



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 11:34 PM UTC

PDB ID : 8Y39 / pdb_00008y39
EMDB ID : EMD-38876
Title : cryo-EM structure of Staphylococcus aureus(ATCC 29213) 70S ribosome in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 3.60 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:

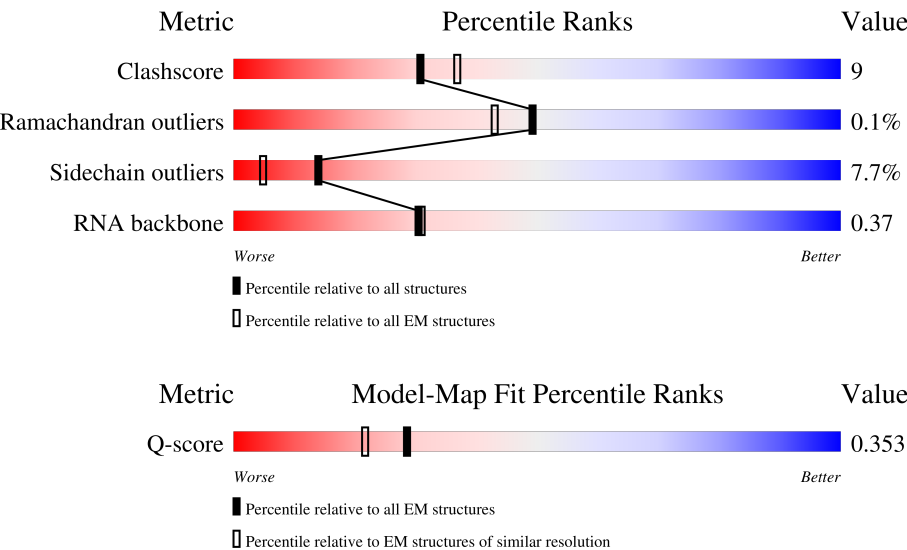
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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.



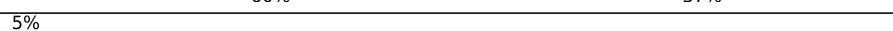
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	2921	53% 38% 8%
2	B	115	48% 44% 8%
3	C	274	70% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	215	
5	E	206	
6	F	175	
7	G	175	
8	H	145	
9	I	122	
10	J	146	
11	K	137	
12	L	120	
13	M	119	
14	N	114	
15	O	116	
16	P	102	
17	Q	117	
18	R	89	
19	S	103	
20	T	94	
21	U	82	
22	V	58	
23	W	67	
24	X	58	
25	Y	59	
26	Z	48	
27	1	47	
28	2	43	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	3	64	
30	4	37	
31	a	1548	
32	b	232	
33	c	217	
34	d	200	
35	e	166	
36	f	98	
37	g	156	
38	h	132	
39	i	130	
40	j	102	
41	k	129	
42	l	149	
43	m	121	
44	n	61	
45	o	89	
46	p	91	
47	q	87	
48	r	80	
49	s	108	
50	t	83	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 138218 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2885	Total	C	N	O	P	0	0
			61859	27619	11312	20043	2885		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	175	Total	C	N	O	S	0	0
			1317	835	223	253	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

- Molecule 8 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 11 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 12 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 13 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 14 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	114	Total	C	N	O	0	0
			889	563	175	151		

- Molecule 15 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 18 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 20 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	94	Total	C	N	O	0	0
			711	456	127	128		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	82	Total	C	N	O	0	0
			615	380	121	114		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	58	Total	C	N	O	0	0
			445	277	96	72		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 25 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	57	Total	C	N	O	0	0
			353	214	65	74		

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	48	Total	C	N	O	S	0	0
			361	222	77	59	3		

- Molecule 27 is a protein called Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1479	Total	C	N	O	P	0	0
			31706	14154	5809	10264	1479		

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	224	Total	C	N	O	S	0	0
			1802	1149	314	332	7		

- Molecule 33 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	199	Total	C	N	O	S	0	0
			1616	1020	302	292	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1160	731	212	215	2		

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			789	498	138	150	3		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	155	Total	C	N	O	S	0	0
			1242	775	239	224	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1031	652	183	192	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			1007	624	201	181	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	97	Total	C	N	O	S	0	0
			773	488	141	143	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			844	520	160	161	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 45 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O	S	0	0
			726	448	149	128	1		

- Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	87	Total	C	N	O	S	0	0
			688	433	127	127	1		

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			657	416	117	123	1		

- Molecule 48 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	64	Total	C	N	O	S	0	0
			525	336	98	88	3		

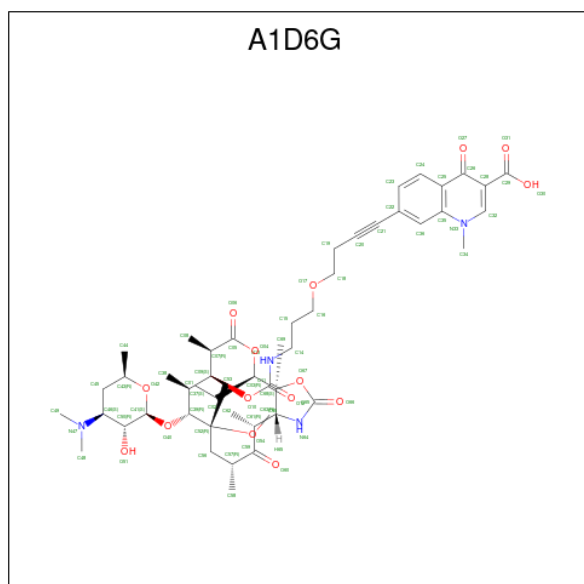
- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			665	427	121	115	2		

- Molecule 50 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 51 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo[1 2.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (CCD ID: A1D6G) (formula: C₅₀H₇₂N₄O₁₅).



Mol	Chain	Residues	Atoms				AltConf
51	A	1	Total	C	N	O	0
			69	50	4	15	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

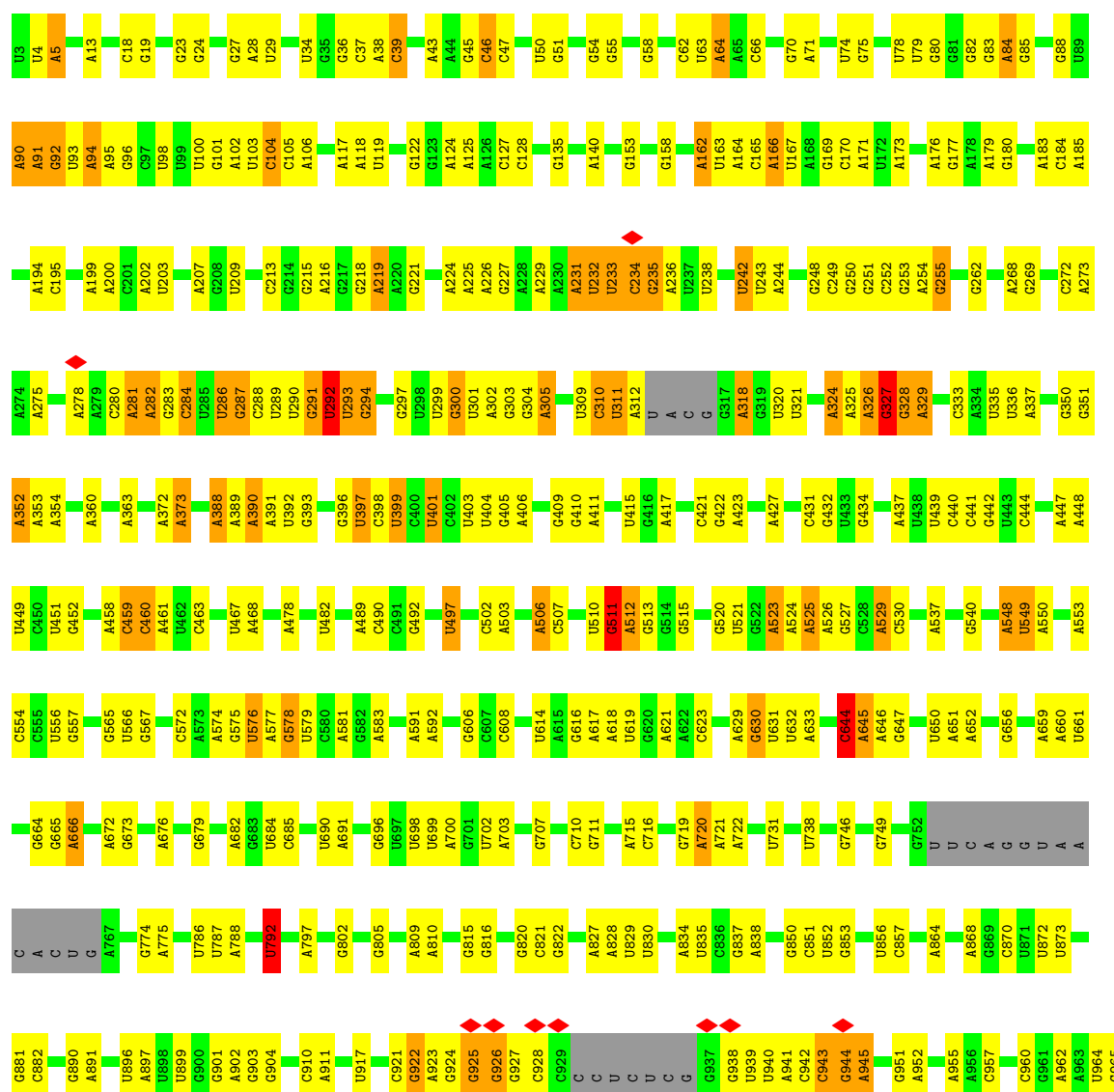
Mol	Chain	Residues	Atoms		AltConf
52	A	12	Total	Mg	0
			12	12	

3 Residue-property plots

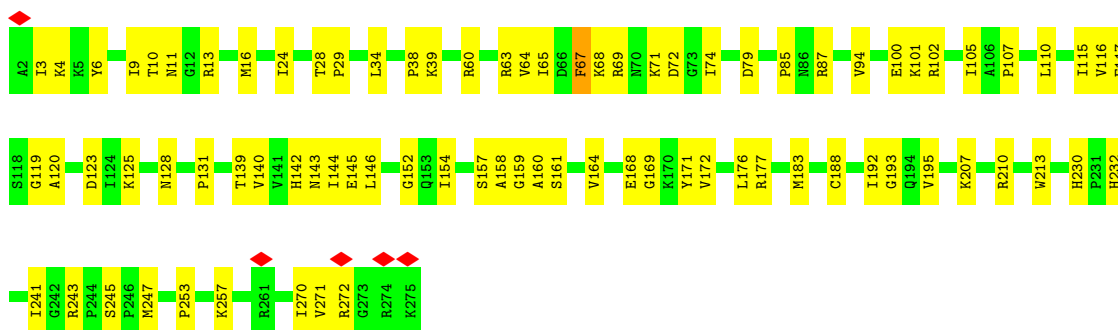
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

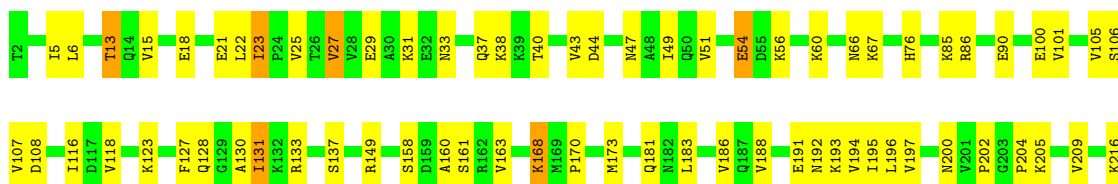
Chain A:  53% 38% 8% .



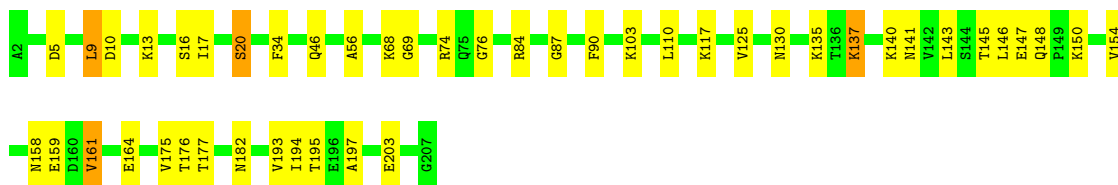
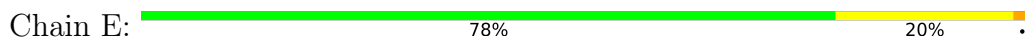
A2008	G1915	A1814	A1726	A1634	G1559	G1486	C1387	G1295	A1200	U1127	U1070	U970
U2009	A1916	C1815	C1727	A1635	A1560	G1487	C1387	C1296	G1201	A1128	A1070	U971
	A1917	C1816		A1636	G1561	A1488	A1390	G1297	C1202	A1129	A1071	U972
U2018	G1918	C1817	U1737	A1637	G1562	A1489	A1390	G1300	U1203	A1130	A1072	A973
G2019	C1919	A1818	C1738	G1639	A1567	G1490	A1396	U1301	G1205	A1131	A1065	A974
U2020	C1920	A1819	G1739	U1640	U1568	U1493	G1397	G1302	U1206	A1132	G1066	U975
C2021		G1820	G1740	G1641	U1569	G1494		A1303	G1207	G1133		U976
U2022	A1923	U1821	G1741	G1651	G1571		C1400	A1304	A1208	U1134	A1070	A977
C2023	A1928	C1822	G1742	A1652	G1574	A1497	G1401	U1305		C1135	A1071	
A2024	C1929	A1823	G1743	A1653	A1575	U1498	A1402	U1306	U1215	C1136	A1072	G984
A2025		G1825	A1744	A1654	A1576	U1499		G1307	U1216	G1137	A1073	A985
C2026	C1827	G1826	G1746	G1655	A1577	G1500	G1405	G1308	U1217	U1138		
G2029	G1933	U1828	G1747	C1656	U1504		A1415	G1309	U1218	A1139	U1077	A989
	G1934	A1829		G1657	C1506		U1416	A1310	G1219	U1140		G990
A2032		A1830	G1751	A1658	A1578	A1507		A1311	U1219	A1141		A991
			G1752	C1659	C1579	C1508	A1421	A1312	U1220	A1142		A992
C2035	U1938	U1835	U1753	A1660	A1580	G1509	A1422		G1225	G1083		C993
G2036	A1939	A1836	G1754	C1661	U1581	U1510	C1423	C1315	U1227	U1084		G1000
G2037	C		U1755	A1662	U1582	U1511	A1432	C1316	A1228	U1085		A1001
A2040	U	U1843	U1756		U1583	U1512	U1433	C1326	G1229	C1087		U1002
A2041	A	G1844	U1757	A1666	U1584	A1513	U1434	C1327	U1230	C1088		A1003
A2042		U1845	G1758		U1585	A1517	C1435	C1328	G1234	C1089		A1004
		A1856	G1760	C1669	U1586		C1436	G1329	C1235	A1090		G1005
G2048	A1945		G1761	A1670	U1587			U1330	G1236	G1091		
U2049	A1946	G1862	G1762	U1671	U1588	G1522	A1440	C1335	U1237	A1092		G1012
A2050	C1947	U1862	U1763	G1672	U1589	G1523	A1443	C1336	U1238	C1093		A1017
G1948	G1948	C1870	A1764	A1678	G1590	C1524		A1337	G1245	U1094		A1018
A2057	U1949	U1871	G1765	A1679	G1591	U1525	A1450	U1338	C1246	A1095		A1019
A2058	U1950	G1872	C1766	U1680	G1592	G1526	U1451	U1339	G1247	U1097		
G2059	C1951	G1873		U1681	U1593	A1527		G1340		G1156		
A2060	A1954	A1874	C1769	A1684	G1595	G1528	U1454	A1341	C1254	A1098		A1024
U2061	A1955	G1875	C1770		G1596	U1529	U1455	U1342	U1157	G1099		
G2062	G1956	G1876	A1771	G1687	U1597	A1530	U1456	U1343	G1158	G1100		A1027
	U1957				U1598	U1531	A1458	U1344	A1159	A1101		G1028
C2070	U1958	A1880	G1783	G1691	G1599	U1532	U1457	U1345	C1260	G1102		C1029
		G1881		G1692		A		G1346	G1261	U1103		G1033
C2074	A1964	G1882	A1789	A1690	U1602	G	A1461	U1347	U1163	U1104		A1034
G2075	A1965	A1883	G1790	G1691		G	A1459	U1348		U1105		C1035
A2076	U1966		G1791	G1693	A1605	C	U1460	U1349	G1166	G1106		G1036
C2077	U1967	A1886			C1606	A1537	G1462					A1037
A2078		A1893	A1796	A1699	G1613	A1538	A1463	G1357	G1169	U1109		C1038
G2082	U1982	G1894	G1797	U1701		A1539	A1464	A1358	U1174	U1110		C1039
			A1800	U1708	A1616	U1540	G1465	A1359	G1175	A1111		A1040
A2087	G1986	U1897	C1801	U1707	A1617	C1542	A1471	G1360	U1176	G1112		U1043
G2088	C1989	C1898	U1802	A1708	A1618		C1472	G1362	G1177	A1113		A1044
A2089	G1991	U1899	G1803	A1709		U1548			C1179	G1115		A1045
C2090	C1992	G1900	U1804		U1623	G1549	G1476	U1366	G1180			G1046
C2091	A1903	U1805	U1806	A1712	C1624	C1550	U1477		A1181	C1116		G1047
C2092	C1904	U1807	A1626	A1713	U1625	U1551	A1478	C1370	G1182	A1117		
G2093	G1905	U1808	G1627	C1714	U1552	U1552	G1479	G1378	G1183	C1118		C1051
G2094	A1908	C1809	A1553	G1717	A1553	A1553	G1480	A1379	G1184	C1119		A1052
U2095	A1996		U1628	U1718	A1554	A1554	A1481	U1381	U1185	A1121		A1053
G2096	A1997	C1909	U1629	U1719	A1555	G1555	U1482	G1380	A1186	U1122		A1054
G2097	C1999		G1631	G1719	G1556	G1556	A1483	U1381	A1192	C1123		U1056
A2098	U2003	A1813	A1632	A1633	C1557	C1557	G1484	G1384		A1124		A1057



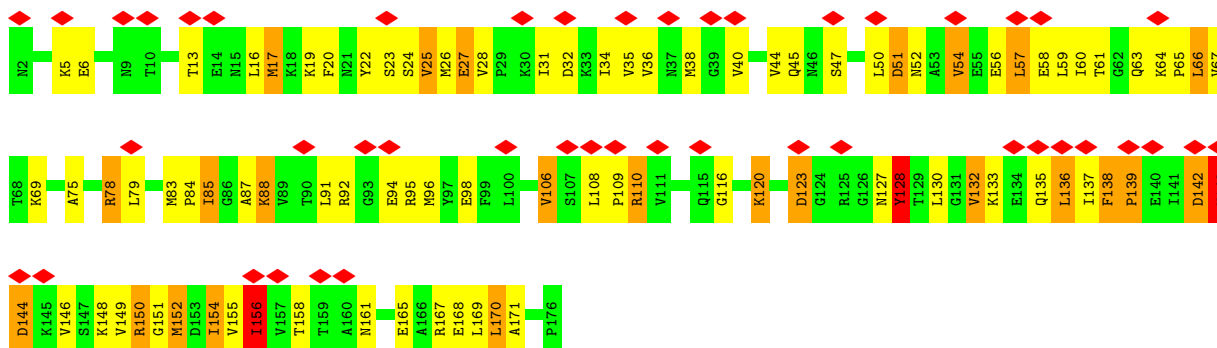
• Molecule 4: Large ribosomal subunit protein uL3



• Molecule 5: Large ribosomal subunit protein uL4

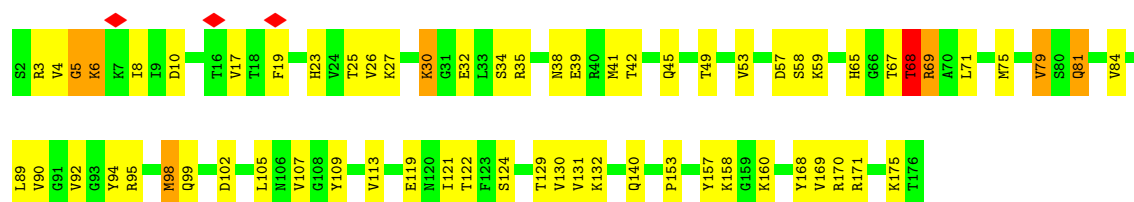


• Molecule 6: Large ribosomal subunit protein uL5



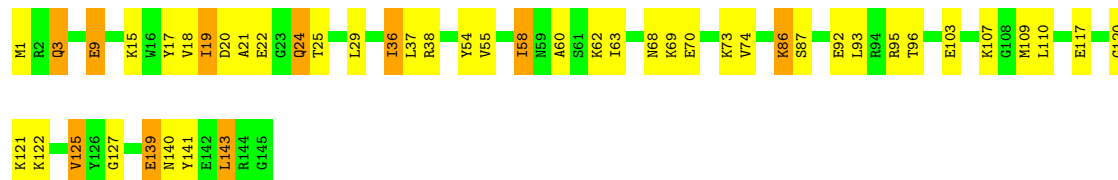
• Molecule 7: Large ribosomal subunit protein uL6





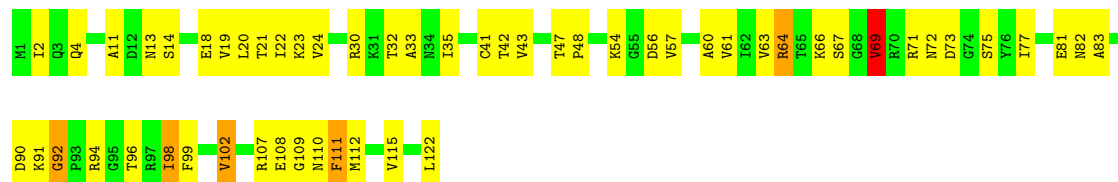
• Molecule 8: Large ribosomal subunit protein uL13

Chain H: 68% 26% 7%



• Molecule 9: Large ribosomal subunit protein uL14

Chain I: 55% 40% . .



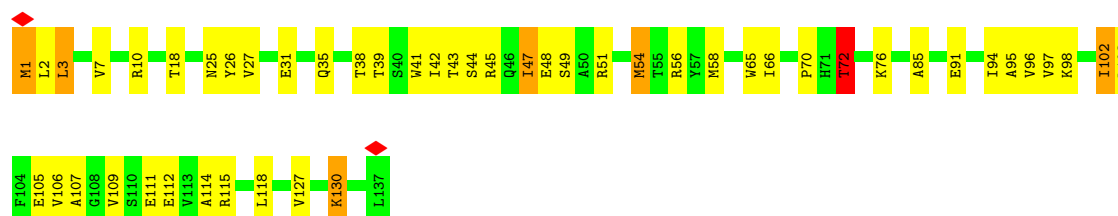
• Molecule 10: Large ribosomal subunit protein uL15

Chain J: 77% 21% .



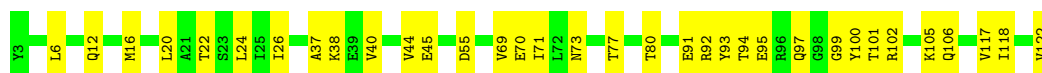
• Molecule 11: Large ribosomal subunit protein uL16

Chain K: 64% 31% . .



• Molecule 12: Large ribosomal subunit protein bL17

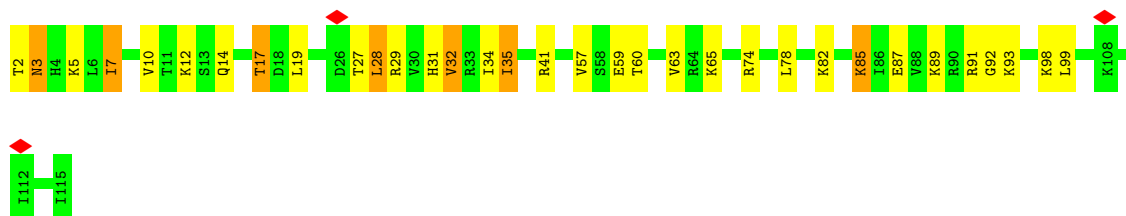
Chain L: 72% 28%



- Molecule 13: Large ribosomal subunit protein uL18



- Molecule 14: Large ribosomal subunit protein bL19



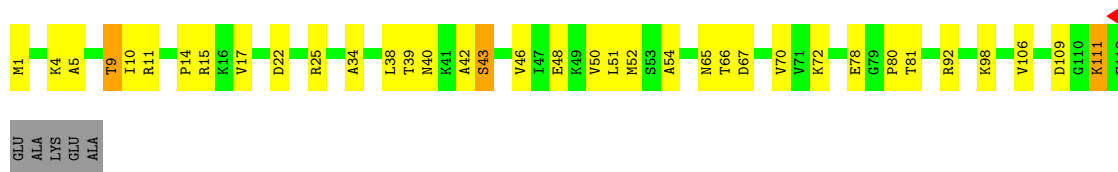
- Molecule 15: Large ribosomal subunit protein bL20



- Molecule 16: Large ribosomal subunit protein bL21



- Molecule 17: Large ribosomal subunit protein uL22



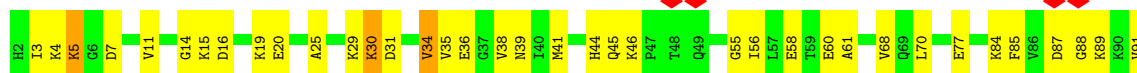
- Molecule 18: Large ribosomal subunit protein uL23

Chain R:  55% 38% 7%



- Molecule 19: Large ribosomal subunit protein uL24

Chain S:  61% 36% 6%



- Molecule 20: Large ribosomal subunit protein bL25

Chain T:  60% 37% 3%



- Molecule 21: Large ribosomal subunit protein bL27

Chain U:  68% 28% 5%



- Molecule 22: Large ribosomal subunit protein bL28

Chain V:  69% 26% 5%



- Molecule 23: Large ribosomal subunit protein uL29

Chain W:  63% 33% 4%



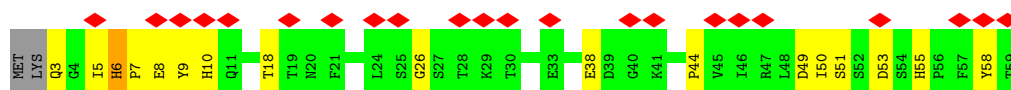
- Molecule 24: Large ribosomal subunit protein uL30

Chain X: 86% 14%



- Molecule 25: Large ribosomal subunit protein bL31B

Chain Y: 37% 68% 27% . .



- Molecule 26: Large ribosomal subunit protein bL32

Chain Z: 79% 21%



- Molecule 27: Large ribosomal subunit protein bL33B

Chain 1: 66% 28% 6%



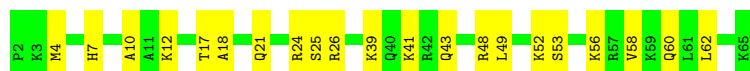
- Molecule 28: Large ribosomal subunit protein bL34

Chain 2: 81% 19%



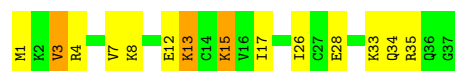
- Molecule 29: Large ribosomal subunit protein bL35

Chain 3: 67% 33%

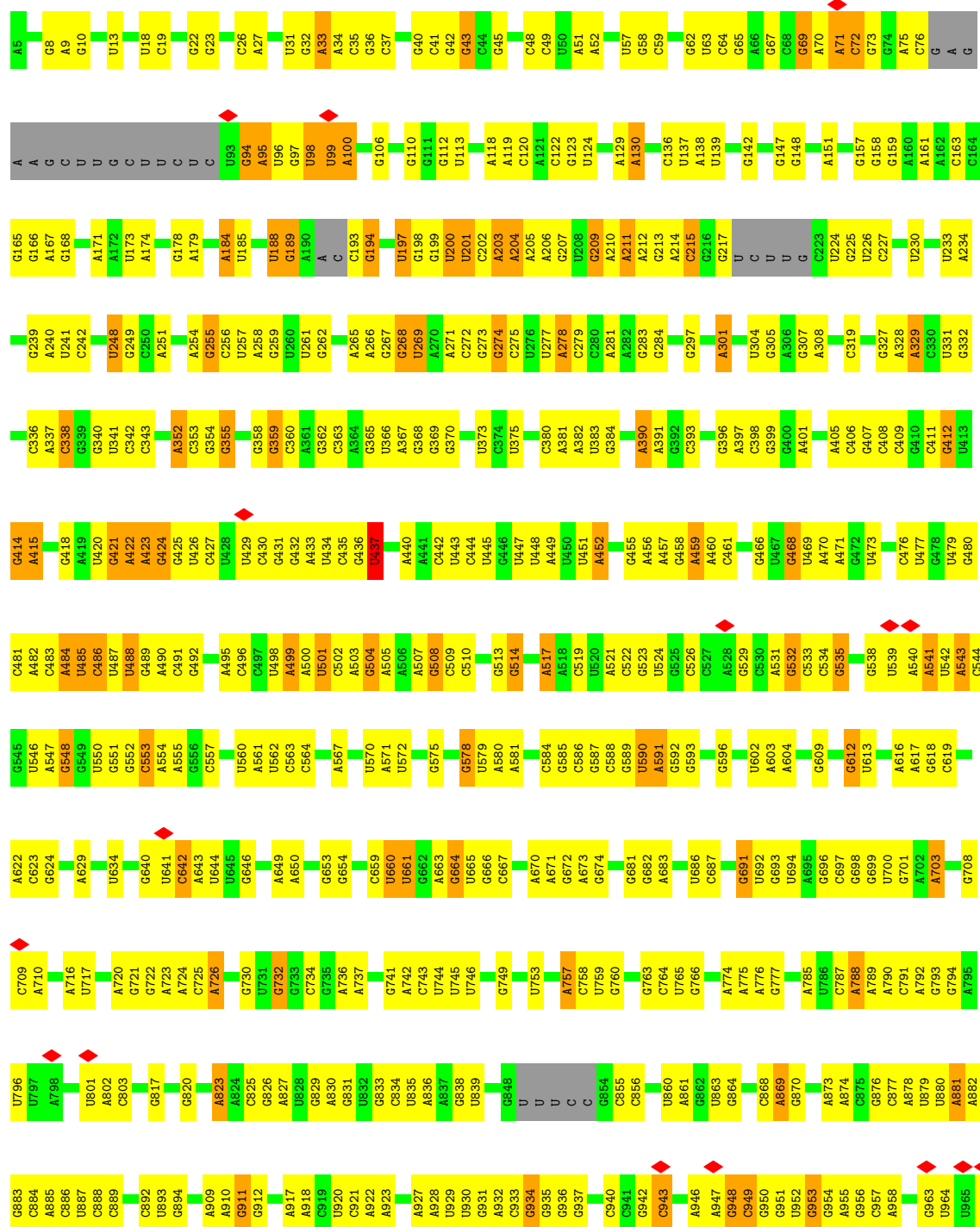


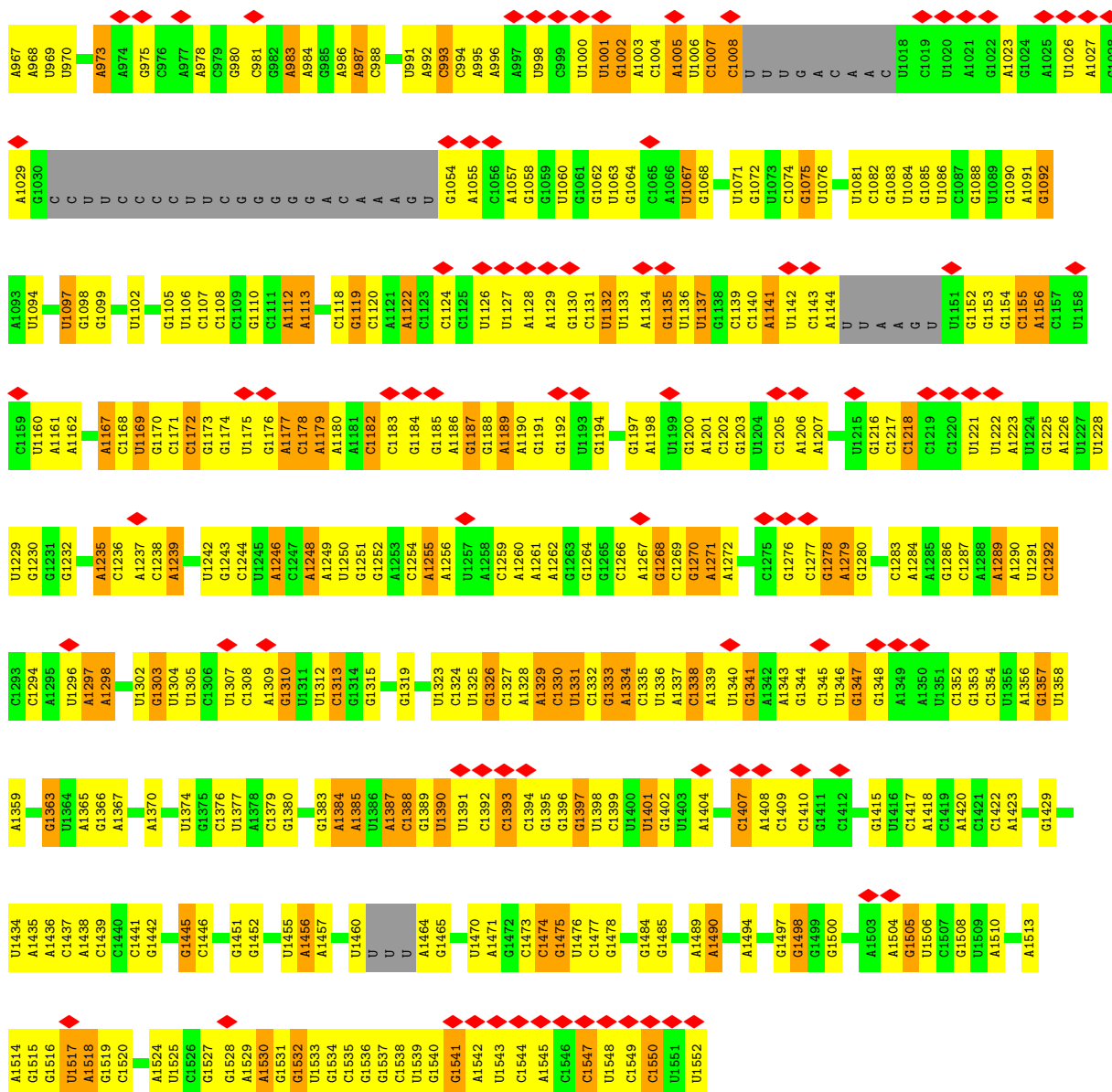
- Molecule 30: Large ribosomal subunit protein bL36

Chain 4: 62% 30% 8%



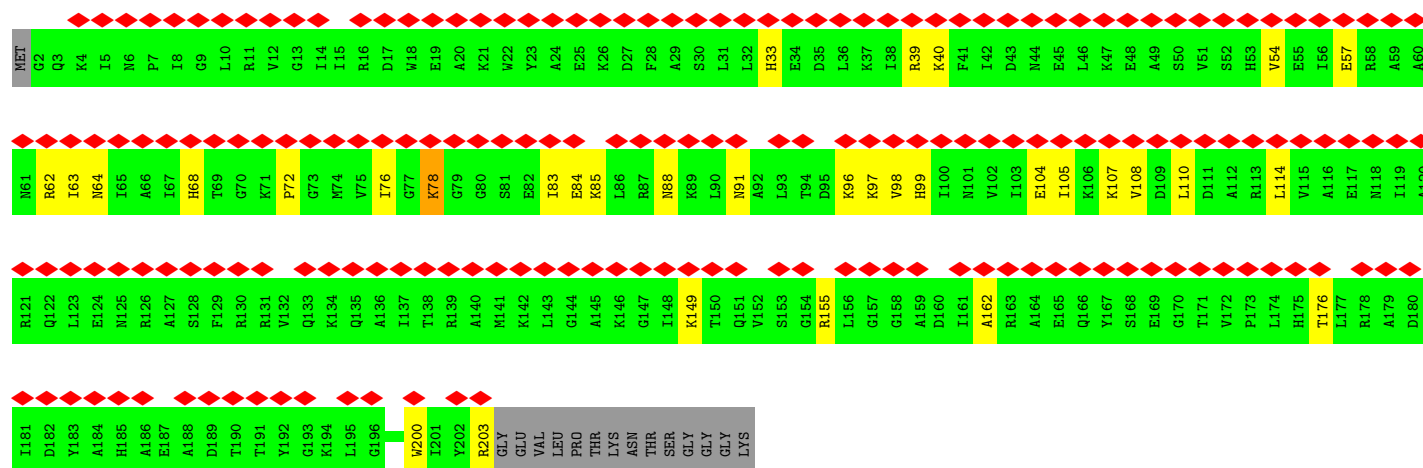
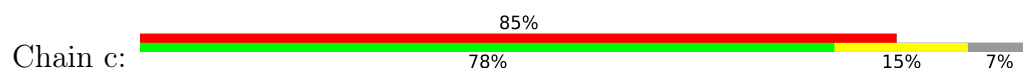
• Molecule 31: 16S ribosomal RNA



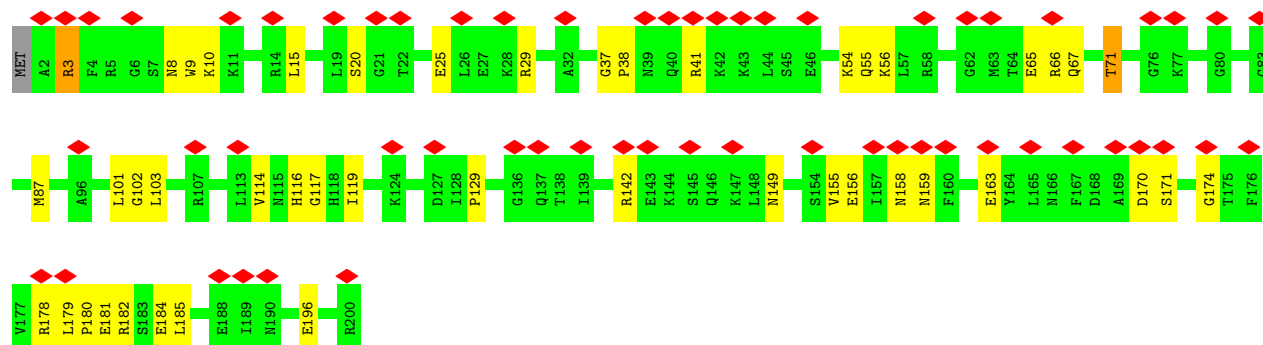
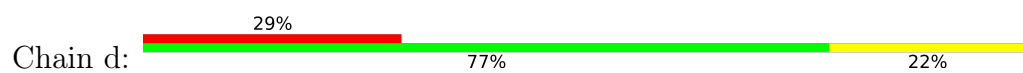




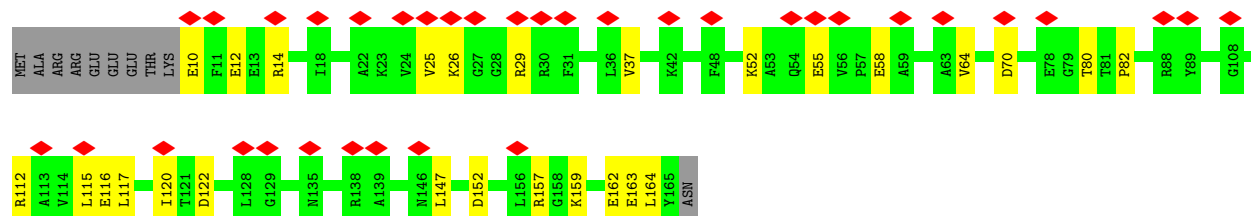
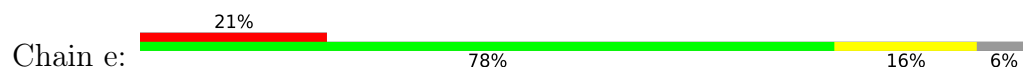
- Molecule 33: Small ribosomal subunit protein uS3



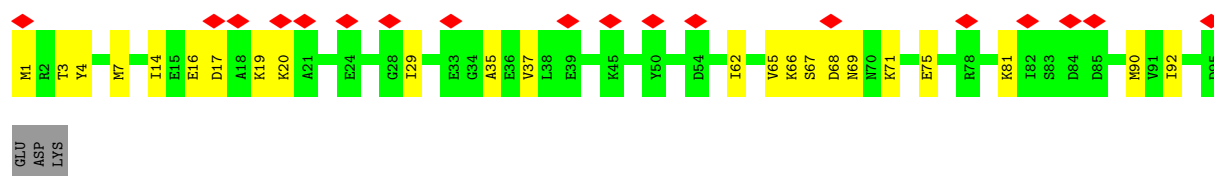
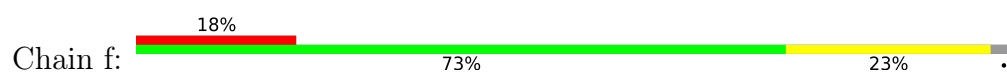
- Molecule 34: Small ribosomal subunit protein uS4



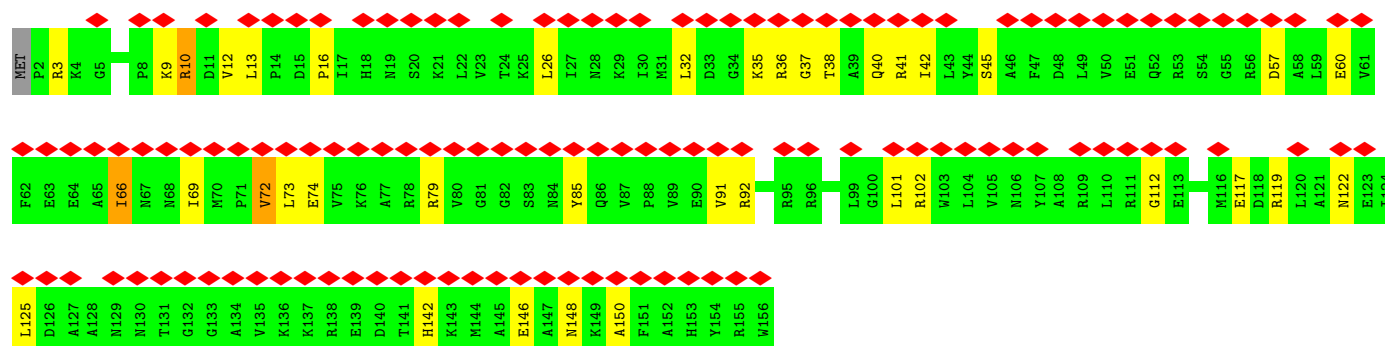
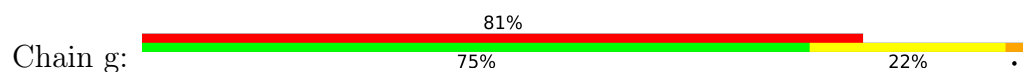
- Molecule 35: Small ribosomal subunit protein uS5



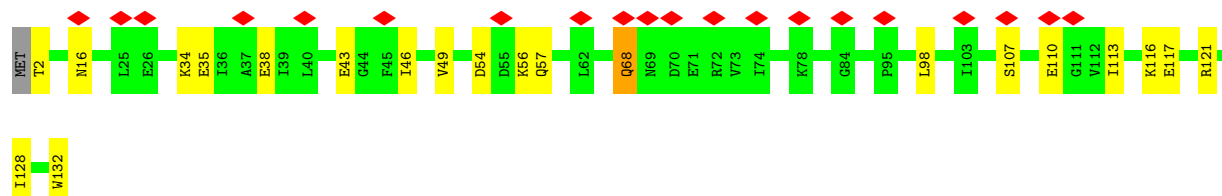
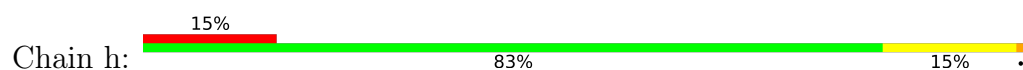
- Molecule 36: Small ribosomal subunit protein bS6



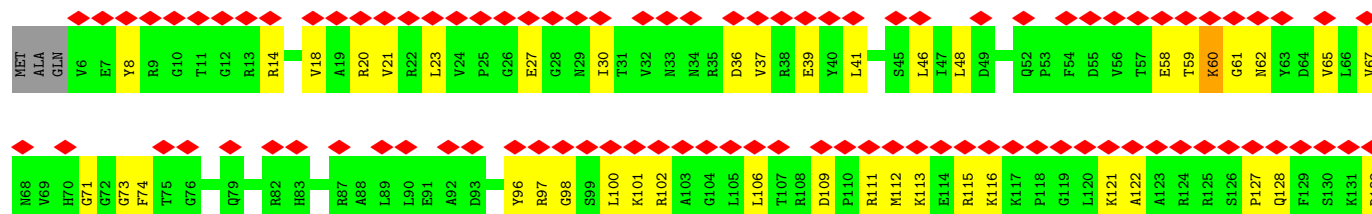
• Molecule 37: Small ribosomal subunit protein uS7



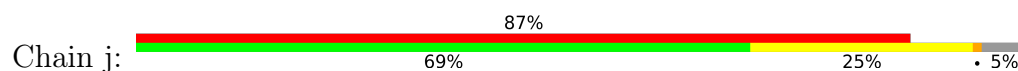
• Molecule 38: Small ribosomal subunit protein uS8



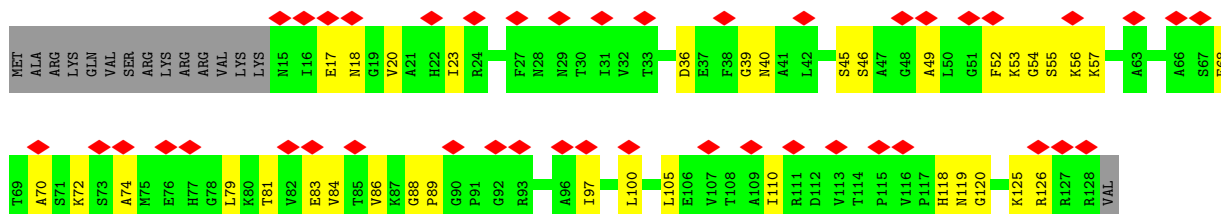
• Molecule 39: Small ribosomal subunit protein uS9



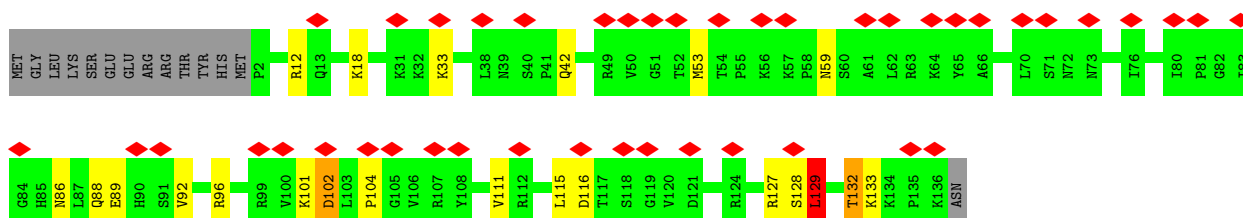
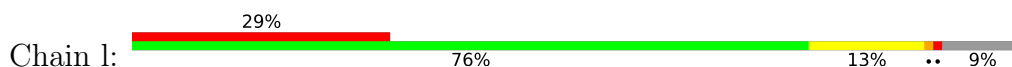
• Molecule 40: Small ribosomal subunit protein uS10



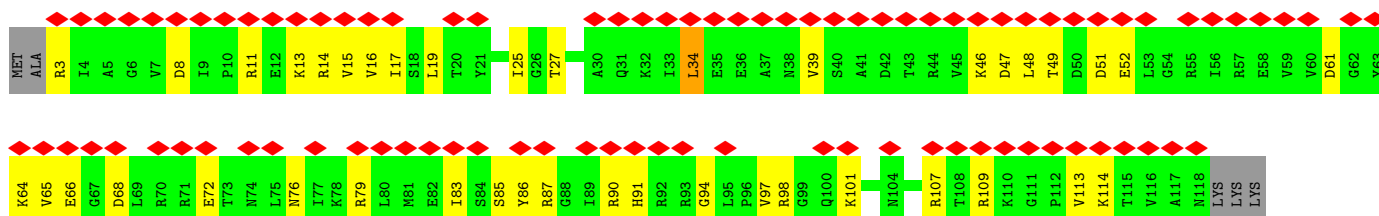
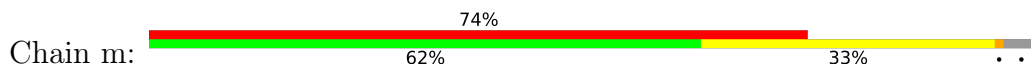
- Molecule 41: Small ribosomal subunit protein uS11



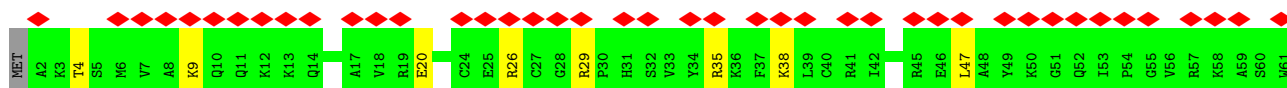
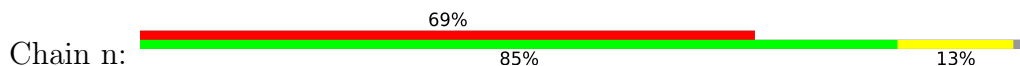
- Molecule 42: Small ribosomal subunit protein uS12



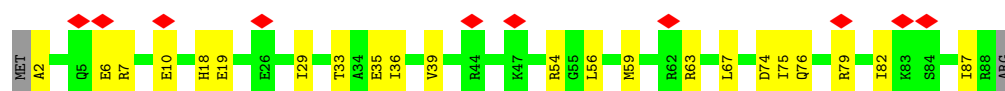
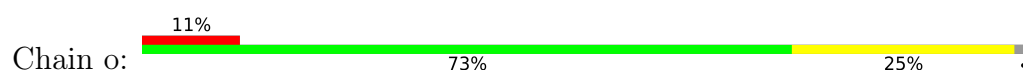
- Molecule 43: Small ribosomal subunit protein uS13



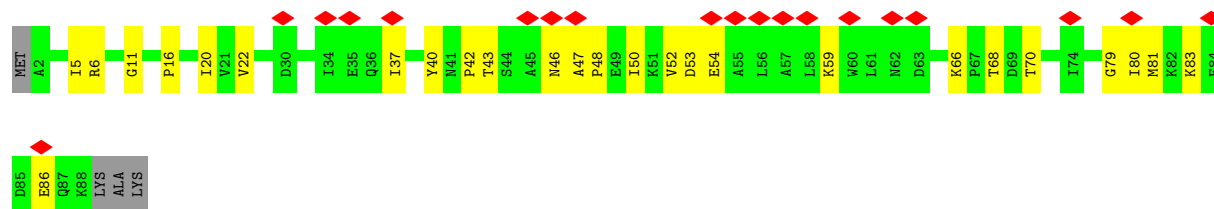
- Molecule 44: Small ribosomal subunit protein uS14B



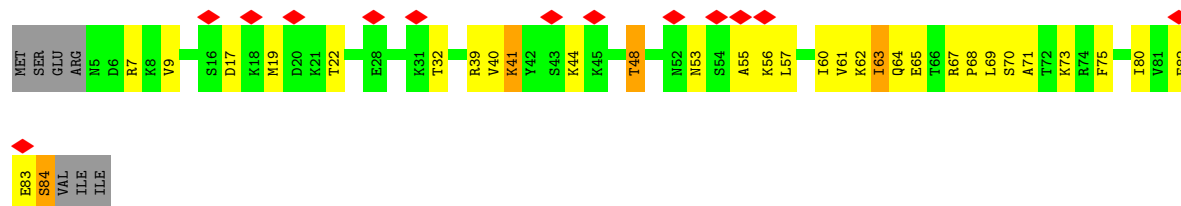
- Molecule 45: Small ribosomal subunit protein uS15



- Molecule 46: Small ribosomal subunit protein bS16



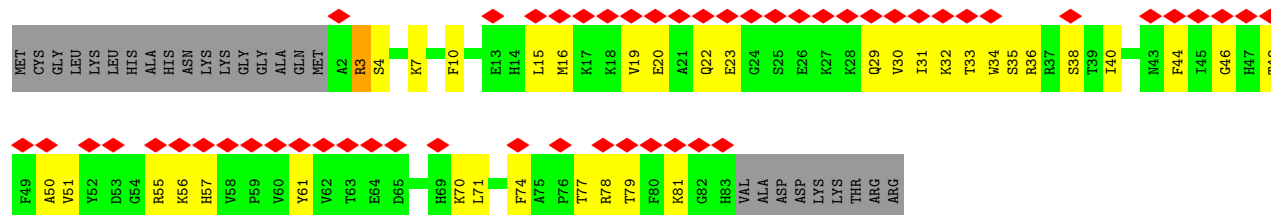
- Molecule 47: Small ribosomal subunit protein uS17



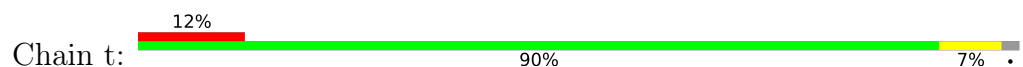
- Molecule 48: Small ribosomal subunit protein bS18

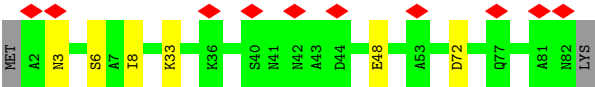


- Molecule 49: Small ribosomal subunit protein uS19



- Molecule 50: Small ribosomal subunit protein bS20





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0023	Depositor
Map size ($\text{\AA}$)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, OMG, MG, A1D6G, 5MU, 2MG

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	0.44	0/69148	0.68	35/107836 (0.0%)
2	B	0.40	0/2733	0.73	1/4257 (0.0%)
3	C	0.96	0/2125	1.23	9/2853 (0.3%)
4	D	1.08	3/1651 (0.2%)	1.18	10/2215 (0.5%)
5	E	0.98	1/1595 (0.1%)	1.21	11/2154 (0.5%)
6	F	0.67	0/1332	1.29	24/1798 (1.3%)
7	G	0.92	1/1277 (0.1%)	1.31	9/1731 (0.5%)
8	H	0.74	0/1165	0.98	5/1570 (0.3%)
9	I	0.93	0/925	1.12	7/1242 (0.6%)
10	J	0.61	0/1100	0.80	3/1467 (0.2%)
11	K	0.96	1/1095 (0.1%)	1.10	10/1472 (0.7%)
12	L	0.63	0/936	0.64	0/1253
13	M	0.90	0/900	1.23	5/1205 (0.4%)
14	N	0.91	1/901 (0.1%)	0.92	3/1209 (0.2%)
15	O	0.54	0/954	0.61	1/1264 (0.1%)
16	P	0.71	0/800	0.96	3/1070 (0.3%)
17	Q	0.97	1/861 (0.1%)	1.02	3/1161 (0.3%)
18	R	0.76	0/723	0.96	2/966 (0.2%)
19	S	0.68	0/779	1.02	4/1043 (0.4%)
20	T	0.68	2/719 (0.3%)	0.89	3/969 (0.3%)
21	U	0.72	0/621	0.89	1/825 (0.1%)
22	V	1.05	1/451 (0.2%)	1.25	4/603 (0.7%)
23	W	0.81	0/542	0.86	1/722 (0.1%)
24	X	0.77	0/451	0.73	2/606 (0.3%)
25	Y	0.48	0/361	0.89	2/500 (0.4%)
26	Z	0.85	0/367	0.99	0/490
27	1	0.90	0/395	1.23	3/530 (0.6%)
28	2	0.51	0/371	0.75	0/484
29	3	0.88	0/526	1.13	5/690 (0.7%)
30	4	1.12	0/299	1.42	6/393 (1.5%)
31	a	0.15	0/35498	0.34	1/55345 (0.0%)
32	b	0.19	0/1829	0.46	0/2455

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.12	0/1618	0.33	0/2173
34	d	0.15	0/1646	0.38	0/2211
35	e	0.25	0/1174	0.47	0/1584
36	f	0.18	0/800	0.45	0/1073
37	g	0.19	0/1262	0.47	1/1698 (0.1%)
38	h	0.22	0/1043	0.41	0/1401
39	i	0.15	0/1023	0.43	0/1374
40	j	0.16	0/785	0.43	0/1060
41	k	0.24	0/859	0.59	0/1161
42	l	0.27	0/1075	0.49	1/1439 (0.1%)
43	m	0.15	0/929	0.40	0/1246
44	n	0.11	0/511	0.33	0/678
45	o	0.12	0/735	0.34	0/982
46	p	0.17	0/699	0.45	0/942
47	q	0.27	0/665	0.48	0/889
48	r	0.25	0/534	0.56	0/715
49	s	0.17	0/683	0.53	1/916 (0.1%)
50	t	0.12	0/611	0.37	0/817
All	All	0.47	11/150082 (0.0%)	0.67	176/224737 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	160	ALA	CA-C	-6.55	1.44	1.52
20	T	76	ASP	CA-C	6.53	1.60	1.52
11	K	97	VAL	C-O	-5.88	1.17	1.24
14	N	59	GLU	CA-C	-5.77	1.45	1.52
4	D	127	PHE	C-O	-5.74	1.17	1.24

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	140	GLN	N-CA-C	-10.41	100.32	113.43
6	F	170	LEU	N-CA-C	-10.37	100.63	113.38
6	F	128	TYR	N-CA-C	10.02	121.96	111.14
8	H	58	ILE	N-CA-C	9.44	122.40	112.96
7	G	69	ARG	N-CA-C	-9.04	102.75	113.88

There are no chirality outliers.

There are no planarity outliers.

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	61859	0	31099	435	0
2	B	2445	0	1240	20	0
3	C	2090	0	2201	49	0
4	D	1627	0	1667	35	0
5	E	1572	0	1619	32	0
6	F	1317	0	1323	62	0
7	G	1259	0	1221	41	0
8	H	1143	0	1134	36	0
9	I	918	0	981	51	0
10	J	1086	0	1125	21	0
11	K	1071	0	1123	25	0
12	L	932	0	983	34	0
13	M	891	0	925	28	0
14	N	889	0	937	23	0
15	O	942	0	1014	37	0
16	P	790	0	830	24	0
17	Q	853	0	905	20	0
18	R	715	0	748	28	0
19	S	770	0	809	35	0
20	T	711	0	740	34	0
21	U	615	0	622	18	0
22	V	445	0	466	9	0
23	W	541	0	563	8	0
24	X	449	0	491	2	0
25	Y	353	0	218	13	0
26	Z	361	0	361	10	0
27	1	390	0	394	4	0
28	2	367	0	415	6	0
29	3	521	0	586	11	0
30	4	296	0	340	7	0
31	a	31706	0	15964	657	0
32	b	1802	0	1866	51	0
33	c	1596	0	1659	24	0
34	d	1616	0	1646	37	0
35	e	1160	0	1223	13	0
36	f	789	0	788	16	0
37	g	1242	0	1276	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	1031	0	1082	15	0
39	i	1007	0	1031	30	0
40	j	773	0	812	19	0
41	k	844	0	851	33	0
42	l	1058	0	1130	15	0
43	m	922	0	970	28	0
44	n	501	0	527	8	0
45	o	726	0	756	16	0
46	p	688	0	713	17	0
47	q	657	0	694	25	0
48	r	525	0	561	11	0
49	s	665	0	668	33	0
50	t	611	0	655	6	0
51	A	69	0	0	0	0
52	A	12	0	0	0	0
All	All	138218	0	91952	2014	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 9.

The worst 5 of 2014 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)
20:T:32:TYR:CE1	20:T:92:LEU:HD21	1.62	1.35
20:T:32:TYR:CD1	20:T:92:LEU:HD23	1.74	1.23
20:T:32:TYR:CD1	20:T:92:LEU:CD2	2.21	1.21
20:T:32:TYR:CE1	20:T:92:LEU:CD2	2.22	1.21
1:A:104:C:H5''	1:A:104:C:H6	1.30	0.96

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	C	272/274 (99%)	245 (90%)	26 (10%)	1 (0%)	30	61
4	D	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	173/175 (99%)	144 (83%)	28 (16%)	1 (1%)	21	54
7	G	173/175 (99%)	157 (91%)	16 (9%)	0	100	100
8	H	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
9	I	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	49
10	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
11	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
12	L	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
13	M	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
14	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
15	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	P	100/102 (98%)	93 (93%)	5 (5%)	2 (2%)	6	32
17	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
18	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
19	S	101/103 (98%)	88 (87%)	13 (13%)	0	100	100
20	T	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
21	U	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
22	V	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
23	W	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
24	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
25	Y	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
26	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
27	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
30	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
32	b	222/232 (96%)	211 (95%)	11 (5%)	0	100	100
33	c	200/217 (92%)	190 (95%)	10 (5%)	0	100	100
34	d	197/200 (98%)	187 (95%)	10 (5%)	0	100	100
35	e	154/166 (93%)	150 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	f	93/98 (95%)	87 (94%)	6 (6%)	0	100	100
37	g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
39	i	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
40	j	95/102 (93%)	89 (94%)	6 (6%)	0	100	100
41	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
42	l	133/149 (89%)	122 (92%)	10 (8%)	1 (1%)	16	49
43	m	114/121 (94%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	o	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
46	p	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
47	q	78/87 (90%)	74 (95%)	4 (5%)	0	100	100
48	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
49	s	80/108 (74%)	73 (91%)	7 (9%)	0	100	100
50	t	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	5323/5563 (96%)	4978 (94%)	339 (6%)	6 (0%)	49	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	51	PRO
9	I	98	ILE
6	F	139	PRO
16	P	50	ALA
42	l	132	THR

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	C	220/221 (100%)	203 (92%)	17 (8%)	12	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	173/173 (100%)	156 (90%)	17 (10%)	7	31
5	E	168/168 (100%)	154 (92%)	14 (8%)	10	35
6	F	139/154 (90%)	100 (72%)	39 (28%)	0	3
7	G	123/153 (80%)	102 (83%)	21 (17%)	2	13
8	H	122/123 (99%)	109 (89%)	13 (11%)	6	28
9	I	100/100 (100%)	91 (91%)	9 (9%)	9	33
10	J	109/112 (97%)	99 (91%)	10 (9%)	8	33
11	K	108/114 (95%)	94 (87%)	14 (13%)	4	21
12	L	96/101 (95%)	96 (100%)	0	100	100
13	M	86/95 (90%)	74 (86%)	12 (14%)	3	19
14	N	93/100 (93%)	74 (80%)	19 (20%)	1	8
15	O	96/96 (100%)	91 (95%)	5 (5%)	21	48
16	P	84/86 (98%)	80 (95%)	4 (5%)	23	50
17	Q	89/94 (95%)	78 (88%)	11 (12%)	4	23
18	R	78/80 (98%)	67 (86%)	11 (14%)	3	19
19	S	81/88 (92%)	74 (91%)	7 (9%)	10	34
20	T	75/82 (92%)	65 (87%)	10 (13%)	4	21
21	U	60/64 (94%)	52 (87%)	8 (13%)	4	21
22	V	44/49 (90%)	38 (86%)	6 (14%)	3	20
23	W	58/60 (97%)	43 (74%)	15 (26%)	0	4
24	X	52/52 (100%)	47 (90%)	5 (10%)	8	32
25	Y	21/56 (38%)	17 (81%)	4 (19%)	1	9
26	Z	36/44 (82%)	36 (100%)	0	100	100
27	1	44/45 (98%)	34 (77%)	10 (23%)	1	6
28	2	39/39 (100%)	38 (97%)	1 (3%)	40	62
29	3	55/55 (100%)	51 (93%)	4 (7%)	13	40
30	4	35/35 (100%)	31 (89%)	4 (11%)	5	26
32	b	194/201 (96%)	192 (99%)	2 (1%)	68	75
33	c	164/175 (94%)	163 (99%)	1 (1%)	78	79
34	d	174/175 (99%)	172 (99%)	2 (1%)	65	74
35	e	122/131 (93%)	117 (96%)	5 (4%)	27	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	83/86 (96%)	81 (98%)	2 (2%)	43	63
37	g	131/132 (99%)	122 (93%)	9 (7%)	14	41
38	h	112/113 (99%)	110 (98%)	2 (2%)	51	68
39	i	105/107 (98%)	102 (97%)	3 (3%)	37	60
40	j	87/91 (96%)	84 (97%)	3 (3%)	32	57
41	k	90/104 (86%)	88 (98%)	2 (2%)	45	65
42	l	117/130 (90%)	111 (95%)	6 (5%)	21	49
43	m	100/104 (96%)	98 (98%)	2 (2%)	48	66
44	n	52/53 (98%)	52 (100%)	0	100	100
45	o	79/81 (98%)	78 (99%)	1 (1%)	61	72
46	p	74/77 (96%)	72 (97%)	2 (3%)	39	61
47	q	75/82 (92%)	68 (91%)	7 (9%)	8	32
48	r	57/68 (84%)	55 (96%)	2 (4%)	32	57
49	s	71/91 (78%)	70 (99%)	1 (1%)	59	71
50	t	67/69 (97%)	67 (100%)	0	100	100
All	All	4438/4709 (94%)	4096 (92%)	342 (8%)	14	38

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	46	VAL
30	4	3	VAL
21	U	82	ARG
23	W	62	ILE
36	f	17	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
27	1	26	ASN
34	d	146	GLN
27	1	45	HIS
32	b	15	HIS
37	g	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2921 (98%)	951 (33%)	78 (2%)
2	B	114/115 (99%)	46 (40%)	4 (3%)
31	a	1470/1548 (94%)	382 (25%)	0
All	All	4463/4584 (97%)	1379 (30%)	82 (1%)

5 of 1379 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	13	A
1	A	18	C
1	A	19	G
1	A	23	G

5 of 82 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1826	G
1	A	2533	U
1	A	2094	G
1	A	2347	A
1	A	2829	A

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	2MG	A	2472	1	23,26,27	1.37	3 (13%)	33,38,41	2.75	12 (36%)
1	2MA	A	2530	1,52	22,25,26	1.47	5 (22%)	32,37,40	2.45	9 (28%)
1	5MU	A	792	1	19,22,23	1.47	5 (26%)	27,32,35	2.28	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	A	2278	1	23,26,27	1.28	4 (17%)	32,38,41	2.07	7 (21%)
1	5MU	A	1966	1	19,22,23	1.66	5 (26%)	27,32,35	2.35	8 (29%)

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
1	2MG	A	2472	1	-	0/9/27/28	0/3/3/3
1	2MA	A	2530	1,52	-	0/7/25/26	0/3/3/3
1	5MU	A	792	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2278	1	-	1/9/27/28	0/3/3/3
1	5MU	A	1966	1	-	0/7/25/26	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2530	2MA	C5-C4	4.00	1.46	1.39
1	A	2472	2MG	C6-N1	-3.40	1.32	1.38
1	A	792	5MU	C4-N3	-3.25	1.32	1.38
1	A	1966	5MU	C4-N3	-3.20	1.32	1.38
1	A	1966	5MU	C6-C5	3.14	1.39	1.34

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2472	2MG	C2-N3-C4	8.90	123.13	112.00
1	A	2530	2MA	C5-C4-N3	-8.26	118.48	127.18
1	A	2472	2MG	N1-C2-N2	7.09	123.80	116.56
1	A	2530	2MA	N3-C4-N9	6.93	135.78	126.99
1	A	2278	OMG	C5-C4-N3	-6.16	118.58	128.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2278	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	792	5MU	1	0
1	A	2278	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	A1D6G	A	3000	52	72,73,73	2.43	25 (34%)	97,107,107	1.84	30 (30%)

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
51	A1D6G	A	3000	52	-	11/82/113/113	0/5/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A	3000	A1D6G	C65-N64	8.81	1.45	1.33
51	A	3000	A1D6G	C11-N13	7.40	1.49	1.34
51	A	3000	A1D6G	O67-C65	4.89	1.43	1.36
51	A	3000	A1D6G	O10-C11	4.81	1.43	1.35
51	A	3000	A1D6G	C22-C21	4.62	1.55	1.44

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A	3000	A1D6G	C63-N64-C65	-4.34	106.72	112.39
51	A	3000	A1D6G	O10-C11-N13	4.31	118.03	111.01
51	A	3000	A1D6G	O42-C43-C45	4.30	115.49	109.34
51	A	3000	A1D6G	C52-C39-C37	-4.09	107.29	113.54
51	A	3000	A1D6G	C02-C03-C68	-3.97	109.76	115.23

There are no chirality outliers.

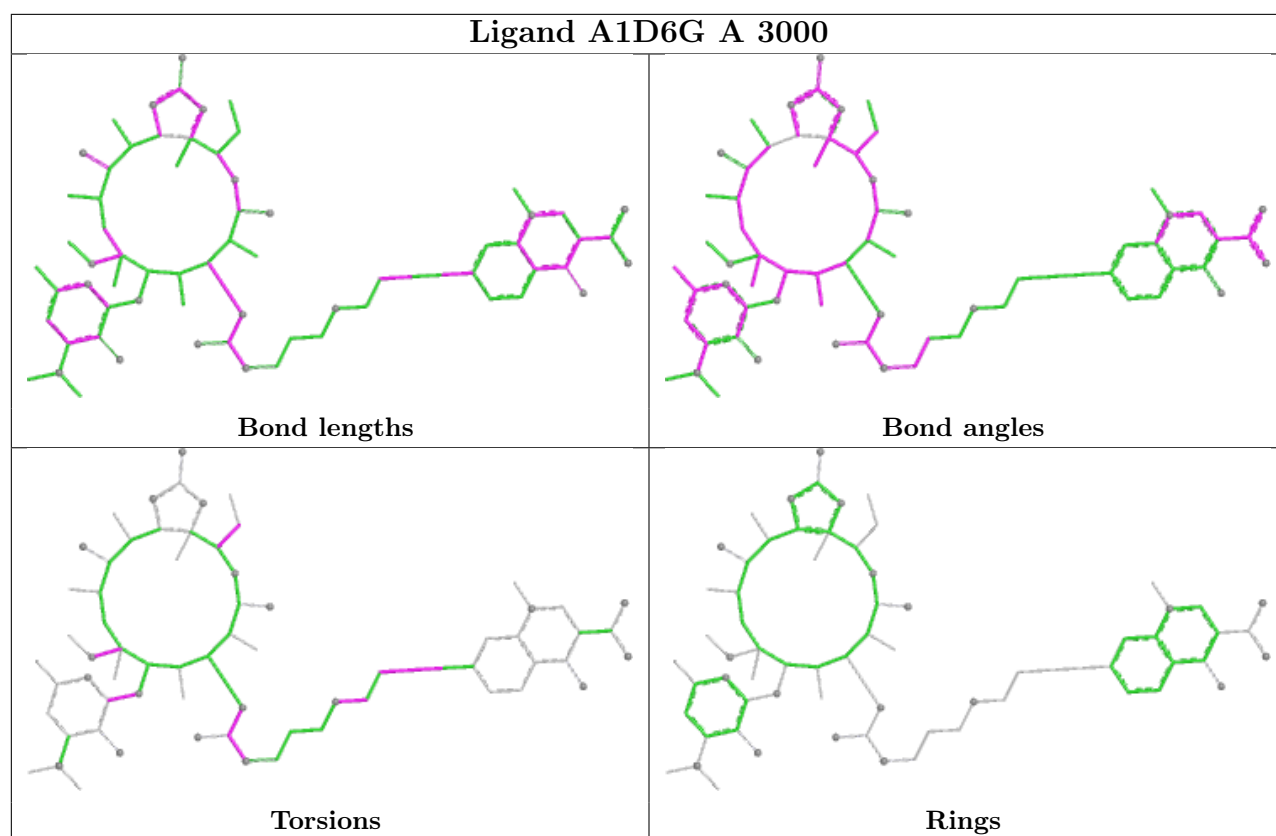
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	A	3000	A1D6G	O10-C11-N13-C14
51	A	3000	A1D6G	O12-C11-N13-C14
51	A	3000	A1D6G	C18-C19-C20-C21
51	A	3000	A1D6G	C19-C20-C21-C22
51	A	3000	A1D6G	N13-C11-O10-C09

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](#)

There are no chain breaks in this entry.

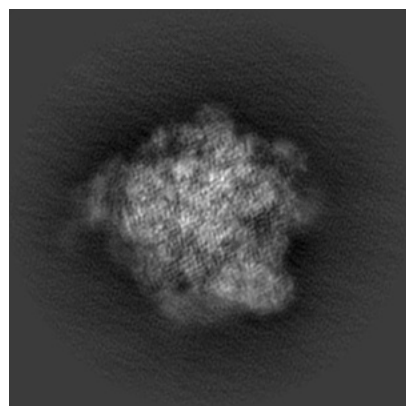
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38876. These allow visual inspection of the internal detail of the map and identification of artifacts.

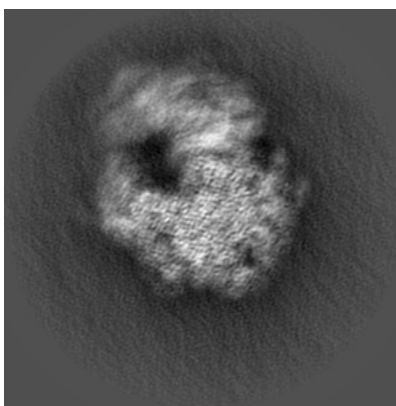
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

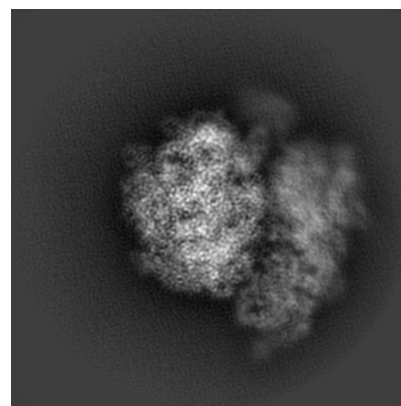
6.1.1 Primary map



X

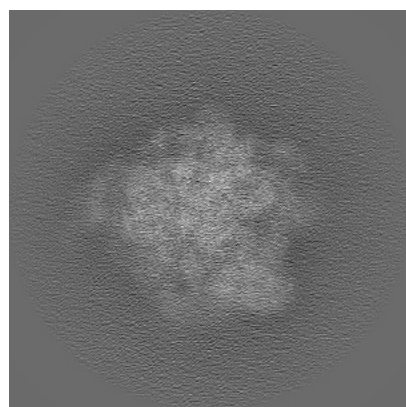


Y

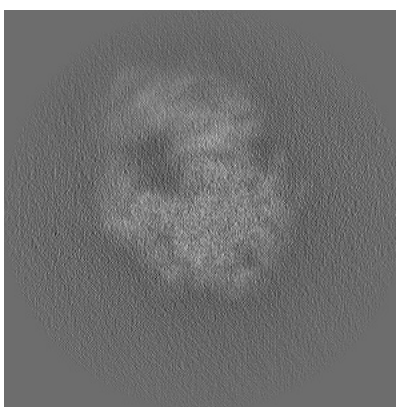


Z

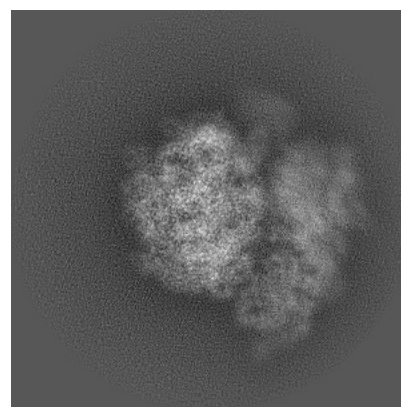
6.1.2 Raw map



X



Y

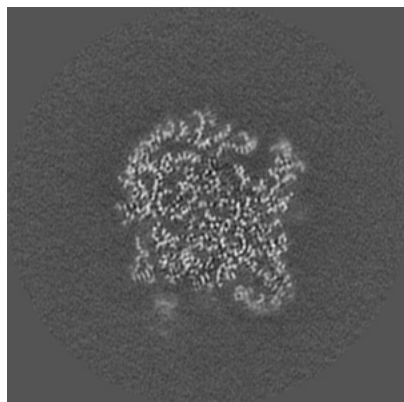


Z

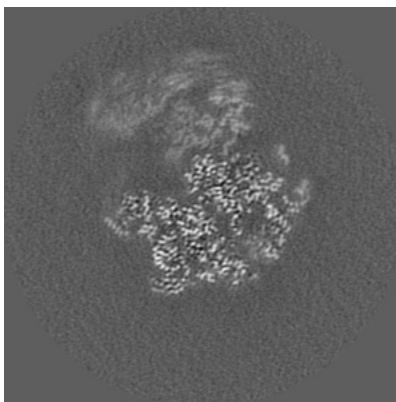
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

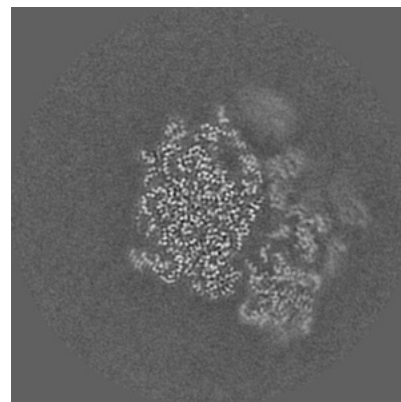
6.2.1 Primary map



X Index: 240

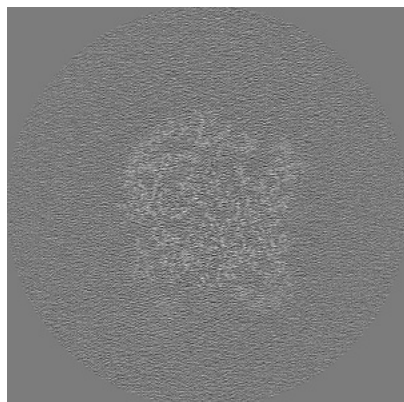


Y Index: 240

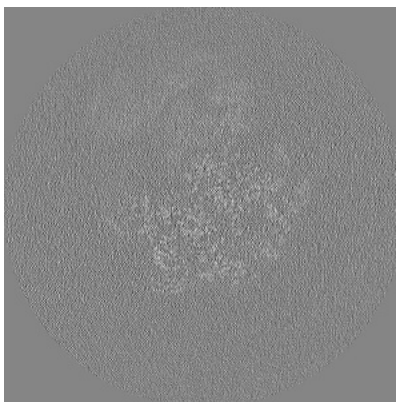


Z Index: 240

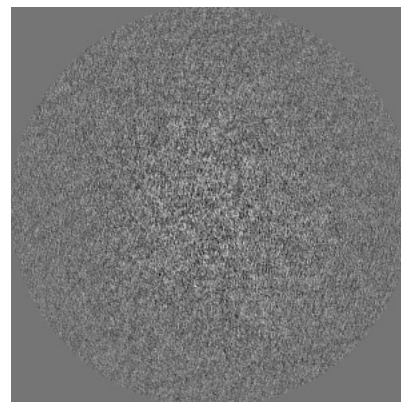
6.2.2 Raw map



X Index: 240



Y Index: 240

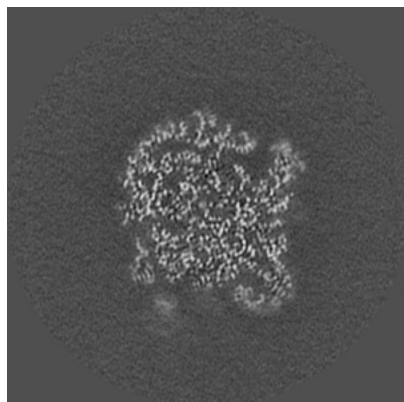


Z Index: 240

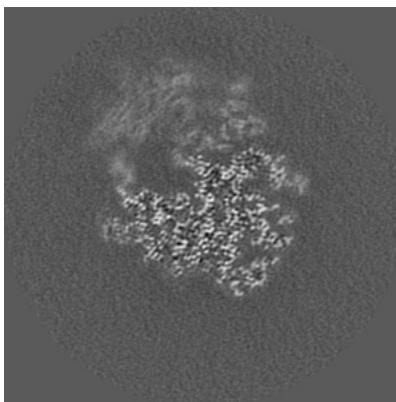
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

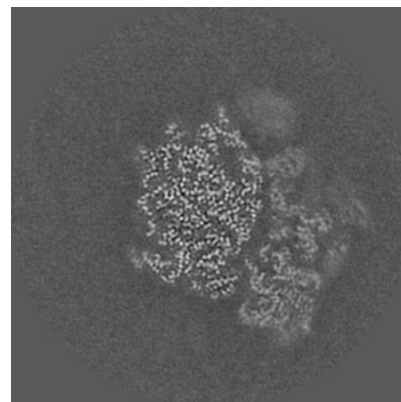
6.3.1 Primary map



X Index: 239

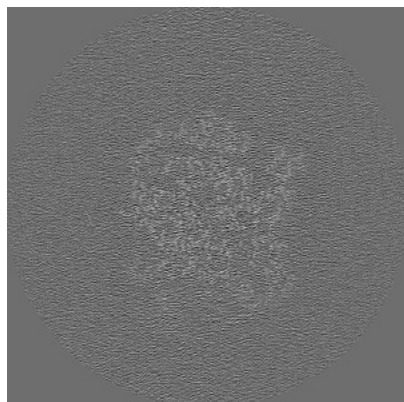


Y Index: 256

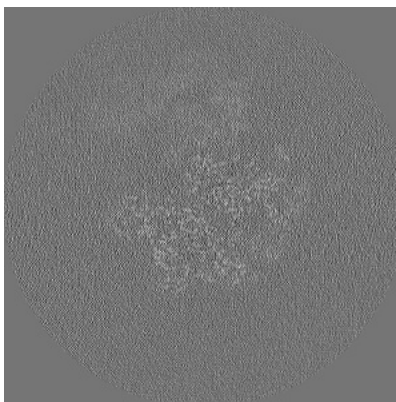


Z Index: 242

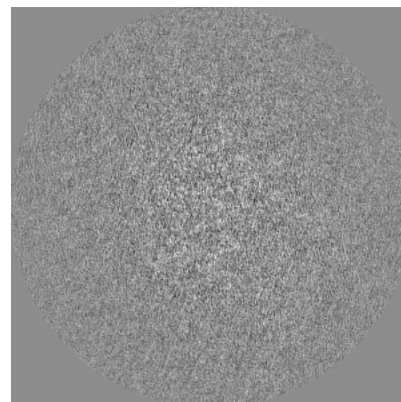
6.3.2 Raw map



X Index: 233



Y Index: 241

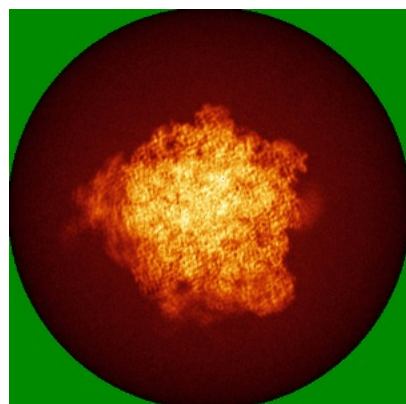


Z Index: 245

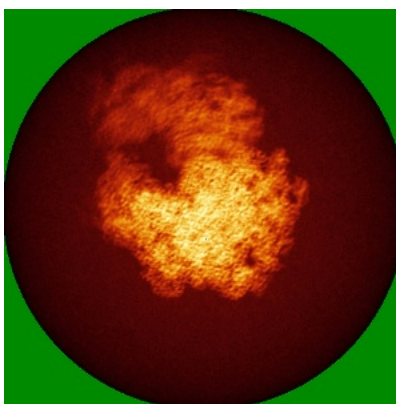
The images above show the largest variance slices of the map in three orthogonal directions.

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

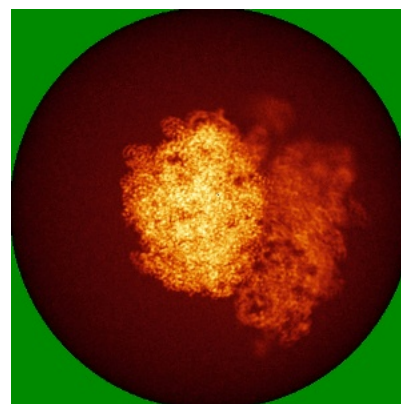
6.4.1 Primary map



X

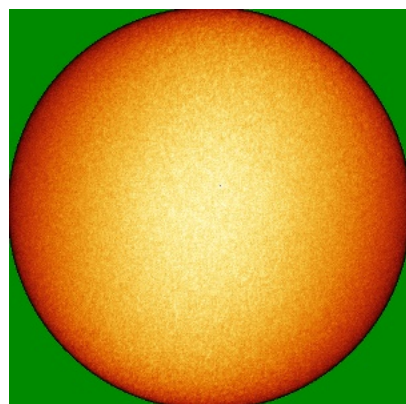


Y

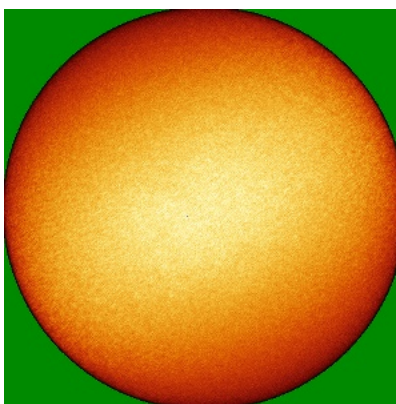


Z

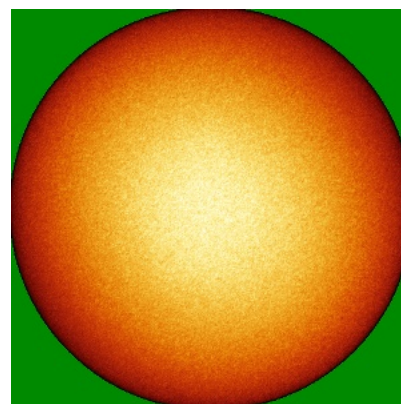
6.4.2 Raw map



X



Y

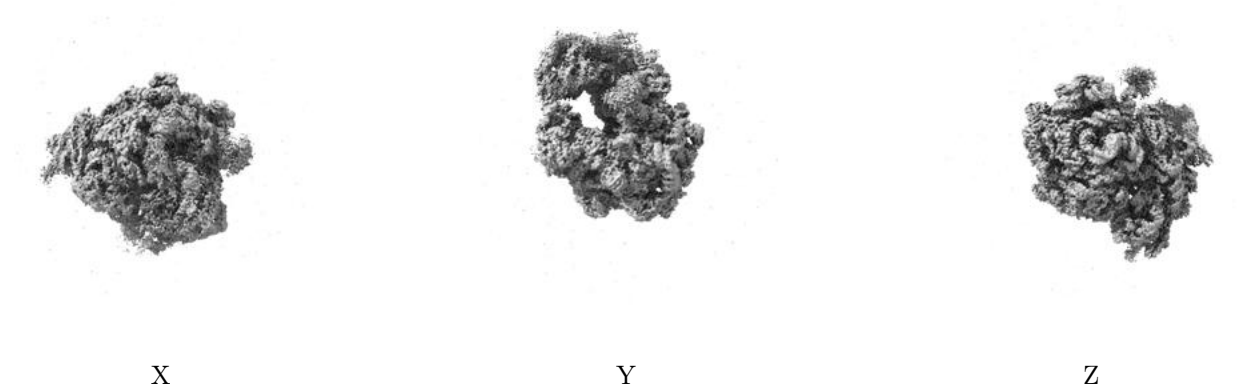


Z

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

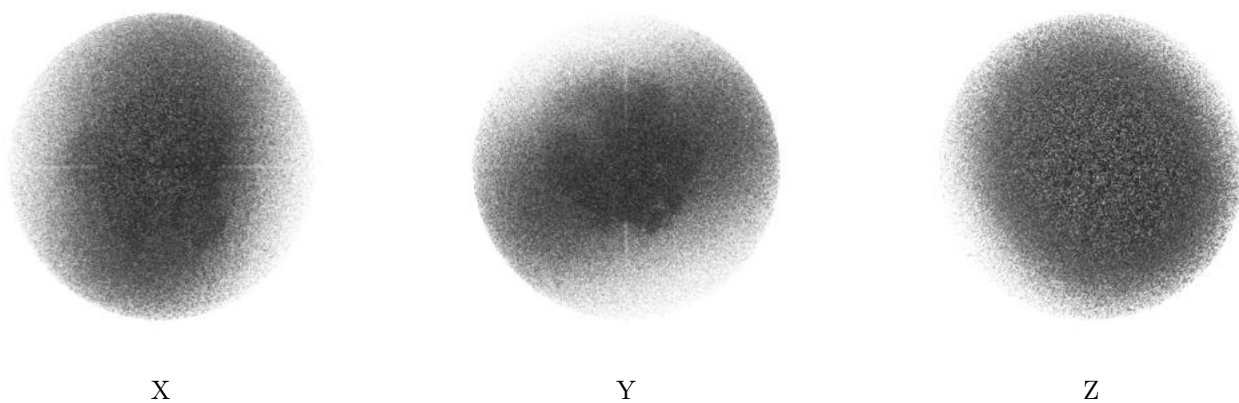
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

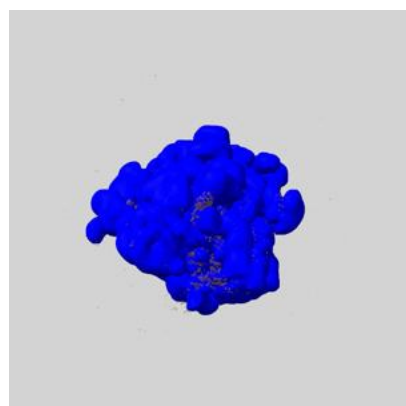
6.6 Mask visualisation [i](#)

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

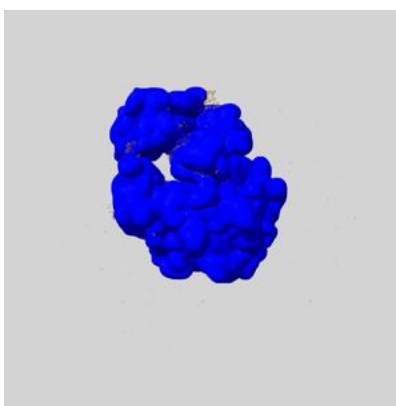
A mask typically either:

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

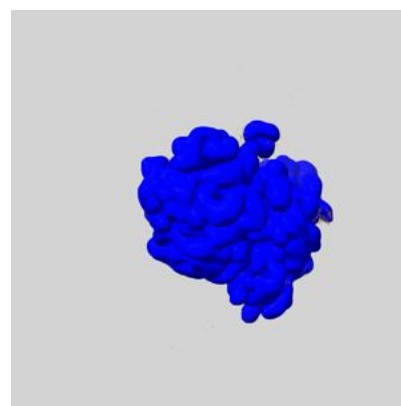
6.6.1 emd_38876_msk_1.map [i](#)



X



Y

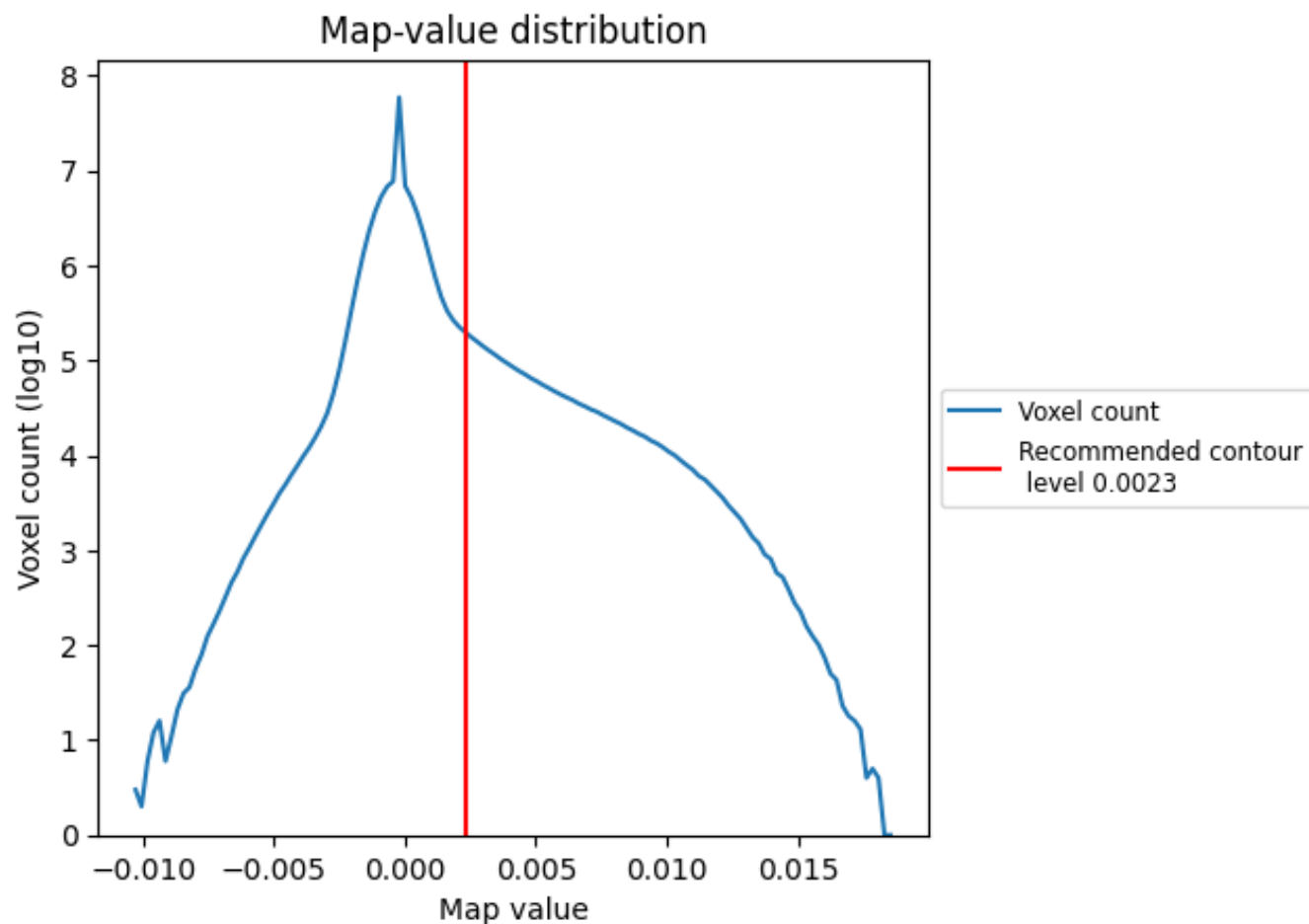


Z

7 Map analysis [i](#)

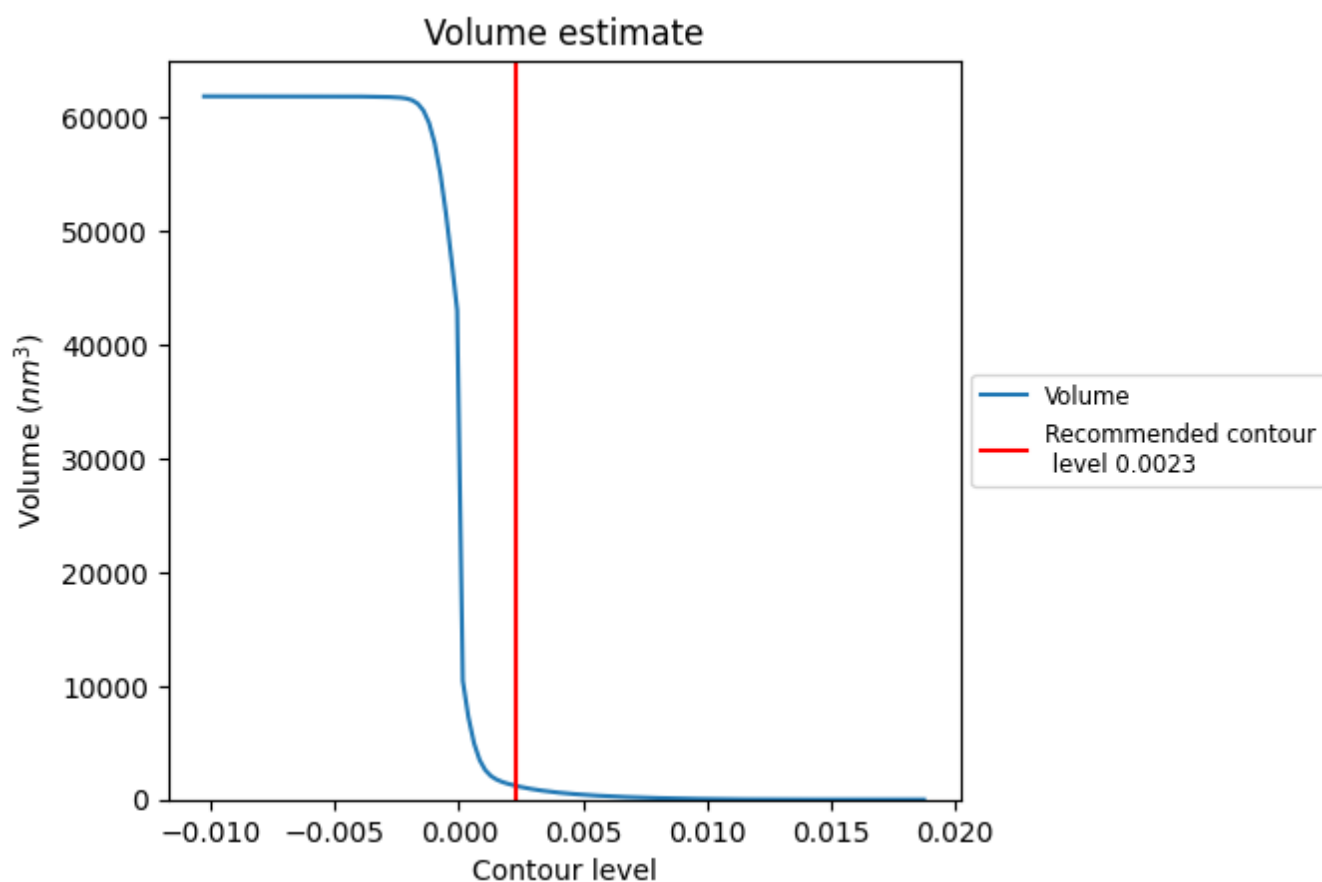
This section contains the results of statistical analysis of the map.

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.

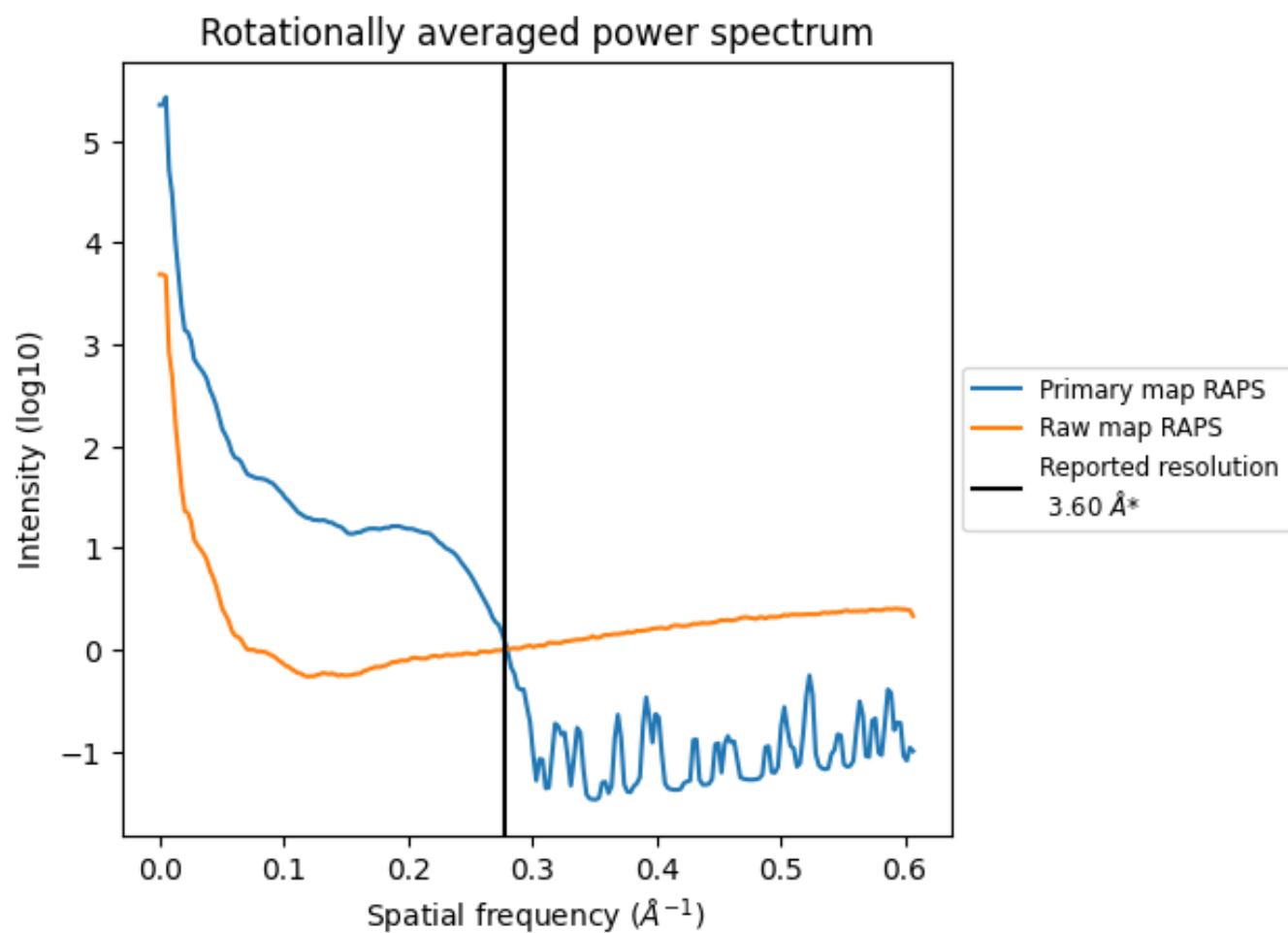
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1208 nm³; this corresponds to an approximate mass of 1091 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 ⓘ

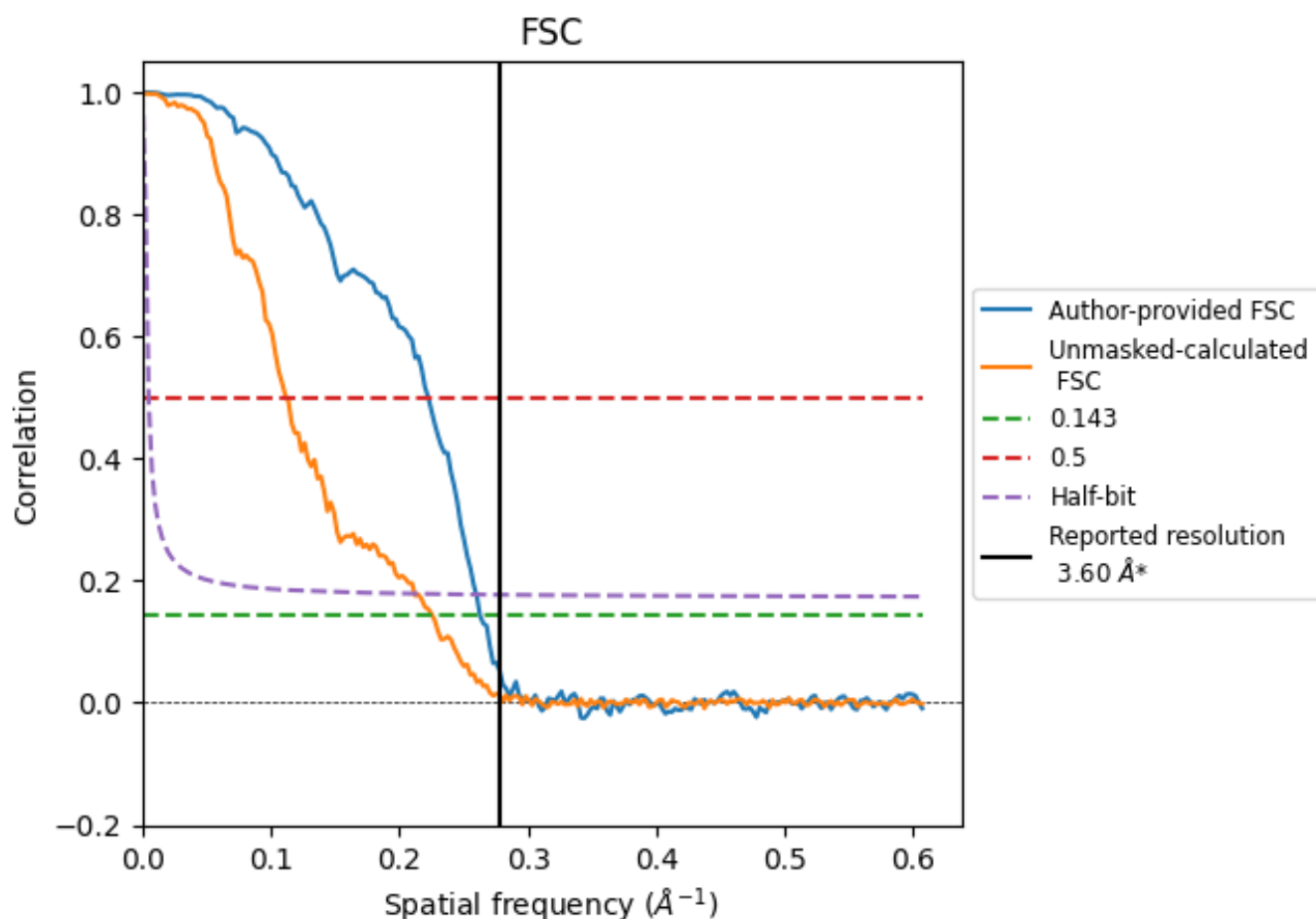


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

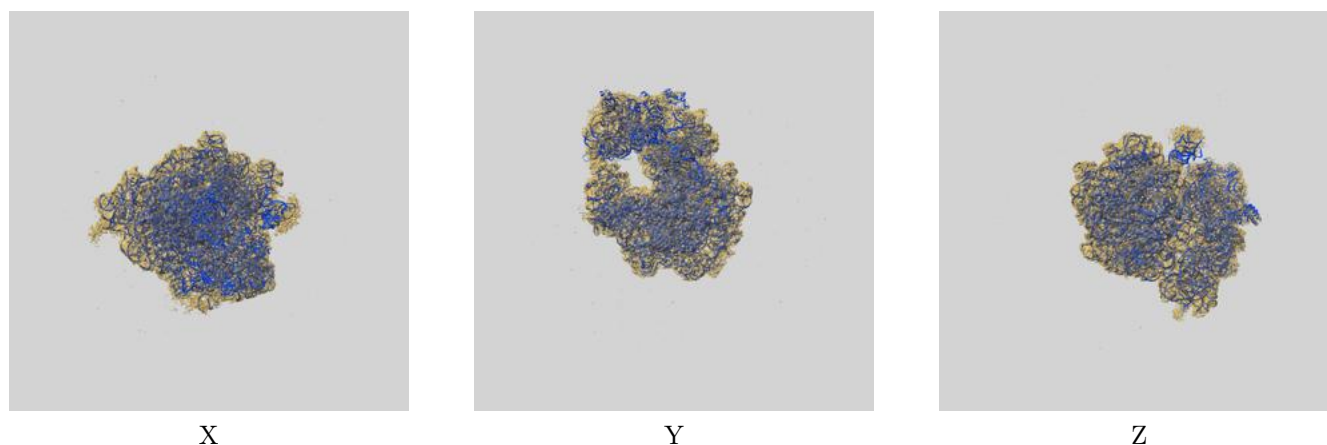
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.80	4.49	3.85
Unmasked-calculated*	4.43	8.90	4.72

*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 4.43 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

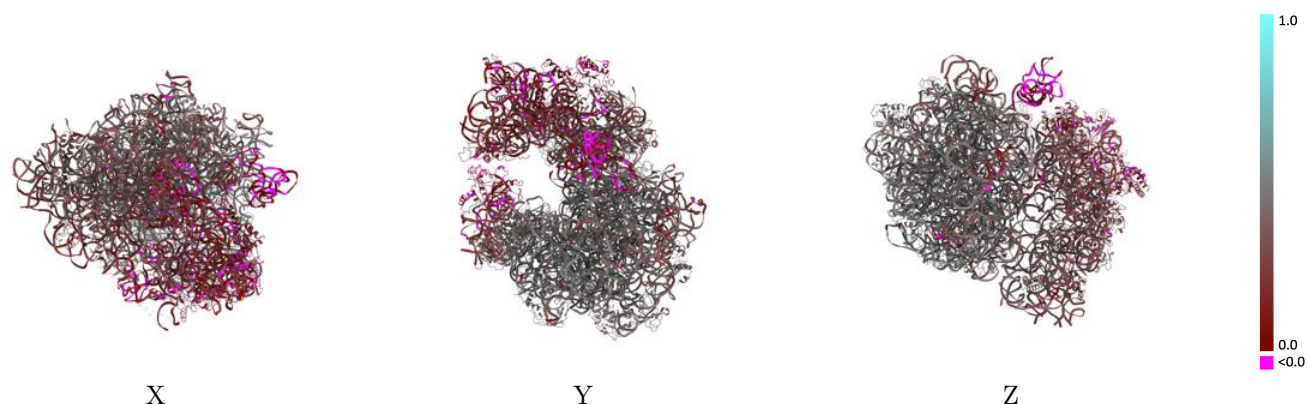
This section contains information regarding the fit between EMDB map EMD-38876 and PDB model 8Y39. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



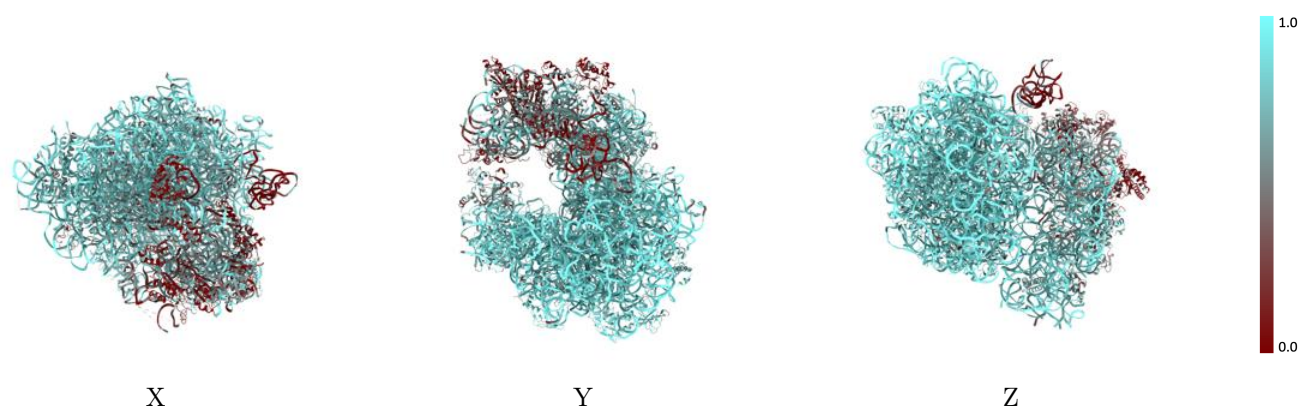
The images above show the 3D surface view of the map at the recommended contour level 0.0023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



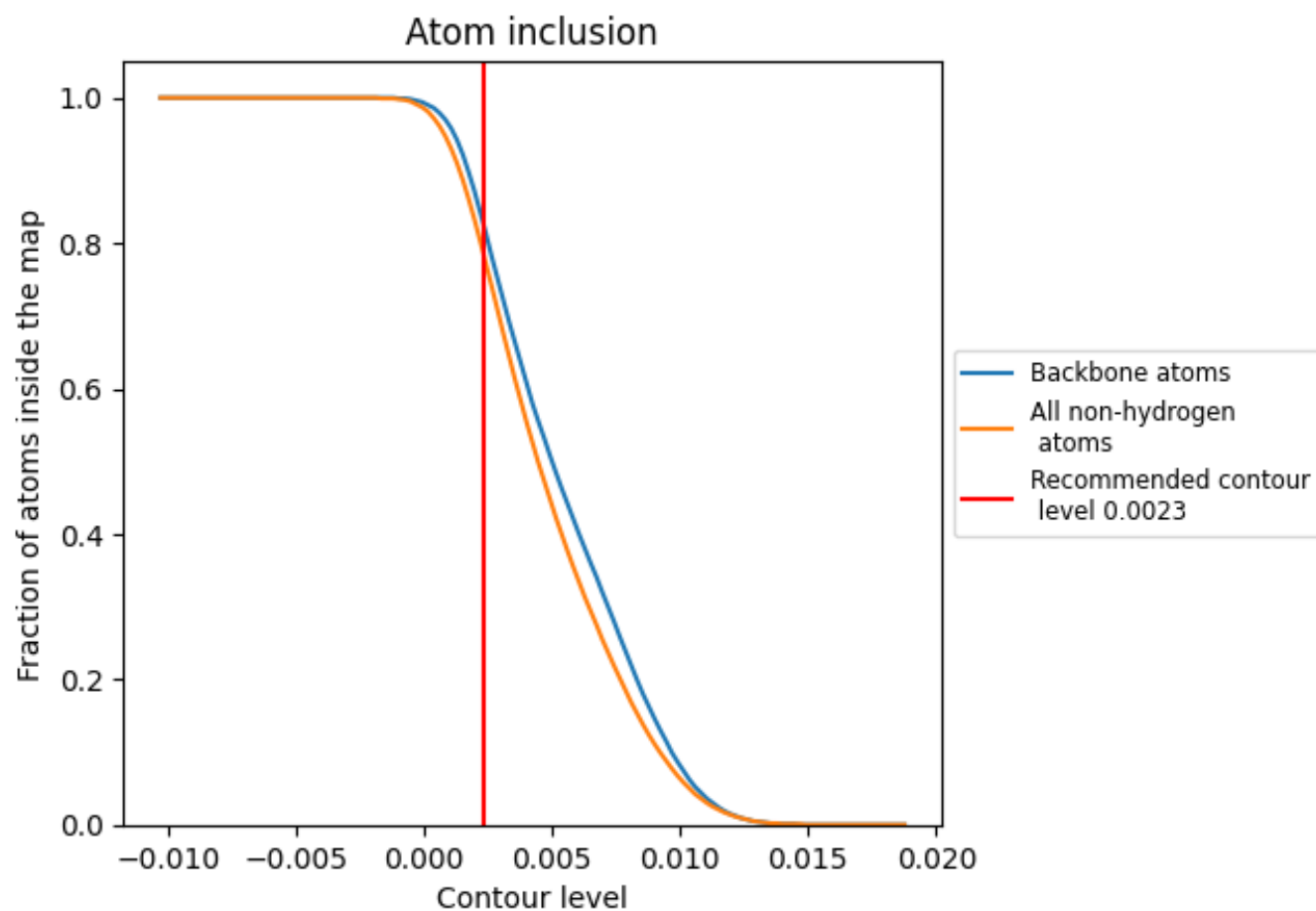
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.0023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.3530
1	 0.8800	 0.4430
2	 0.8320	 0.4650
3	 0.8630	 0.4810
4	 0.8410	 0.4670
A	 0.8940	 0.3980
B	 0.8810	 0.3200
C	 0.8170	 0.4580
D	 0.8650	 0.4710
E	 0.8380	 0.4500
F	 0.5710	 0.1650
G	 0.8380	 0.3990
H	 0.8600	 0.4600
I	 0.8040	 0.4570
J	 0.8710	 0.4650
K	 0.8670	 0.4650
L	 0.8410	 0.4630
M	 0.7790	 0.3250
N	 0.8170	 0.4400
O	 0.8910	 0.4530
P	 0.8550	 0.4650
Q	 0.8350	 0.4530
R	 0.7940	 0.4240
S	 0.7880	 0.4100
T	 0.7760	 0.3820
U	 0.8370	 0.4330
V	 0.8370	 0.4500
W	 0.7730	 0.3910
X	 0.8440	 0.4680
Y	 0.5380	 0.0990
Z	 0.8850	 0.4820
a	 0.7660	 0.2860
b	 0.1700	 0.1330
c	 0.1650	 0.2070
d	 0.5540	 0.2560



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.5530	 0.2670
f	 0.6340	 0.3250
g	 0.1960	 0.1510
h	 0.6320	 0.3110
i	 0.2380	 0.0840
j	 0.1470	 0.1500
k	 0.5070	 0.2320
l	 0.5110	 0.3050
m	 0.2340	 0.1690
n	 0.3020	 0.1990
o	 0.6880	 0.3160
p	 0.6290	 0.3350
q	 0.6230	 0.3290
r	 0.6590	 0.2740
s	 0.3360	 0.1510
t	 0.6480	 0.3450