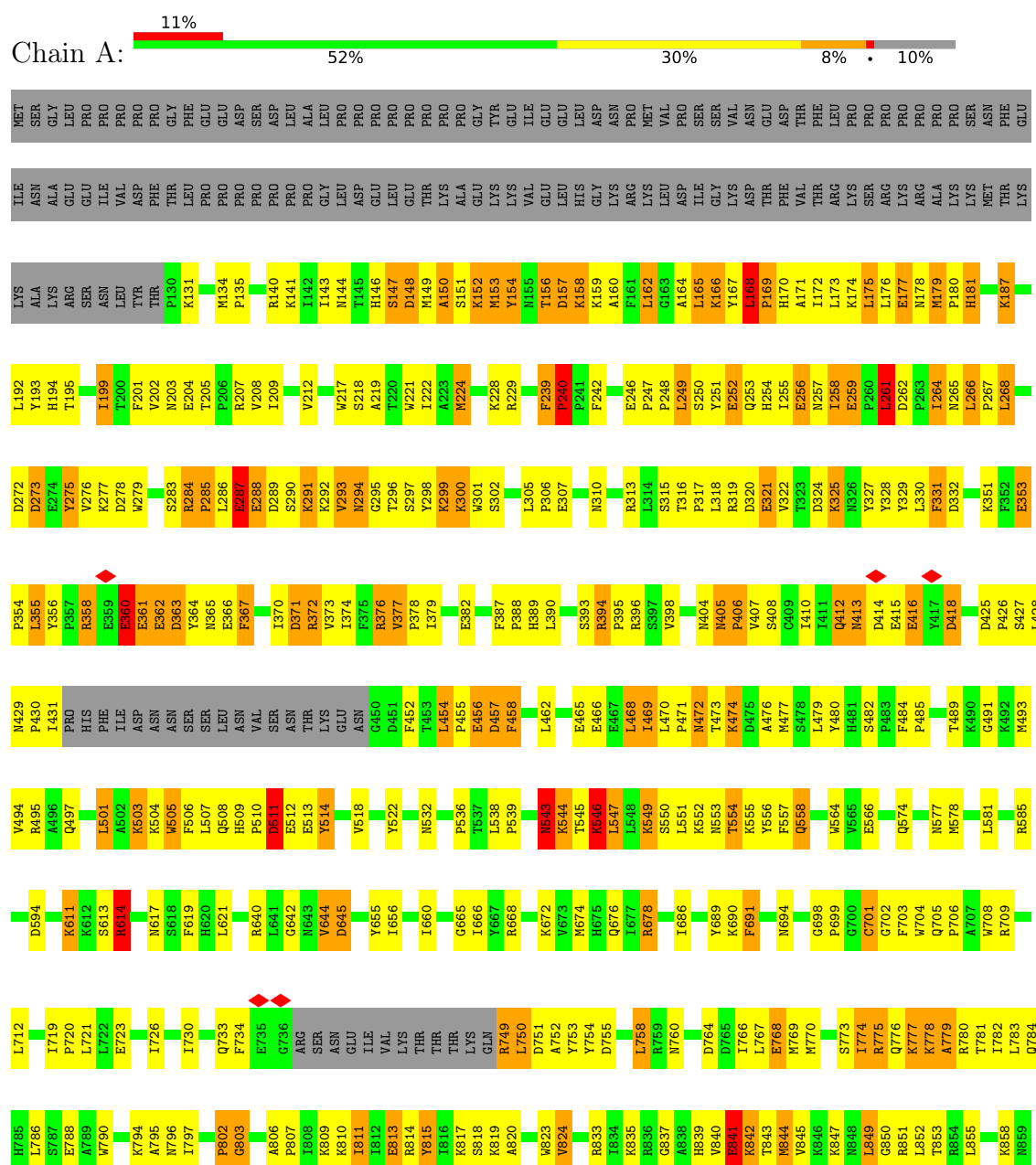


Mol	Chain	Residues	Atoms					AltConf
29	E	1	Total	C	N	O	P	0
			31	13	5	11	2	

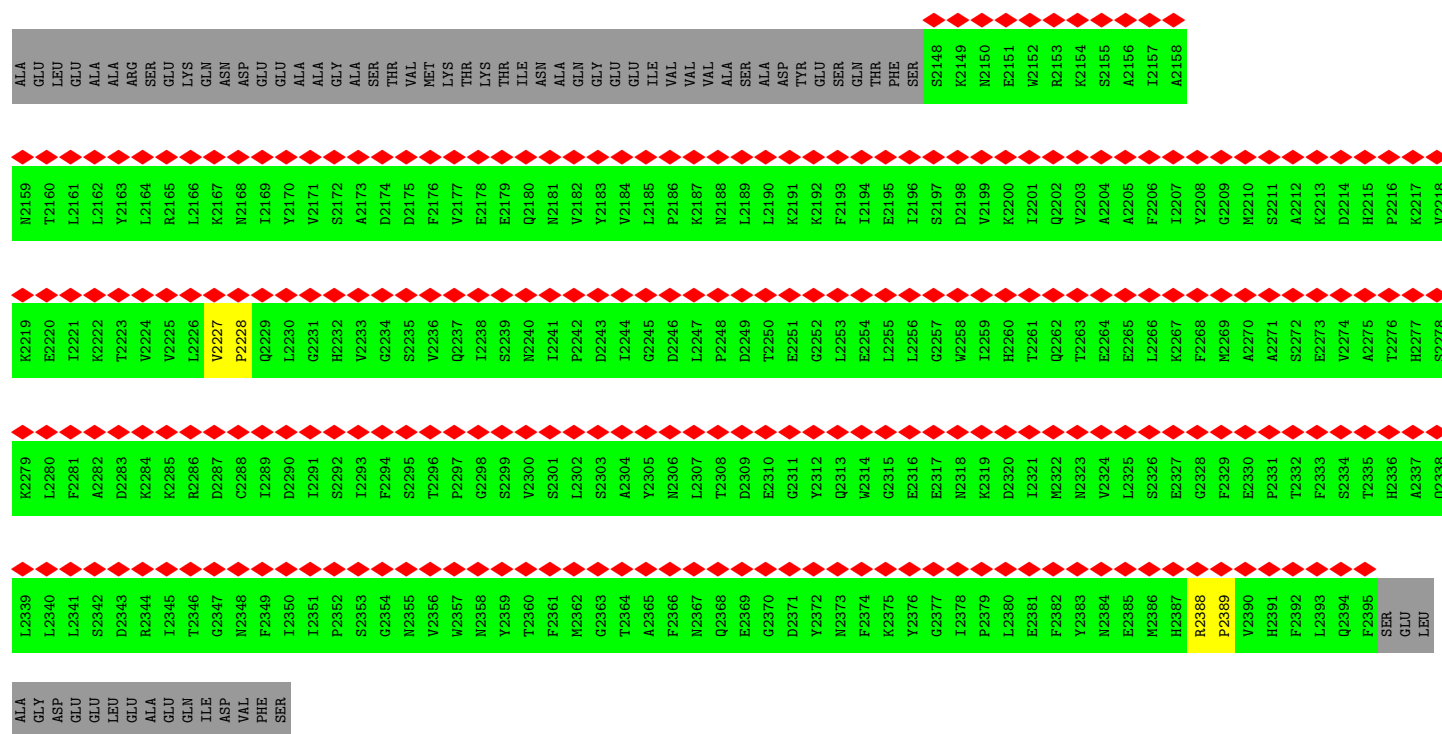
3 Residue-property plots

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.

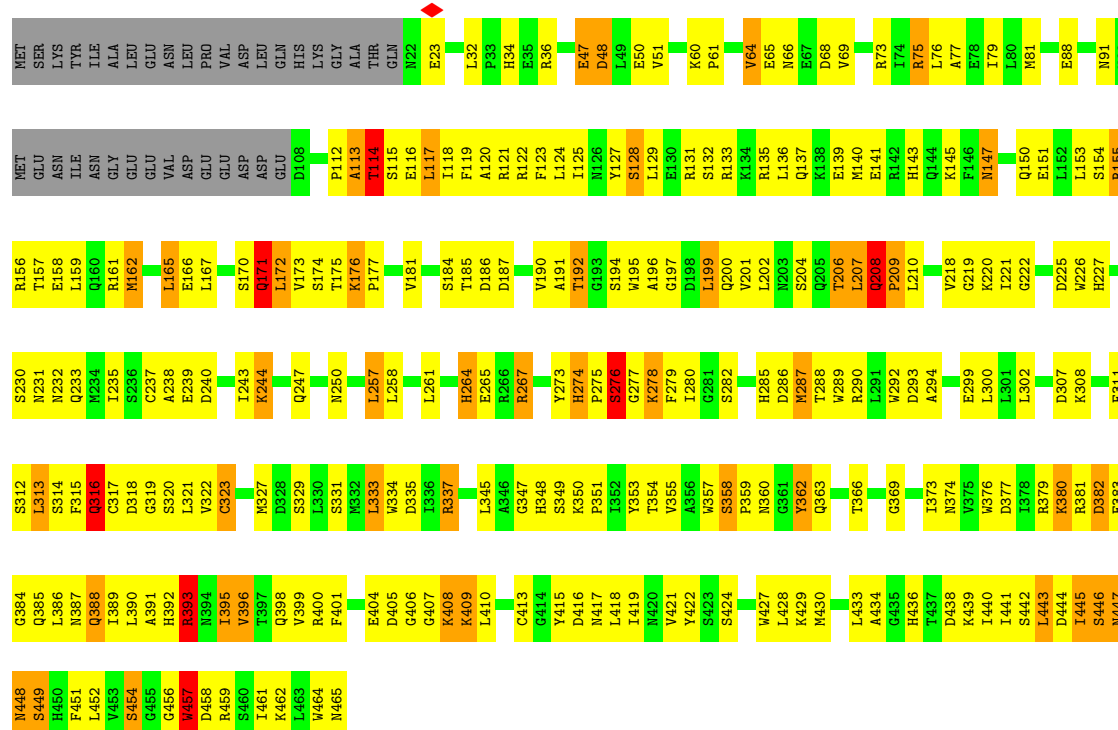
• Molecule 1: Pre-mRNA-splicing factor 8







• Molecule 2: U4/U6 small nuclear ribonucleoprotein PRP4

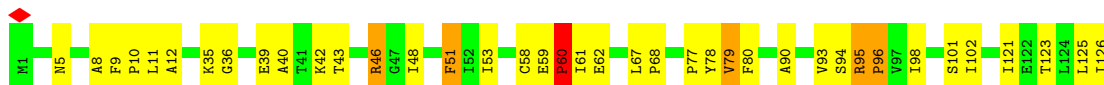


• Molecule 3: Pre-mRNA-processing factor 31

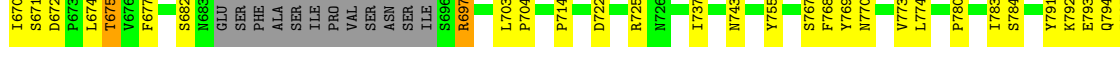
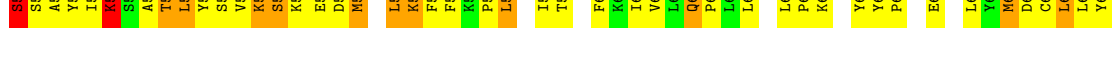
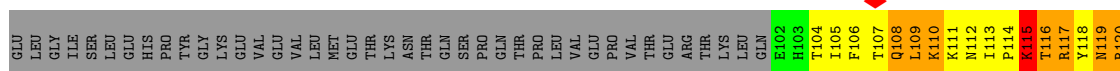
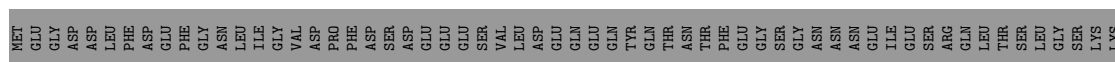


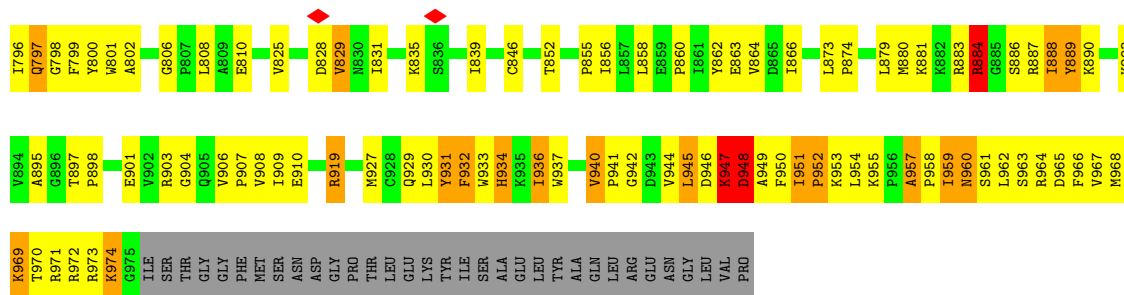


- Molecule 7: 13 kDa ribonucleoprotein-associated protein

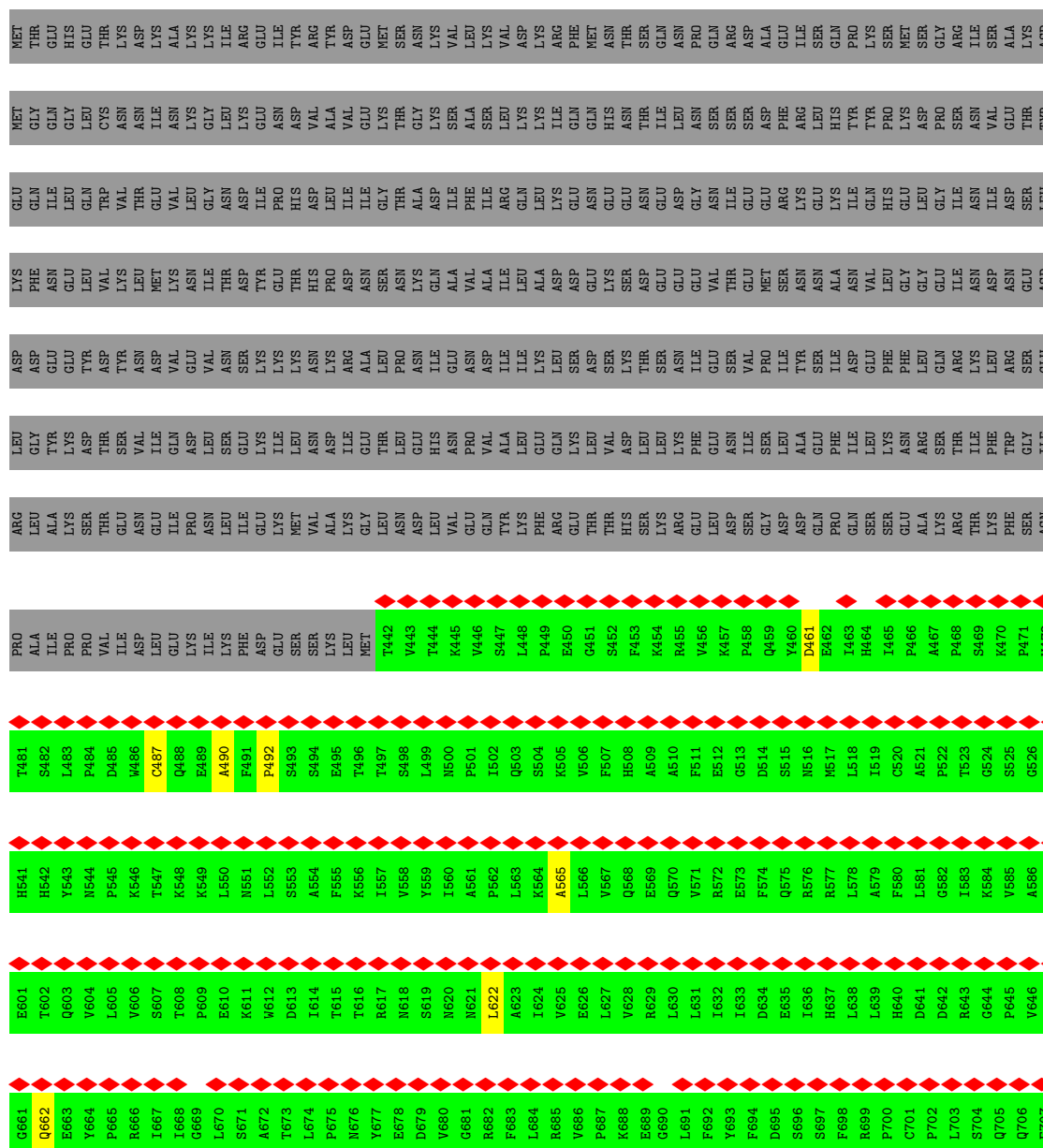
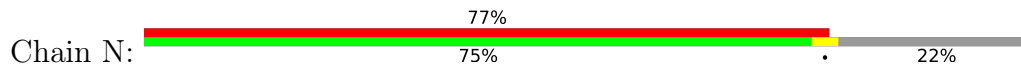


- Molecule 8: Pre-mRNA-splicing factor SNU114





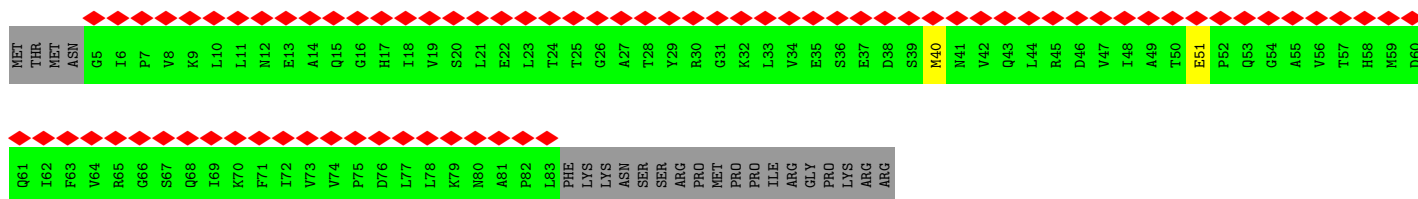
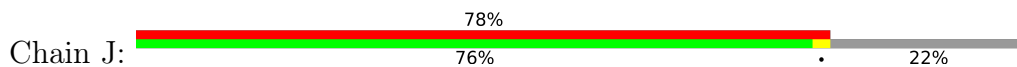
• Molecule 9: Pre-mRNA-splicing helicase BRR2



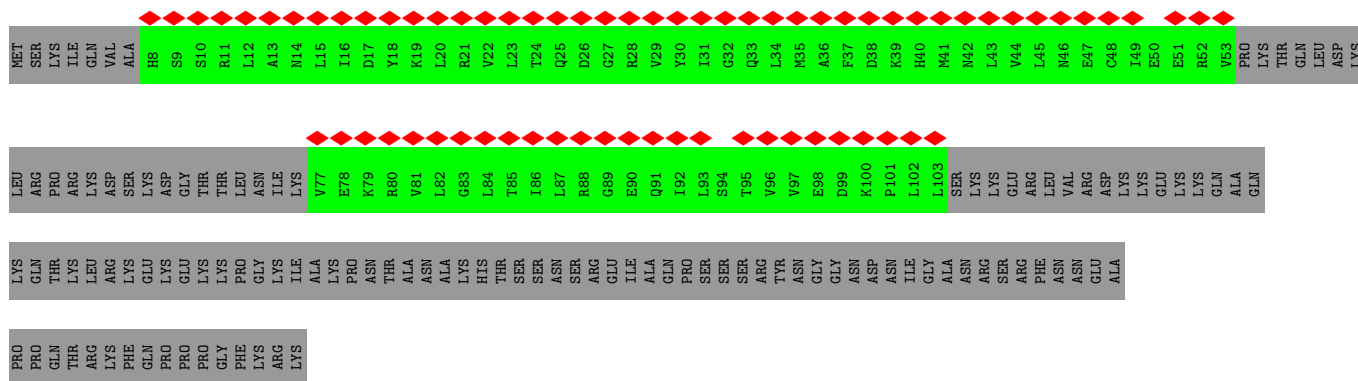
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E1381	L1382	A1383	L1384	L1385	N1386	H1387	W1388	N1389	Q1390	K1391	K1392	G1393	R1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	W1412	W1413	K1414	R1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422	K1423	I1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	P1432	S1433	L1434	M1435	L1436	F1437	L1438	L1439	A1440	
T1321	P1322	L1323	L1324	E1325	N1326	I1327	E1328	I1329	S1330	T1331	S1332	E1333	L1334	G1335	N1336	D1337	D1338	F1339	S1340	E1341	V1342	F1343	E1344	F1346	K1346	T1347	F1348	N1349	K1350	L1351	Q1352	S1353	Q1354	V1355	F1356	E1357	S1358	L1359	Y1360	M1361	S1362	M1363	I1424	S1365	V1366	F1367	V1368	G1369	S1370	G1371	K1372	G1373	T1374	G1375	K1376	T1377	A1378	M1379	A1380	
P1261	D1262	I1263	V1264	G1265	H1266	E1267	F1268	L1269	L1270	S1271	F1272	L1273	Y1274	E1275	L1276	K1277	Q1278	H1279	M1280	Q1281	M1282	M1283	L1284	P1285	P1286	M1287	F1288	L1289	M1290	L1291	L1292	L1293	S1294	E1295	M1296	W1297	W1298	H1299	S1300	E1301	F1302	E1303	I1304	P1305	V1306	S1307	F1308	ASN	GLY	PHE	LYS	LEU	PRO	LYS	F1317	P1318	P1319	P1320		
K1201	M1202	S1203	V1204	T1205	C1206	N1207	A1208	Q1209	P1210	I1211	T1212	L1213	S1214	V1215	M1216	L1217	F1218	N1219	I1220	E1221	I1222	F1223	A1224	D1225	W1226	I1227	W1228	D1229	M1230	N1231	W1232	W1233	G1234	S1235	L1236	E1237	P1238	F1239	L1240	L1241	M1242	L1243	E1244	D1245	T1246	D1247	G1248	D1249	S1250	I1251	Y1252	Y1253	Y1254	D1255	V1256	F1257	F1258	I1259	T1260	
P1261	D1262	I1263	V1264	K1265	H1266	E1267	F1268	L1269	L1270	S1271	F1272	L1273	Y1274	E1275	L1276	K1277	Q1278	H1279	M1280	Q1281	M1282	M1283	L1284	P1285	P1286	M1287	F1288	L1289	M1290	I1291	L1292	L1293	S1294	E1295	M1296	W1297	W1298	H1299	S1300	E1301	F1302	E1303	I1304	P1305	V1306	S1307	F1308	ASN	GLY	PHE	LYS	LEU	PRO	LYS	F1317	P1318	P1319	P1320		
T1321	P1322	L1323	L1324	E1325	N1326	I1327	E1328	I1329	S1330	T1331	S1332	E1333	L1334	G1335	N1336	D1337	D1338	F1339	S1340	E1341	V1342	F1343	E1344	F1346	K1346	T1347	F1348	N1349	K1350	L1351	Q1352	S1353	Q1354	V1355	F1356	E1357	S1358	L1359	Y1360	M1361	S1362	M1363	I1424	S1365	V1366	F1367	V1368	G1369	S1370	G1371	K1372	G1373	T1374	G1375	K1376	T1377	A1378	M1379	A1380	
E1381	L1382	A1383	L1384	L1385	N1386	H1387	W1388	N1389	Q1390	K1391	K1392	G1393	R1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	W1412	W1413	K1414	R1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422	K1423	I1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	P1432	S1433	L1434	M1435	L1436	F1437	L1438	L1439	A1440	
L781	K782	T783	E784	A785	I786	N787	V788	L789	D790	P791	S792	L793	R794	K795	L796	I797	E798	S799	G800	I801	G802	T803	H804	H805	S806	G807	L808	T809	R810	S811	D812	R813	S814	T755	L756	L757	K758	N759	K760	F761	A762	E763	E764	N765	I766	T767	H768	K769	L770	K771	K772	N773	D774	A775	G776	S777	K778	Q779	I780	
P841	A842	H843	T844	V845	I846	I847	K848	G849	T850	D851	V852	Y853	S854	P855	E856	K857	G858	S859	W860	E861	Q862	L863	S864	P865	Q866	D867	V868	L869	Q870	M871	L872	G873	R874	A875	G876	R877	P878	R879	Y880	D881	T882	F883	G884	L885	E886	I887	I888	I889	T890	C830	T831	A832	N773	L833	A835	W836	S777	V838	N839	I780
V901	L902	ASN	GLN	L906	P907	I908	E909	S910	Q911	F912	V913	S914	K915	L916	V917	D918	N919	S959	W860	E861	Q862	L863	S864	P865	Q866	D867	V868	L869	Q870	M871	R832	N933	D934	A935	V936	N937	W938	L939	A940	D1000	Y941	T942	Y943	L944	Y945	V946	R947	M948	L949	A950	S951	P952	M953	L954	Y955	K956	V957	P958	D959	I960
S961	S962	D963	G964	Q965	L966	K967	K968	F969	A970	E971	S972	L973	V974	H975	S976	A977	L978	C979	I980	L981	K982	E983	Q984	E985	L986	V987	L988	Y989	D990	A991	E992	N993	D994	V995	I996	E997	A998	T999	D1000	L1001	G1002	M1003	I1004	A1005	S1006	S1007	F1008	Y1009	I1010	M1011	H1012	M953	L954	Y955	K956	V957	Y958	L959	S900	
E1021	L1022	ASP	GLU	H1025	T1026	T1027	Q1028	I1029	D1030	L1031	F1032	R1033	I1034	F1035	M1036	S1037	S1038	E1039	E1040	F1041	K1042	Y1043	V1044	S1045	V1046	R1047	Y1048	E1049	E1050	K1051	R1052	E1053	L1054	K1055	Q1056	L1057	L1058	E1059	K1060	A1061	P1062	I1063	P1064	I1065	R1066	E1067	D1068	I1069	D1070	D1071	P1072	L1073	A1074	K1075	V1076	M1077	V1078	L1079	L1080	
Q1081	S1082	Y1083	F1084	S1085	Q1086	L1087	K1088	F1089	E1090	G1091	F1092	A1093	L1094	M1095	S1096	D1097	I1098	V1099	F1100	I1101	K1102	Q1103	V1104	M1105	G1106	R1107	L1108	L1109	R1110	A1111	M1112	F1113	E1114	I1115	C1116	L1117	K1118	R1119	G1120	W1121	G1122	H1123	P1124	T1125	R1126	M1127	L1128	L1129	M1130	L1131	C1132	K1133	S1134	A1135	T1136	T1137	K1138	M1139	W1140	
PRO	THR	M1143	C1144	P1145	L1146	R1147	Q1148	F1149	K1150	T1151	C1152	P1153	V1154	E1155	V1156	I1157	K1158	R1159	L1160	E1161	A1162	S1163	T1164	V1165	P1166	W1167	G1168	D1169	Y1170	L1171	Q1172	L1173	E1174	T1175	P1176	E1177	E1178	V1179	G1180	R1181	A1182	I1183	R1184	S1185	E1186	K1187	L1188	G1189	K1190	Q1191	V1192	Y1193	D1194	L1195	L1196	K1197	R1198	F1199	P1200	
K1201	M1202	S1203	V1204	T1205	C1206	N1207	A1208	Q1209	P1210	I1211	T1212	L1213	S1214	V1215	M1216	L1217	F1218	N1219	I1220	E1221	I1222	F1223	A1224	D1225	W1226	I1227	W1228	D1229	M1230	N1231	W1232	W1233	G1234	S1235	L1236	E1237	P1238	F1239	L1240	L1241	M1242	L1243	E1244	D1245	T1246	D1247	G1248	D1249	S1250	I1251	Y1252	Y1253	Y1254	D1255	V1256	F1257	F1258	I1259	T1260	



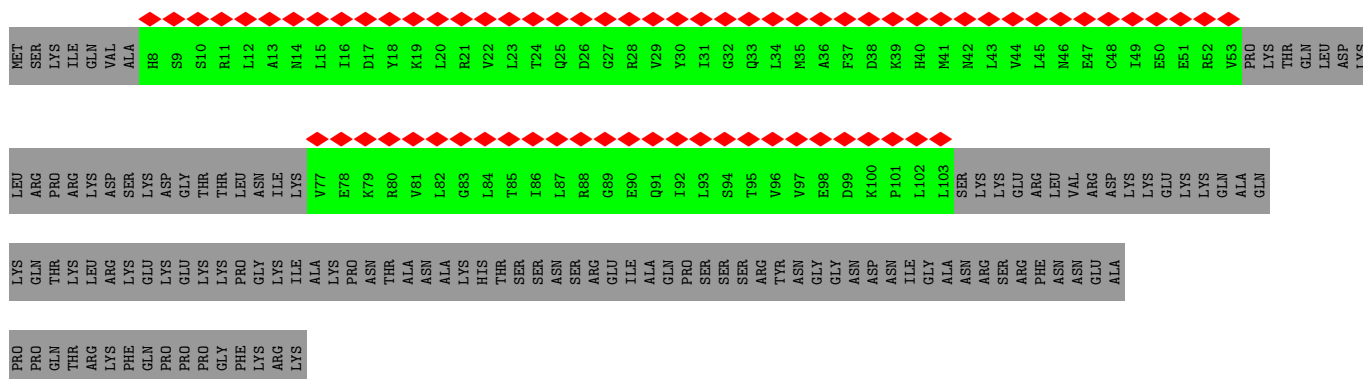
- Molecule 10: Small nuclear ribonucleoprotein Sm D3



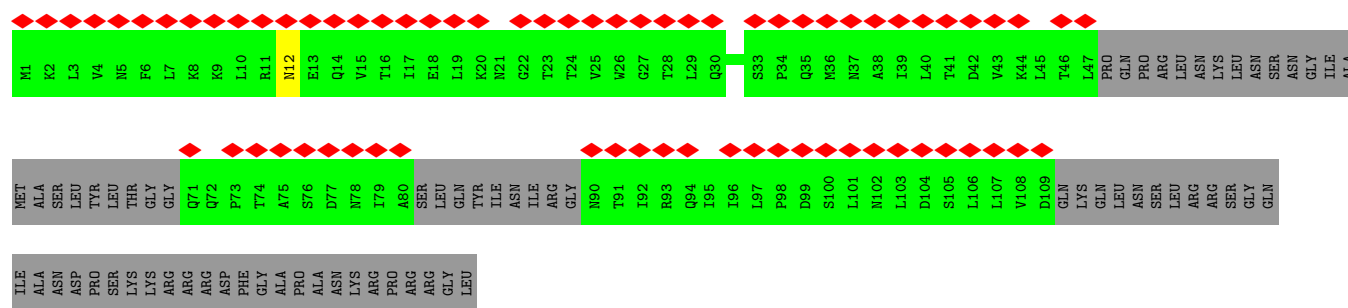
- Molecule 11: Small nuclear ribonucleoprotein-associated protein B



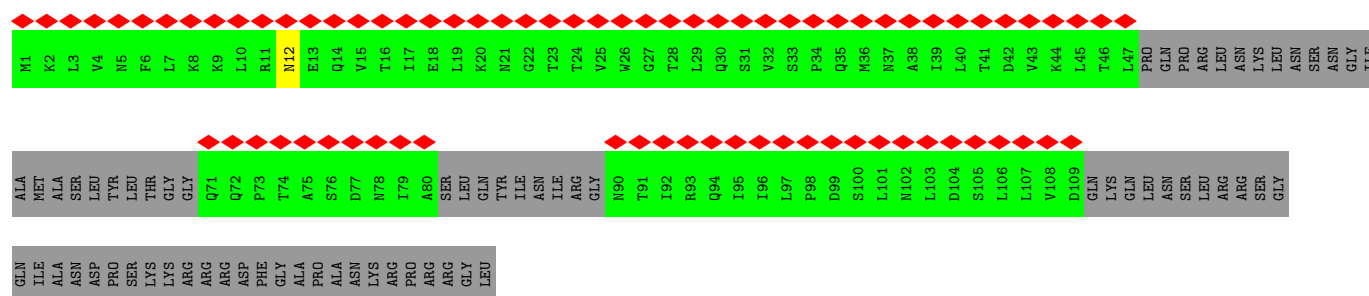
- Molecule 11: Small nuclear ribonucleoprotein-associated protein B



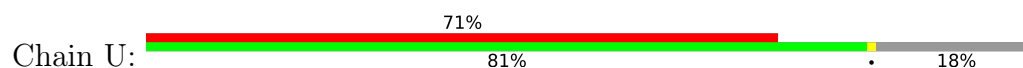
- Molecule 12: Small nuclear ribonucleoprotein Sm D1



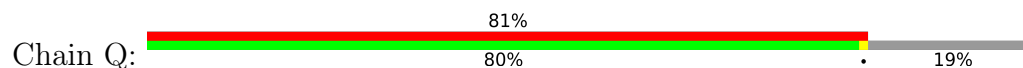
- Molecule 12: Small nuclear ribonucleoprotein Sm D1



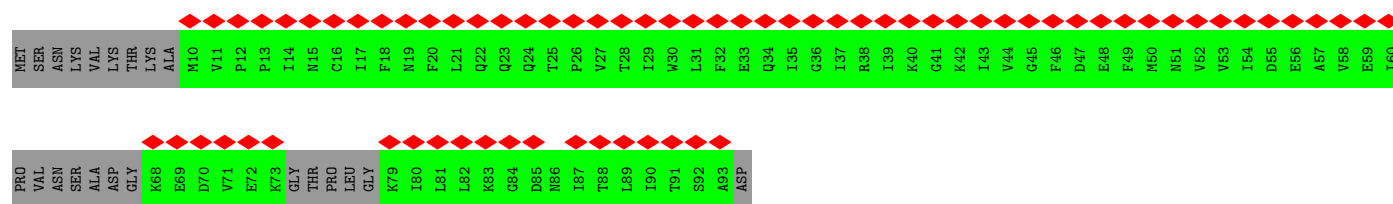
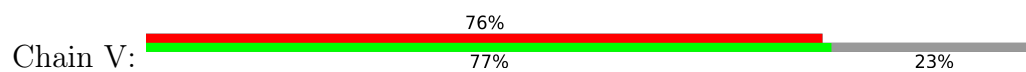
- Molecule 13: Small nuclear ribonucleoprotein Sm D2



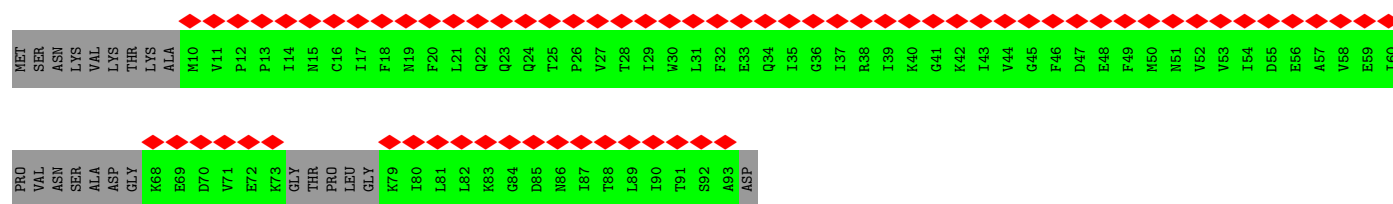
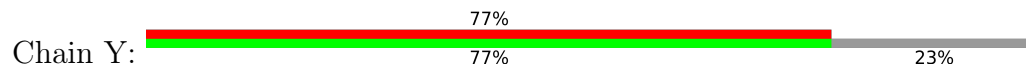
- Molecule 13: Small nuclear ribonucleoprotein Sm D2



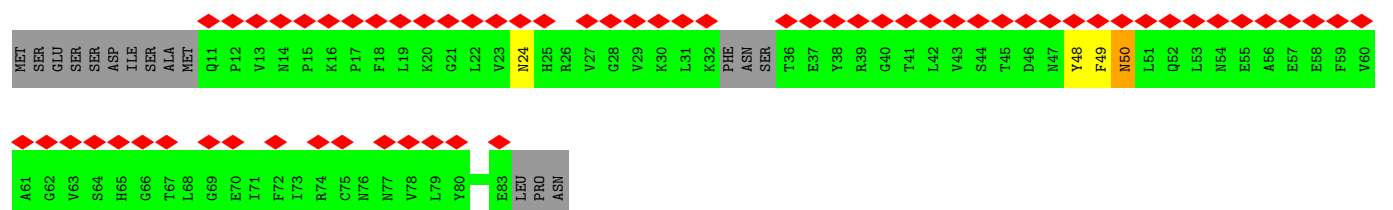
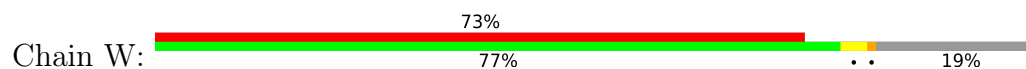
- Molecule 14: Small nuclear ribonucleoprotein E



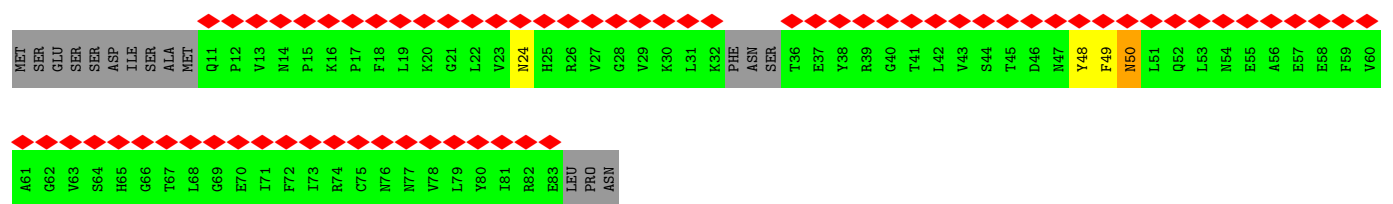
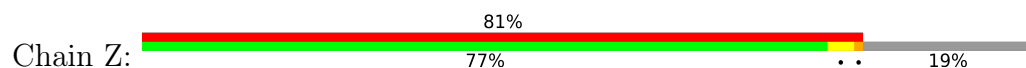
• Molecule 14: Small nuclear ribonucleoprotein E



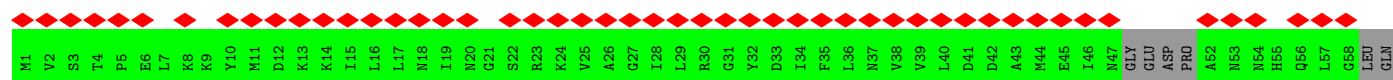
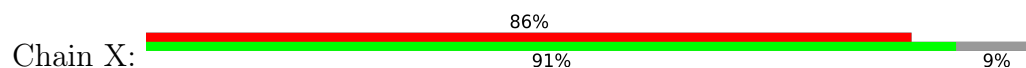
• Molecule 15: Small nuclear ribonucleoprotein F



• Molecule 15: Small nuclear ribonucleoprotein F

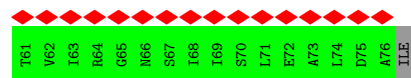
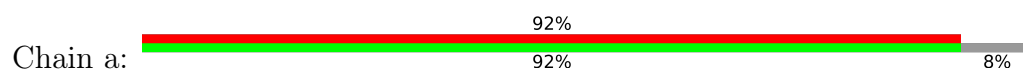


• Molecule 16: Small nuclear ribonucleoprotein G

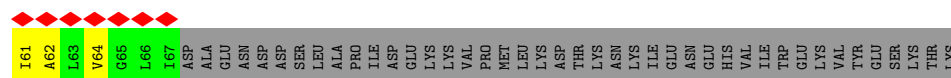
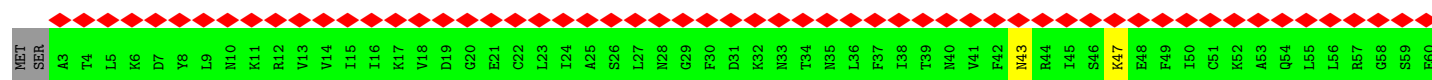




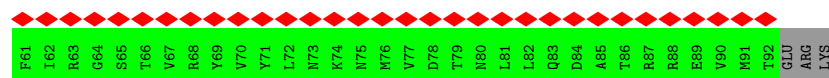
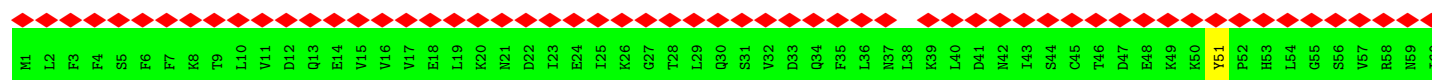
- Molecule 16: Small nuclear ribonucleoprotein G



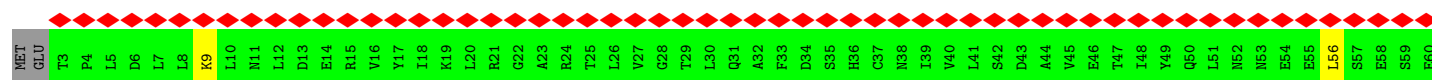
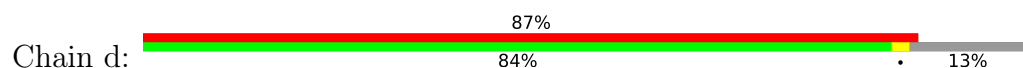
- Molecule 17: U6 snRNA-associated Sm-like protein LSm8



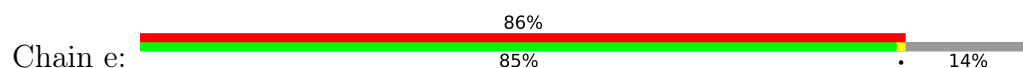
- Molecule 18: U6 snRNA-associated Sm-like protein LSm2

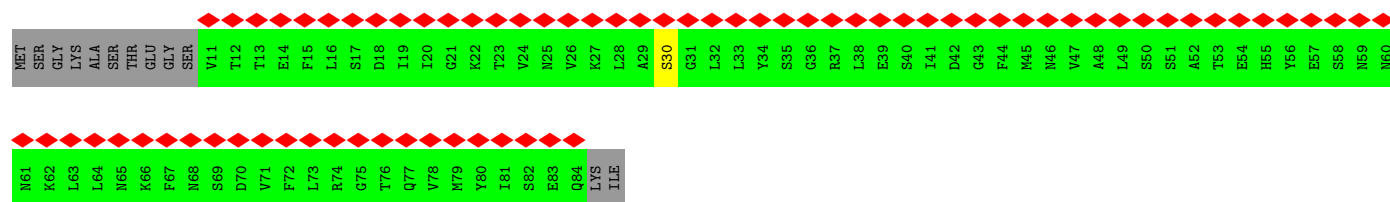


- Molecule 19: U6 snRNA-associated Sm-like protein LSm3

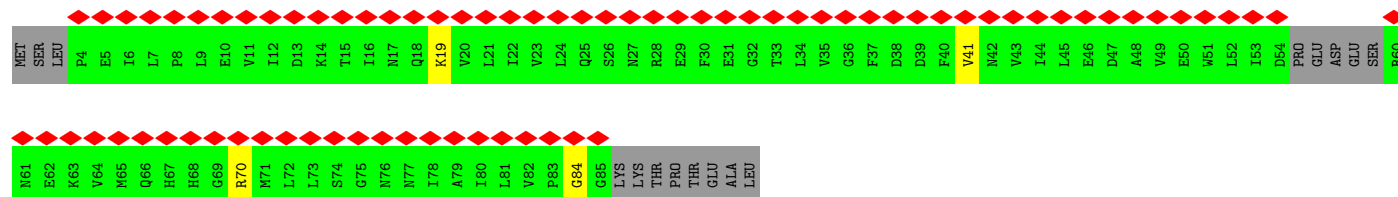
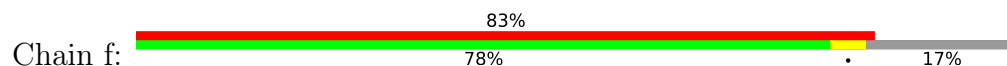


- Molecule 20: U6 snRNA-associated Sm-like protein LSm6

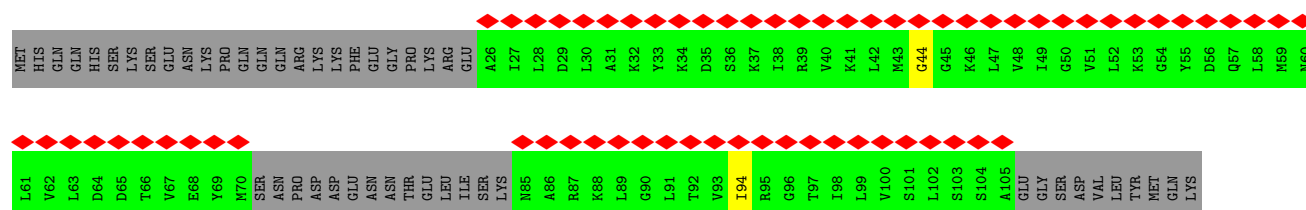




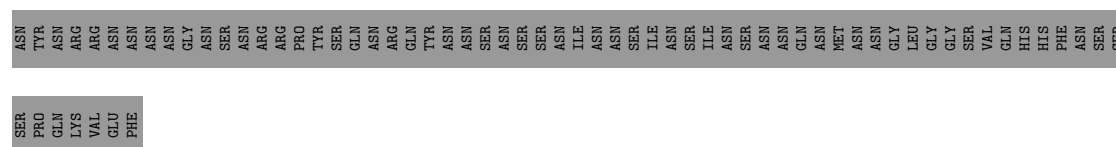
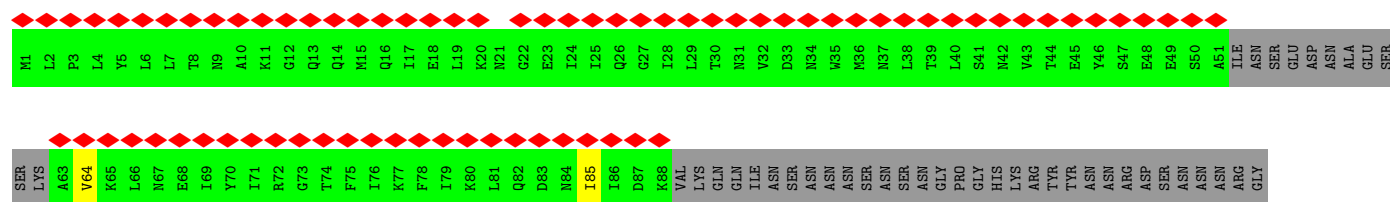
• Molecule 21: U6 snRNA-associated Sm-like protein LSm5



• Molecule 22: U6 snRNA-associated Sm-like protein LSm7



• Molecule 23: U6 snRNA-associated Sm-like protein LSm4



• Molecule 24: pre-mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172134	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0147	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	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, M7M

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	1.10	42/17296 (0.2%)	1.18	66/23336 (0.3%)
2	B	0.96	3/3434 (0.1%)	1.10	11/4635 (0.2%)
3	I	1.12	3/3219 (0.1%)	1.24	10/4332 (0.2%)
4	G	0.83	5/4967 (0.1%)	1.17	29/6746 (0.4%)
5	K	0.88	1/2376 (0.0%)	1.10	8/3183 (0.3%)
6	L	0.98	1/1167 (0.1%)	1.04	1/1571 (0.1%)
7	M	1.40	6/963 (0.6%)	1.27	6/1310 (0.5%)
8	H	0.74	8/6874 (0.1%)	1.18	47/9305 (0.5%)
9	N	0.91	0/6738	1.21	13/8412 (0.2%)
10	J	0.47	0/315	0.92	0/392
10	R	0.47	0/315	0.92	0/392
11	O	0.50	0/290	0.86	0/359
11	S	0.50	0/290	0.86	0/359
12	P	0.49	0/305	0.89	0/376
12	T	0.49	0/305	0.89	0/376
13	Q	0.49	0/354	0.95	2/439 (0.5%)
13	U	0.49	0/358	0.95	2/444 (0.5%)
14	V	0.52	0/285	0.85	0/351
14	Y	0.52	0/285	0.85	0/351
15	W	0.53	0/278	0.80	0/344
15	Z	0.53	0/278	0.80	0/344
16	X	0.42	0/277	0.83	0/341
16	a	0.44	0/281	0.83	0/346
17	b	0.77	0/259	1.35	4/322 (1.2%)
18	c	0.83	0/367	1.31	2/457 (0.4%)
19	d	0.98	0/307	1.46	2/382 (0.5%)
20	e	0.82	0/295	1.41	2/367 (0.5%)
21	f	0.81	0/306	1.26	1/379 (0.3%)
22	g	0.83	0/262	1.22	2/324 (0.6%)
23	h	0.79	0/306	1.39	2/379 (0.5%)
24	C	0.41	0/481	0.74	0/747
25	D	0.60	0/1054	0.87	0/1634

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	E	0.71	3/2016 (0.1%)	0.96	13/3136 (0.4%)
27	F	0.50	2/2659 (0.1%)	0.87	2/4131 (0.0%)
All	All	0.92	74/59562 (0.1%)	1.13	225/80302 (0.3%)

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	3
2	B	0	2
3	I	0	1
4	G	0	7
5	K	0	1
7	M	0	4
8	H	0	2
All	All	0	20

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1608	LEU	CA-C	-9.28	1.41	1.52
4	G	148	ALA	CA-C	-8.04	1.43	1.53
1	A	1335	TRP	CG-CD2	-7.95	1.29	1.43
4	G	147	ALA	CA-C	-7.94	1.43	1.52
7	M	79	VAL	CA-C	-7.93	1.42	1.52

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	852	LEU	N-CA-C	15.26	132.89	112.90
5	K	142	LEU	N-CA-C	14.01	130.59	114.62
4	G	853	GLY	N-CA-C	13.53	145.25	113.18
4	G	143	ARG	N-CA-C	11.96	124.32	111.28
1	A	1383	PHE	CA-C-N	-10.18	112.23	119.66

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1867	GLU	Peptide
1	A	694	ASN	Peptide
2	B	208	GLN	Peptide
2	B	316	GLN	Peptide

5.2 Too-close contacts

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	16889	0	16134	1167	0
2	B	3378	0	3342	377	0
3	I	3171	0	3140	285	0
4	G	4927	0	4006	395	0
5	K	2328	0	2314	164	0
6	L	1146	0	1133	127	0
7	M	950	0	1004	28	0
8	H	6732	0	6904	888	0
9	N	6744	0	1759	36	0
10	J	316	0	86	0	0
10	R	316	0	86	2	0
11	O	292	0	78	0	0
11	S	292	0	78	0	0
12	P	308	0	78	0	0
12	T	308	0	78	0	0
13	Q	356	0	88	0	0
13	U	360	0	89	0	0
14	V	288	0	74	0	0
14	Y	288	0	74	0	0
15	W	280	0	77	1	0
15	Z	280	0	77	1	0
16	X	280	0	79	0	0
16	a	284	0	82	0	0
17	b	260	0	72	1	0
18	c	368	0	99	0	0
19	d	308	0	80	0	0
20	e	296	0	83	0	0
21	f	308	0	85	3	0
22	g	264	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	h	308	0	85	0	0
24	C	429	0	214	48	0
25	D	945	0	478	73	0
26	E	1806	0	907	49	0
27	F	2385	0	1209	209	0
28	H	32	0	12	10	0
29	E	31	0	20	6	0
All	All	58253	0	44280	3674	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 36.

The worst 5 of 3674 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:856:ILE:HA	8:H:944:VAL:CG1	1.17	1.58
4:G:672:LEU:HD21	4:G:704:LEU:CD2	1.29	1.58
8:H:168:VAL:HG13	8:H:173:LYS:CD	1.09	1.56
8:H:364:PHE:CB	8:H:369:LYS:HG3	1.34	1.54
4:G:672:LEU:CD2	4:G:704:LEU:CD2	1.82	1.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2166/2413 (90%)	2019 (93%)	110 (5%)	37 (2%)	7	34
2	B	425/465 (91%)	380 (89%)	36 (8%)	9 (2%)	5	31
3	I	410/494 (83%)	380 (93%)	24 (6%)	6 (2%)	8	36
4	G	684/899 (76%)	604 (88%)	64 (9%)	16 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	273/469 (58%)	247 (90%)	21 (8%)	5 (2%)	6	33
6	L	137/143 (96%)	129 (94%)	6 (4%)	2 (2%)	8	36
7	M	124/126 (98%)	118 (95%)	4 (3%)	2 (2%)	7	35
8	H	837/1008 (83%)	770 (92%)	47 (6%)	20 (2%)	4	29
9	N	1674/2163 (77%)	1555 (93%)	109 (6%)	10 (1%)	21	54
10	J	77/101 (76%)	69 (90%)	6 (8%)	2 (3%)	4	27
10	R	77/101 (76%)	69 (90%)	6 (8%)	2 (3%)	4	27
11	O	69/196 (35%)	63 (91%)	6 (9%)	0	100	100
11	S	69/196 (35%)	63 (91%)	6 (9%)	0	100	100
12	P	71/146 (49%)	66 (93%)	4 (6%)	1 (1%)	9	37
12	T	71/146 (49%)	66 (93%)	4 (6%)	1 (1%)	9	37
13	Q	85/110 (77%)	82 (96%)	3 (4%)	0	100	100
13	U	86/110 (78%)	83 (96%)	3 (4%)	0	100	100
14	V	66/94 (70%)	62 (94%)	4 (6%)	0	100	100
14	Y	66/94 (70%)	62 (94%)	4 (6%)	0	100	100
15	W	66/86 (77%)	59 (89%)	4 (6%)	3 (4%)	2	18
15	Z	66/86 (77%)	60 (91%)	3 (4%)	3 (4%)	2	18
16	X	64/77 (83%)	58 (91%)	6 (9%)	0	100	100
16	a	65/77 (84%)	59 (91%)	6 (9%)	0	100	100
17	b	63/109 (58%)	61 (97%)	2 (3%)	0	100	100
18	c	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
19	d	75/89 (84%)	71 (95%)	4 (5%)	0	100	100
20	e	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
21	f	73/93 (78%)	69 (94%)	3 (4%)	1 (1%)	9	37
22	g	62/115 (54%)	62 (100%)	0	0	100	100
23	h	73/187 (39%)	72 (99%)	1 (1%)	0	100	100
All	All	8236/10574 (78%)	7611 (92%)	505 (6%)	120 (2%)	11	36

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ALA
1	A	157	ASP

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Mol	Chain	Res	Type
1	A	239	PHE
1	A	240	PRO
1	A	259	GLU

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	1749/2182 (80%)	1541 (88%)	208 (12%)	5	22
2	B	374/410 (91%)	317 (85%)	57 (15%)	3	16
3	I	327/445 (74%)	259 (79%)	68 (21%)	1	7
4	G	361/813 (44%)	292 (81%)	69 (19%)	1	9
5	K	253/436 (58%)	225 (89%)	28 (11%)	6	24
6	L	129/132 (98%)	112 (87%)	17 (13%)	4	19
7	M	104/104 (100%)	99 (95%)	5 (5%)	23	47
8	H	757/910 (83%)	632 (84%)	125 (16%)	2	14
All	All	4054/5432 (75%)	3477 (86%)	577 (14%)	5	17

5 of 577 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	129	ILE
8	H	960	ASN
8	H	189	LEU
8	H	124	LEU
8	H	465	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	160	ASN
6	L	87	HIS

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Mol	Chain	Res	Type
4	G	285	HIS
5	K	283	ASN
8	H	135	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	C	19/20 (95%)	17 (89%)	2 (10%)
25	D	41/112 (36%)	22 (53%)	4 (9%)
26	E	85/160 (53%)	28 (32%)	7 (8%)
27	F	111/214 (51%)	51 (45%)	14 (12%)
All	All	256/506 (50%)	118 (46%)	27 (10%)

5 of 118 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	C	-5	A
24	C	-4	A
24	C	-3	A
24	C	-2	A
24	C	-1	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	F	33	U
27	F	81	A
27	F	166	U
27	F	77	A
27	F	83	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are 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
28	GTP	H	1500	-	33,34,34	1.09	3 (9%)	50,54,54	1.71	7 (14%)
29	M7M	E	201	26	31,33,33	1.38	4 (12%)	37,52,52	1.77	5 (13%)

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
28	GTP	H	1500	-	-	4/22/38/38	0/3/3/3
29	M7M	E	201	26	-	6/20/48/48	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	201	M7M	CBG-CBO	3.82	1.46	1.36
28	H	1500	GTP	C5-C4	3.15	1.47	1.38
29	E	201	M7M	CBF-NBE	-2.92	1.33	1.38
29	E	201	M7M	CBG-NBH	-2.91	1.32	1.35
28	H	1500	GTP	C6-N1	-2.44	1.34	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	1500	GTP	C5-C4-N3	-6.09	118.69	128.39
29	E	201	M7M	NBP-CBI-NBH	-5.85	95.09	103.37
28	H	1500	GTP	C2-N3-C4	4.83	120.62	112.30
29	E	201	M7M	PBK-OBV-CBT	4.60	147.72	121.35
28	H	1500	GTP	N9-C4-N3	4.29	134.54	125.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	E	201	M7M	NBE-CBM-NBV-CBW
29	E	201	M7M	NBE-CBM-NBV-CBZ
29	E	201	M7M	NBN-CBM-NBV-CBZ
29	E	201	M7M	CBS-CBT-OBV-PBK
28	H	1500	GTP	O4'-C4'-C5'-O5'

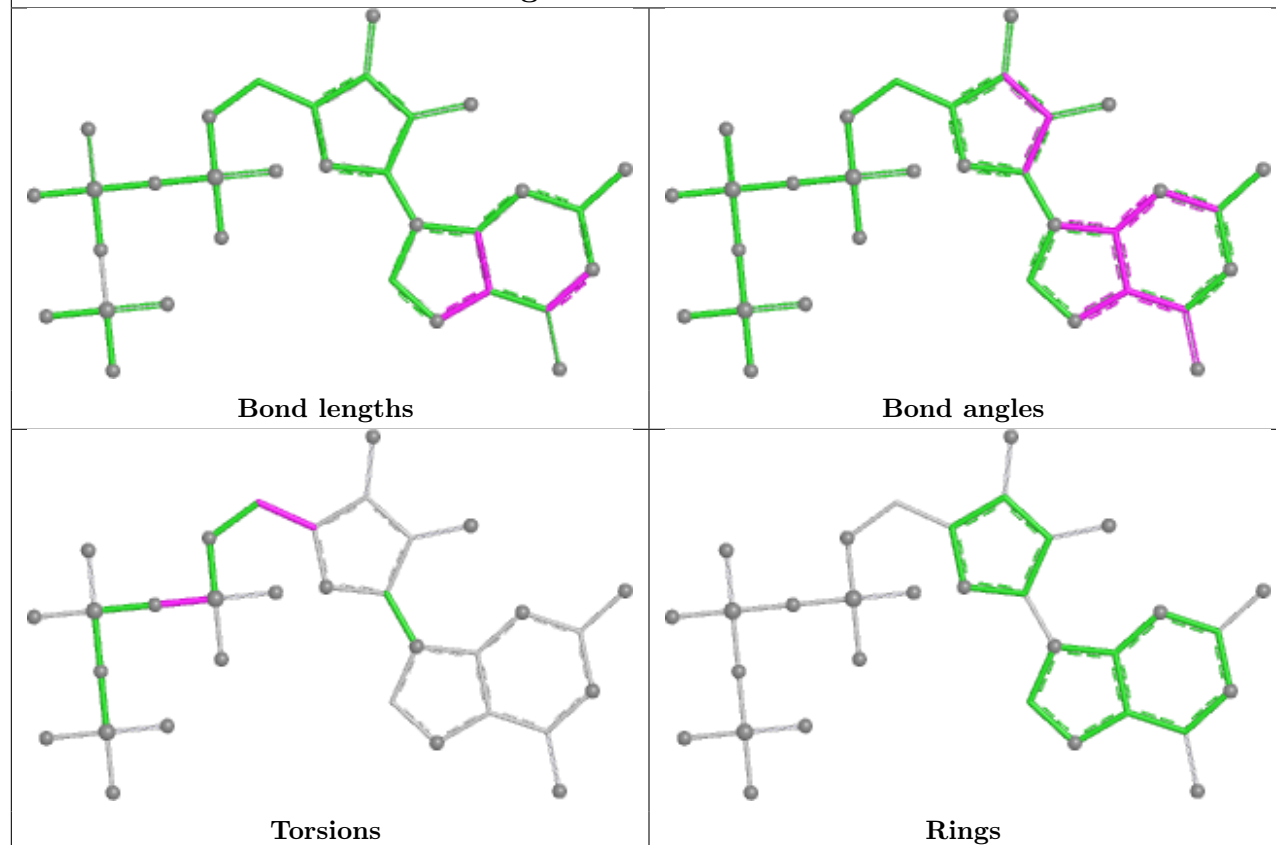
There are no ring outliers.

2 monomers are involved in 16 short contacts:

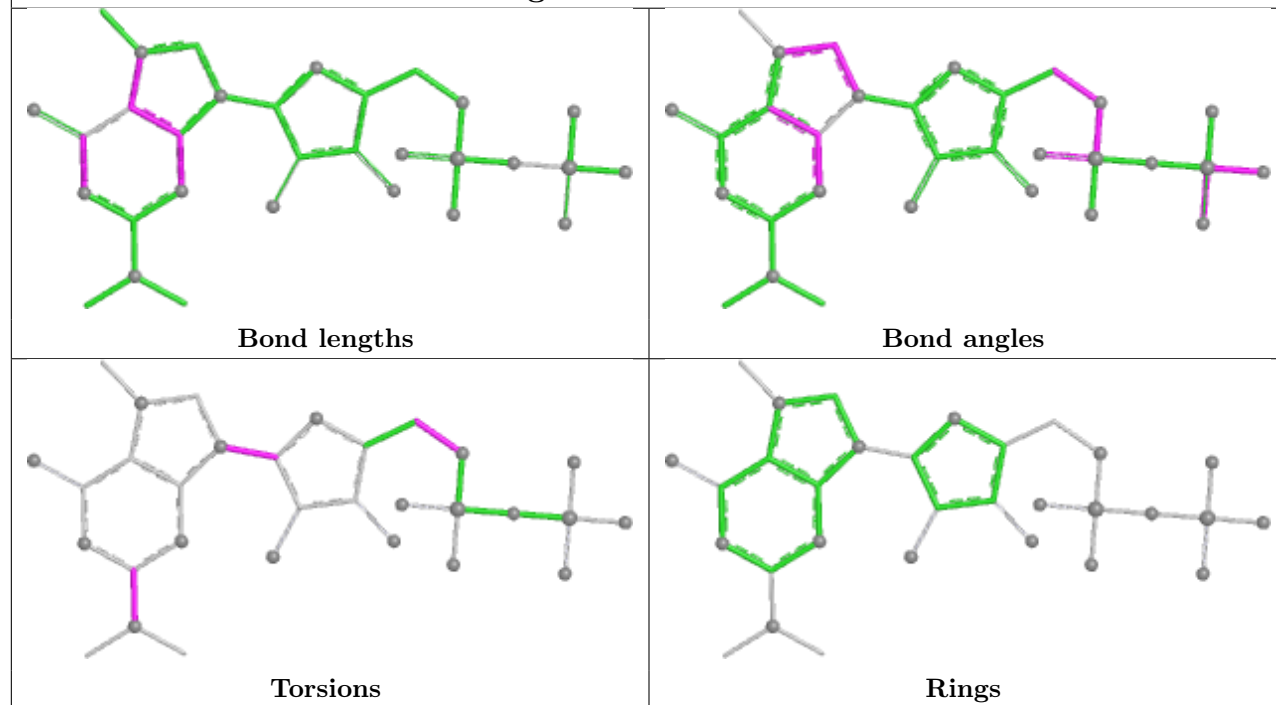
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	H	1500	GTP	10	0
29	E	201	M7M	6	0

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

Ligand GTP H 1500



Ligand M7M E 201



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

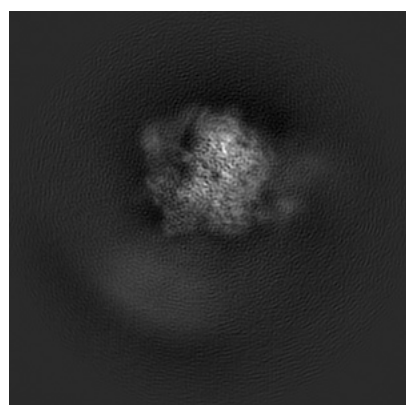
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6561. These allow visual inspection of the internal detail of the map and identification of artifacts.

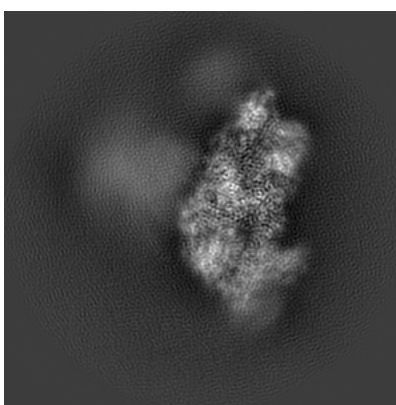
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

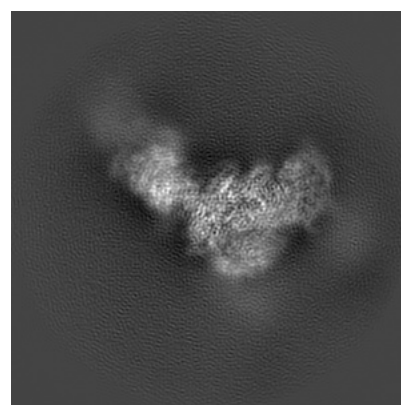
6.1.1 Primary map



X



Y

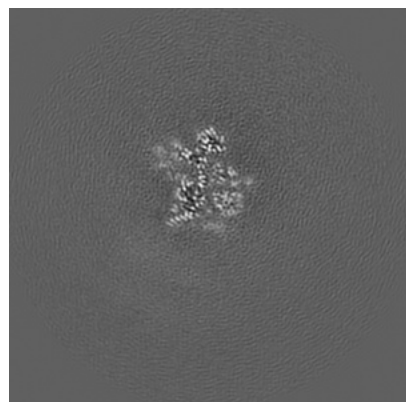


Z

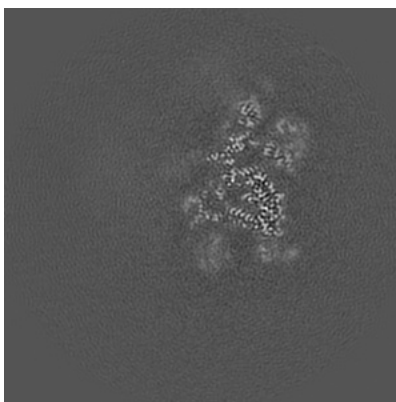
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

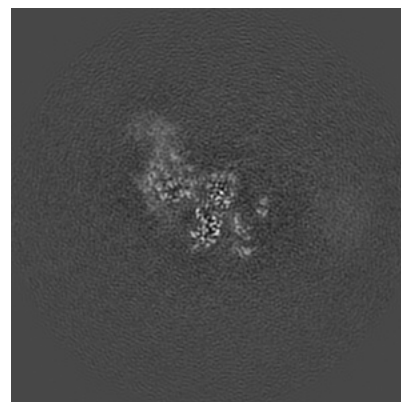
6.2.1 Primary map



X Index: 160



Y Index: 160

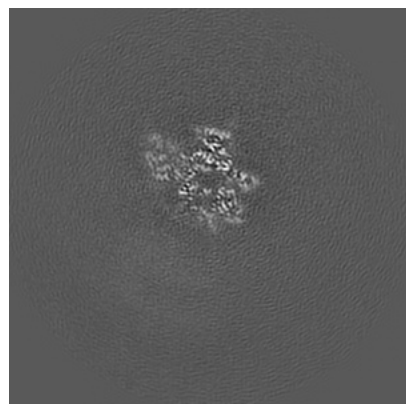


Z Index: 160

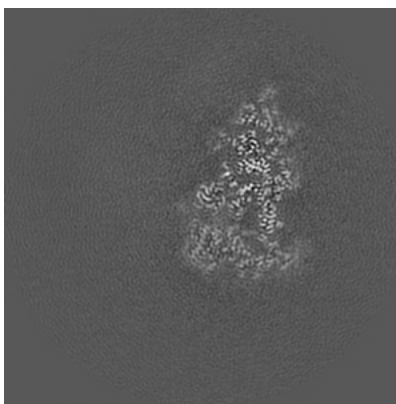
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

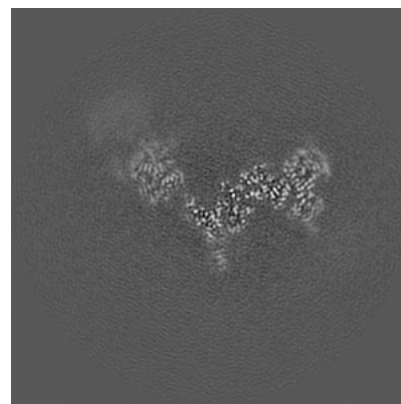
6.3.1 Primary map



X Index: 167



Y Index: 171

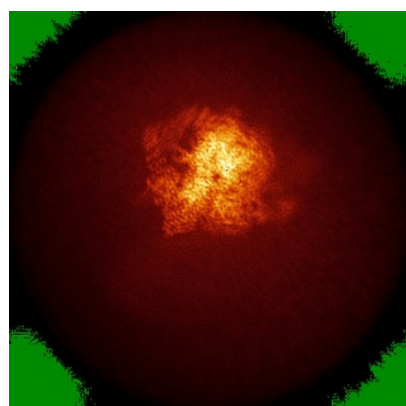


Z Index: 199

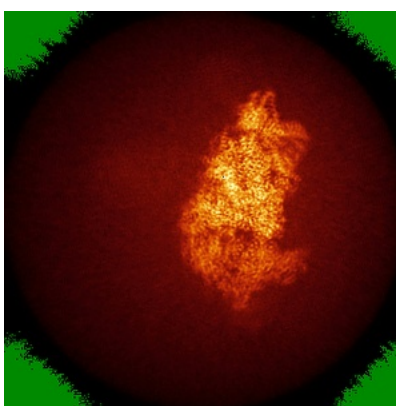
The images above show the largest variance slices of the map in three orthogonal directions.

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

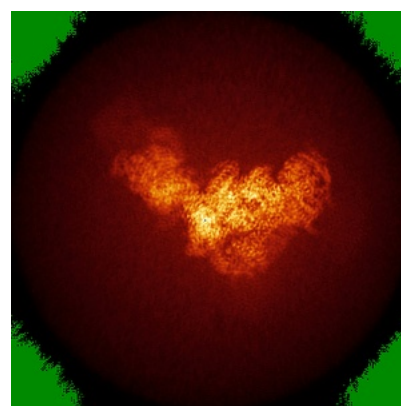
6.4.1 Primary map



X



Y

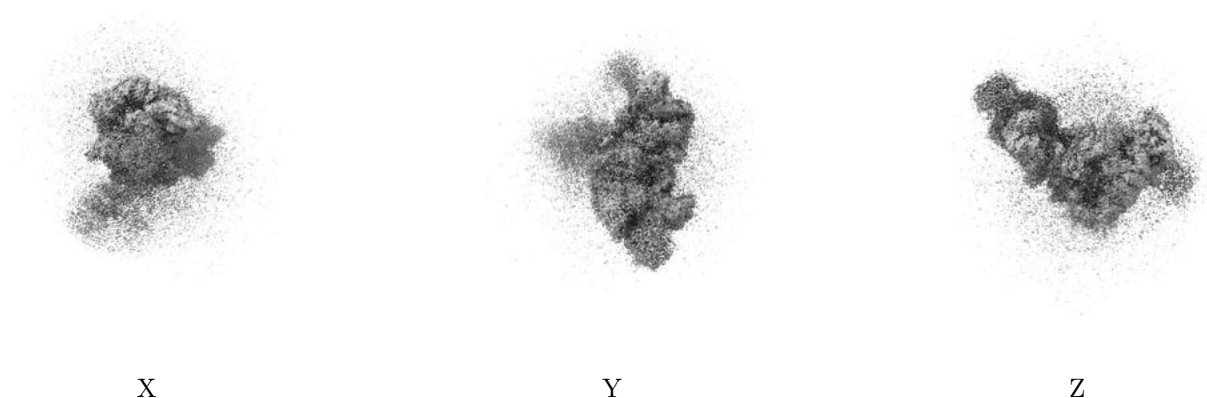


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0147. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

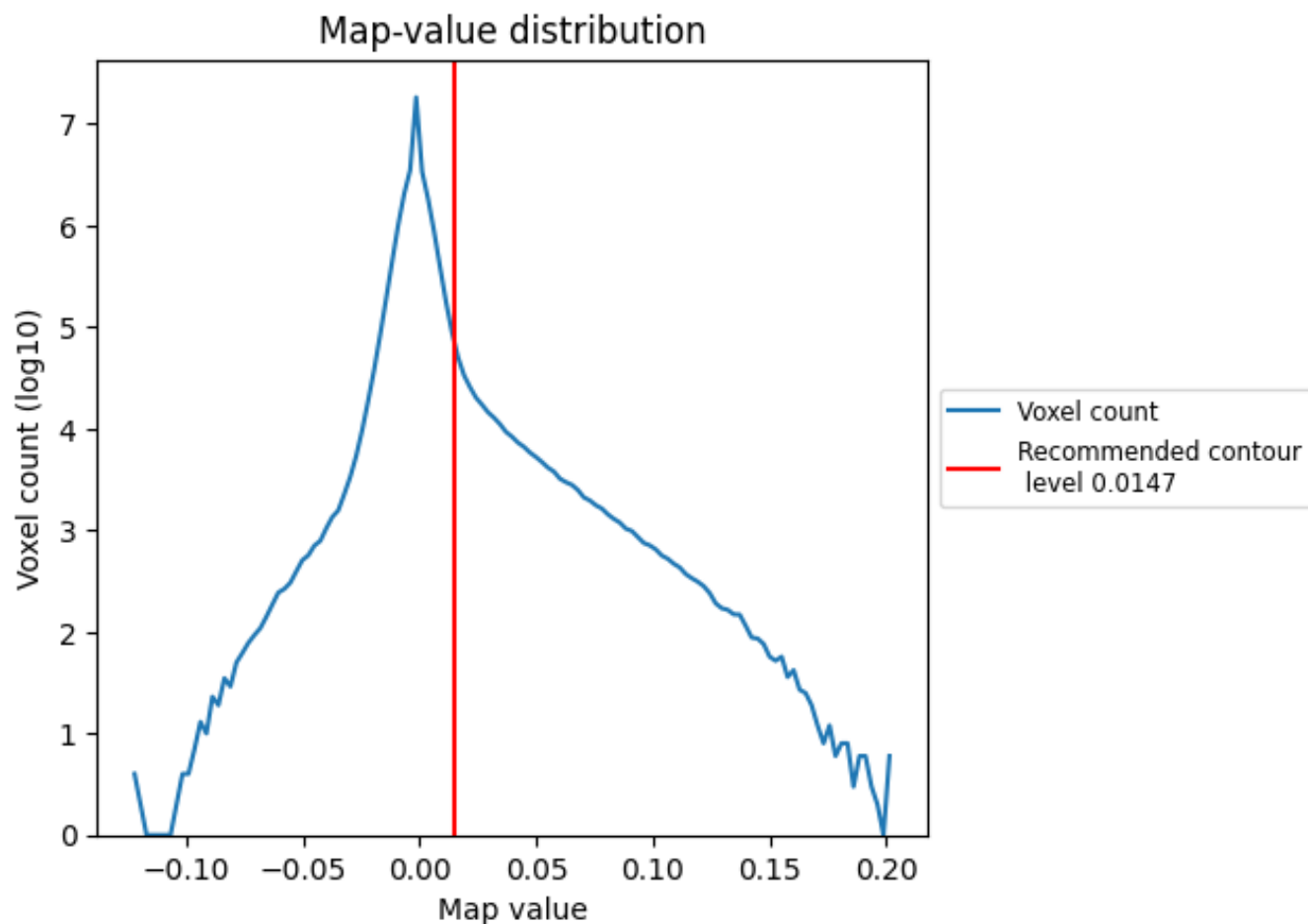
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

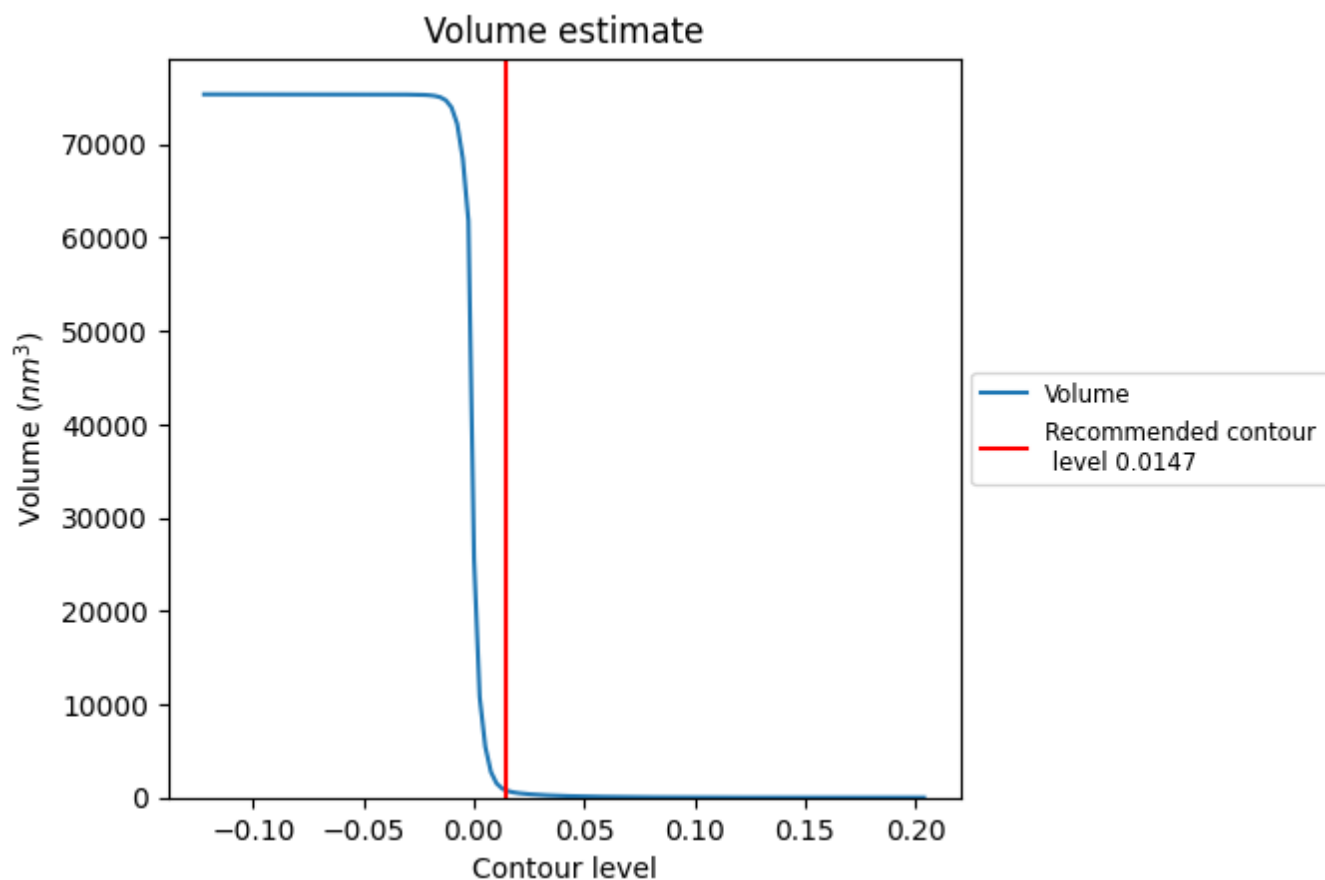
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

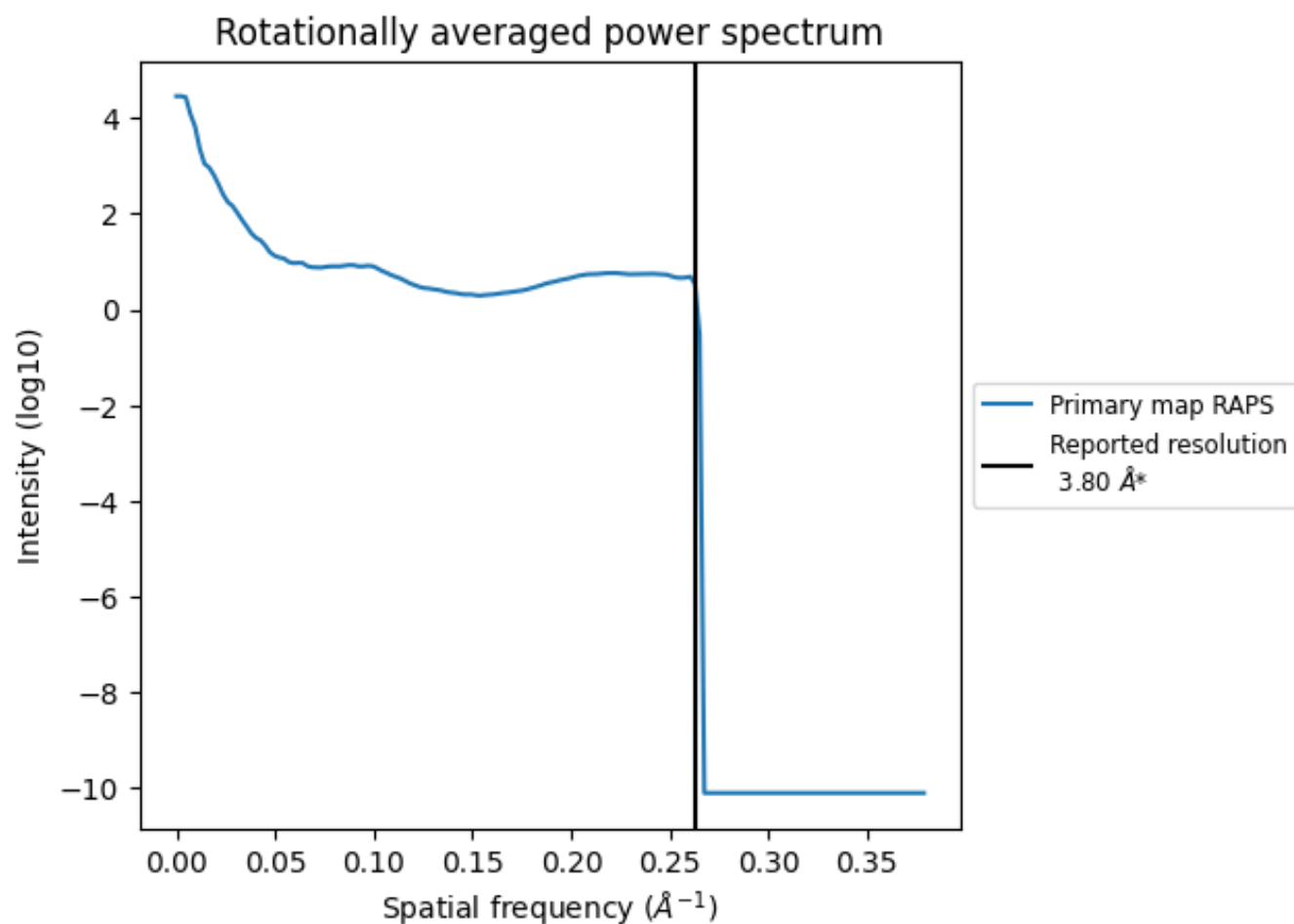
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 773 nm^3 ; this corresponds to an approximate mass of 699 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 0.263 $\text{\AA}^{-1}$

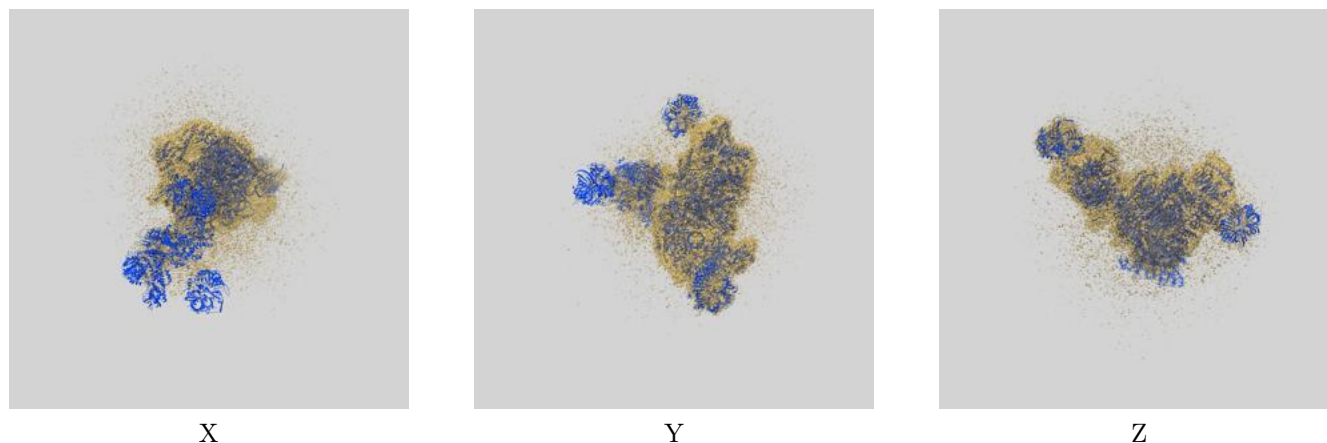
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

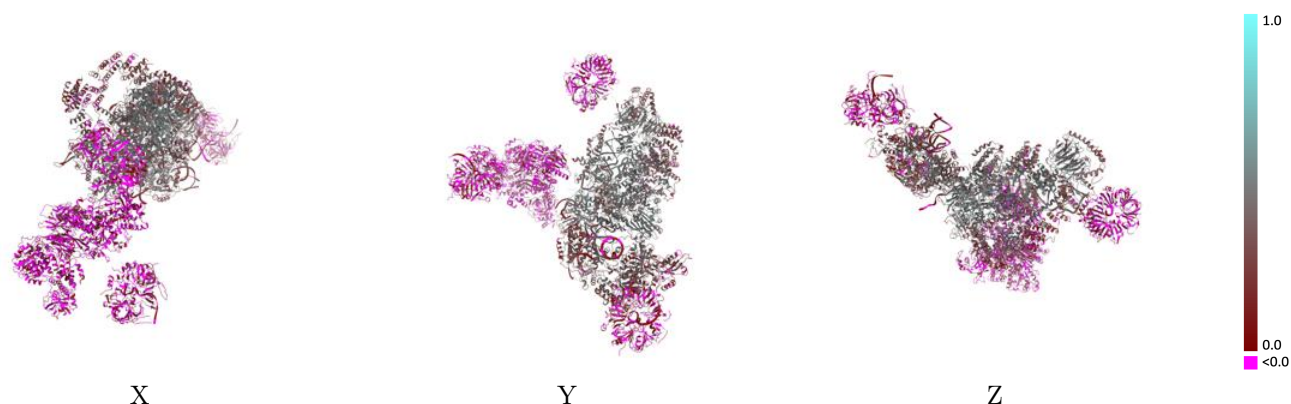
This section contains information regarding the fit between EMDB map EMD-6561 and PDB model 3JCM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



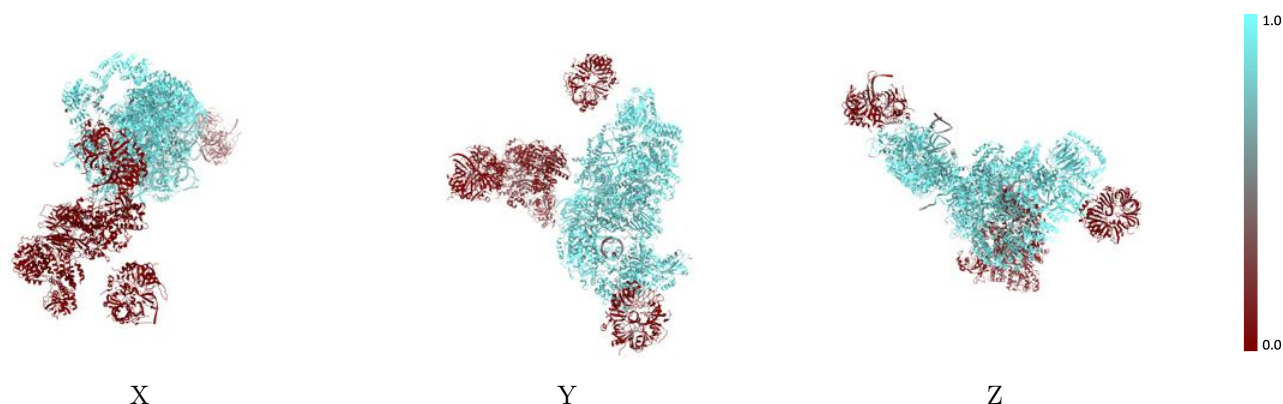
The images above show the 3D surface view of the map at the recommended contour level 0.0147 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



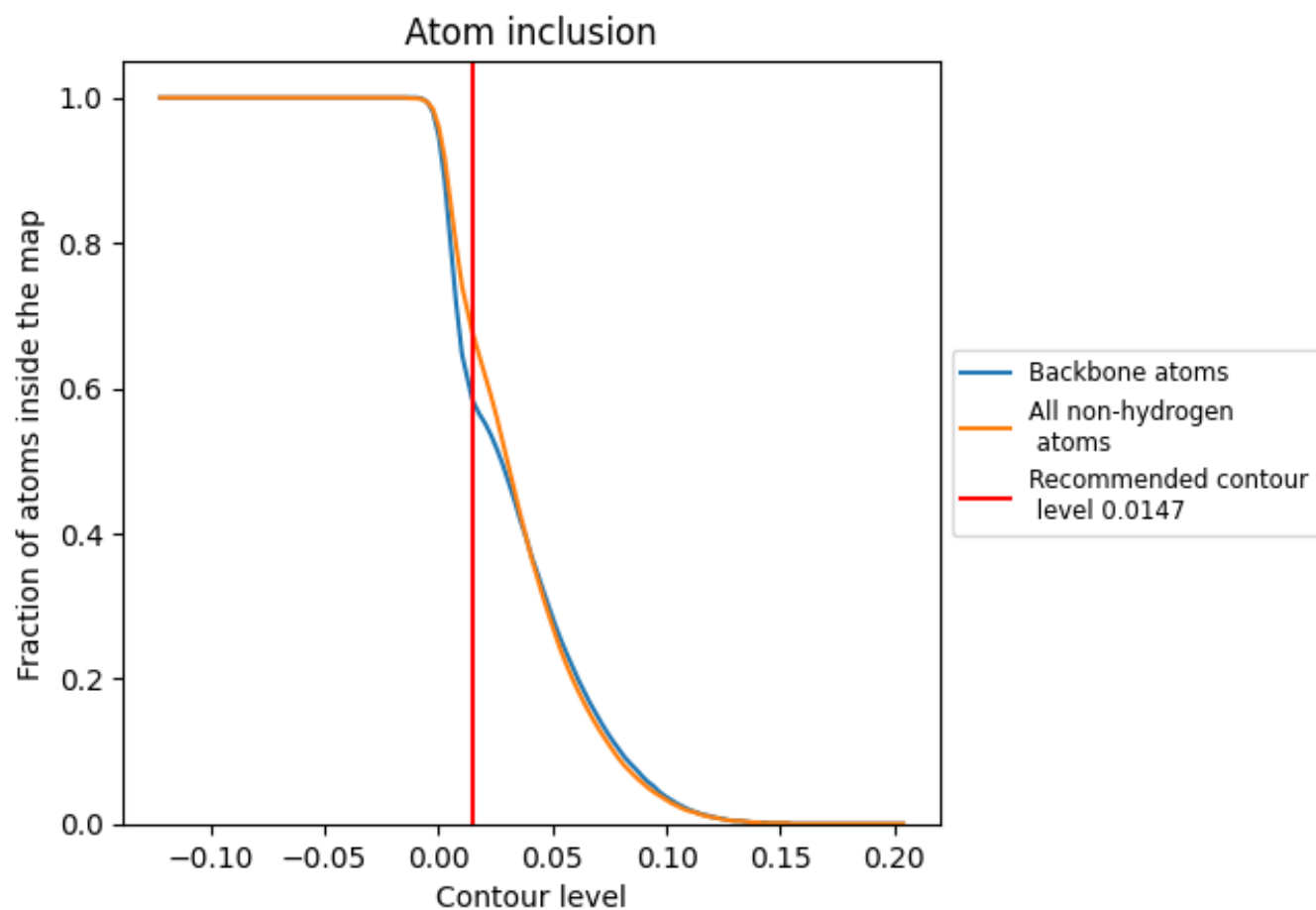
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0147).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 68% 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 (0.0147) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.2940
A	 0.8560	 0.3990
B	 0.9060	 0.4200
C	 0.8700	 0.2880
D	 0.8910	 0.3730
E	 0.7470	 0.3630
F	 0.7110	 0.2090
G	 0.9070	 0.3400
H	 0.8910	 0.3210
I	 0.9220	 0.4400
J	 0.0000	 -0.0190
K	 0.9070	 0.4070
L	 0.9240	 0.4570
M	 0.9270	 0.4890
N	 0.0230	 0.0020
O	 0.0000	 0.0160
P	 0.0030	 0.0440
Q	 0.0000	 0.0460
R	 0.1490	 0.0620
S	 0.0510	 0.0240
T	 0.0910	 0.0940
U	 0.1220	 0.0370
V	 0.0490	 -0.0010
W	 0.1320	 0.0400
X	 0.0500	 0.0310
Y	 0.0000	 -0.0070
Z	 0.0040	 0.0190
a	 0.0000	 0.0330
b	 0.0110	 0.0180
c	 0.0110	 0.0280
d	 0.0100	 0.0140
e	 0.0270	 0.0190
f	 0.0130	 0.0250
g	 0.0110	 0.0220
h	 0.0160	 -0.0580

