



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 05:45 PM UTC

PDB ID : 7VCI / pdb_00007vci
EMDB ID : EMD-31891
Title : Structure of Xenopus laevis NPC nuclear ring asymmetric unit
Authors : Tai, L.; Zhu, Y.; Sun, F.
Deposited on : 2021-09-03
Resolution : 8.10 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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

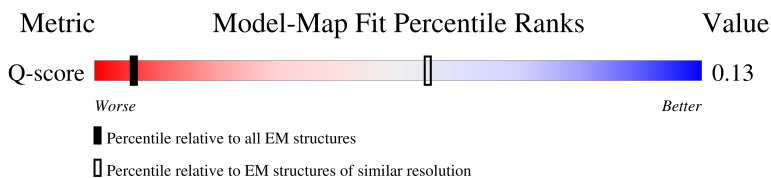
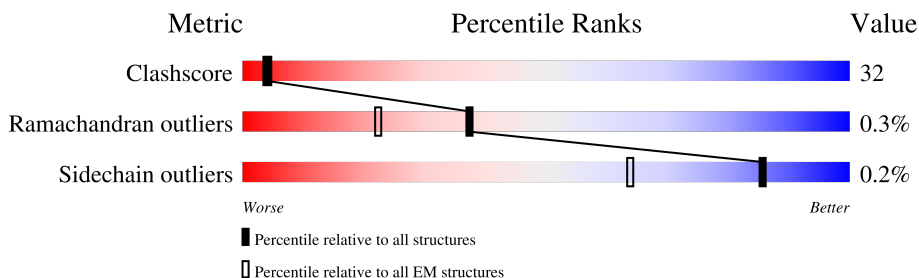
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

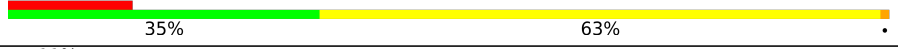
The reported resolution of this entry is 8.10 Å.

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.



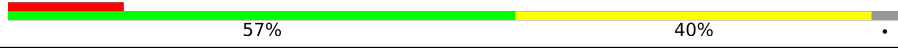
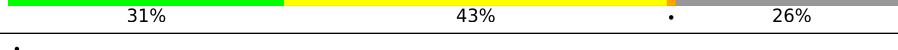
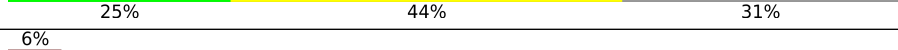
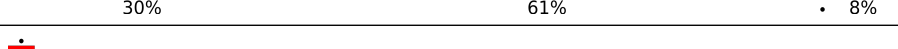
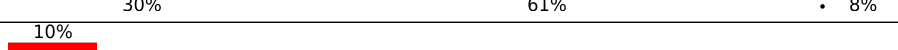
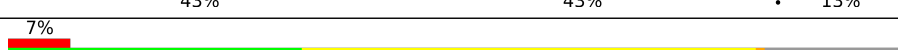
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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	653	
1	J	653	
2	B	375	
2	K	375	

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Mol	Chain	Length	Quality of chain
3	C	360	
3	L	360	
4	D	1439	
4	M	1439	
5	E	326	
5	N	326	
6	F	924	
6	O	924	
7	G	320	
7	P	320	
8	H	916	
8	Q	916	
9	I	1140	
9	R	1140	
10	S	2011	
11	T	2408	
12	U	820	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 124700 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 Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	653	Total	C	N	O	S	0	0
			5268	3341	904	984	39		
1	J	653	Total	C	N	O	S	0	0
			5268	3341	904	984	39		

- Molecule 2 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	375	Total	C	N	O	S	0	0
			2927	1813	524	571	19		
2	K	375	Total	C	N	O	S	0	0
			2927	1813	524	571	19		

- Molecule 3 is a protein called Nucleoporin SEH1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	333	Total	C	N	O	S	0	0
			2607	1632	466	491	18		
3	L	325	Total	C	N	O	S	0	0
			2546	1592	455	482	17		

- Molecule 4 is a protein called Nup160.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1394	Total	C	N	O	S	0	0
			11118	7052	1912	2086	68		
4	M	1394	Total	C	N	O	S	0	0
			11118	7052	1912	2086	68		

- Molecule 5 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	326	Total	C	N	O	S	0	0
			2573	1640	443	473	17		
5	N	326	Total	C	N	O	S	0	0
			2573	1640	443	473	17		

- Molecule 6 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	687	Total	C	N	O	S	0	0
			5560	3525	979	1024	32		
6	O	637	Total	C	N	O	S	0	0
			5168	3282	911	946	29		

- Molecule 7 is a protein called GATOR complex protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	294	Total	C	N	O	S	0	0
			2300	1454	394	440	12		
7	P	294	Total	C	N	O	S	0	0
			2300	1454	394	440	12		

- Molecule 8 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	798	Total	C	N	O	S	0	0
			6494	4126	1096	1240	32		
8	Q	780	Total	C	N	O	S	0	0
			6351	4034	1076	1210	31		

- Molecule 9 is a protein called outer Nup133.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1076	Total	C	N	O	S	0	0
			8482	5362	1409	1661	50		
9	R	1082	Total	C	N	O	S	0	0
			8536	5397	1420	1669	50		

- Molecule 10 is a protein called MGC83295 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	2011	Total	C	N	O	S	0	0
			15974	10112	2785	2978	99		

- Molecule 11 is a protein called Protein ELYS.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	1013	Total	C	N	O	S	0	0
			8041	5095	1388	1518	40		

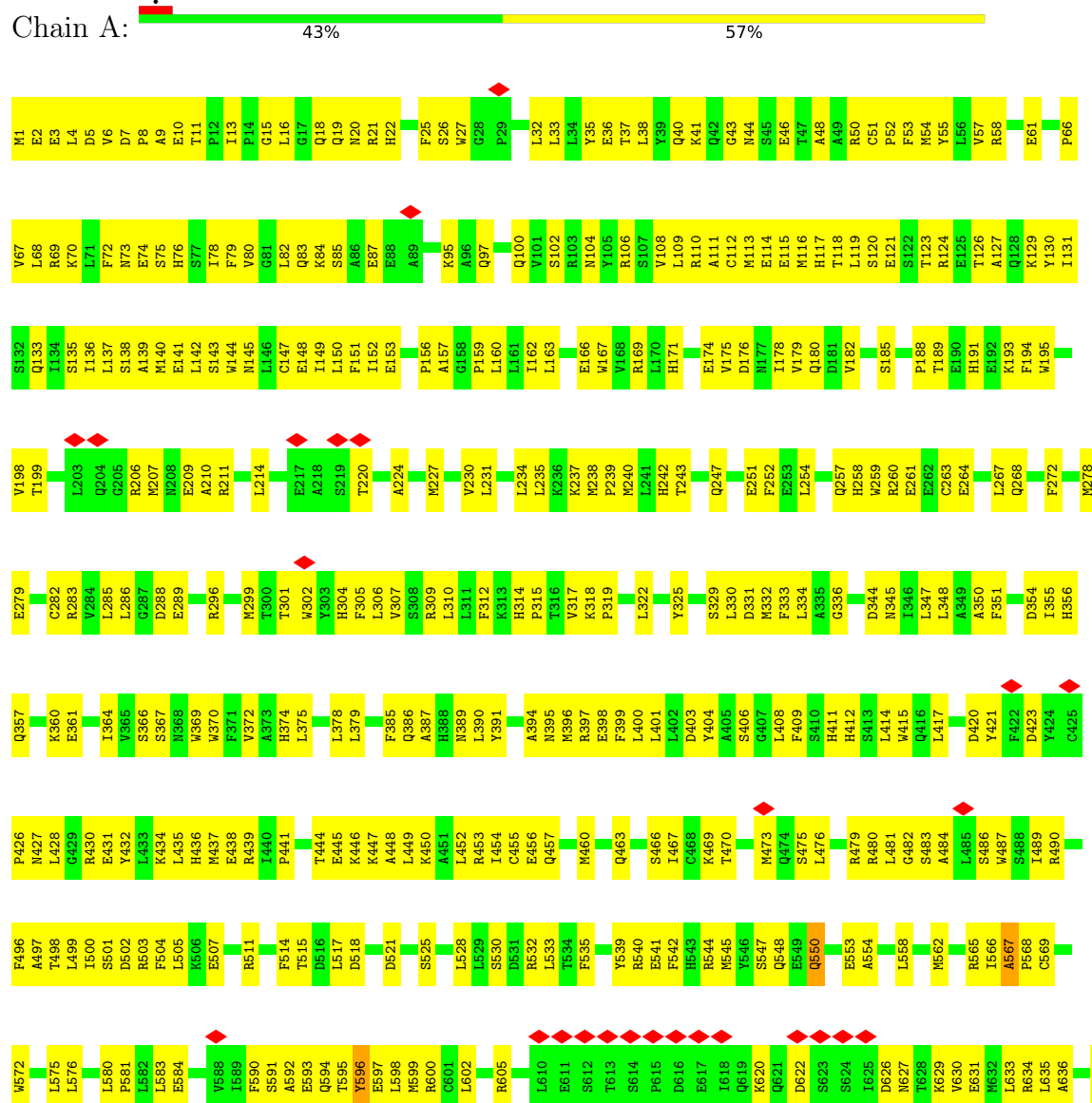
- Molecule 12 is a protein called Nuclear pore complex protein Nup93.

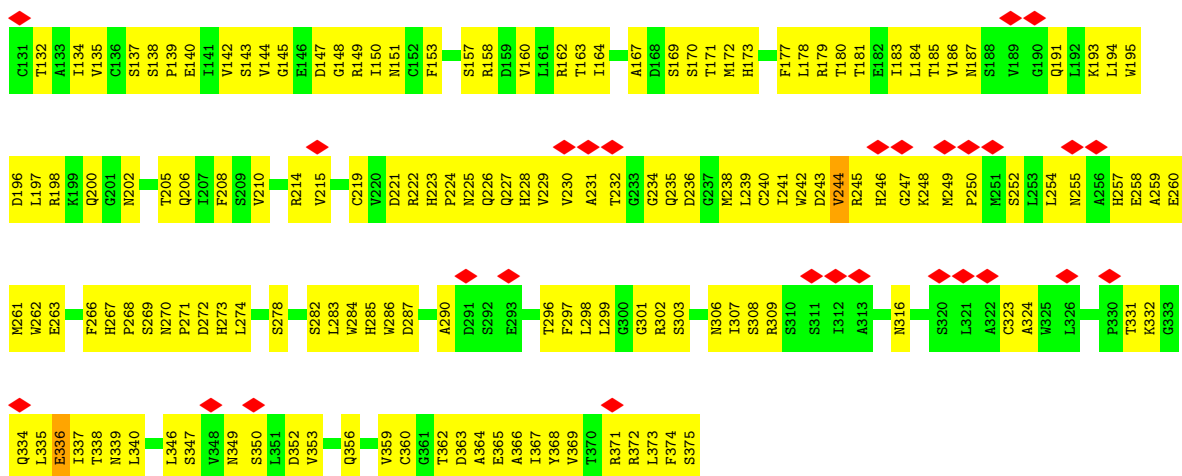
Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	820	Total	C	N	O	S	0	0
			6569	4132	1146	1259	32		

3 Residue-property plots

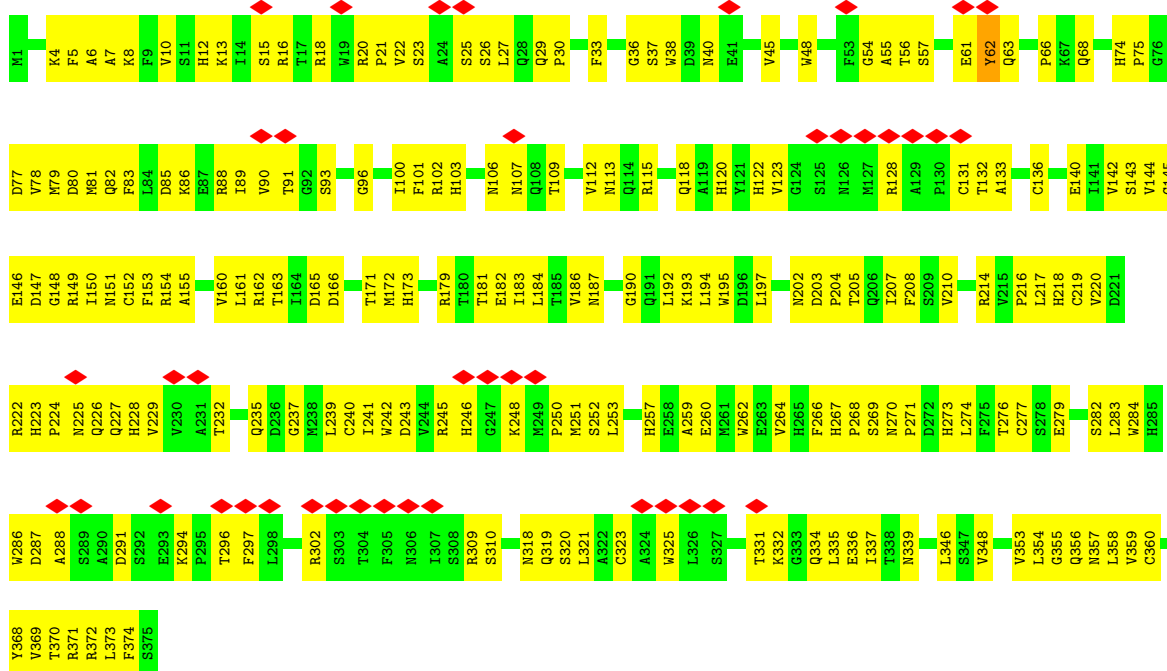
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nuclear pore complex protein Nup85

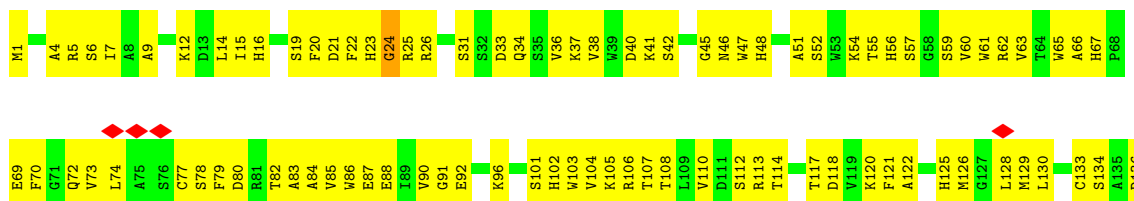


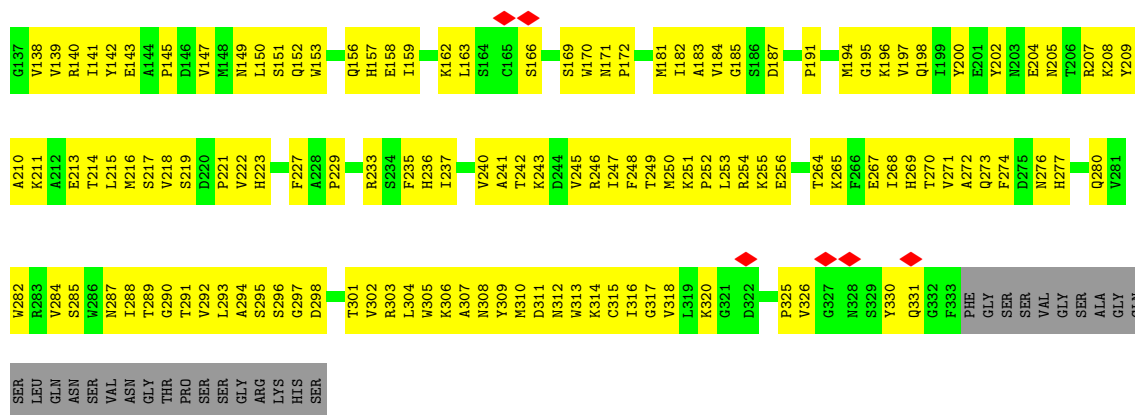


• Molecule 2: MGC154553 protein

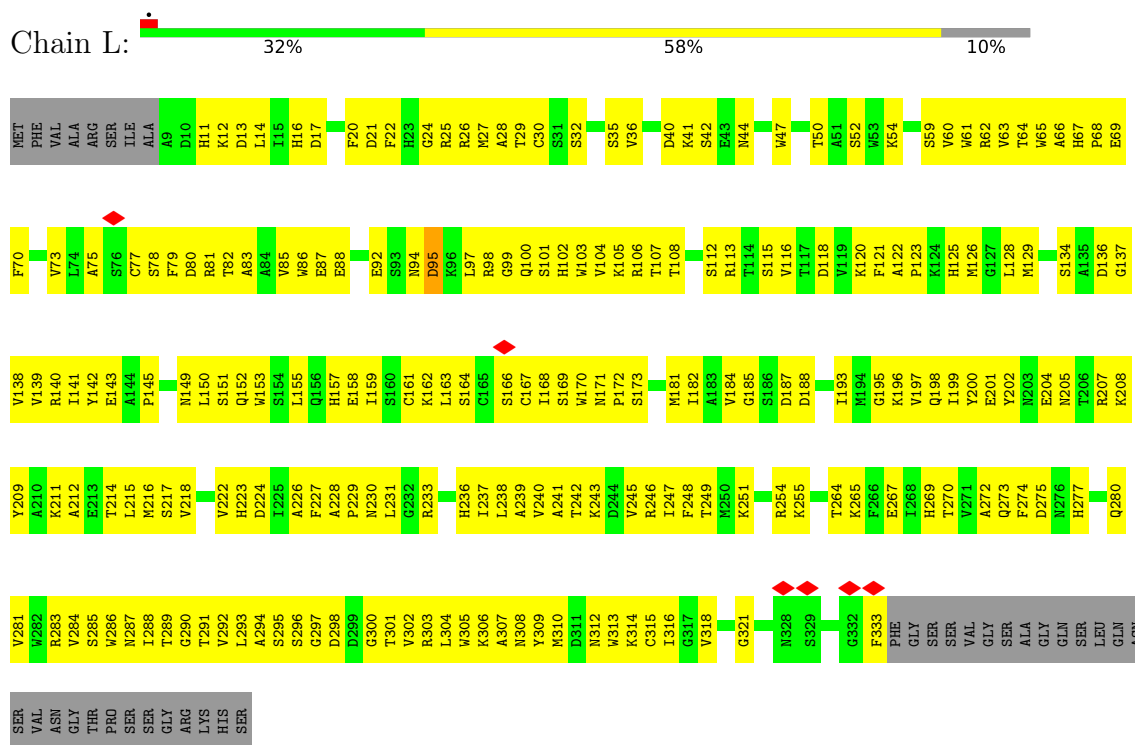


• Molecule 3: Nucleoporin SEH1-A

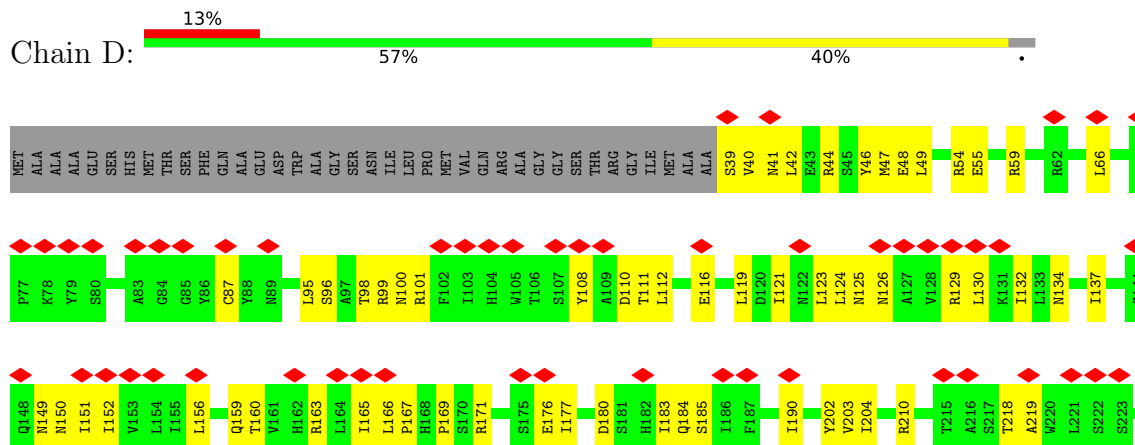




• Molecule 3: Nucleoporin SEH1-A



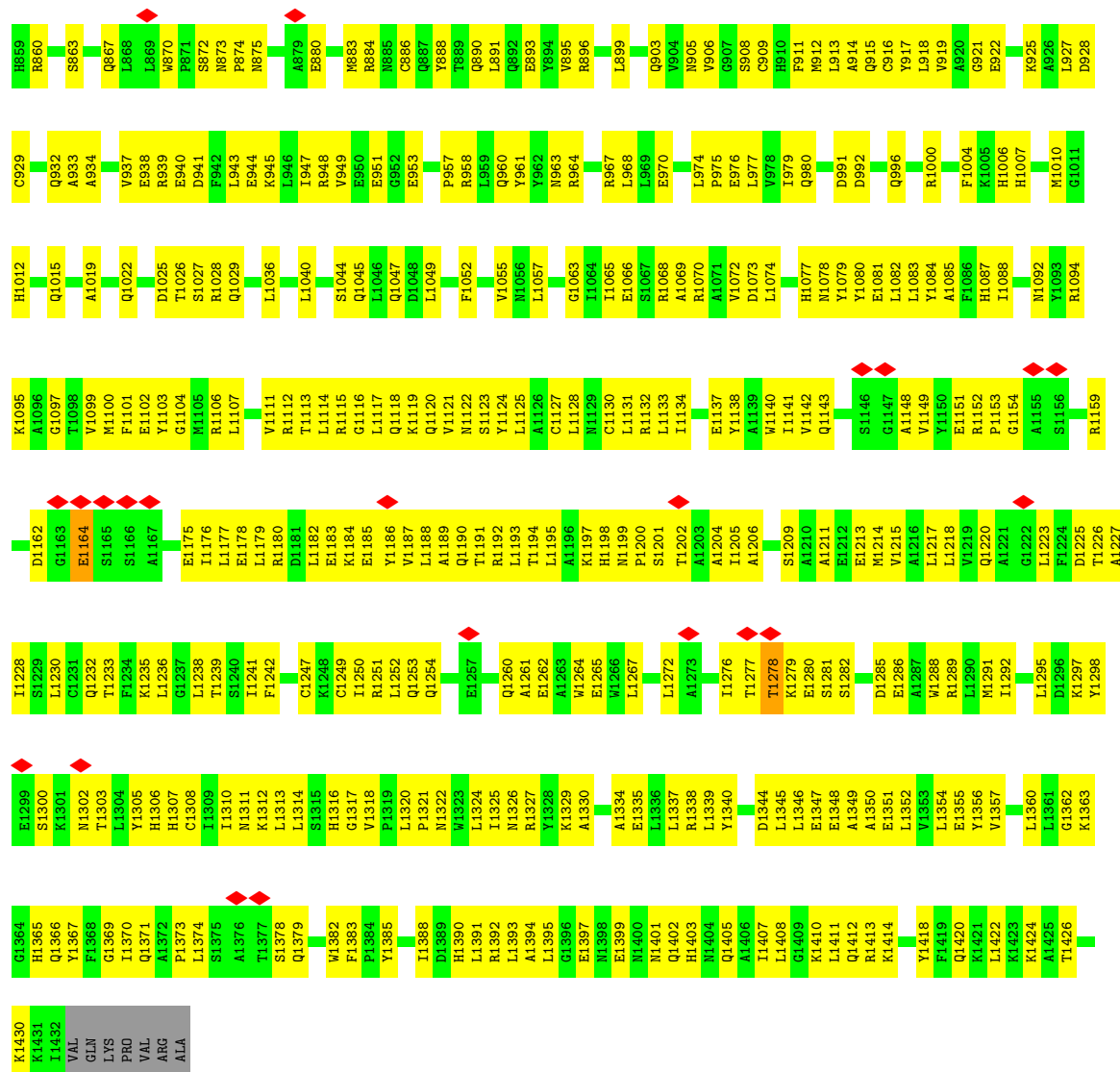
• Molecule 4: Nup160



H1316	H1317	H1318	H1319	H1320	H1321	H1322	H1323	H1324	H1325	H1326	H1327	H1328	H1329	H1330	H1331	H1332	H1333	H1334	H1335	H1336	H1337	H1338	H1339	H1340	H1341	H1342	H1343	E1347	E1348	A1349	A1350	A1351	L1352	L1353	L1354	L1355	E1355	E1356	Y1357	D1358	A1359	L1360	L1361	G1362	K1363	G1364	H1365	Q1366	Y1367	A1372	P1373	L1374	L1380	V1381	H1382	F1383	P1384	Y1385	S1386
F1242	K1248	C1249	T1250	R1251	L1252	Q1253	Q1254	E1257	Q1260	W1264	L1267	M1270	Q1271	L1272	A1273	T1274	V1275	I1276	T1277	T1278	K1279	S1282	A1283	E1286	R1289	L1290	M1291	I1292	S1293	Y1294	L1295	D1296	K1297	Y1298	E1299	S1300	K1301	N1302	T1303	L1304	Y1305	H1306	C1307	C1308	I1309	L1310	M1311	K1312	L1313										
E1175	L1176	F1086	H1087	I1088	D1181	N1092	Y1093	K1184	E1185	Y1186	V1187	L1188	A1189	Q1190	T1191	L1192	L1193	T1194	L1195	K1196	K1197	N1199	T1202	I1205	A1206	G1207	S1208	S1209	A1210	A1211	M1214	V1215	L1218	G1222	L1223	F1224	D1225	T1226	A1227	I1228	S1229	L1230	C1231	Q1232	T1233	F1234	K1235	L1236	G1237	L1238	T1239	S1240	I1241						
Y1084	A1085	F1086	H1087	I1088	M1092	Y1093	R1094	K1095	A1096	V1099	M1100	F1101	E1102	R1106	L1107	R1115	Q1118	K1119	Q1120	V1121	S1122	Y1124	L1125	A1126	C1127	L1128	M1129	C1130	L1131	R1132	L1133	T1134	R1135	P1136	E1137	Y1138	A1139	W1140	I1141	V1142	Q1143	S1146	G1147	A1148	V1149	Y1150	E1151	R1152	S1166	I1174									
L999	R1000	T1001	I1002	F1004	K1005	H1006	M1010	G1011	H1012	N1013	Q1014	Q1015	A1016	Y1017	D1018	T1021	Q1022	H1023	L1036	L1040	R1043	S1044	Q1045	L1046	Q1047	D1048	L1049	E1050	E1051	F1052	V1055	N1056	L1057	H1058	N1059	E1060	V1061	L1062	I1065	R1070	L1074	H1077	N1078	E1081	L1082	L1083													
R829	K830	H831	F832	P833	Q834	V835	F836	A837	H838	T841	G844	S845	V848	H849	R850	S851	L852	R853	H854	Q857	L858	L859	H870	N873	P874	H875	A879	E880	C881	L882	R883	R884	N885	Y888	T889	Q890	L891	Q892	E893	Y894	V895	R896	Y906	C909	H910	F911	N912	L913	A914	Q915									
C916	Y917	L918	E922	G923	H924	K925	A926	C929	A933	A934	S935	E936	R939	E940	D941	F942	L943	L946	E950	E953	S954	V955	S956	Q960	Y961	R964	R967	L968	V972	G973	L974	P975	E976	L977	V978	Y979	A982	Y986	S987	E988	A989	S990	D991	Q996															
L740	R741	D744	L747	V748	G749	A750	L754	Q757	Q758	L767	L768	L769	S770	Y771	Y772	M773	L774	R775	W776	C780	L781	N787	P787	H785	E791	S792	N793	L794	Q795	H796	L797	S798	L800	E801	L802	S803	D804	S805	Q806	H807	E808	K809	R810	R811	T812	T813	S814	C815	T816	L819	V820	E821							
L665	Q666	R669	N670	P671	L672	Q673	L675	S676	F677	L678	Q680	N681	M682	D689	M690	E691	Q692	S693	Q694	R698	L699	N700	M624	A625	Y626	Q627	M628	E629	S630	A631	Q636	S637	R640	V641	I645	L646	E647	D648	L649	I650	A651	N652	D653	I654	D655	M658	E659	N660	Q662	N663	K664								
G487	R488	V489	L490	D491	L492	S493	H494	E495	K498	V501	E506	E522	F523	R524	Q525	I526	N530	W531	K533	F534	Y535	T536	L539	Q540	Y541	R547	L551	V552	H553	P555	N556	N558	M559	V560	C561	L562	K565	Q566	F567	F570	L571	A572	P573	C574	G585														
M407	M408	W410	A411	L412	W413	L414	D415	D416	D417	M418	W421	H424	I425	N426	F427	E428	R429	M430	Q431	A432	G433	H434	W435	V438	F439	W440	N441	P444	D445	D452	Y460	L461	E462	F465	G468	R469	F470	T471	I472	Q476	K477	A478	I479	Q480	I481	K484	G485	S486											
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K242	M243	P244	M248	E249	V252	T253	I254	Q259	V262	M263	Q264	R265	G269	V270	M271	P272	S273	S274	L275	R276	P285	V286	S287	L288	A289	V290	L293	D294	H295	Y298	L299	F300	A301	L302	C303	H306	K307	L308	R309	M310	D315	Q316	M317	M320	V321	A322	D323												

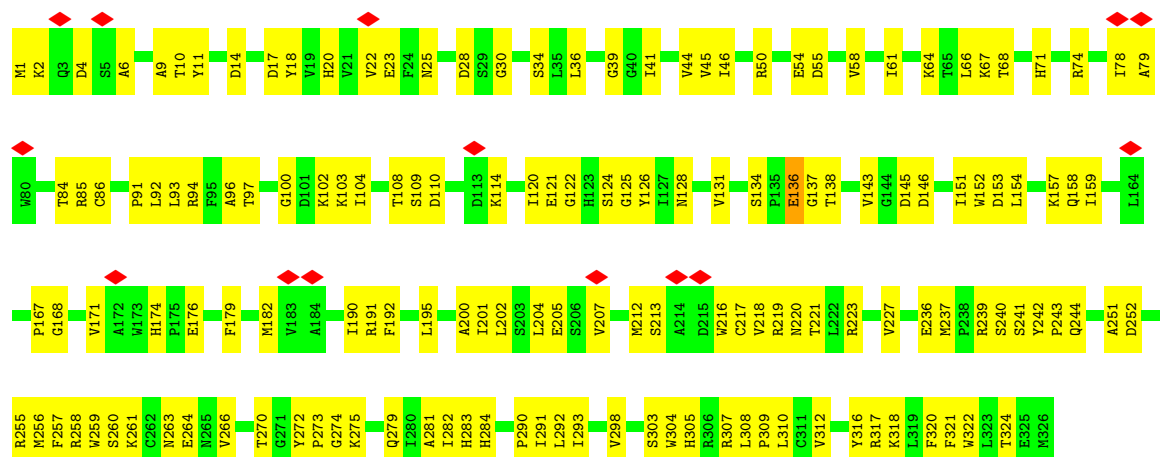
Chain M:



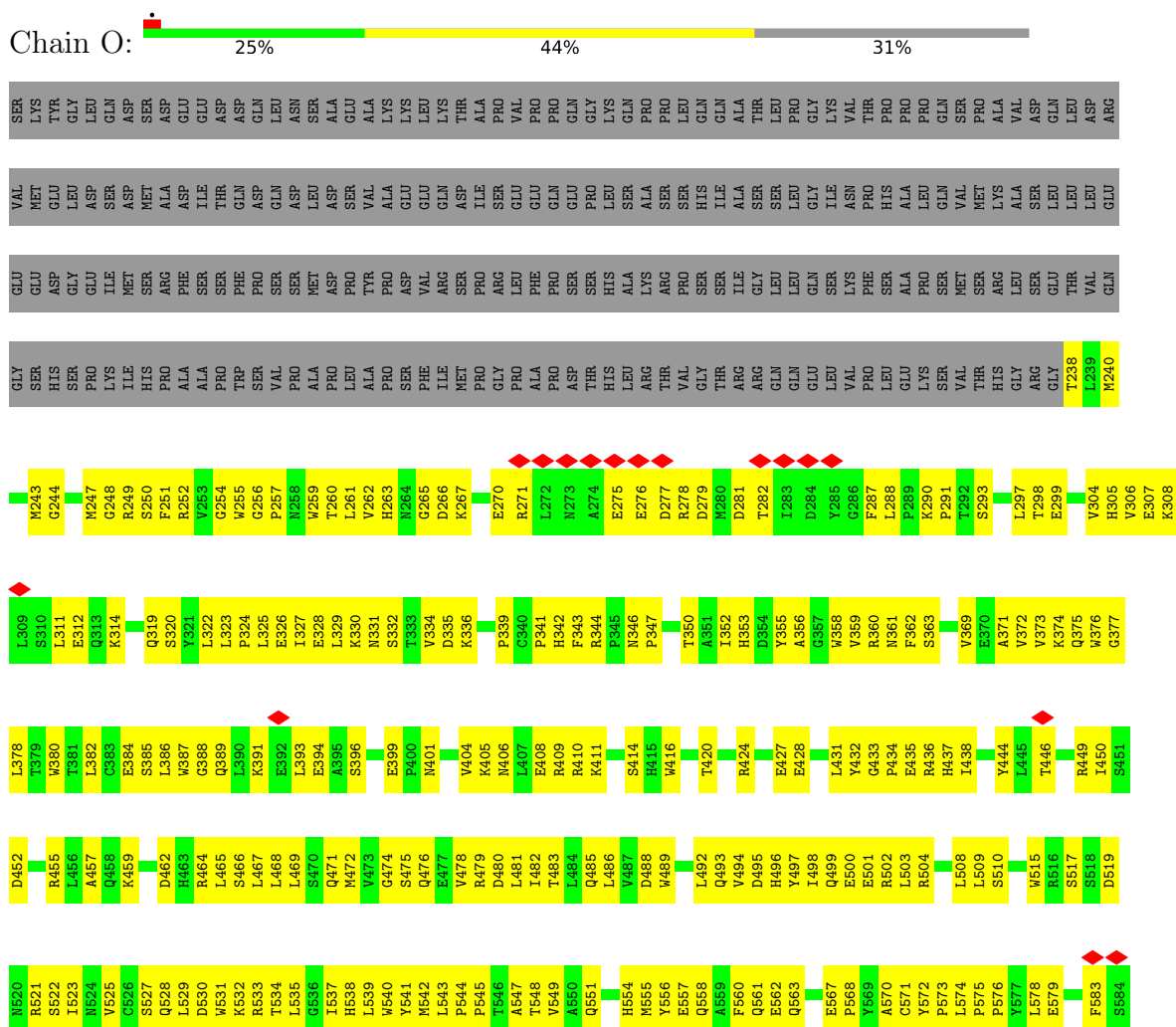


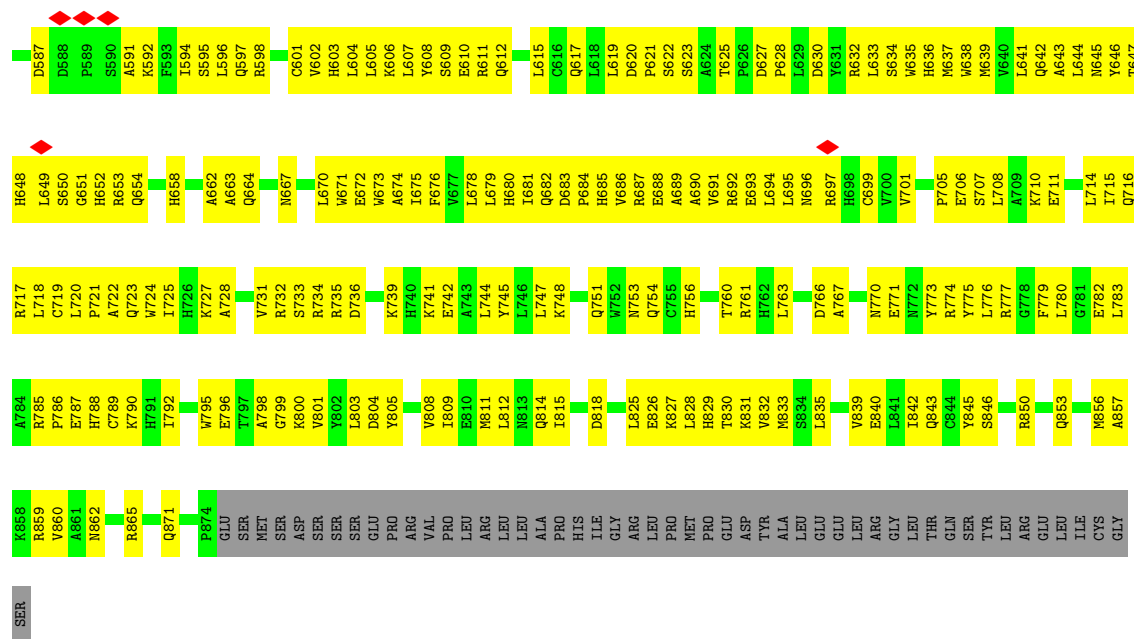
• Molecule 5: MGC83926 protein

Chain E: 53% 46%

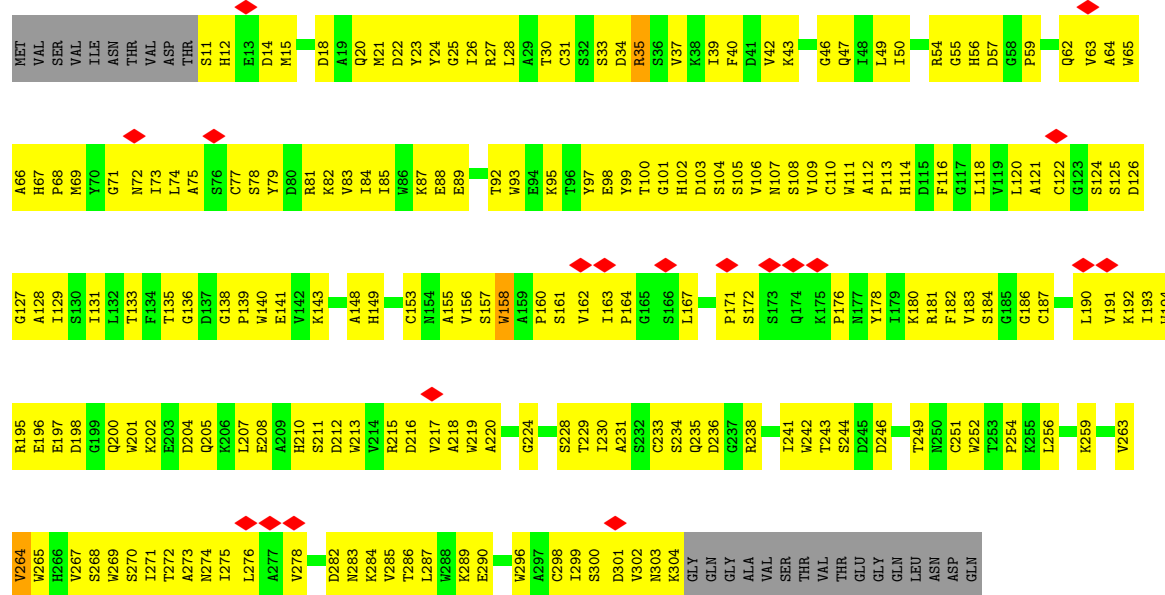


- Molecule 6: Nuclear pore complex protein Nup96

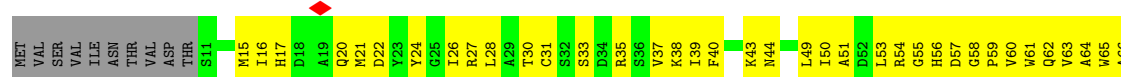




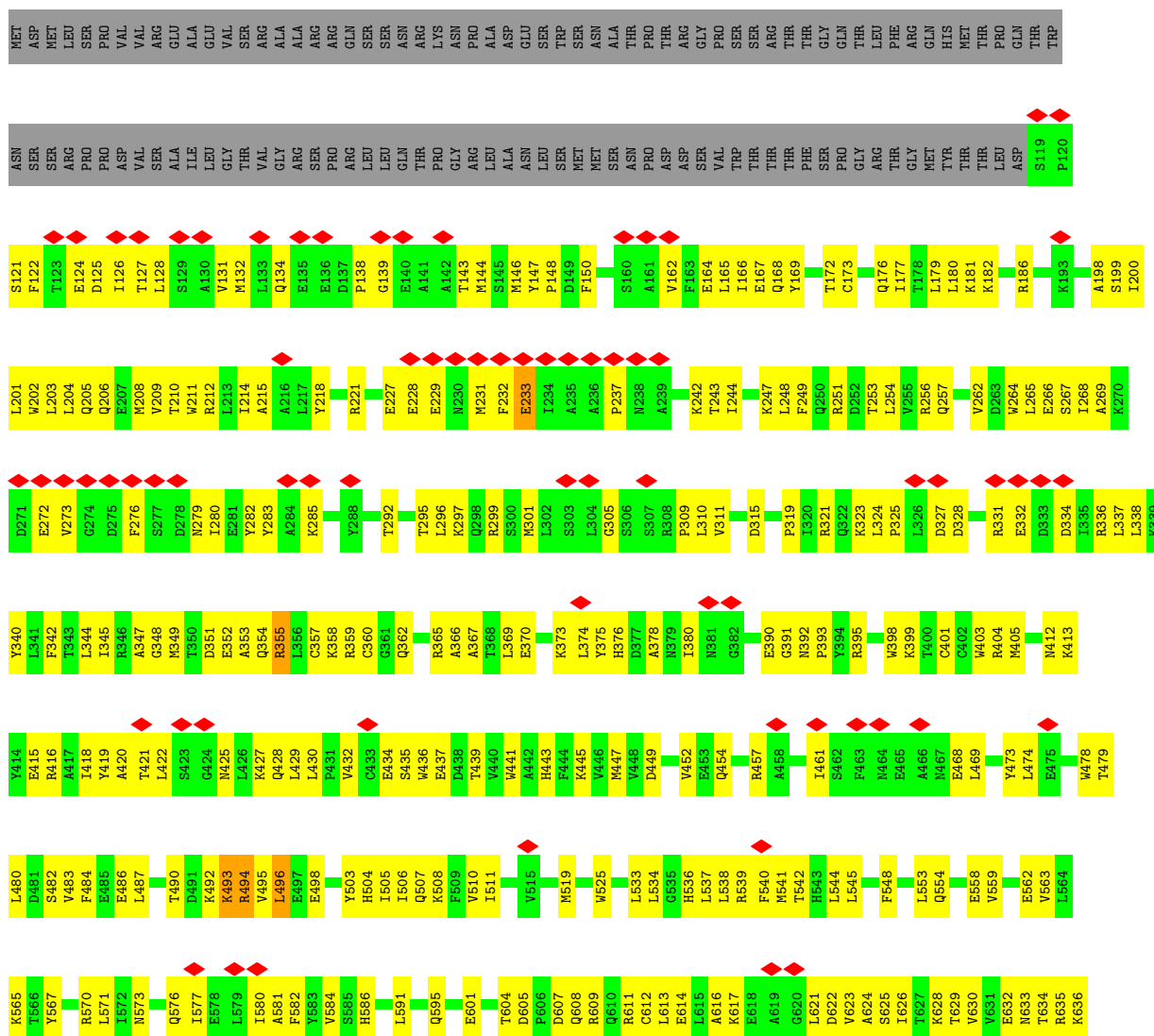
• Molecule 7: GATOR complex protein SEC13

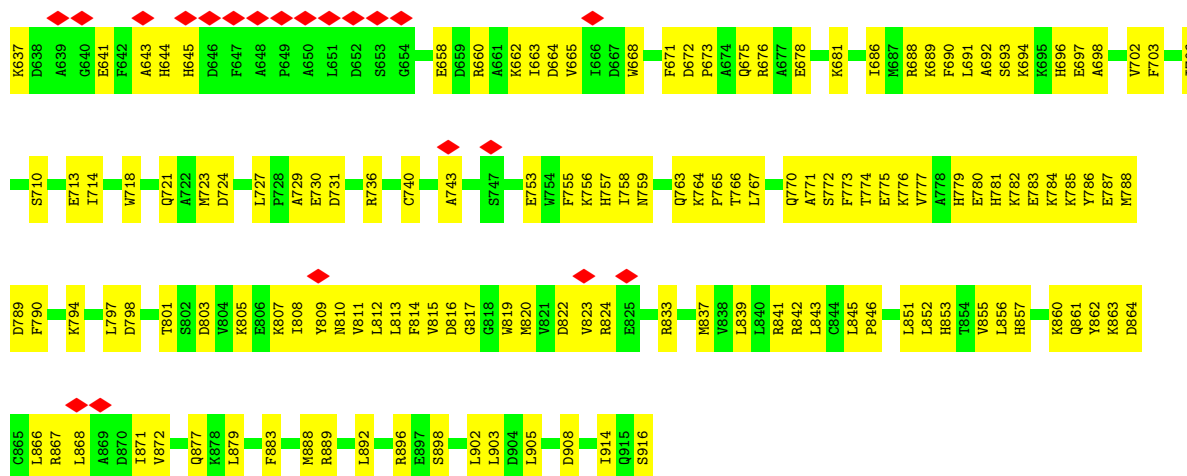


• Molecule 7: GATOR complex protein SEC13

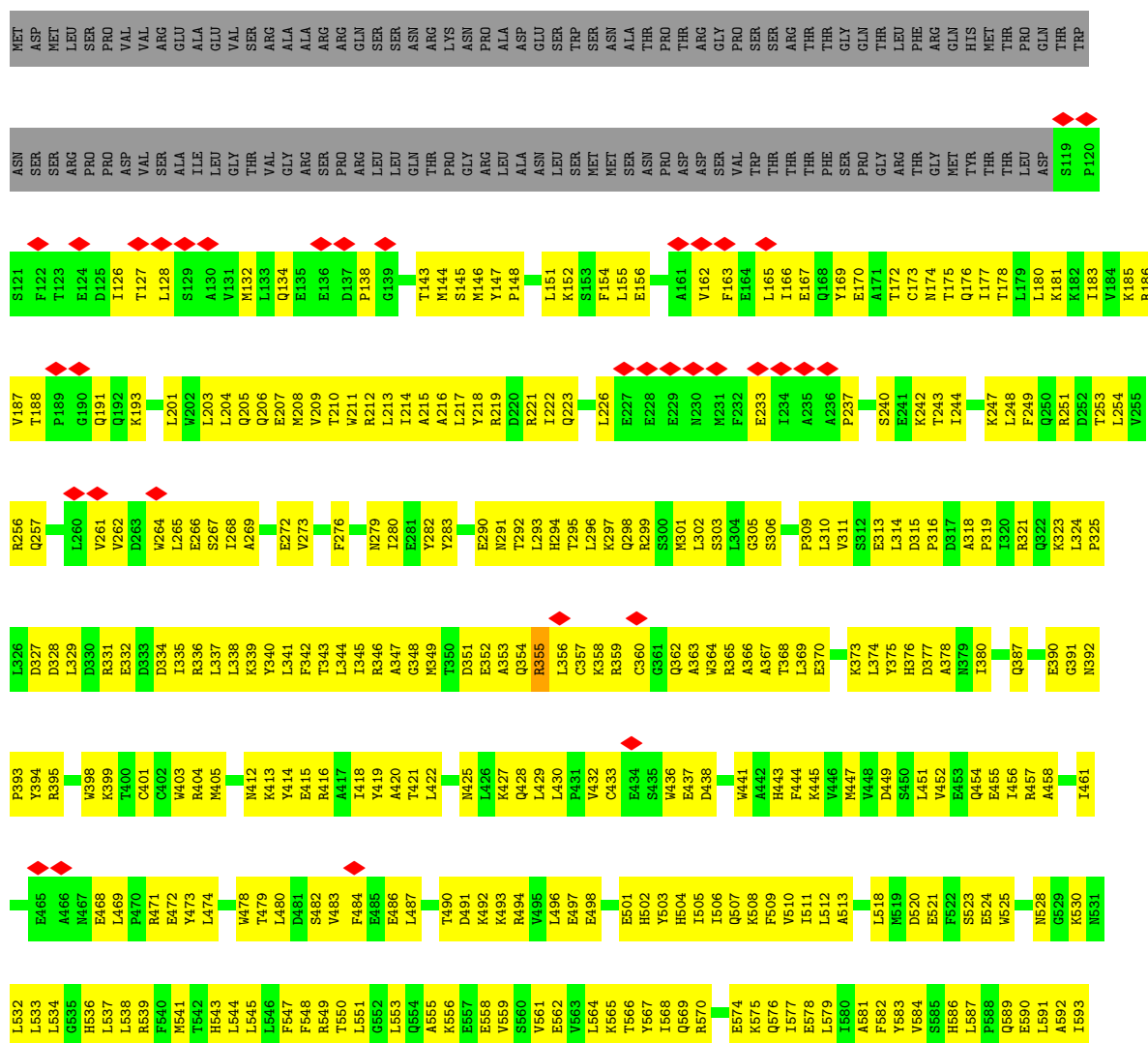


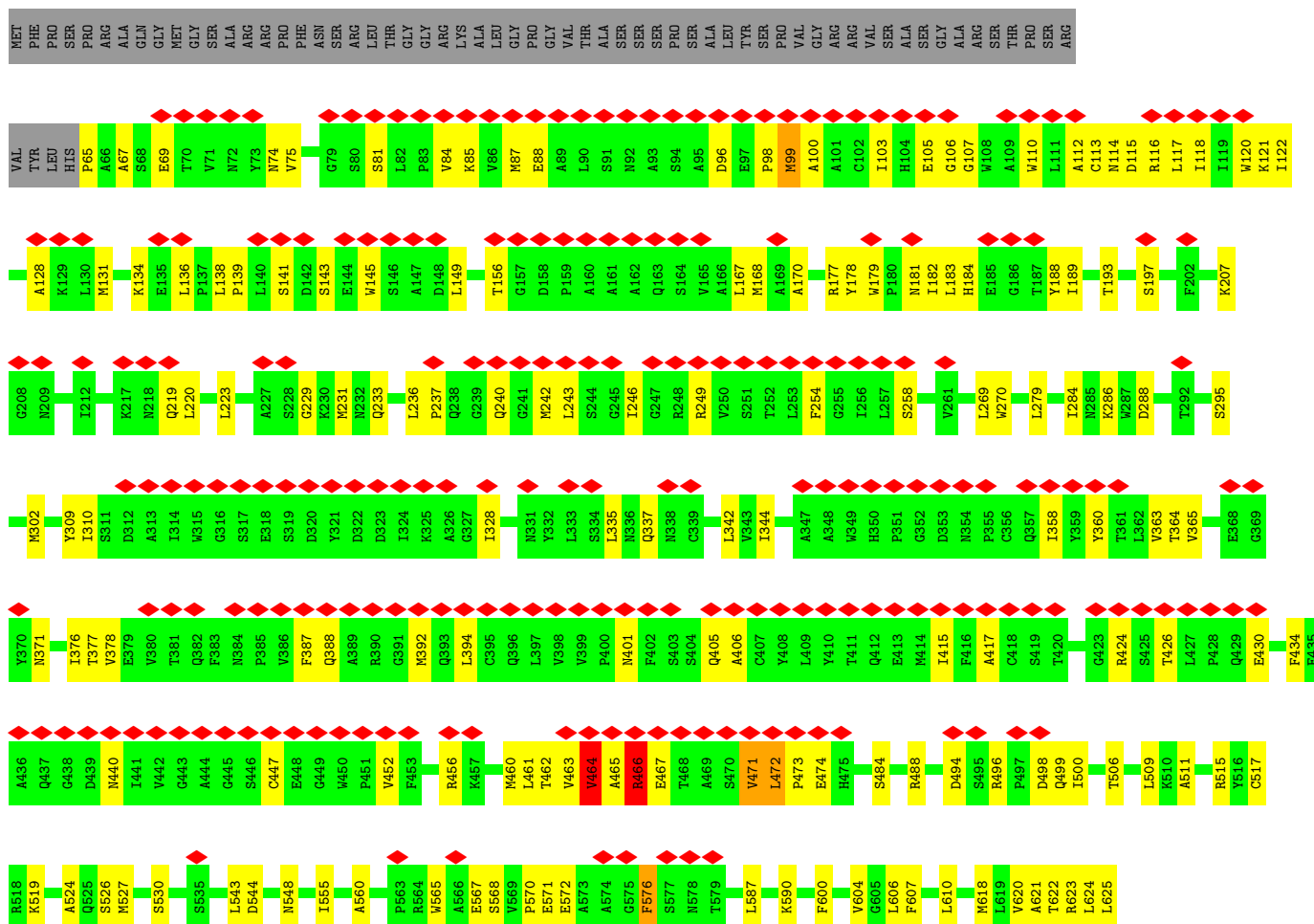
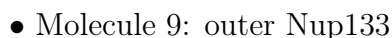
- Molecule 8: Nuclear pore complex protein

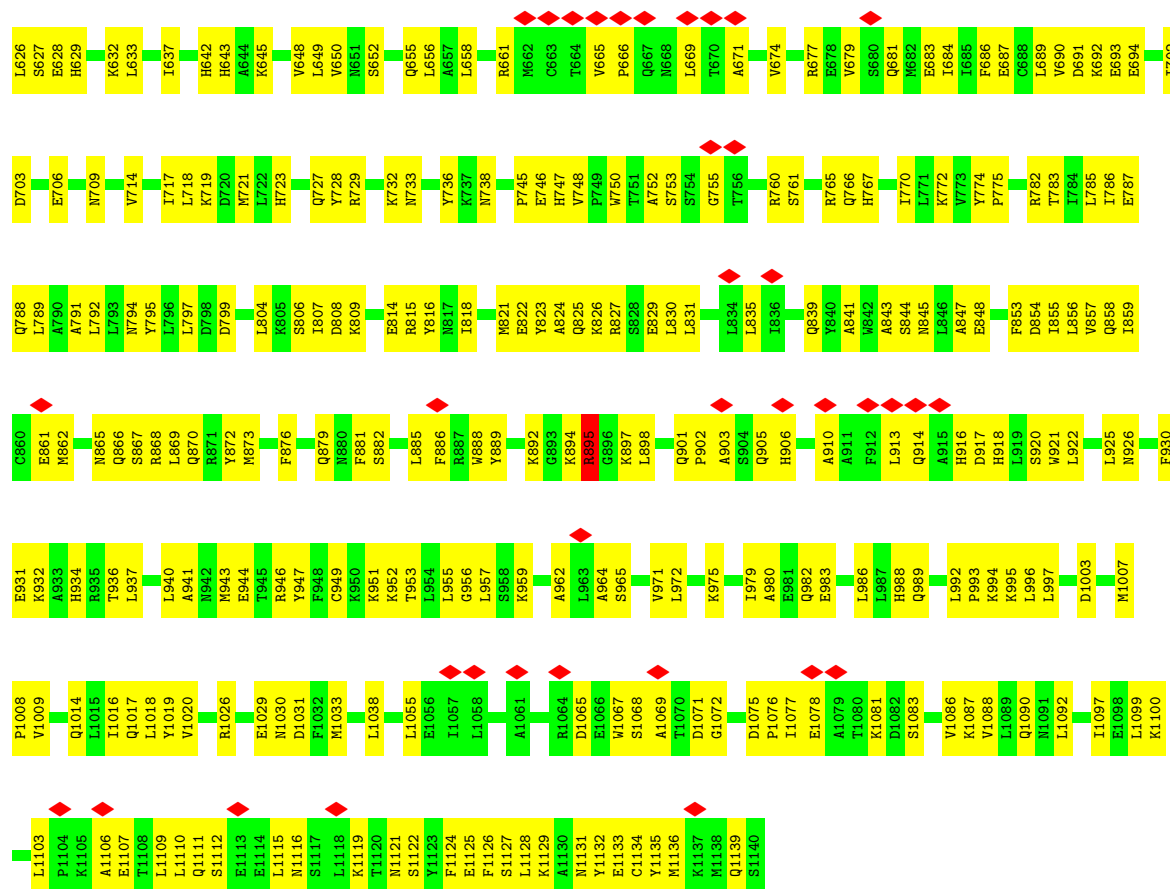




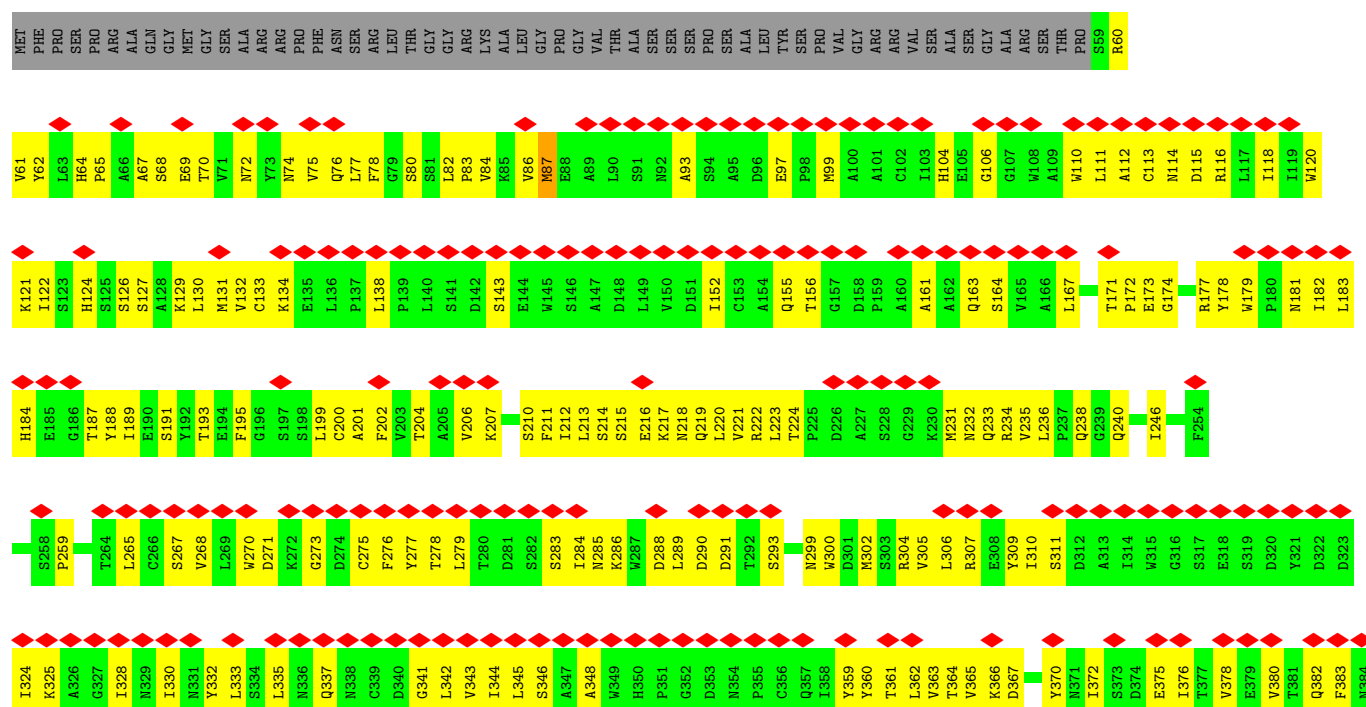
• Molecule 8: Nuclear pore complex protein

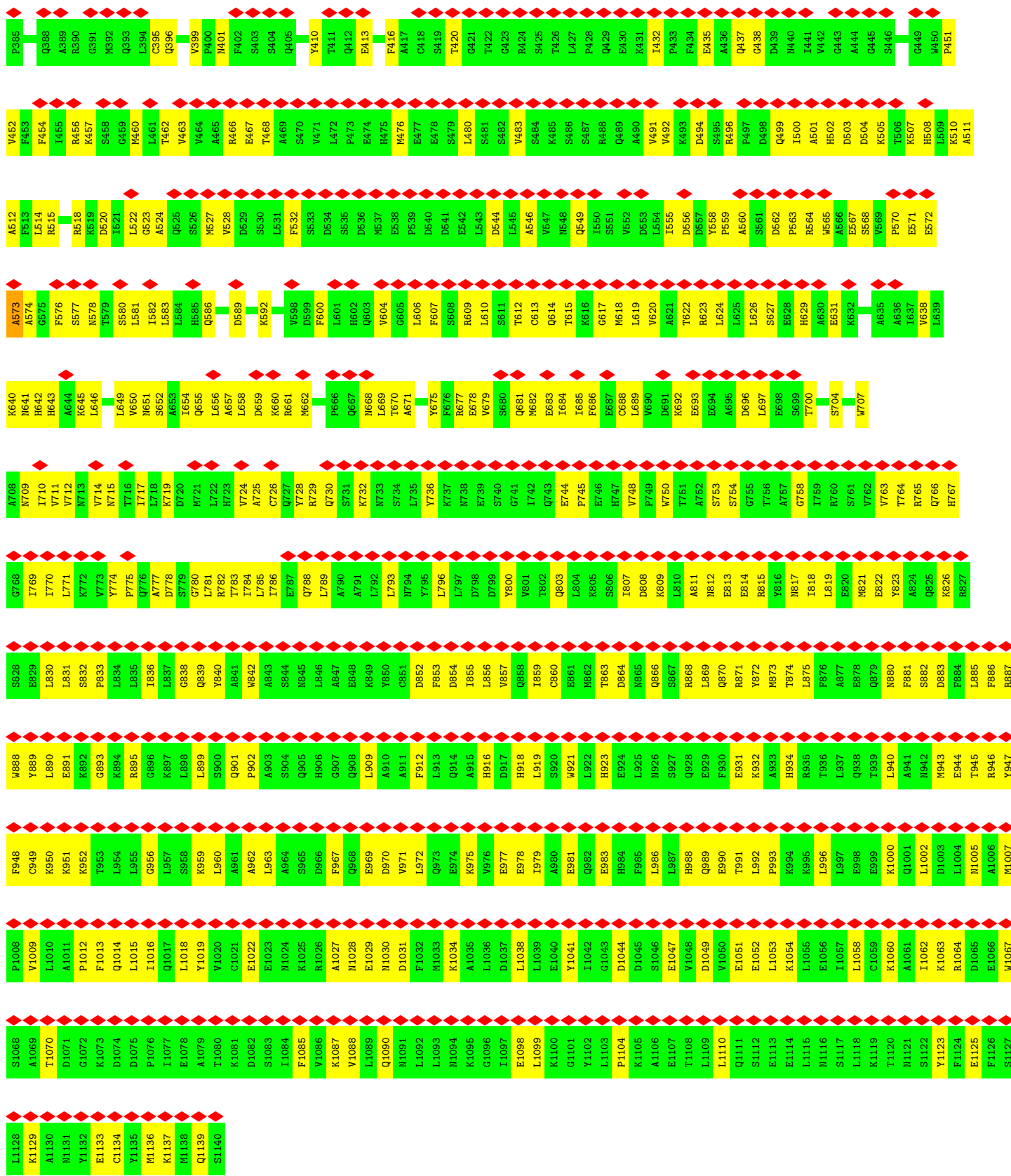




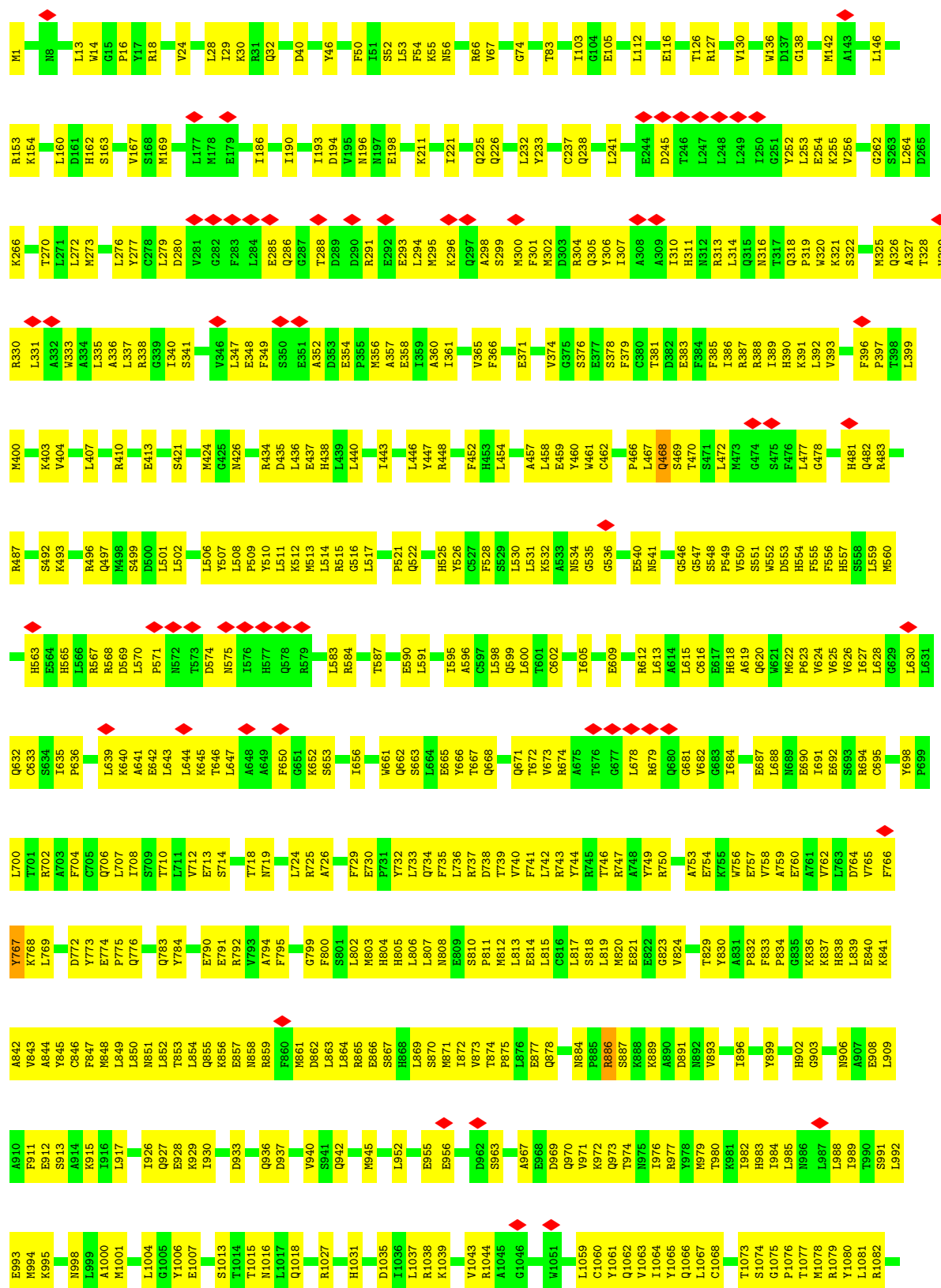


• Molecule 9: outer Nup133



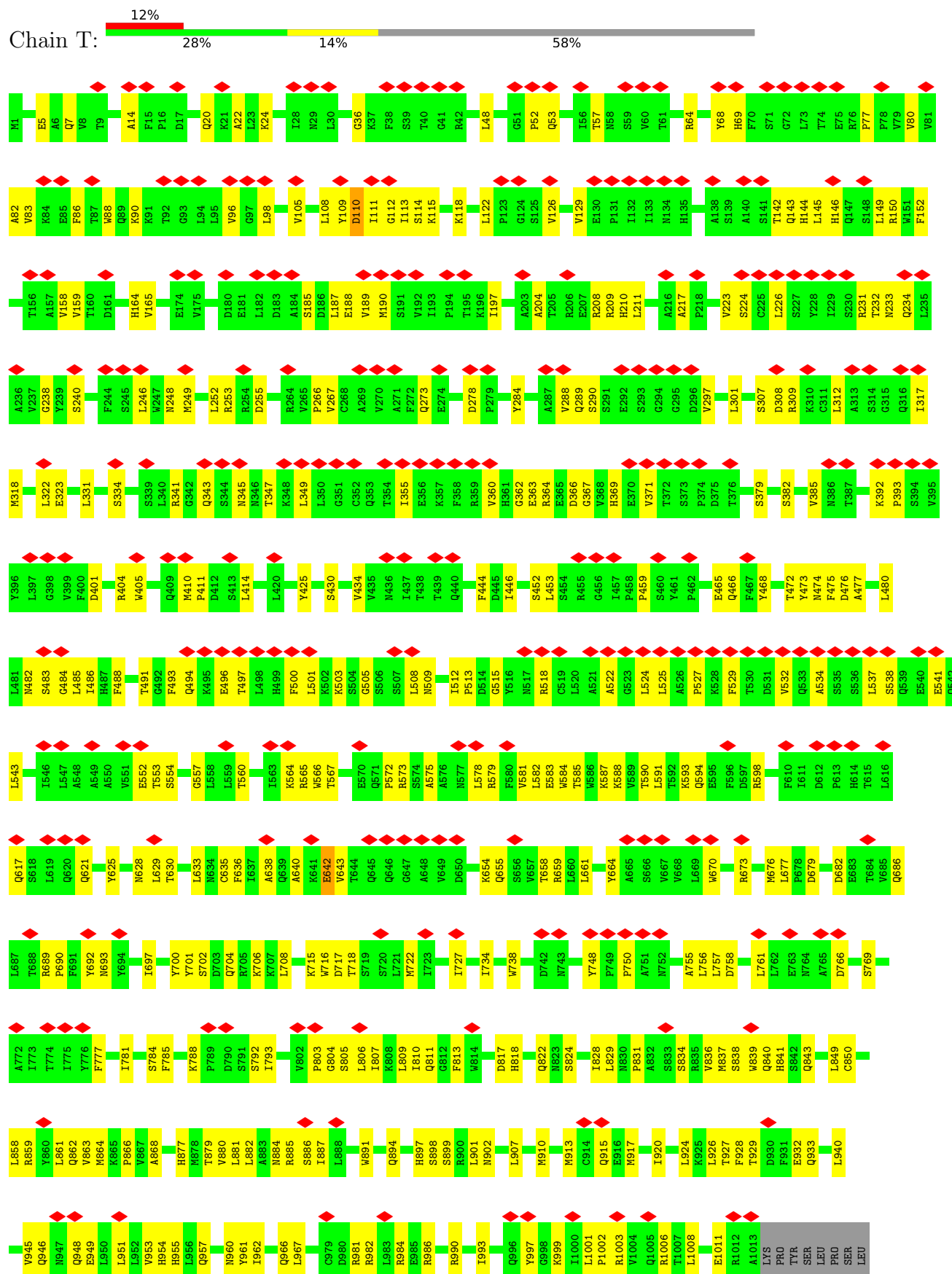


- Molecule 10: MGC83295 protein

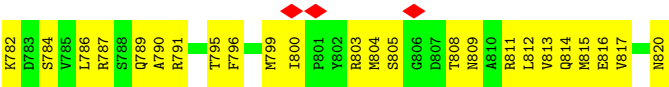


R2000	Y1904	F1826	M1752	L1672	E1592	V1505	D1435	L1370	L1367	M1244	S1163	F1087
R2001	R1905	T1827	Q1753	A1673	T1593	D1506	E1436	L1371	I1308	A1245	F1167	L1068
R2002	H1906	Y1828	Q1754	L1674	D1594	R1507	P1437	G1372	I1309	A1246	L1168	F1089
R2003	L1907	L1675		L1676		Q1508	D1438		R1310	Q1247	Q1091	Q1091
G2004	Y1910	T1831	S1757	T1676	G1597	Q1510	T1439	A1375	D1311	G1248	T1173	L1092
L2005	H1832	G1677	M1758	G1677	V1598	W1511		A1376	L1312	R1177		L1092
L2006	H1832	T1678	W1759	T1678	F1599	L1512		A1377	L1313	R1178		Q1093
R2007	G1837	G1679	M1760	L1679		L1514	H1444	P1377	Q1314	R1250		H1094
V2008	K1838	S1680	W1761	S1680	R1602	Y1514	H1445	P1378	D1315	L1252		L1095
L1912	L1839	Y1762	Y1762	L1515	E1603	Y1515	K1445	G1379	L1316	L1253		H1094
L1913	Q1840	C1763	C1763	S1516	T1604	S1516	S1446	T1380	L1317	M1254		F1096
D1918	N1841	A1682	Q1764	A1683			W1447	E1381	H1317	F1097		F1097
Y1928	V1842	A1683			P1609	Y1520	M1447	E1382	I1320	I1098		S1098
L1845	L1688	L1688	M1767		P1609		E1448	M1382	L1321	L1181		V1099
L1850	N1689	N1689	Q1776		A1610	D1526	E1449	I1383	D1322	I1182		S1102
L1851	E1690	E1690	P1776		P1611		R1450	S1384	D1323	I1183		E1103
E1852	L1691	L1691	C1779		D1531		L1451	S1385	D1324	L1184		T1104
L1853	L1695	L1695	F1780		Y1614	V1534	T1462	A1386	A1325	I1187		S1105
E1857	M1700	M1700	T1781		Y1615	L1535	A1463	Q1386	V1264	Q1188		A1106
M1858	L1707	L1707	F1782		L1619	R1536	P1464	Q1327	V1265	F1189		M1107
P1859	T1708	T1708	S1784		L1620	N1537	T1464	E1328	E1266	S1190		N1108
V1860	G1708	G1708	L1785		Q1624	L1538	E1465	I1390	R1267	Q1109		Q1109
A1862	F1710	F1710	A1789		Q1627	L1539	D1466	L1395	M1268	M1110		Y1111
A1866	R1711	R1711	S1790		L1628	Q1542	V1467	H1396	M1330	M1112		W1112
S1866	Q1712	Q1712	R1791		L1630	P1544	F1468	W1397	L1329	W1114		M1114
T1867	Q1713	Q1713	Q1793		S1633	L1545	D1464	I1398	M1327	T1116		T1116
Q1869	A1716	A1716	G1795		Q1636	L1546	S1467	R1400	H1275	F1201		F1201
K1870	L1717	L1717	L1796		L1637	K1547	F1468	N1401	L1274	D1203		D1203
Y1871	L1718	L1718	Q1796		L1638	K1555	F1469	L1402	A1276	R1204		R1204
R1876	R1719	R1719	D1797		Q1639	T1559		L1403	L1276	I1119		I1119
L1877	F1720	F1720	Q1798		L1639	R1560	Y1472	E1404	K1277	E1205		E1205
V1878	S1724	S1724	Q1799		G1642	T1560	T1474	I1406	R1278	Q1206		Q1206
K1880	D1725	D1725	V1800		Q1643	R1561		K1408	R1279	L1121		L1121
L1881	R1728	R1728	S1801		V1644	K1564		T1409	A1280	R1122		R1122
L1882	Q1729	Q1729	I1802		L1645		M1477	G1410	E1215	I1123		I1123
N1883	L1730	L1730	L1803		L1646	Q1567	E1478	G1411	H1216	S1131		S1131
S1884	S1731	S1731	S1905		F1647	Q1568	Y1479	F1413	K1217	R1135		R1135
R1885	W1806	W1806	W1905		L1648	A1569	V1480	Q1414	N1218	L1136		L1136
L1888	R1807	R1807	R1906		H1651	E1571	A1484	R1415	R1219	L1137		L1137
L1889	L1732	L1732	L1808		S1652	L1572	C1485	R1416	R1220	H1138		H1138
S1890	Q1733	Q1733	P1809		D1653	L1573	D1486	A1418	G1221	L1139		L1139
L1891	D1735	D1735	S1910		T1654		G1487	H1419	Q1222	L1140		L1140
Y1894	S1736	S1736	L1811		I1655	G1576	H1488	L1420	E1289	D1141		D1141
I1895	S1737	S1737	G1812		Q1656	V1577	D1489	Y1421	I1291	C1225		C1225
T1898	R1738	R1738	V1813		L1659	I1578	I1490	G1422	L1292	M1144		M1144
C1899	L1739	L1739	S1665		S1665	V1579	G1491	S1423	L1293	P1145		P1145
L1900	K1744	K1744	L1666		L1666	L1581	H1498	L1424	M1356	T1146		T1146
Y1901	D1747	D1747	G1667		G1667	Y1587	A1497	L1425	C1295	R1147		R1147
I1902	M1748	M1748	S1668		S1668	R1590	L1499	L1426		H1230		H1230
L1903	E1749	E1749	L1669		Q1670	P1591	D1500	Y1427	D1298	P1148		P1148
A1907	L1750	L1750	Q1671		E1671		R1501	Q1363	L1299	Y1149		Y1149
	A1751	A1751					S1504	S1364	E1303	M1157		M1157
								Q1365	E1304	E1158		E1158
								Y1366	R1304	D1159		D1159
								V1367	R1305	E1160		E1160
								Q1368	Q1306	S1161		S1161
								M1369	G1243	R1162		R1162

● Molecule 11: Protein ELYS







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.301	Depositor
Minimum map value	-2.133	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.24, 2.24, 2.24	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	1/5377 (0.0%)	0.63	1/7265 (0.0%)
1	J	0.24	0/5377	0.55	0/7265
2	B	0.31	0/2996	0.68	4/4074 (0.1%)
2	K	0.22	0/2996	0.56	0/4074
3	C	0.30	0/2674	0.63	1/3628 (0.0%)
3	L	0.25	0/2612	0.56	0/3545
4	D	0.22	0/11349	0.50	1/15414 (0.0%)
4	M	0.26	1/11349 (0.0%)	0.53	5/15414 (0.0%)
5	E	0.20	0/2643	0.51	1/3587 (0.0%)
5	N	0.20	0/2643	0.49	0/3587
6	F	0.34	0/5699	0.64	1/7730 (0.0%)
6	O	0.29	0/5299	0.63	1/7189 (0.0%)
7	G	0.35	0/2367	0.72	2/3231 (0.1%)
7	P	0.32	0/2367	0.66	2/3231 (0.1%)
8	H	0.26	0/6628	0.54	1/8968 (0.0%)
8	Q	0.31	0/6483	0.59	2/8772 (0.0%)
9	I	0.80	6/8647 (0.1%)	0.52	4/11720 (0.0%)
9	R	0.25	1/8703 (0.0%)	0.53	6/11797 (0.1%)
10	S	0.23	0/16272	0.51	6/22021 (0.0%)
11	T	0.37	1/8213 (0.0%)	0.49	5/11150 (0.0%)
12	U	0.24	0/6685	0.56	4/9025 (0.0%)
All	All	0.33	10/127379 (0.0%)	0.56	47/172687 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
6	F	0	4
7	G	0	2
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Q	0	1
9	I	0	2
11	T	0	1
12	U	0	1
All	All	0	13

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	576	PHE	CD2-CE2	34.59	2.42	1.38
9	I	576	PHE	CD1-CE1	34.33	2.41	1.38
9	I	576	PHE	CE1-CZ	30.22	2.29	1.38
9	I	576	PHE	CE2-CZ	29.30	2.26	1.38
11	T	642	GLU	CA-C	28.94	1.86	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	902	PRO	N-CD-CG	-15.00	80.70	103.20
4	M	786	PRO	N-CD-CG	-13.51	82.93	103.20
11	T	642	GLU	O-C-N	-12.80	106.22	123.12
11	T	642	GLU	CB-CA-C	11.13	127.43	110.62
11	T	642	GLU	N-CA-CB	-11.12	93.93	110.84

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	VAL	Peptide
6	F	248	GLY	Peptide
6	F	250	SER	Peptide
6	F	409	ARG	Sidechain
6	F	598	ARG	Sidechain

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	5268	0	5226	450	0
1	J	5268	0	5226	412	0
2	B	2927	0	2800	276	0
2	K	2927	0	2800	221	0
3	C	2607	0	2513	298	0
3	L	2546	0	2444	213	0
4	D	11118	0	11035	533	0
4	M	11118	0	11035	676	0
5	E	2573	0	2503	144	0
5	N	2573	0	2503	140	0
6	F	5560	0	5469	577	0
6	O	5168	0	5080	454	0
7	G	2300	0	2180	242	0
7	P	2300	0	2180	268	0
8	H	6494	0	6413	434	0
8	Q	6351	0	6268	562	0
9	I	8482	0	8354	399	0
9	R	8536	0	8407	460	0
10	S	15974	0	16156	922	0
11	T	8041	0	7961	312	0
12	U	6569	0	6537	427	0
All	All	124700	0	123090	7873	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 32.

The worst 5 of 7873 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)
9:I:576:PHE:CD1	9:I:576:PHE:CG	1.84	1.65
9:I:576:PHE:CG	9:I:576:PHE:CD2	1.83	1.64
6:F:612:GLN:HA	12:U:183:MET:CG	1.11	1.58
8:Q:869:ALA:CB	8:Q:895:LEU:CD2	1.84	1.54
6:F:612:GLN:CA	12:U:183:MET:HG2	1.41	1.50

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	651/653 (100%)	594 (91%)	56 (9%)	1 (0%)	43	78
1	J	651/653 (100%)	607 (93%)	44 (7%)	0	100	100
2	B	373/375 (100%)	314 (84%)	57 (15%)	2 (0%)	24	63
2	K	373/375 (100%)	333 (89%)	37 (10%)	3 (1%)	16	54
3	C	331/360 (92%)	280 (85%)	50 (15%)	1 (0%)	36	72
3	L	323/360 (90%)	286 (88%)	35 (11%)	2 (1%)	21	59
4	D	1392/1439 (97%)	1294 (93%)	95 (7%)	3 (0%)	43	78
4	M	1392/1439 (97%)	1293 (93%)	95 (7%)	4 (0%)	36	72
5	E	324/326 (99%)	299 (92%)	25 (8%)	0	100	100
5	N	324/326 (99%)	299 (92%)	25 (8%)	0	100	100
6	F	685/924 (74%)	612 (89%)	69 (10%)	4 (1%)	21	59
6	O	635/924 (69%)	556 (88%)	79 (12%)	0	100	100
7	G	292/320 (91%)	262 (90%)	30 (10%)	0	100	100
7	P	292/320 (91%)	253 (87%)	38 (13%)	1 (0%)	36	72
8	H	796/916 (87%)	745 (94%)	50 (6%)	1 (0%)	48	83
8	Q	778/916 (85%)	719 (92%)	55 (7%)	4 (0%)	24	63
9	I	1074/1140 (94%)	989 (92%)	77 (7%)	8 (1%)	18	56
9	R	1080/1140 (95%)	1013 (94%)	66 (6%)	1 (0%)	48	83
10	S	2009/2011 (100%)	1874 (93%)	133 (7%)	2 (0%)	48	83
11	T	1011/2408 (42%)	960 (95%)	50 (5%)	1 (0%)	48	83
12	U	818/820 (100%)	756 (92%)	53 (6%)	9 (1%)	11	46
All	All	15604/18145 (86%)	14338 (92%)	1219 (8%)	47 (0%)	37	72

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	ALA
2	B	61	GLU
3	C	217	SER
6	F	597	GLN
6	F	615	LEU

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	580/580 (100%)	580 (100%)	0	100	100
1	J	580/580 (100%)	580 (100%)	0	100	100
2	B	329/329 (100%)	329 (100%)	0	100	100
2	K	329/329 (100%)	329 (100%)	0	100	100
3	C	288/309 (93%)	288 (100%)	0	100	100
3	L	282/309 (91%)	282 (100%)	0	100	100
4	D	1230/1262 (98%)	1229 (100%)	1 (0%)	88	89
4	M	1230/1262 (98%)	1229 (100%)	1 (0%)	88	89
5	E	275/275 (100%)	275 (100%)	0	100	100
5	N	275/275 (100%)	275 (100%)	0	100	100
6	F	608/816 (74%)	603 (99%)	5 (1%)	73	80
6	O	563/816 (69%)	563 (100%)	0	100	100
7	G	250/272 (92%)	250 (100%)	0	100	100
7	P	250/272 (92%)	250 (100%)	0	100	100
8	H	712/816 (87%)	708 (99%)	4 (1%)	78	83
8	Q	695/816 (85%)	685 (99%)	10 (1%)	59	72
9	I	944/993 (95%)	940 (100%)	4 (0%)	84	84
9	R	950/993 (96%)	950 (100%)	0	100	100
10	S	1779/1779 (100%)	1778 (100%)	1 (0%)	88	89
11	T	895/2166 (41%)	895 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	U	721/721 (100%)	721 (100%)	0	100	100
All	All	13765/15970 (86%)	13739 (100%)	26 (0%)	85	87

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	441	ASN
8	Q	870	ASP
8	Q	881	THR
8	Q	867	ARG
8	Q	871	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 261 such sidechains are listed below:

Mol	Chain	Res	Type
10	S	1636	GLN
11	T	728	ASN
12	U	814	GLN
8	H	861	GLN
8	H	763	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

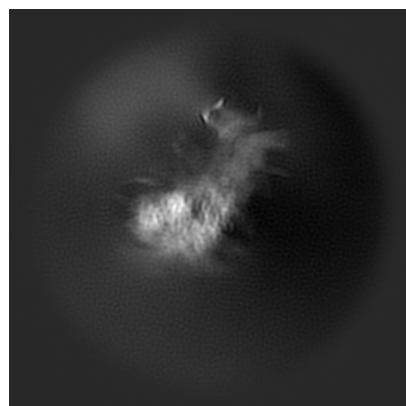
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31891. These allow visual inspection of the internal detail of the map and identification of artifacts.

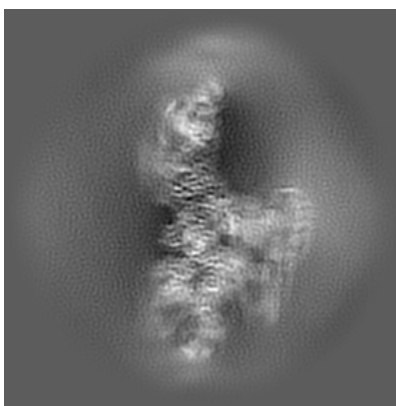
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

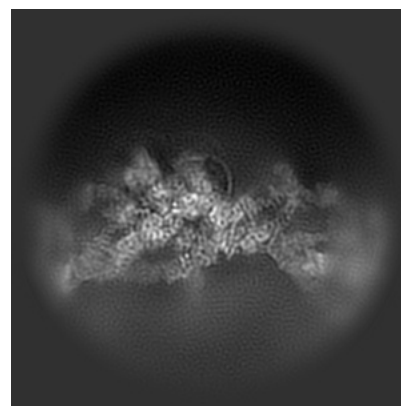
6.1.1 Primary map



X

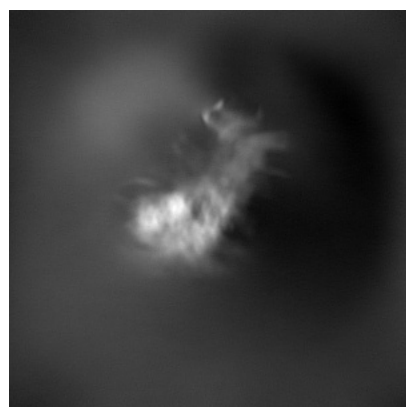


Y

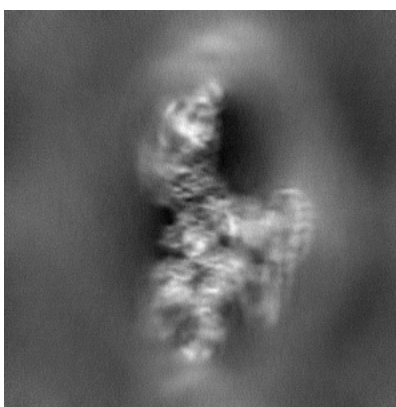


Z

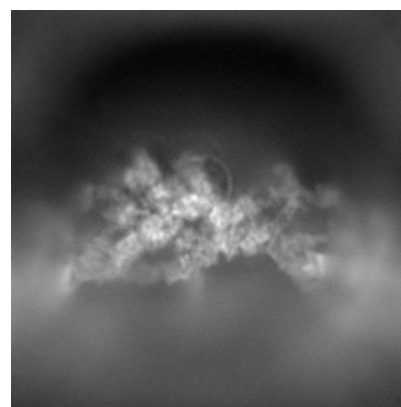
6.1.2 Raw map



X



Y

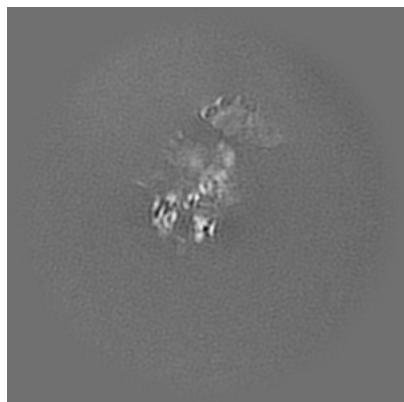


Z

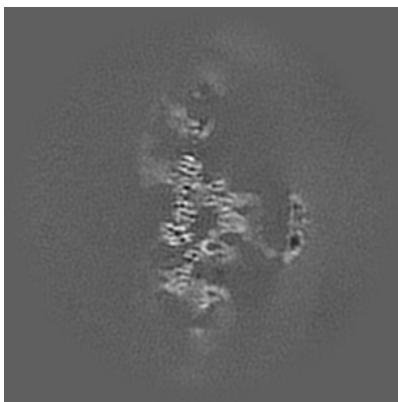
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

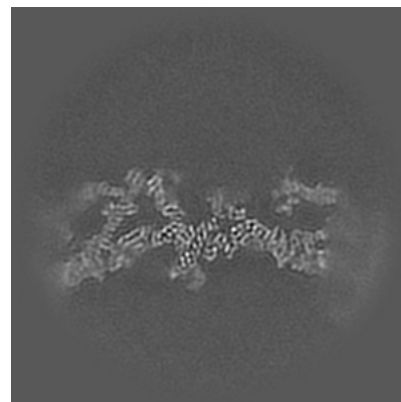
6.2.1 Primary map



X Index: 160

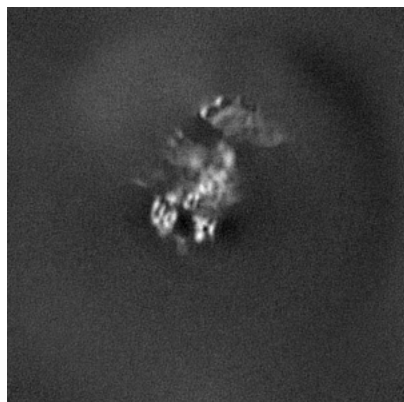


Y Index: 160

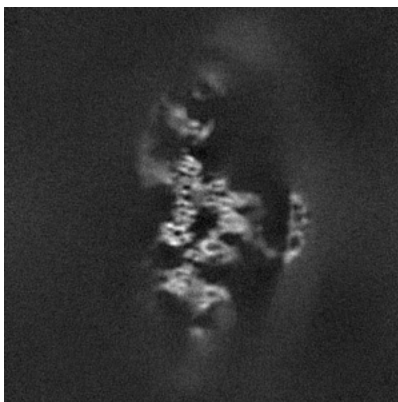


Z Index: 160

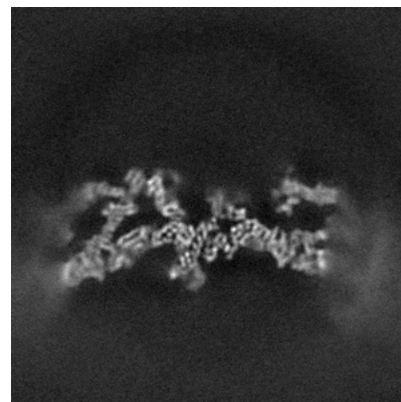
6.2.2 Raw map



X Index: 160



Y Index: 160

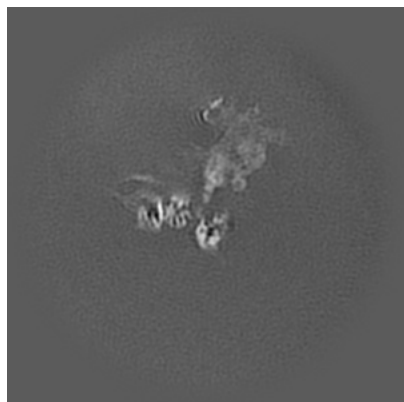


Z Index: 160

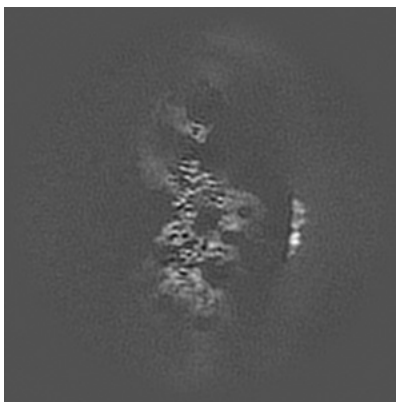
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

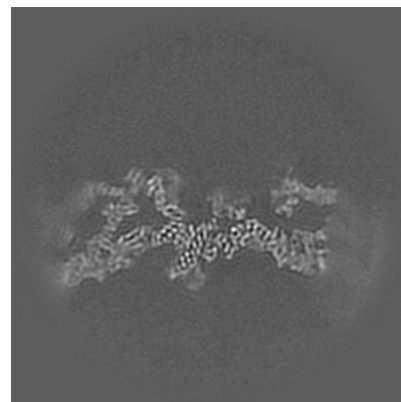
6.3.1 Primary map



X Index: 140



Y Index: 157

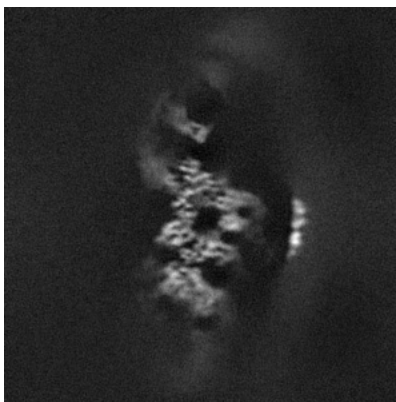


Z Index: 159

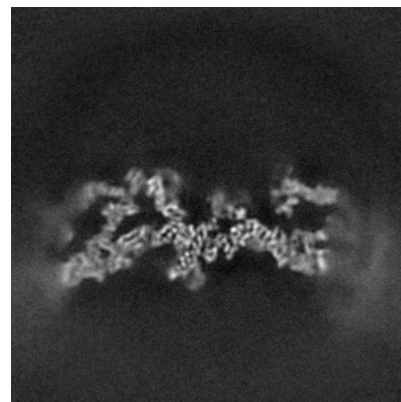
6.3.2 Raw map



X Index: 146



Y Index: 157

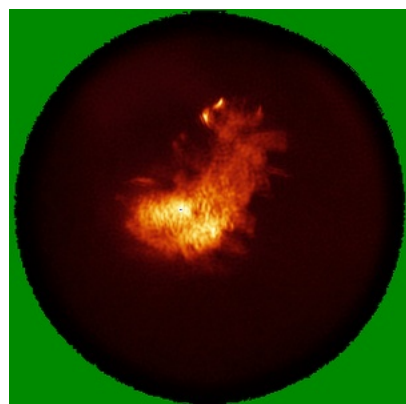


Z Index: 159

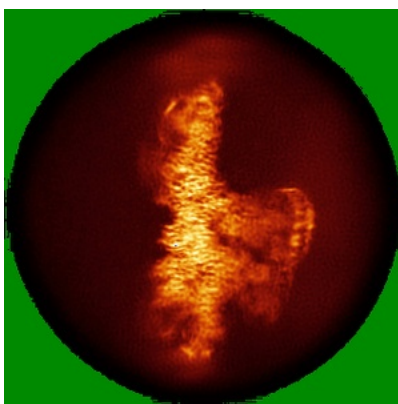
The images above show the largest variance slices of the map in three orthogonal directions.

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

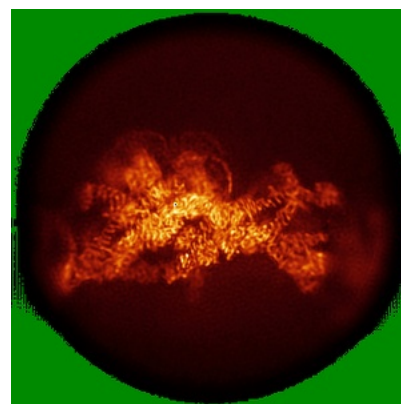
6.4.1 Primary map



X

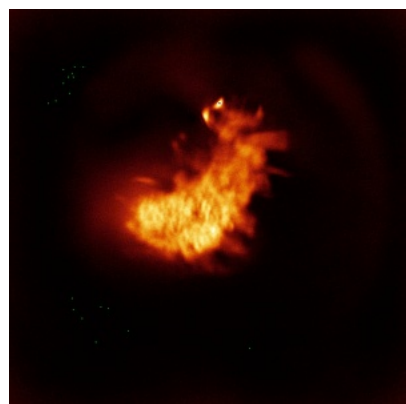


Y

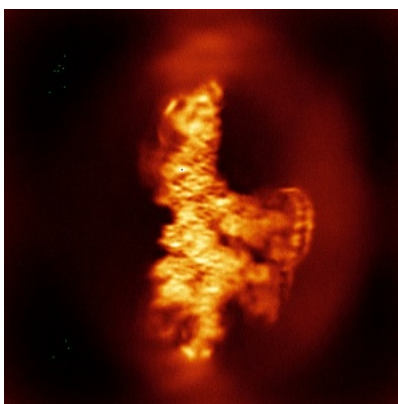


Z

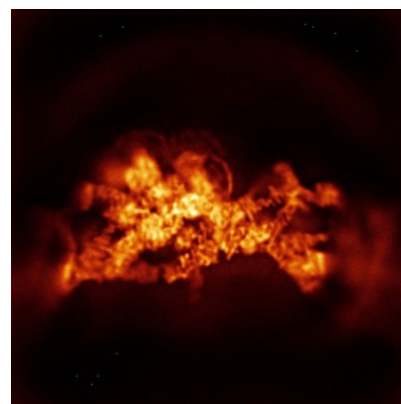
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



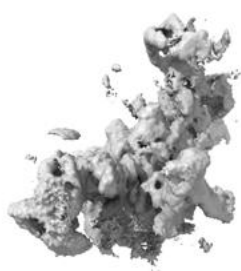
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

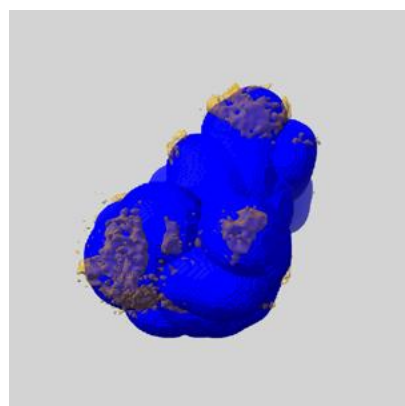
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

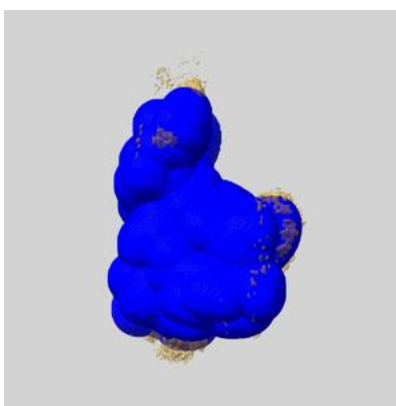
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

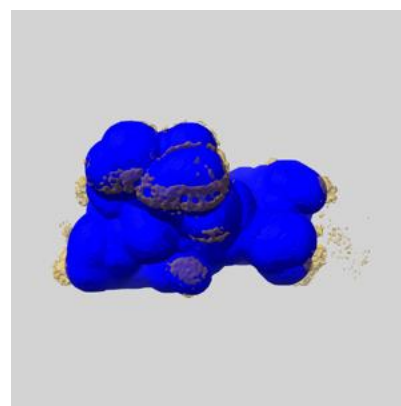
6.6.1 emd_31891_msk_1.map [i](#)



X



Y

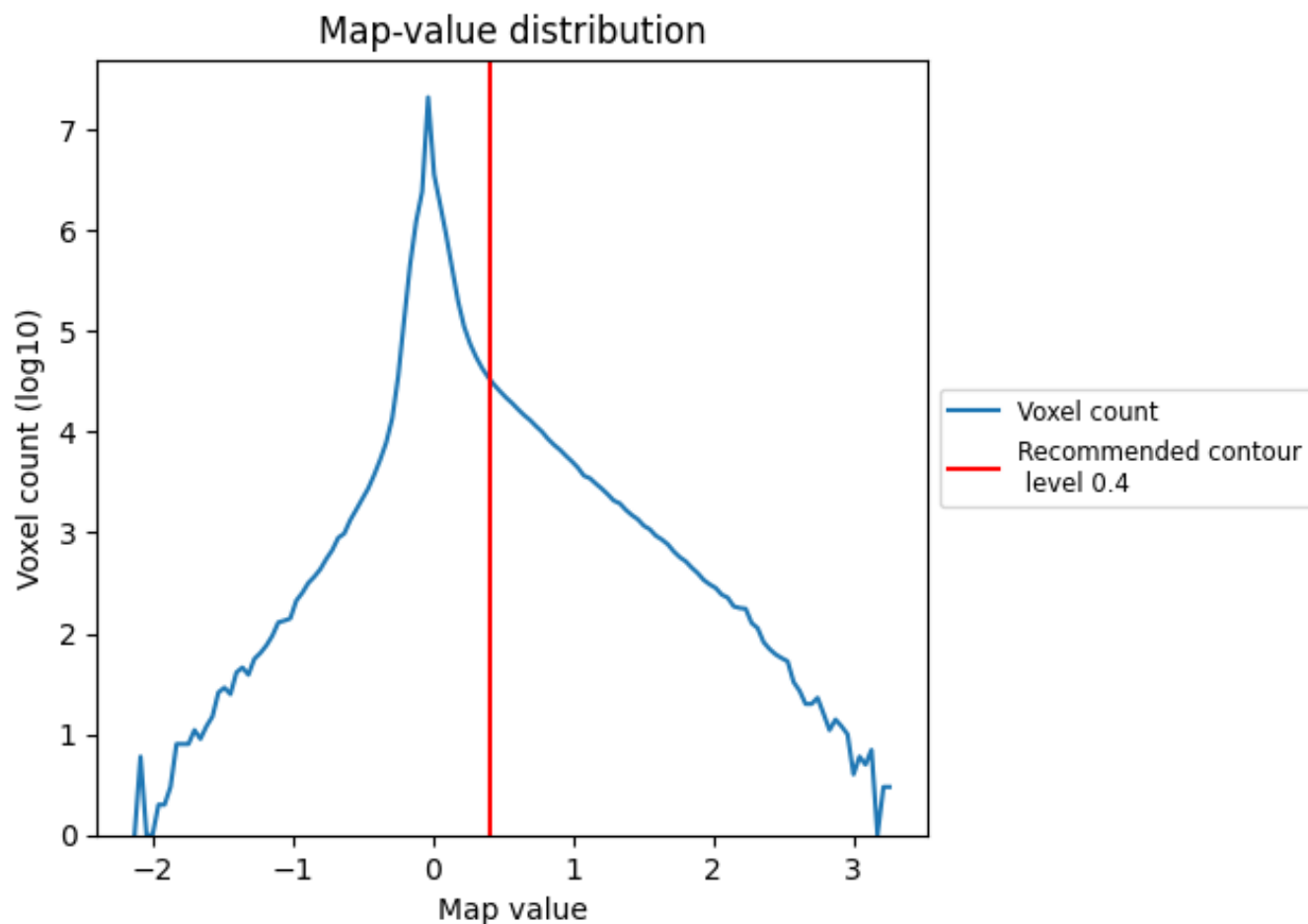


Z

7 Map analysis [i](#)

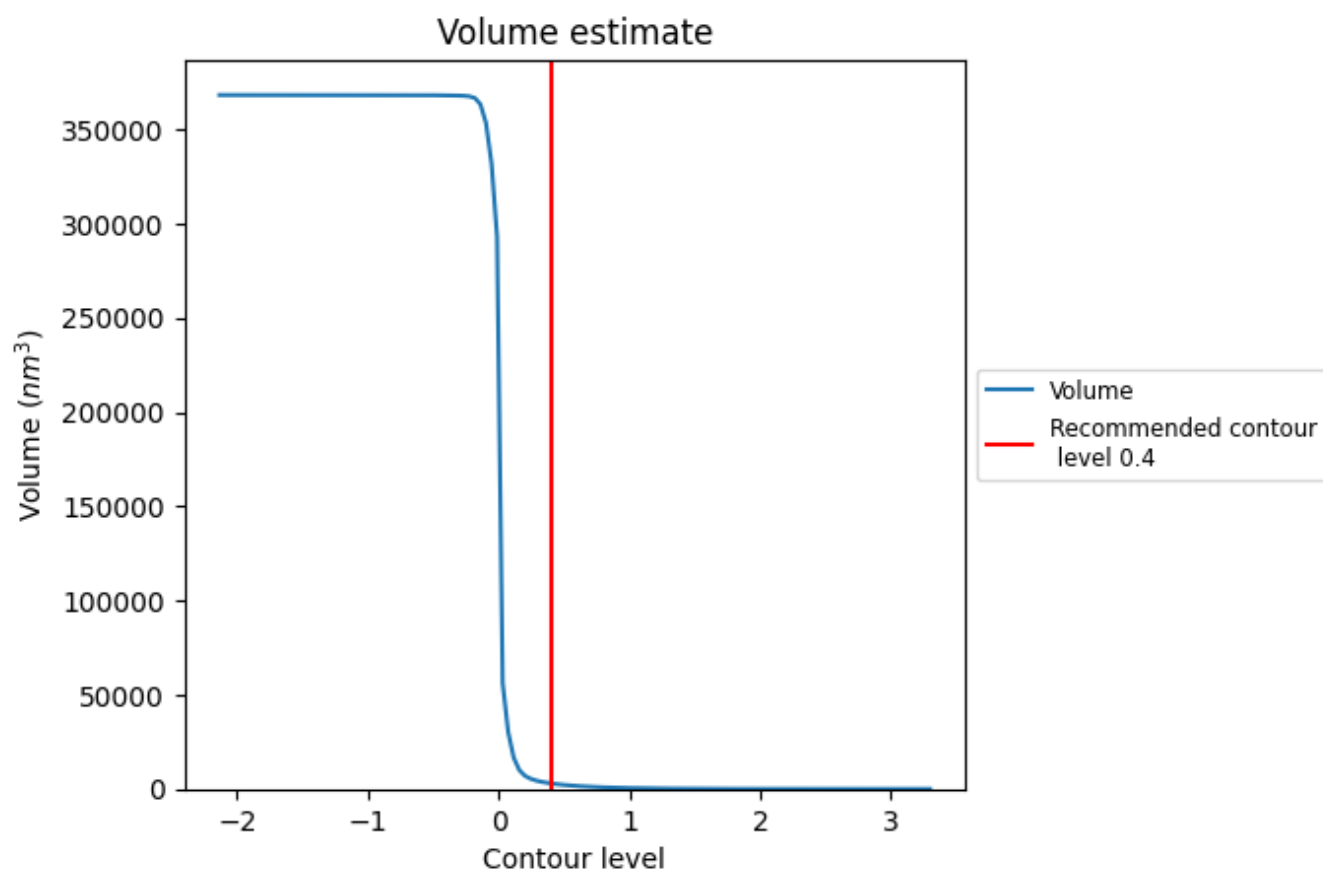
This section contains the results of statistical analysis of the map.

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.

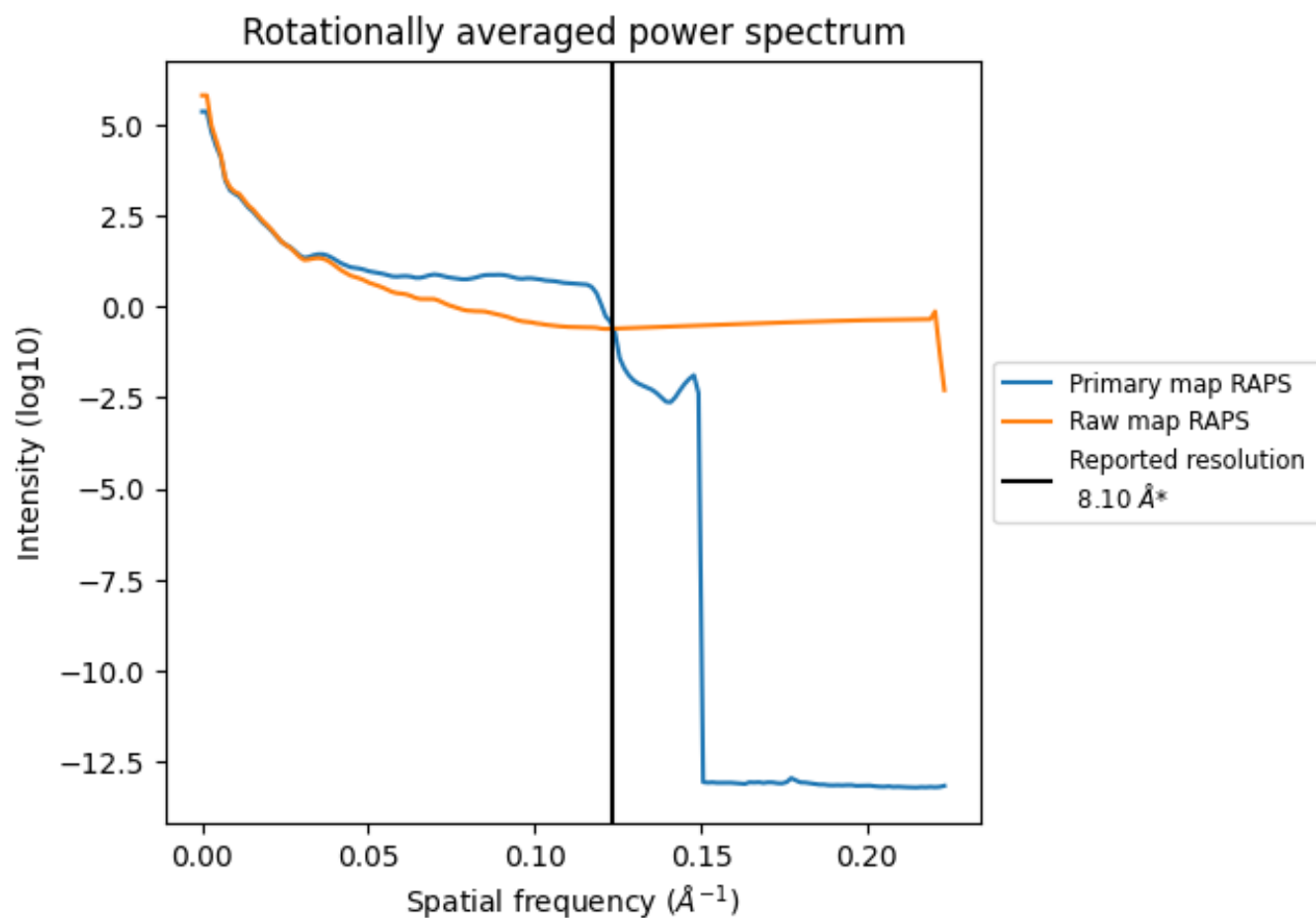
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2954 nm³; this corresponds to an approximate mass of 2669 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 ⓘ

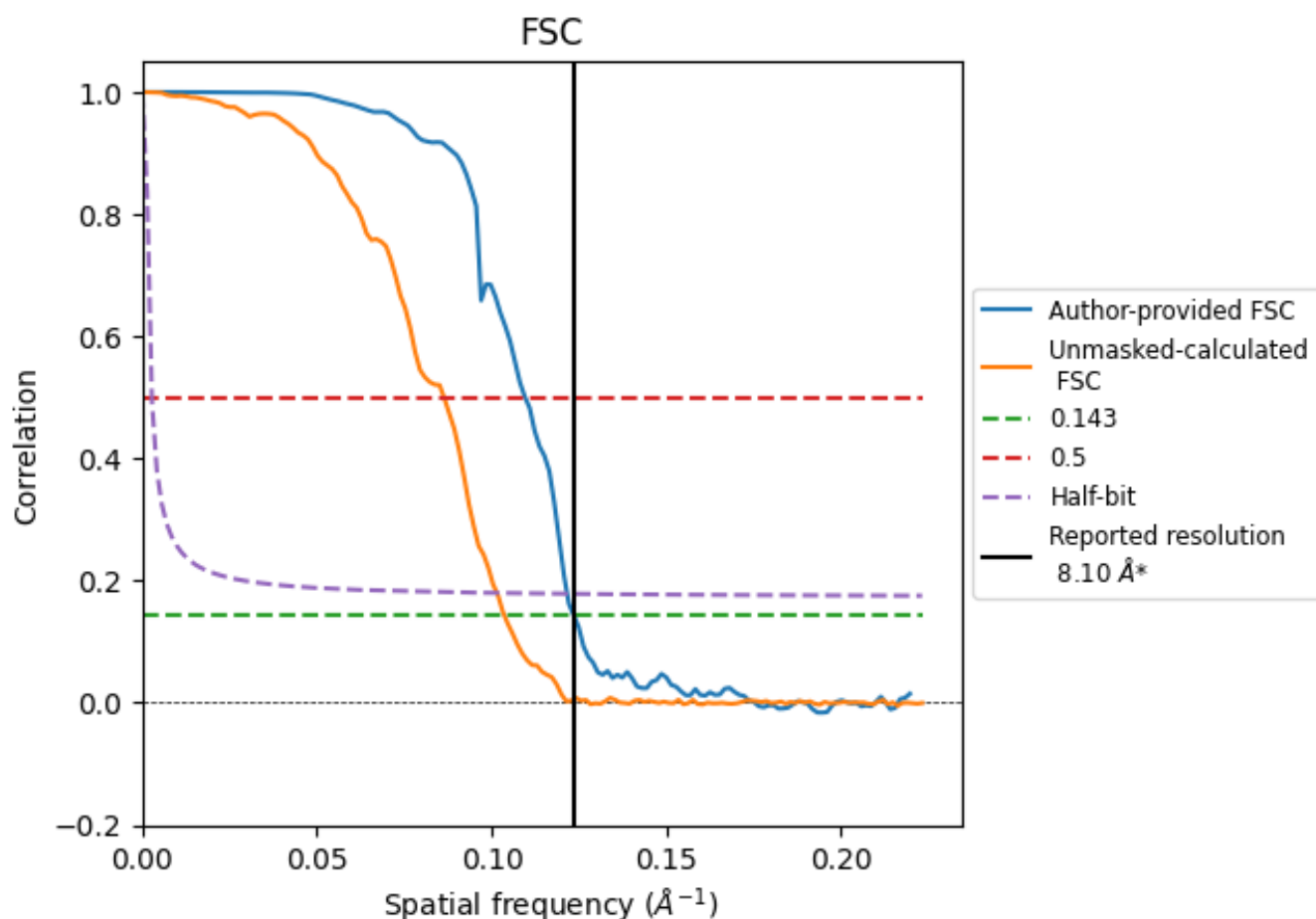


*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

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 $0.123 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

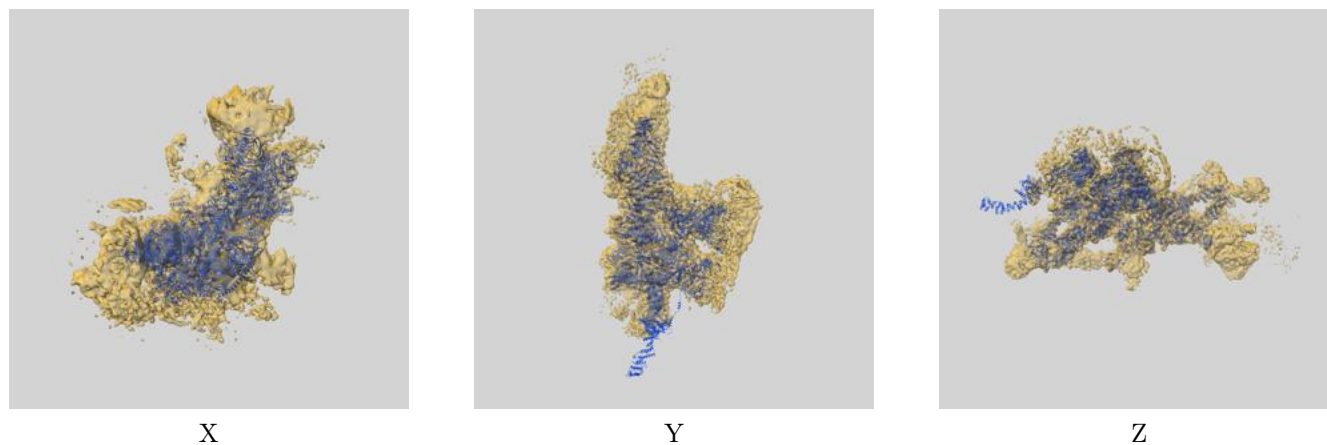
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.10	9.12	8.22
Unmasked-calculated*	9.64	11.57	9.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.64 differs from the reported value 8.1 by more than 10 %

9 Map-model fit [i](#)

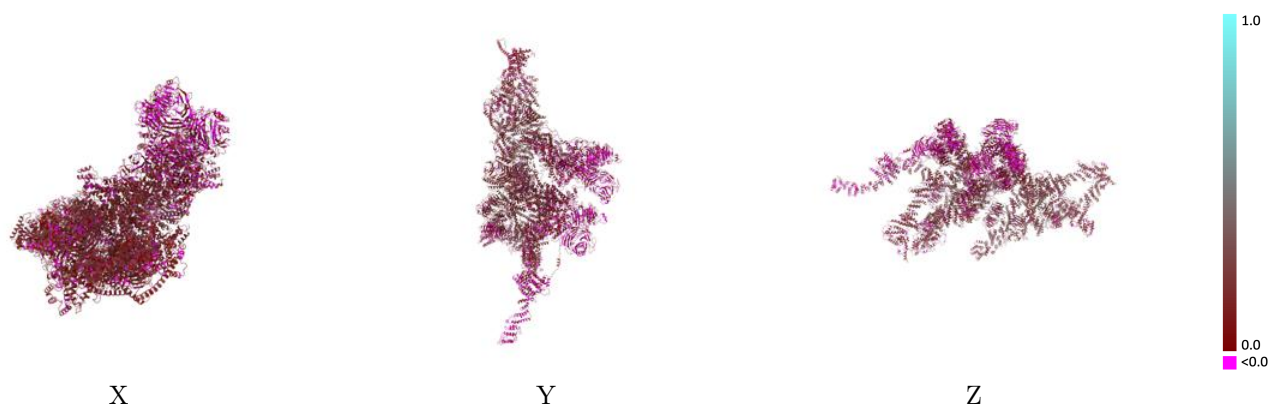
This section contains information regarding the fit between EMDB map EMD-31891 and PDB model 7VCI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



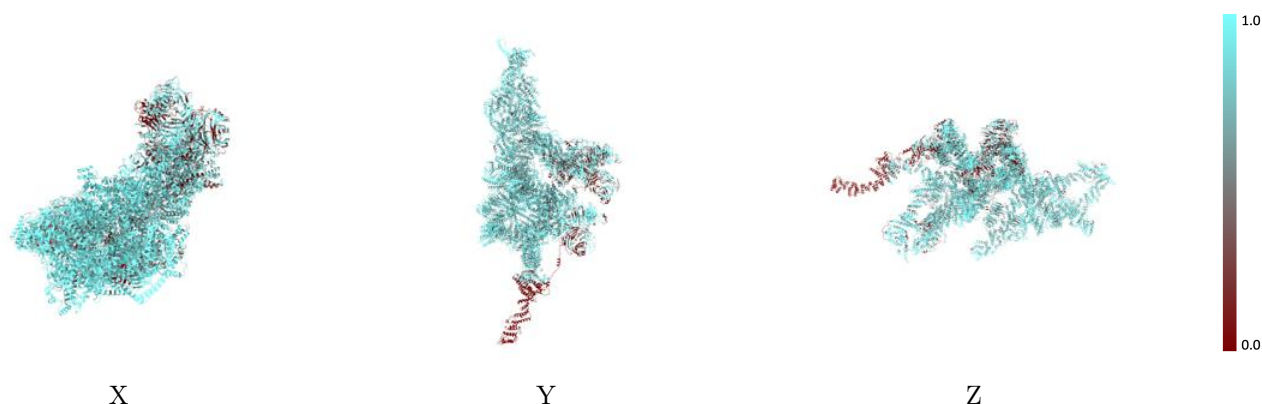
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



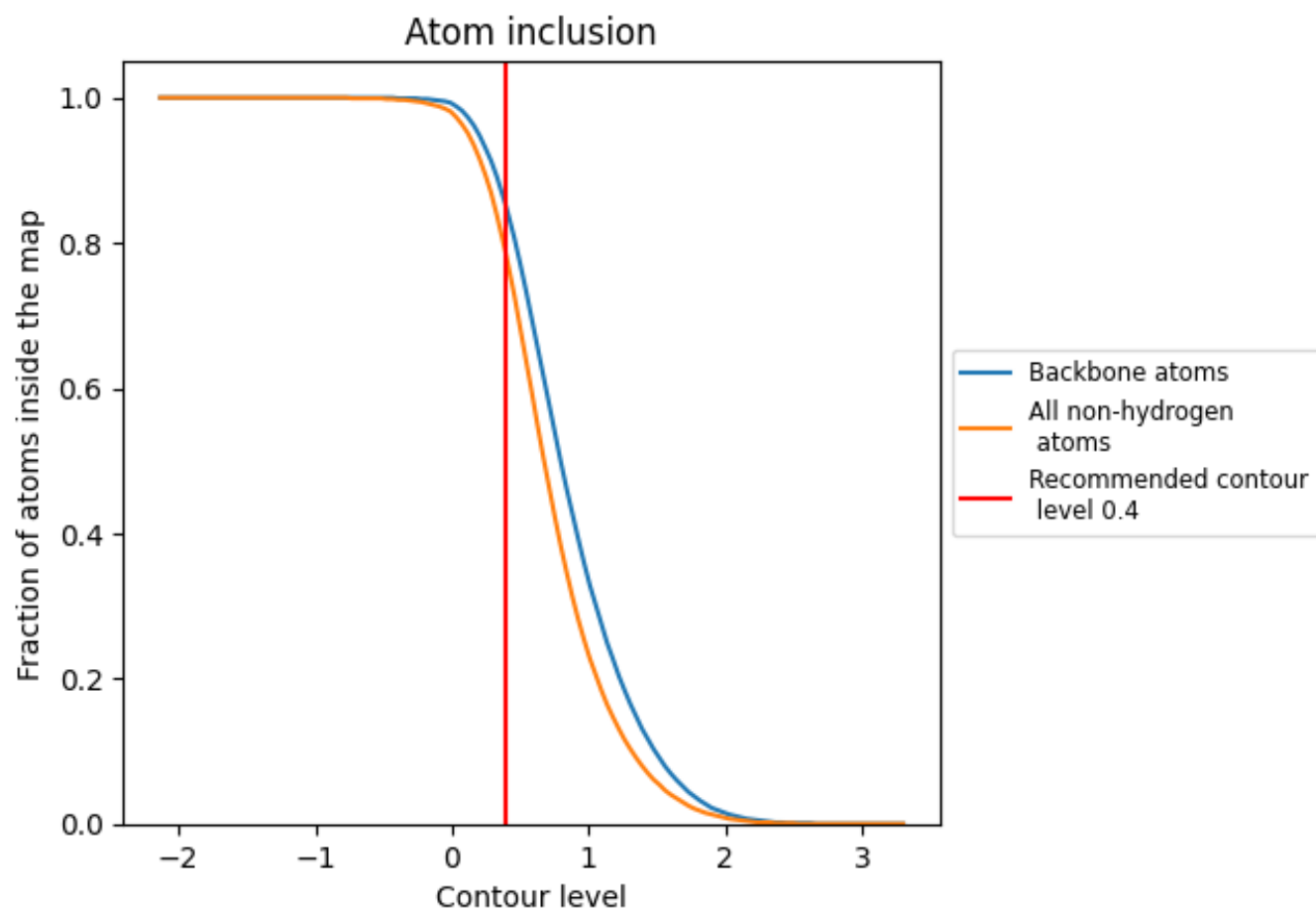
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.1300
A	 0.8540	 0.1760
B	 0.7860	 0.1290
C	 0.9010	 0.1700
D	 0.7970	 0.1160
E	 0.9200	 0.1150
F	 0.8320	 0.1610
G	 0.8570	 0.1570
H	 0.8030	 0.1390
I	 0.6720	 0.0990
J	 0.8920	 0.1590
K	 0.8480	 0.1030
L	 0.9230	 0.1560
M	 0.8340	 0.1070
N	 0.8670	 0.1180
O	 0.8610	 0.1840
P	 0.9080	 0.1580
Q	 0.8180	 0.1640
R	 0.2590	 0.0390
S	 0.8480	 0.1480
T	 0.6470	 0.0980
U	 0.8870	 0.1570

