



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 05:12 PM EST

PDB ID : 3J8G  
EMDB ID : EMD-6149  
Title : Electron cryo-microscopy structure of EngA bound with the 50S ribosomal subunit  
Authors : Zhang, X.; Yan, K.; Zhang, Y.; Li, N.; Ma, C.; Li, Z.; Zhang, Y.; Feng, B.; Liu, J.; Sun, Y.; Xu, Y.; Lei, J.; Gao, N.  
Deposited on : 2014-10-24  
Resolution : 5.00 Å (reported)  
Based on initial models : 2HJG, 2WWQ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

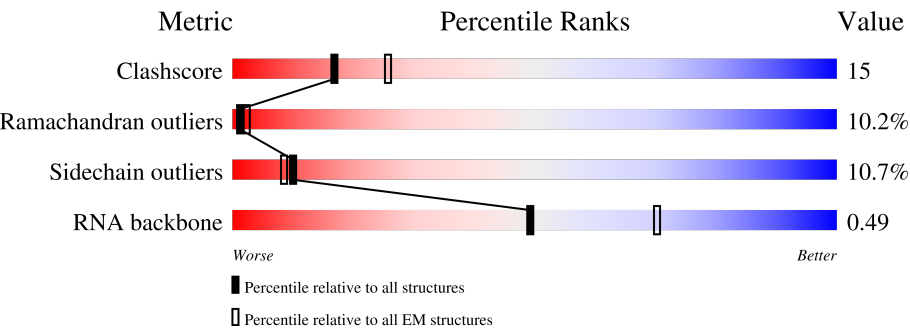
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 5.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	117	<div><div>6%</div><div>13%</div><div>42%</div><div>44%</div><div>.</div></div>
2	B	2903	<div><div>9%</div><div>11%</div><div>38%</div><div>50%</div><div>.</div></div>
3	O	78	<div><div>51%</div><div>58%</div><div>23%</div><div>15%</div><div>..</div></div>
4	K	123	<div><div>18%</div><div>56%</div><div>33%</div><div>7%</div><div>..</div></div>
5	L	144	<div><div>47%</div><div>57%</div><div>22%</div><div>16%</div><div>..</div></div>
6	1	63	<div><div>48%</div><div>68%</div><div>24%</div><div>5%</div><div>.</div></div>
7	M	136	<div><div>14%</div><div>54%</div><div>34%</div><div>12%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
8	N	127	
9	O	117	
10	P	115	
11	Q	118	
12	R	103	
13	S	110	
14	D	209	
15	T	100	
16	2	59	
17	U	104	
18	W	94	
19	X	490	
20	E	201	
21	Y	85	
22	3	57	
23	5	234	
24	6	46	
25	7	65	
26	8	38	
27	C	273	
28	F	179	
29	G	177	
30	H	149	
31	I	142	
32	J	142	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 94855 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 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	P	0	0
			2455	1097	451	795	112		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2874	Total	C	N	O	P	0	0
			61689	27523	11353	19941	2872		

- Molecule 3 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 4 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	121	Total	C	N	O	S	0	0
			931	582	179	164	6		

- Molecule 5 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 6 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 7 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 8 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 9 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 10 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 11 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 12 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 13 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 14 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 16 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	99	Total	C	N	O		0	0
			755	479	140	136			

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 19 is a protein called GTPase Der.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	418	Total	C	N	O	S	0	0
			3280	2074	582	610	14		

- Molecule 20 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	G	175	Total	C	N	O	S	0	0
			1316	827	242	245	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

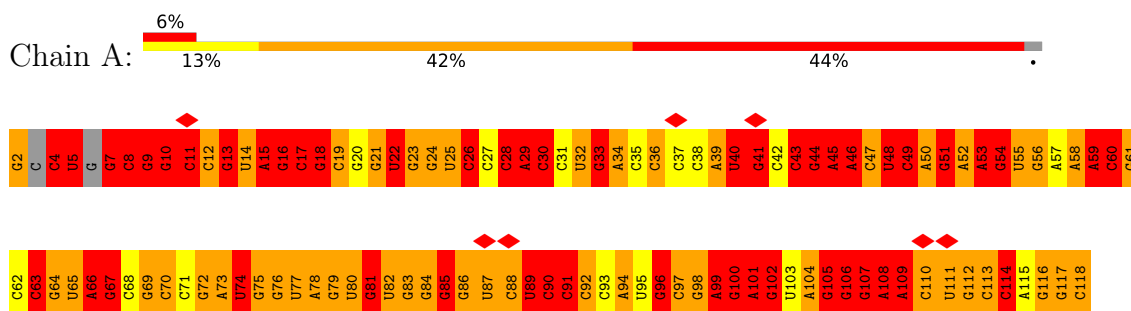
Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		



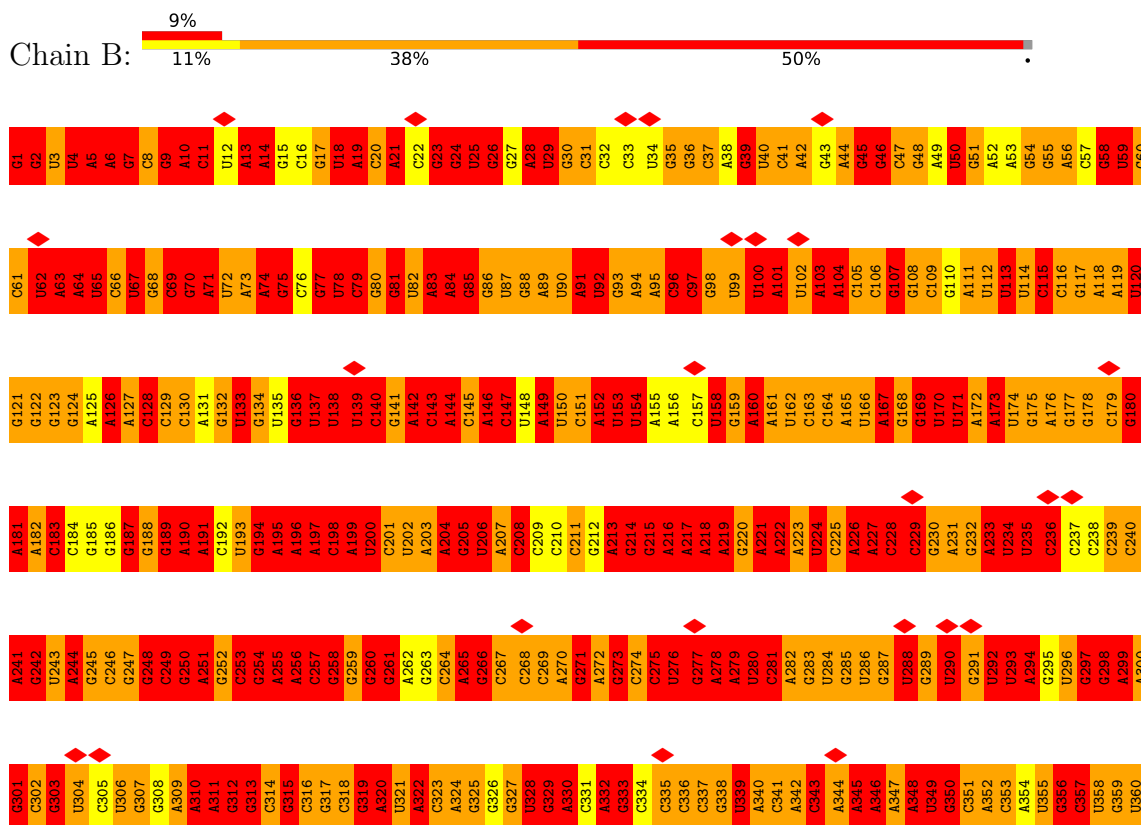
### 3 Residue-property plots [i](#)

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: 5S rRNA



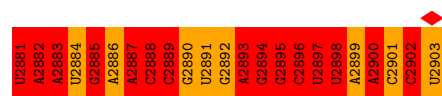
#### • Molecule 2: 23S rRNA



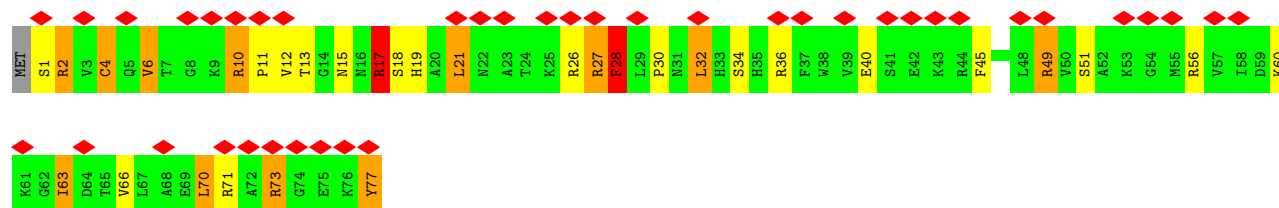
U1141	A1021	G841	A781	A721	A541	G481	C421	G361
A1142	G1022	U842	A782	A722	C541	A482	A422	A362
U1082	U1023	G843	A783	C723	G663	A483	G423	G363
A1084	G1024	A844	G784	U724	G664	C484	A24	C364
C1145	A1085	A845	G785	G725	U665	C485	G425	U365
C1146	G1026	U846	G786	G726	A666	C486	C426	C366
A1147	A1027	U847	C787	A727	U667	C487	U427	G367
U1088	A1028	C908	A788	G728	A668	A488	A428	A368
G1149	U1029	G909	A789	G729	G669	A489	A429	U369
C1150	C1030	A910	U790	A730	C510	G490	A430	G370
A1151	G1031	U850	C791	A731	C511	G491	A431	A371
C1152	A1032	C851	A792	C732	G672	A492	A432	G372
G1091	U1033	U852	A793	G733	C673	G493	C433	U373
C1153	C1034	C853	A794	A734	G674	A494	U434	A374
G1154	U1035	C854	C795	A735	A675	G495	C435	G375
A1155	U1036	G855	G796	C736	A676	G496	C436	G376
A1156	G1037	G856	G797	G737	A677	A497	U437	G377
C1157	A1038	U857	G798	G738	G678	G498	G378	C378
U1097	A1039	G858	G799	A739	C679	U499	G379	G379
A1098	A1040	G859	A800	C740	C680	G500	C440	G380
C1161	G1041	U860	G801	U741	G681	A501	U441	G381
G1162	U1042	A861	A802	A742	G682	A502	G442	C382
C1163	C1043	G862	U803	A743	U683	A503	A443	C383
A1164	U1044	G863	A804	U744	C684	A504	A444	C384
G1165	C1045	G864	G805	G745	G685	A505	C445	C385
A1166	U1046	C865	C806	U746	U686	G506	G446	G386
C1167	A1047	A866	U807	U747	C687	A507	A447	U387
G1168	U1048	G867	G808	G748	U688	A508	G448	G388
A1169	C1049	U868	G809	A749	G689	G509	U449	G389
C1170	U1050	G869	U810	A750	G690	C510	U450	U390
G1171	G1051	U870	U811	A751	C691	G570	A451	A391
U1108	C1052	U871	C812	A752	C692	U571	C461	A402
C1172	U1053	G872	A813	A753	A693	G572	G462	U403
U1173	G1054	C873	C814	U754	U694	A513	G463	A404
A1174	U1055	G874	C815	U755	G695	A514	U464	U405
C1175	C1056	G875	C816	A756	G696	A515	G465	G406
U1176	U1057	C876	C817	G757	G697	A516	G466	G407
G1177	A1058	A877	G818	C758	C698	C517	G467	G408
C1178	U1059	U878	A819	G759	G699	G518	G468	G409
U1179	G1060	G879	A820	U760	G700	U519	A470	G410
A1180	U1061	C880	A821	A761	C641	G520	A471	G411
U1181	C1062	G881	G822	U762	U642	C581	A472	C413
C1182	U1063	G882	C823	G763	U643	A522	G473	C414
U1183	G1064	G883	U824	A764	G644	G523	G474	A415
A1184	U1065	U884	A825	C765	A645	C524	C475	U416
G1185	C1066	C885	U826	U766	G646	G525	G476	C417
U1186	U1067	G886	U827	G767	A586	A526	A477	C418
G1187	A1068	U887	U828	G768	C587	C527	G478	U419
U1188	U1069	C888	A829	U769	G648	A528	A479	C420
C1189	G1070	G889	G830	G770	G649	A529	G480	
U1190	A1071	C890	G831	G771	C650	G530		
G1191	U1072	G891	U832	C772	G651	A591		
C1192	C1073	C892	G833	U773	U652	A592		
U1193	U1074	G893	G834	G774	U653	A593		
G1194	G1075	C894	C835	G775	A654	U594		
A1195	U1076	U895	G836	G776	A655	G595		
C1196	C1077	G896	C837	G777	G656	U596		
U1197	U1078	U897	C838	G778	C717	G597		
G1198	C1079	C898	U839	G779	A718	U598		
U1199	U1080	A899	C840	G780	C719	A599		
C1200		C897		G780	U720	G600		

A1981	U1982	G1983	G1984	C1985	C1986	A1987	G1988	G1989	C1990	U1991	G1992	U1993	C1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	C2002	A2003	C2004	C2005	C2006	U2007	C2008	A2009	C2010	U2011	C2012	A2013	A2014	A2015	U2016	G1948	G1949	G1950	U1951	A1952	A1953	G1954	U1955	U1956	C1957	G1958	G1959	A1960	C1961	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970	U1971	C1972	G1973	C1974	G1975	U1976	A1977	A1978	U1979	G1980																																																			
A1801	A1802	A1803	C1804	A1805	A1806	G1807	A1808	A1809	A1810	G1811	A1812	G1813	A1814	A1815	A1816	G1817	A1818	A1819	A1820	A1821	C1822	G1823	G1824	U1825	G1826	G1827	G1828	A1829	C1830	A1831	C1832	C1833	U1834	G1835	C1836	C1837	C1838	G1839	G1840	U1841	G1842	C1843	C1844	G1845	G1846	A1847	A1848	G1905	G1906	G1907	C1908	C1909	G1910	U1911	A1912	A1913	C1914	U1915	A1916	U1917	A1918	A1919	U1976	A1977	A1978	U1979	G1980																																																				
C1741	U1742	G1743	A1744	A1745	A1746	U1747	C1748	A1749	G1750	U1751	C1752	G1753	A1754	U1755	G1756	A1757	U1758	A1759	C1760	C1761	A1762	G1763	C1764	U1765	G1766	G1767	C1768	U1769	G1770	C1771	A1772	U1773	C1774	U1775	G1776	U1777	U1778	U1779	A1780	U1781	U1782	A1783	A1784	U1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	A1794	G1795	U1796	G1797	U1798	G1799	C1800																																																												
G1681	G1682	U1683	C1684	C1685	C1686	G1687	U1688	A1689	A1690	C1691	U1692	G1693	C1694	G1695	G1696	A1697	A1698	G1699	A1700	A1701	G1642	G1643	C1644	G1645	C1646	U1647	U1648	U1649	A1650	G1651	A1652	C1653	A1654	A1655	C1656	U1657	C1658	G1659	G1660	G1661	U1662	G1663	A1664	A1665	G1666	G1667	C1668	A1669	C1670	U1671	C1672	G1673	G1674	C1675	A1676	A1677	U1678	A1679	U1680																																																												
C1561	U1562	U1563	C1564	C1565	A1566	G1567	U1568	A1569	A1570	C1571	A1572	G1573	C1574	U1575	G1576	C1577	U1578	A1579	A1580	G1581	A1582	C1583	U1584	C1585	A1586	G1587	U1588	U1589	A1590	A1591	C1592	C1593	U1594	A1595	A1596	C1597	A1598	U1599	C1600	G1601	U1602	A1603	C1604	C1605	G1606	C1607	A1608	A1609	A1610	C1611	G1612	G1613	A1614	C1615	A1616	C1617	A1618	G1619	G1620																																																												
G1501	A1502	A1503	C1504	A1505	U1506	C1507	A1508	A1509	G1510	C1511	U1512	A1513	G1514	U1515	G1516	C1517	U1518	G1519	U1520	A1521	C1522	G1523	U1524	A1525	C1526	G1527	U1528	G1529	C1530	C1531	A1532	C1533	U1534	A1535	C1536	G1537	U1538	G1539	C1540	G1541	U1542	G1543	A1544	U1545	G1546	C1547	A1548	A1549	C1550	A1551	A1552	U1553	U1554	G1555	C1556	C1557	C1558	U1559	G1560																																																												
U1442	U1443	U1444	G1445	A1446	C1447	G1448	U1449	G1450	C1451	U1452	A1453	C1454	G1455	U1456	G1457	U1458	G1459	U1460	C1461	C1462	G1463	G1464	U1465	U1466	U1467	U1468	A1469	A1470	U1471	C1472	G1473	U1474	U1475	U1476	G1477	U1478	C1479	C1480	U1481	U1482	G1483	U1484	U1485	U1486	U1487	C1488	G1489	A1490	C1491	G1492	C1493	A1494	U1495	A1496	U1497	C1498	U1499	C1500																																																													
G1381	G1382	A1383	C1384	A1385	U1386	A1387	G1388	A1389	C1390	U1391	A1392	G1393	U1394	A1395	U1396	G1397	C1398	G1399	U1400	U1401	C1402	A1403	C1404	U1405	U1406	G1407	U1408	A1409	C1410	C1411	U1412	A1413	U1414	U1415	G1416	C1417	G1418	A1419	A1420	G1421	C1422	G1423	G1424	G1425	G1426	A1427	C1428	G1429	G1430	A1431	G1432	A1433	A1434	G1435	G1436	C1437	U1438	A1439	U1440																																																												
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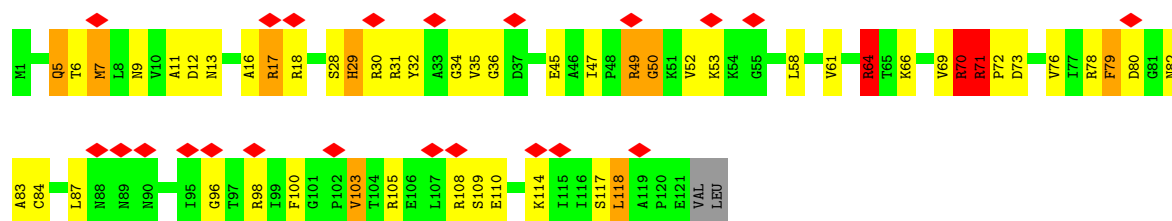




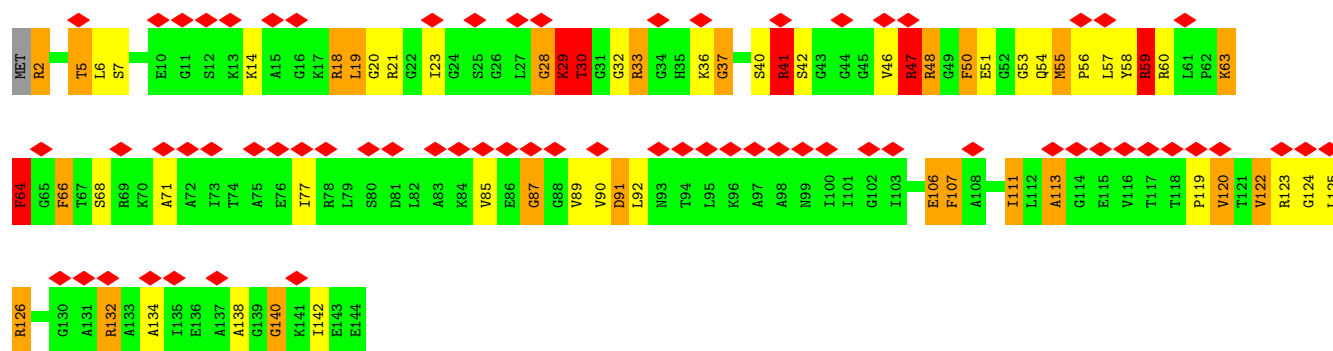
• Molecule 3: 50S ribosomal protein L28



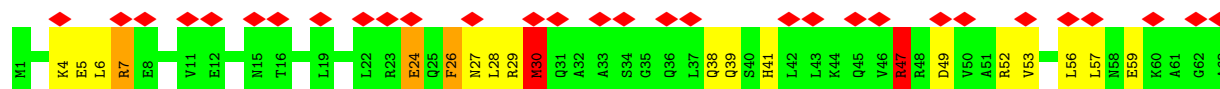
• Molecule 4: 50S ribosomal protein L14



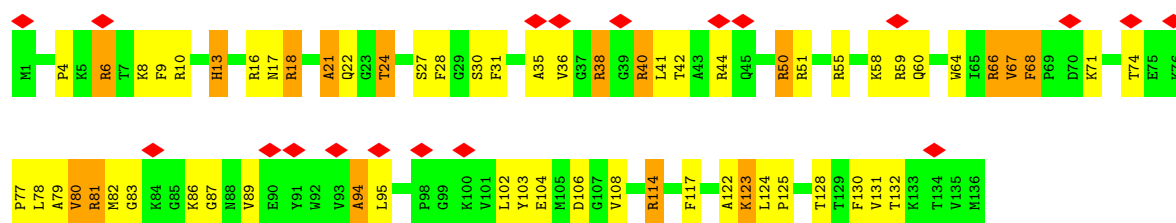
• Molecule 5: 50S ribosomal protein L15



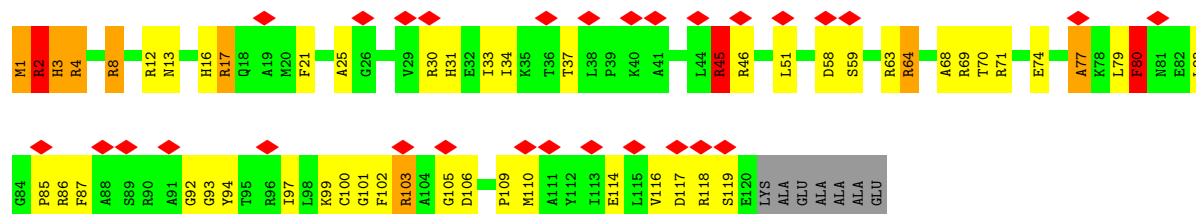
• Molecule 6: 50S ribosomal protein L29



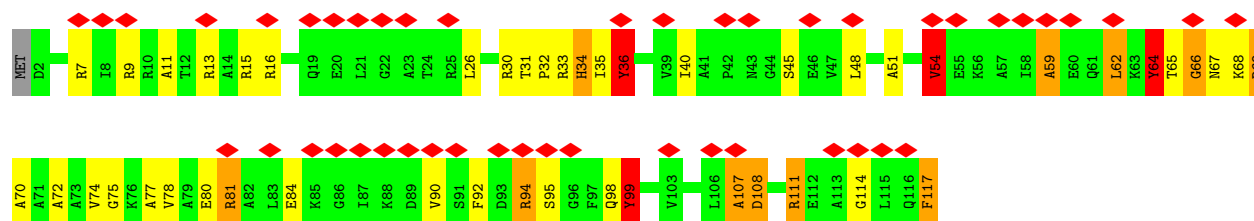
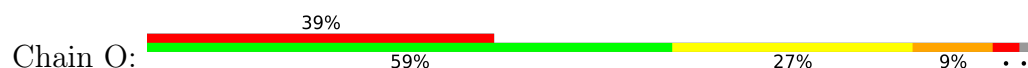
• Molecule 7: 50S ribosomal protein L16



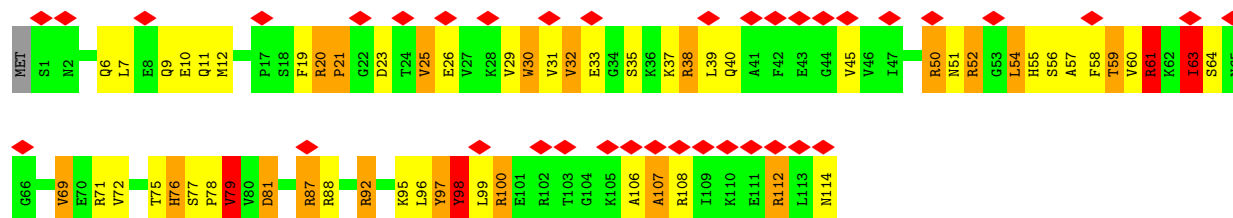
• Molecule 8: 50S ribosomal protein L17



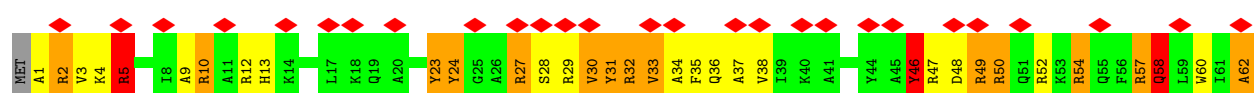
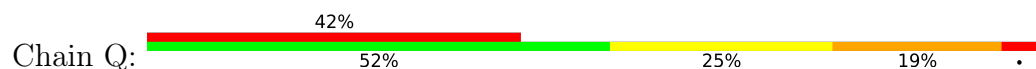
• Molecule 9: 50S ribosomal protein L18

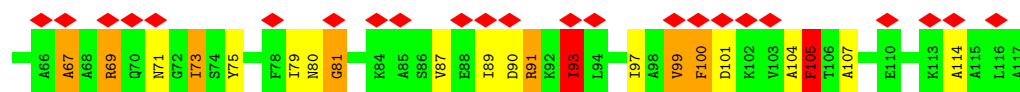


• Molecule 10: 50S ribosomal protein L19

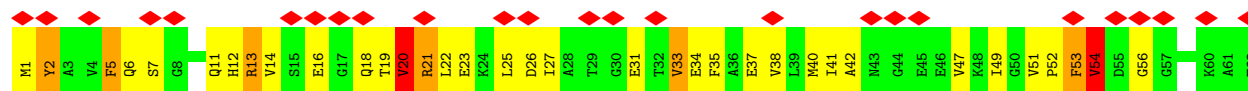
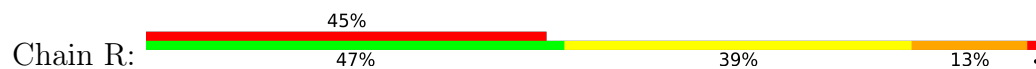


• Molecule 11: 50S ribosomal protein L20





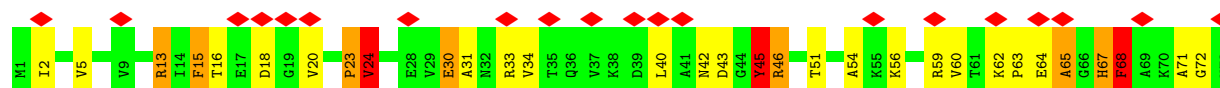
• Molecule 12: 50S ribosomal protein L21



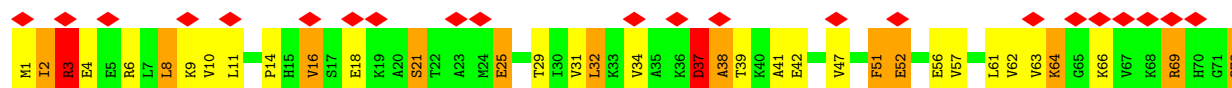
• Molecule 13: 50S ribosomal protein L22



• Molecule 14: 50S ribosomal protein L3

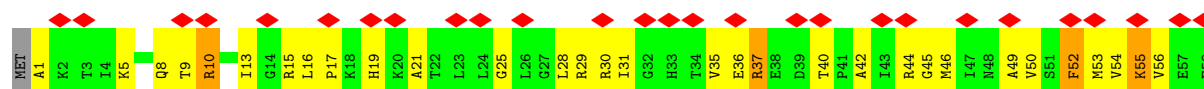


• Molecule 15: 50S ribosomal protein L23

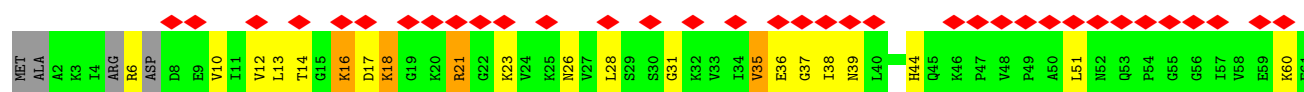




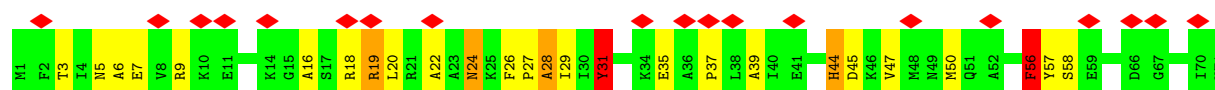
• Molecule 16: 50S ribosomal protein L30



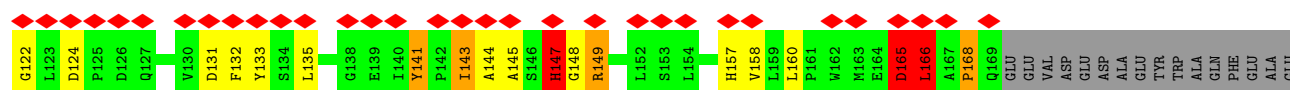
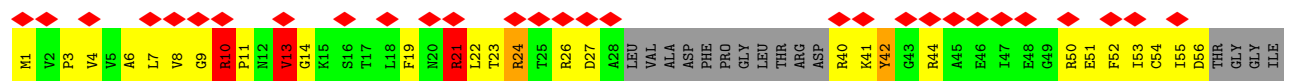
• Molecule 17: 50S ribosomal protein L24



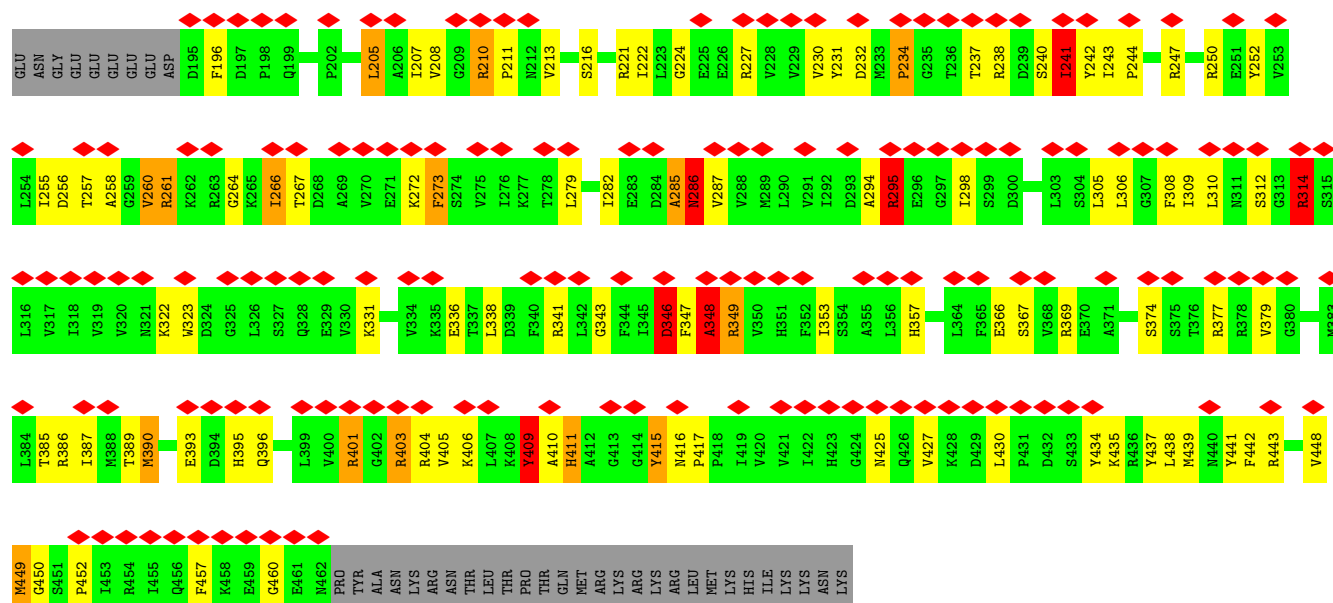
• Molecule 18: 50S ribosomal protein L25



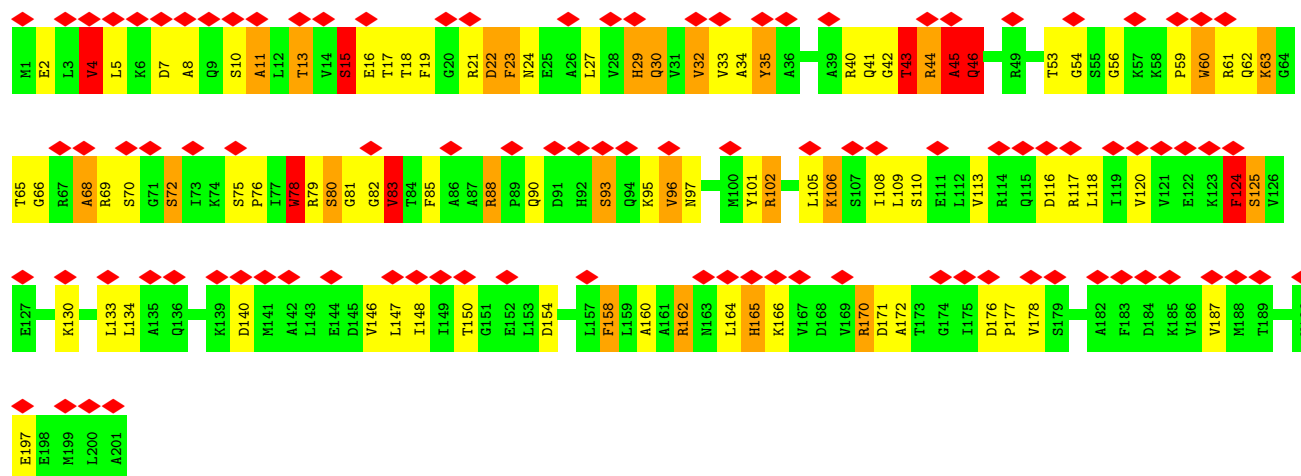
• Molecule 19: GTPase Der



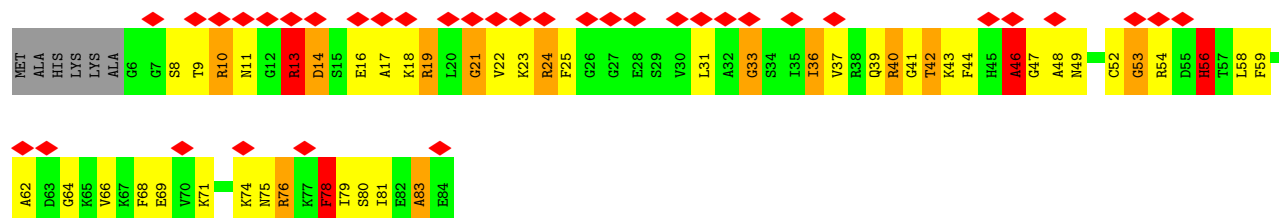




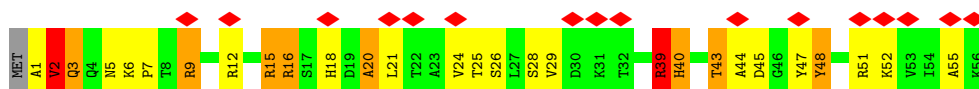
• Molecule 20: 50S ribosomal protein L4



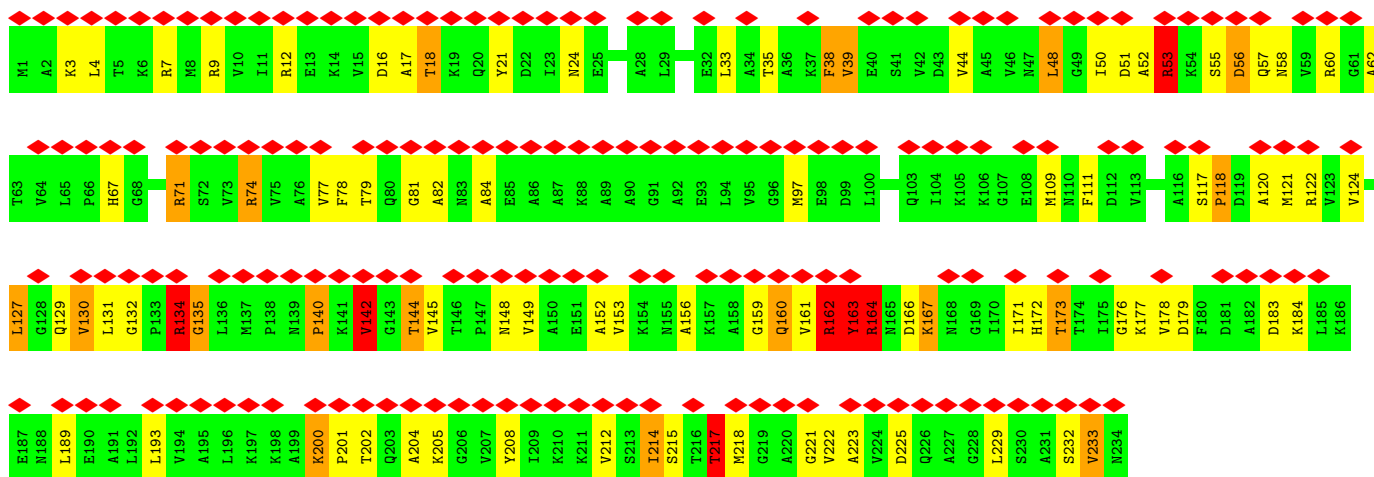
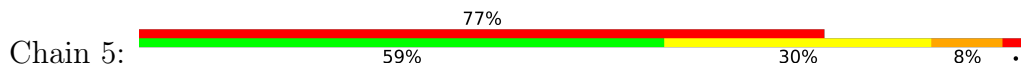
• Molecule 21: 50S ribosomal protein L27



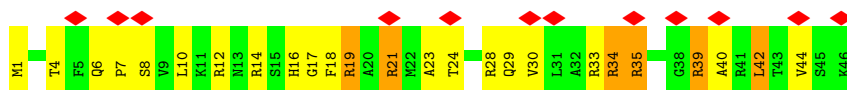
• Molecule 22: 50S ribosomal protein L32



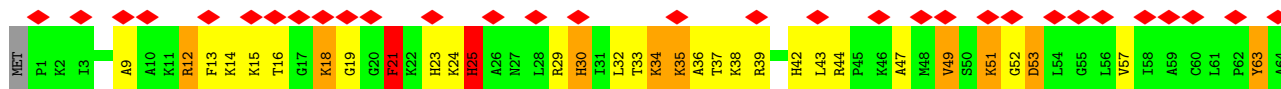
• Molecule 23: 50S ribosomal protein L1



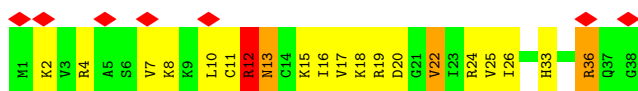
• Molecule 24: 50S ribosomal protein L34



• Molecule 25: 50S ribosomal protein L35

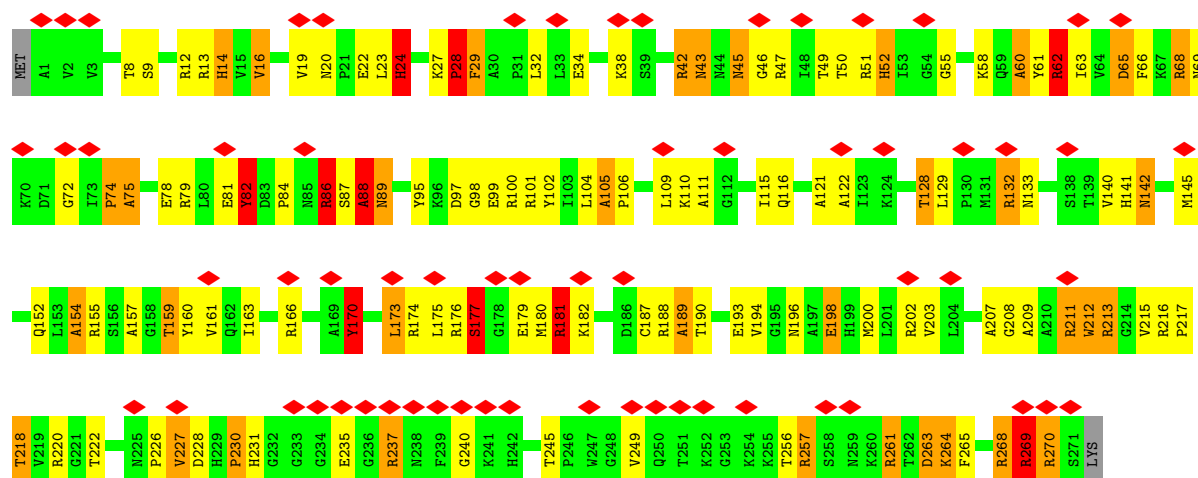


• Molecule 26: 50S ribosomal protein L36

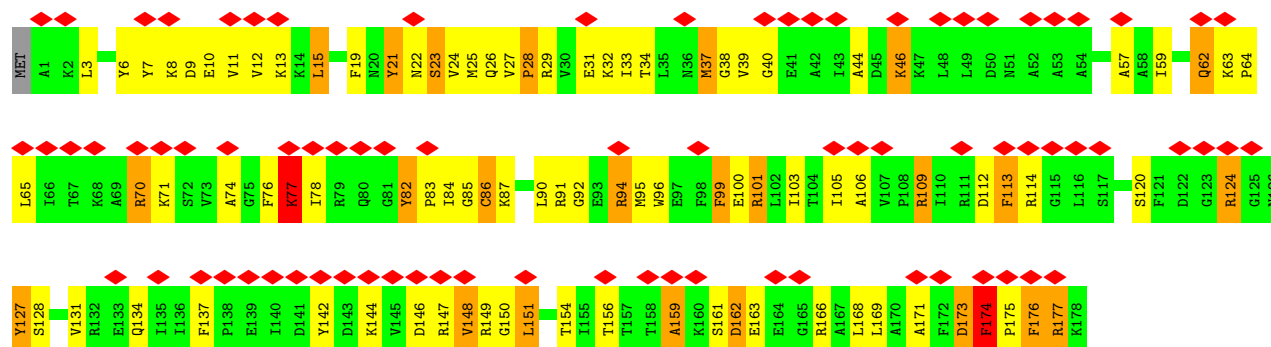


• Molecule 27: 50S ribosomal protein L2

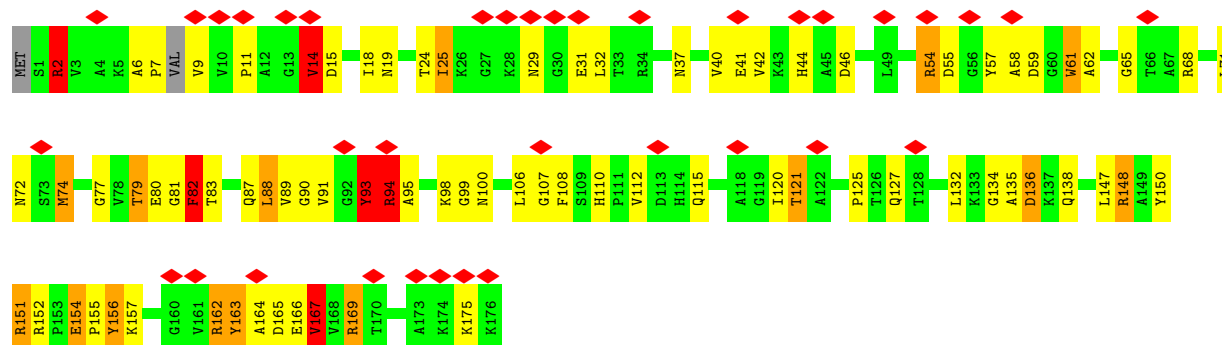




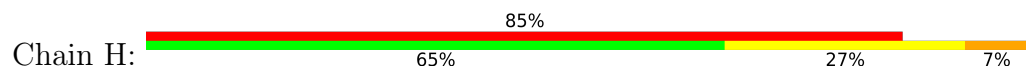
• Molecule 28: 50S ribosomal protein L5

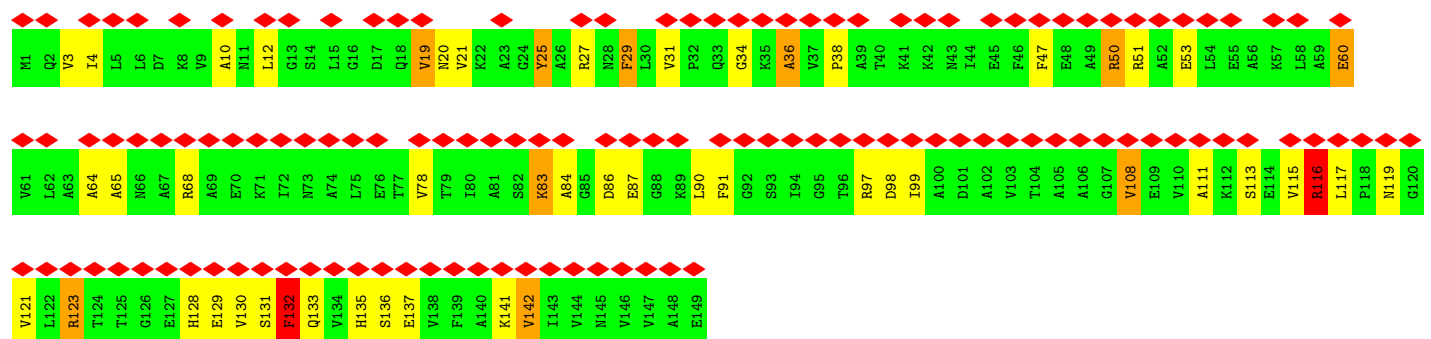


• Molecule 29: 50S ribosomal protein L6

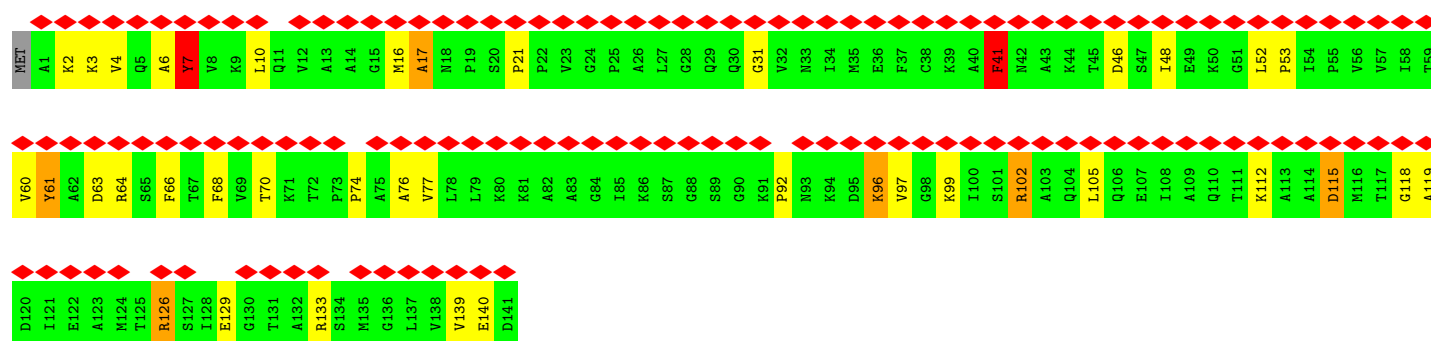
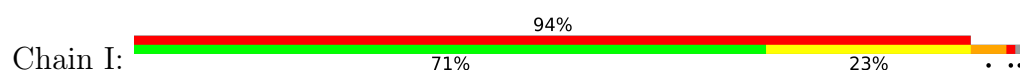


• Molecule 30: 50S ribosomal protein L9

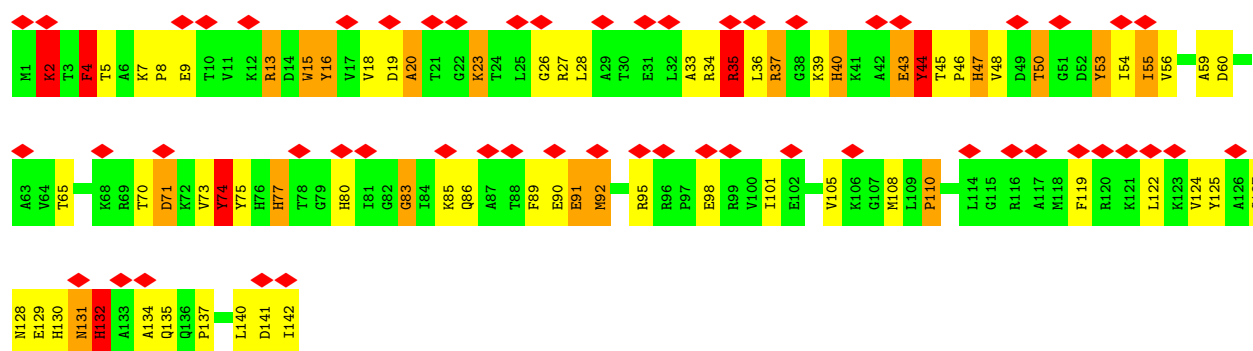
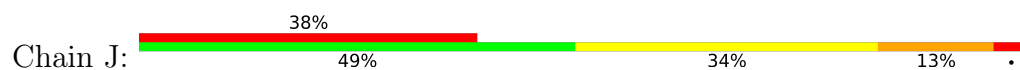




• Molecule 31: 50S ribosomal protein L11



• Molecule 32: 50S ribosomal protein L13



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	189614	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.045	Depositor
Map size ( $\text{\AA}$ )	373.088, 373.088, 373.088	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1659, 1.1659, 1.1659	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	3.57	414/2744 (15.1%)	3.75	637/4276 (14.9%)
2	B	3.66	11120/69092 (16.1%)	3.80	17069/107787 (15.8%)
3	0	1.89	7/635 (1.1%)	2.19	18/848 (2.1%)
4	K	1.72	6/940 (0.6%)	2.04	23/1258 (1.8%)
5	L	1.89	18/1054 (1.7%)	2.13	35/1403 (2.5%)
6	1	1.66	2/510 (0.4%)	1.81	4/677 (0.6%)
7	M	1.78	7/1093 (0.6%)	2.07	34/1460 (2.3%)
8	N	1.83	10/973 (1.0%)	2.11	35/1301 (2.7%)
9	O	1.84	12/902 (1.3%)	2.08	26/1209 (2.2%)
10	P	1.83	13/929 (1.4%)	2.13	26/1242 (2.1%)
11	Q	1.81	9/960 (0.9%)	2.35	47/1278 (3.7%)
12	R	1.75	4/829 (0.5%)	2.09	26/1107 (2.3%)
13	S	1.83	9/864 (1.0%)	2.06	22/1156 (1.9%)
14	D	1.81	19/1586 (1.2%)	2.12	48/2134 (2.2%)
15	T	1.88	7/744 (0.9%)	2.05	24/994 (2.4%)
16	2	1.84	8/453 (1.8%)	2.15	14/605 (2.3%)
17	U	1.71	2/761 (0.3%)	1.94	13/1013 (1.3%)
18	W	1.74	5/766 (0.7%)	2.12	22/1025 (2.1%)
19	X	1.73	26/3334 (0.8%)	2.01	98/4502 (2.2%)
20	E	1.83	25/1571 (1.6%)	2.01	44/2113 (2.1%)
21	Y	1.84	8/603 (1.3%)	2.19	20/797 (2.5%)
22	3	1.85	2/450 (0.4%)	2.17	18/599 (3.0%)
23	5	1.68	18/1748 (1.0%)	1.99	52/2355 (2.2%)
24	6	1.97	5/380 (1.3%)	2.15	17/498 (3.4%)
25	7	1.82	6/513 (1.2%)	2.15	14/676 (2.1%)
26	8	1.72	3/303 (1.0%)	2.04	3/397 (0.8%)
27	C	1.87	34/2121 (1.6%)	2.07	66/2852 (2.3%)
28	F	1.75	16/1444 (1.1%)	2.21	59/1937 (3.0%)
29	G	1.77	12/1335 (0.9%)	2.13	40/1803 (2.2%)
30	H	1.71	8/1122 (0.7%)	1.87	17/1515 (1.1%)
31	I	1.65	5/1046 (0.5%)	1.92	28/1410 (2.0%)
32	J	1.79	12/1152 (1.0%)	2.02	36/1551 (2.3%)
All	All	3.21	11852/102957 (11.5%)	3.42	18635/153778 (12.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	69
2	B	0	1764
3	O	0	5
4	K	0	4
5	L	0	10
6	1	0	6
7	M	0	9
8	N	0	4
9	O	0	5
10	P	0	7
11	Q	0	11
12	R	0	8
13	S	0	3
14	D	0	11
15	T	0	3
16	2	0	4
17	U	0	4
18	W	0	2
19	X	0	25
20	E	0	7
21	Y	0	6
22	3	0	4
23	5	0	7
24	6	0	3
25	7	0	3
26	8	0	1
27	C	0	11
28	F	0	6
29	G	0	9
30	H	0	9
31	I	0	3
32	J	0	9
All	All	0	2032

The worst 5 of 11852 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	159	G	N7-C5	-23.28	1.25	1.39
2	B	1674	G	N7-C5	-21.28	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	770	G	N7-C5	-20.77	1.26	1.39
2	B	1626	A	N7-C5	-20.30	1.27	1.39
2	B	1641	A	N7-C5	-19.84	1.27	1.39

The worst 5 of 18635 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1784	A	N1-C6-N6	27.35	135.01	118.60
2	B	319	G	N1-C6-O6	25.96	135.47	119.90
2	B	332	A	N1-C6-N6	25.93	134.16	118.60
2	B	909	A	N1-C6-N6	25.56	133.93	118.60
2	B	2270	A	N1-C6-N6	25.05	133.63	118.60

There are no chirality outliers.

5 of 2032 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	G	Sidechain
1	A	4	C	Sidechain
1	A	5	U	Sidechain
1	A	7	G	Sidechain
1	A	8	C	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	1253	65	0
2	B	61689	0	30889	2037	0
3	O	625	0	655	7	0
4	K	931	0	1003	12	0
5	L	1045	0	1117	16	0
6	1	509	0	543	8	0
7	M	1074	0	1157	17	0
8	N	960	0	1000	14	0
9	O	892	0	923	10	0
10	P	917	0	965	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Q	947	0	1022	16	0
12	R	816	0	839	13	0
13	S	857	0	922	18	0
14	D	1565	0	1616	24	0
15	T	738	0	807	9	0
16	2	449	0	491	4	0
17	U	755	0	807	6	0
18	W	753	0	780	11	0
19	X	3280	0	3334	47	0
20	E	1552	0	1619	27	0
21	Y	596	0	610	14	0
22	3	444	0	461	7	0
23	5	1733	0	1824	19	0
24	6	377	0	418	4	0
25	7	504	0	574	8	0
26	8	302	0	343	8	0
27	C	2082	0	2157	31	0
28	F	1420	0	1460	18	0
29	G	1316	0	1364	15	0
30	H	1111	0	1148	13	0
31	I	1032	0	1088	3	0
32	J	1129	0	1162	30	0
All	All	94855	0	64351	2462	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 15.

The worst 5 of 2462 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)
19:X:347:PHE:CD2	19:X:449:MET:CG	2.00	1.45
19:X:347:PHE:CD2	19:X:449:MET:HG2	1.49	1.26
19:X:347:PHE:CD2	19:X:449:MET:HG3	1.84	0.97
19:X:449:MET:HA	19:X:449:MET:CE	1.97	0.94
19:X:347:PHE:HD2	19:X:449:MET:HG2	0.77	0.90

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	
3	0	75/78 (96%)	54 (72%)	11 (15%)	10 (13%)	0	4
4	K	119/123 (97%)	84 (71%)	21 (18%)	14 (12%)	0	6
5	L	141/144 (98%)	108 (77%)	23 (16%)	10 (7%)	1	16
6	1	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
7	M	134/136 (98%)	97 (72%)	18 (13%)	19 (14%)	0	4
8	N	118/127 (93%)	91 (77%)	20 (17%)	7 (6%)	1	19
9	O	114/117 (97%)	96 (84%)	12 (10%)	6 (5%)	2	21
10	P	112/115 (97%)	81 (72%)	18 (16%)	13 (12%)	0	6
11	Q	115/118 (98%)	87 (76%)	17 (15%)	11 (10%)	0	10
12	R	101/103 (98%)	71 (70%)	23 (23%)	7 (7%)	1	16
13	S	108/110 (98%)	83 (77%)	16 (15%)	9 (8%)	1	13
14	D	207/209 (99%)	143 (69%)	42 (20%)	22 (11%)	0	8
15	T	91/100 (91%)	58 (64%)	17 (19%)	16 (18%)	0	3
16	2	56/59 (95%)	46 (82%)	7 (12%)	3 (5%)	2	21
17	U	94/104 (90%)	66 (70%)	16 (17%)	12 (13%)	0	5
18	W	92/94 (98%)	77 (84%)	10 (11%)	5 (5%)	2	21
19	X	410/490 (84%)	329 (80%)	46 (11%)	35 (8%)	1	12
20	E	199/201 (99%)	145 (73%)	28 (14%)	26 (13%)	0	4
21	Y	77/85 (91%)	43 (56%)	15 (20%)	19 (25%)	0	1
22	3	54/57 (95%)	36 (67%)	10 (18%)	8 (15%)	0	4
23	5	232/234 (99%)	185 (80%)	23 (10%)	24 (10%)	0	9
24	6	44/46 (96%)	33 (75%)	7 (16%)	4 (9%)	1	12
25	7	62/65 (95%)	44 (71%)	11 (18%)	7 (11%)	0	7
26	8	36/38 (95%)	26 (72%)	6 (17%)	4 (11%)	0	8
27	C	269/273 (98%)	201 (75%)	35 (13%)	33 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	F	176/179 (98%)	119 (68%)	41 (23%)	16 (9%)	1	12
29	G	171/177 (97%)	128 (75%)	26 (15%)	17 (10%)	0	10
30	H	147/149 (99%)	109 (74%)	25 (17%)	13 (9%)	1	12
31	I	139/142 (98%)	114 (82%)	16 (12%)	9 (6%)	1	18
32	J	140/142 (99%)	102 (73%)	21 (15%)	17 (12%)	0	6
All	All	3894/4078 (96%)	2905 (75%)	593 (15%)	396 (10%)	1	9

5 of 396 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	0	15	ASN
3	0	28	PHE
3	0	70	LEU
5	L	29	LYS
5	L	41	ARG

### 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	0	67/68 (98%)	62 (92%)	5 (8%)	13	39
4	K	102/104 (98%)	92 (90%)	10 (10%)	8	28
5	L	102/103 (99%)	89 (87%)	13 (13%)	4	20
6	1	55/55 (100%)	50 (91%)	5 (9%)	9	31
7	M	109/109 (100%)	105 (96%)	4 (4%)	34	58
8	N	100/103 (97%)	93 (93%)	7 (7%)	15	41
9	O	86/87 (99%)	73 (85%)	13 (15%)	3	16
10	P	99/100 (99%)	87 (88%)	12 (12%)	5	22
11	Q	89/90 (99%)	81 (91%)	8 (9%)	9	32
12	R	84/84 (100%)	69 (82%)	15 (18%)	2	11
13	S	93/93 (100%)	88 (95%)	5 (5%)	22	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	D	164/164 (100%)	143 (87%)	21 (13%)	4	20
15	T	80/84 (95%)	69 (86%)	11 (14%)	3	19
16	2	48/49 (98%)	44 (92%)	4 (8%)	11	36
17	U	81/85 (95%)	72 (89%)	9 (11%)	6	24
18	W	78/78 (100%)	71 (91%)	7 (9%)	9	32
19	X	357/419 (85%)	324 (91%)	33 (9%)	9	31
20	E	165/165 (100%)	152 (92%)	13 (8%)	12	38
21	Y	59/63 (94%)	55 (93%)	4 (7%)	16	42
22	3	47/48 (98%)	40 (85%)	7 (15%)	3	16
23	5	181/181 (100%)	158 (87%)	23 (13%)	4	20
24	6	38/38 (100%)	35 (92%)	3 (8%)	12	38
25	7	51/52 (98%)	44 (86%)	7 (14%)	3	19
26	8	34/34 (100%)	31 (91%)	3 (9%)	10	33
27	C	216/218 (99%)	190 (88%)	26 (12%)	5	22
28	F	149/150 (99%)	131 (88%)	18 (12%)	5	22
29	G	136/138 (99%)	115 (85%)	21 (15%)	2	15
30	H	114/114 (100%)	105 (92%)	9 (8%)	12	38
31	I	109/110 (99%)	100 (92%)	9 (8%)	11	36
32	J	116/116 (100%)	99 (85%)	17 (15%)	3	16
All	All	3209/3302 (97%)	2867 (89%)	342 (11%)	10	26

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

Mol	Chain	Res	Type
24	6	34	ARG
29	G	14	VAL
25	7	37	THR
27	C	213	ARG
29	G	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
29	G	110	HIS

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Mol	Chain	Res	Type
30	H	128	HIS
32	J	86	GLN
14	D	136	ASN
14	D	134	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	112/117 (95%)	20 (17%)	4 (3%)
2	B	2873/2903 (98%)	580 (20%)	122 (4%)
All	All	2985/3020 (98%)	600 (20%)	126 (4%)

5 of 600 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	13	G
1	A	14	U
1	A	15	A
1	A	16	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1284	A
2	B	2402	U
2	B	1730	C
2	B	2336	A
2	B	2601	C

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

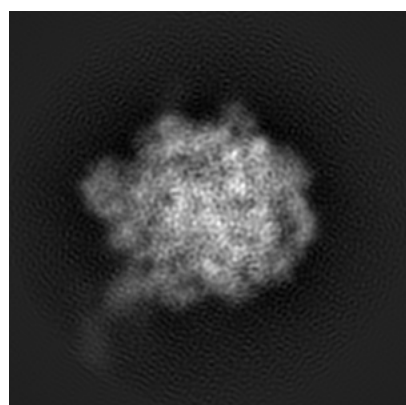
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6149. These allow visual inspection of the internal detail of the map and identification of artifacts.

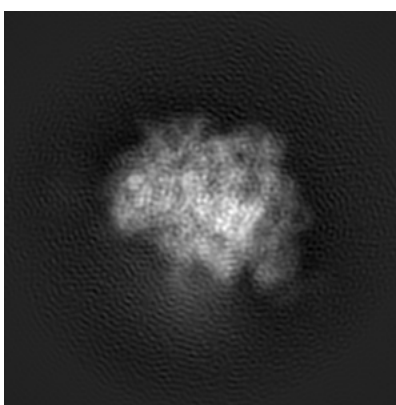
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

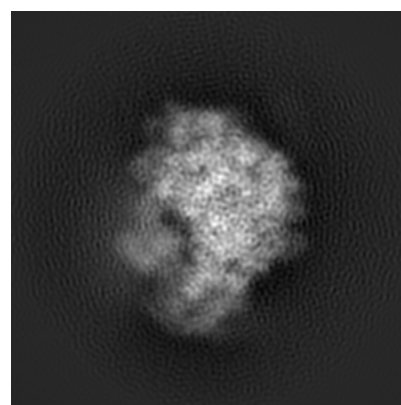
#### 6.1.1 Primary map



X



Y

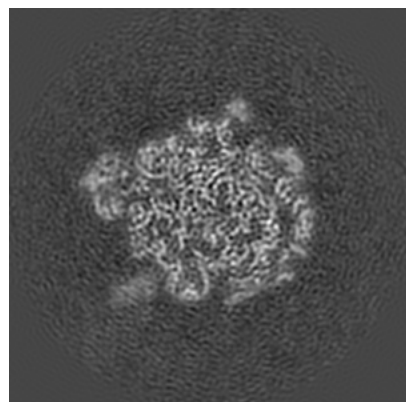


Z

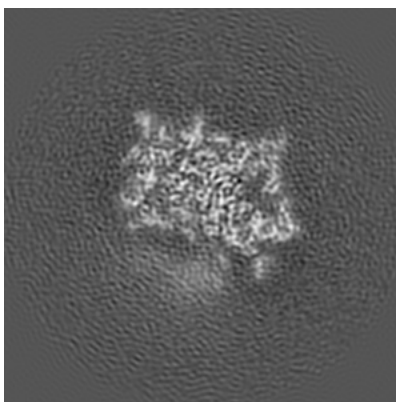
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

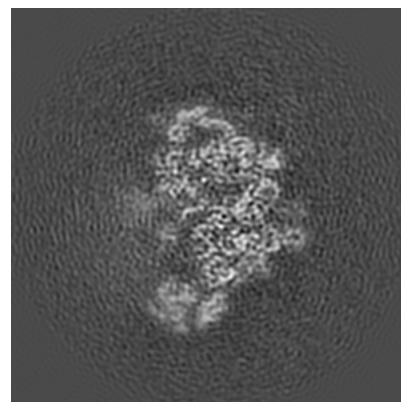
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

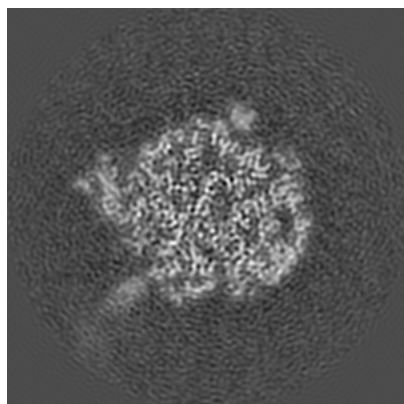


Z Index: 160

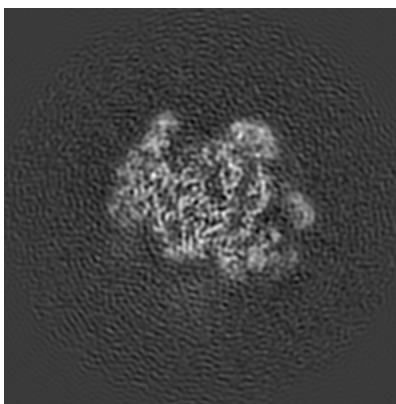
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

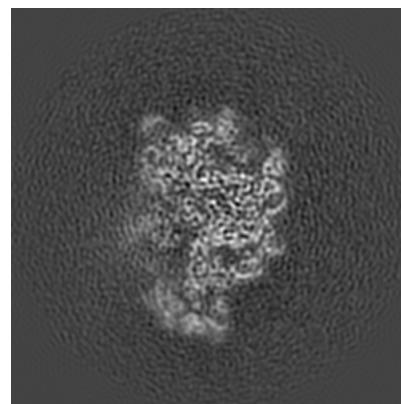
### 6.3.1 Primary map



X Index: 166



Y Index: 181

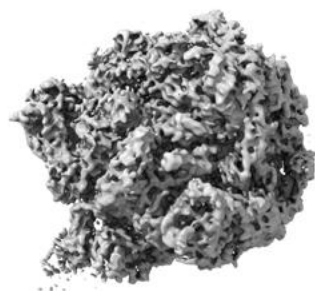


Z Index: 176

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

## 6.4 Orthogonal surface views [i](#)

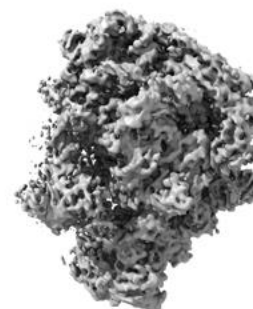
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



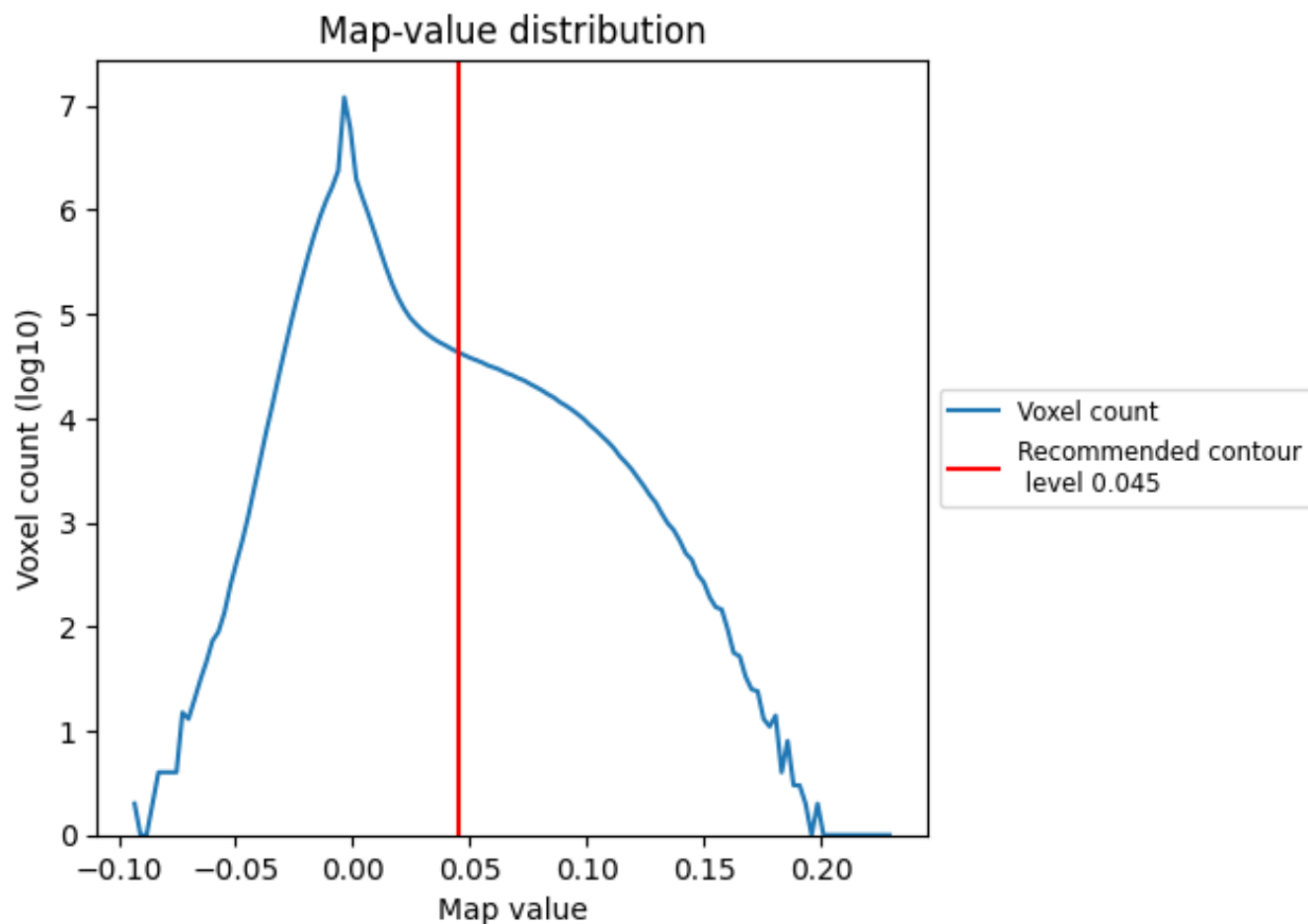
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

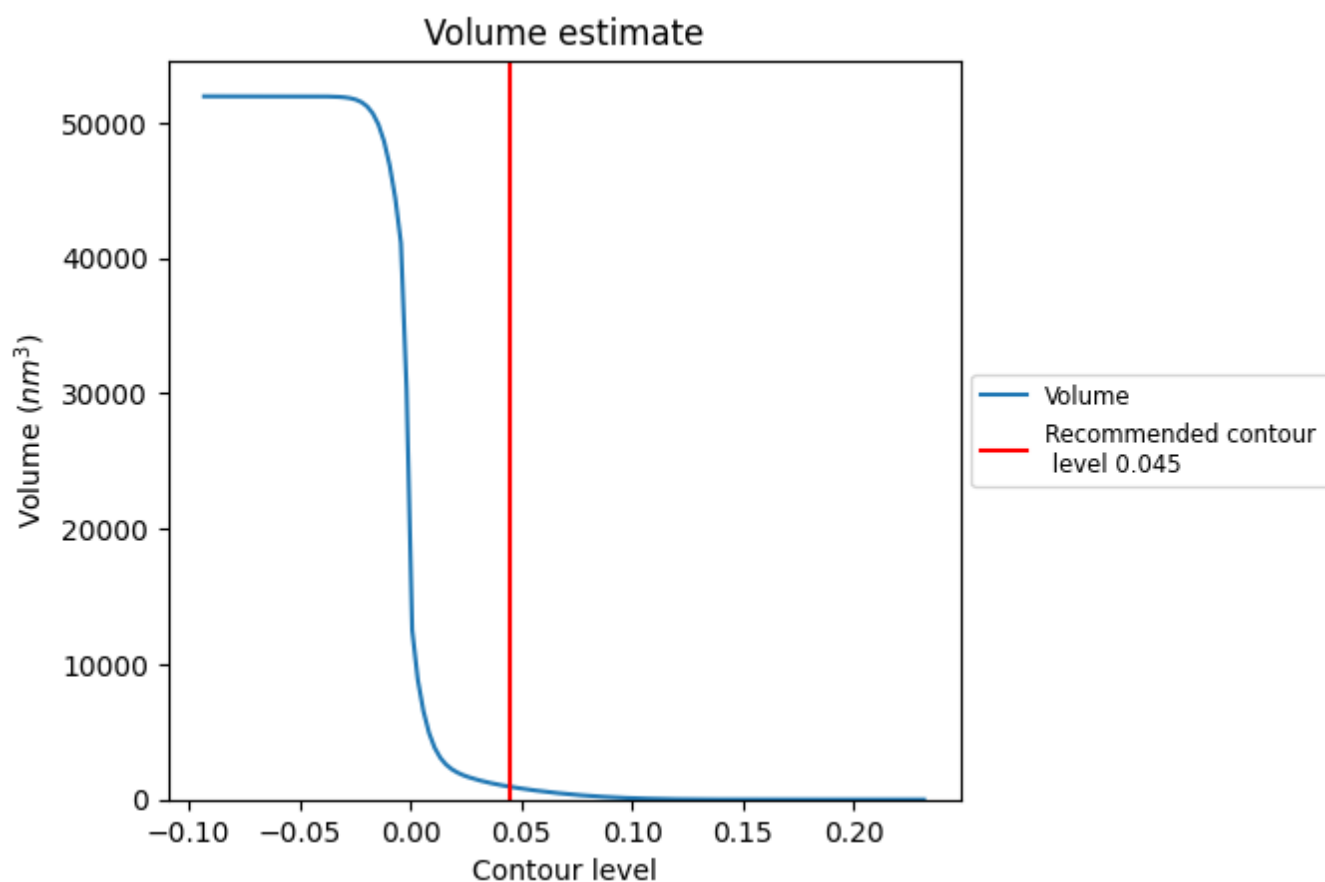
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

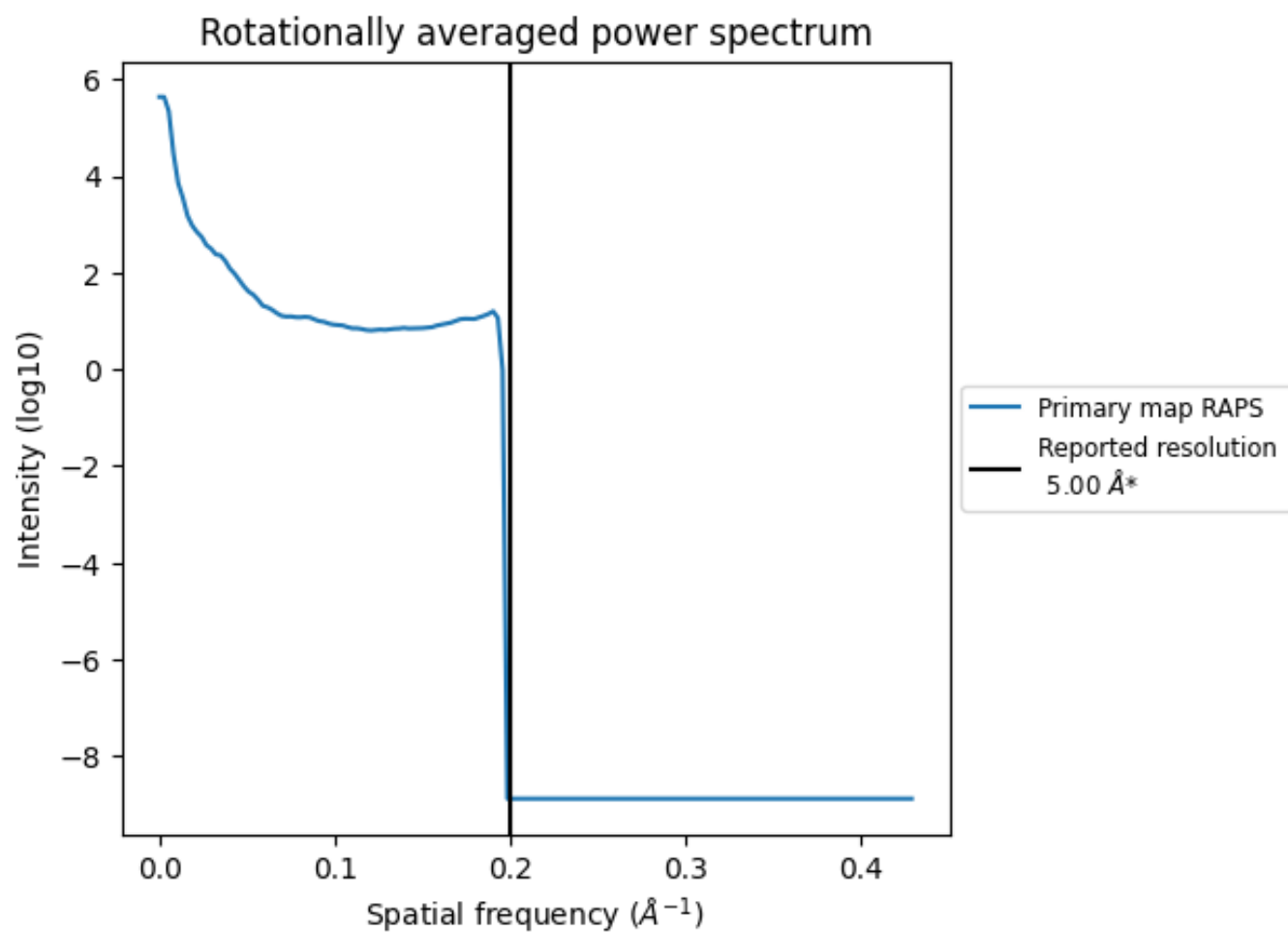
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 946 nm<sup>3</sup>; this corresponds to an approximate mass of 854 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 ⓘ

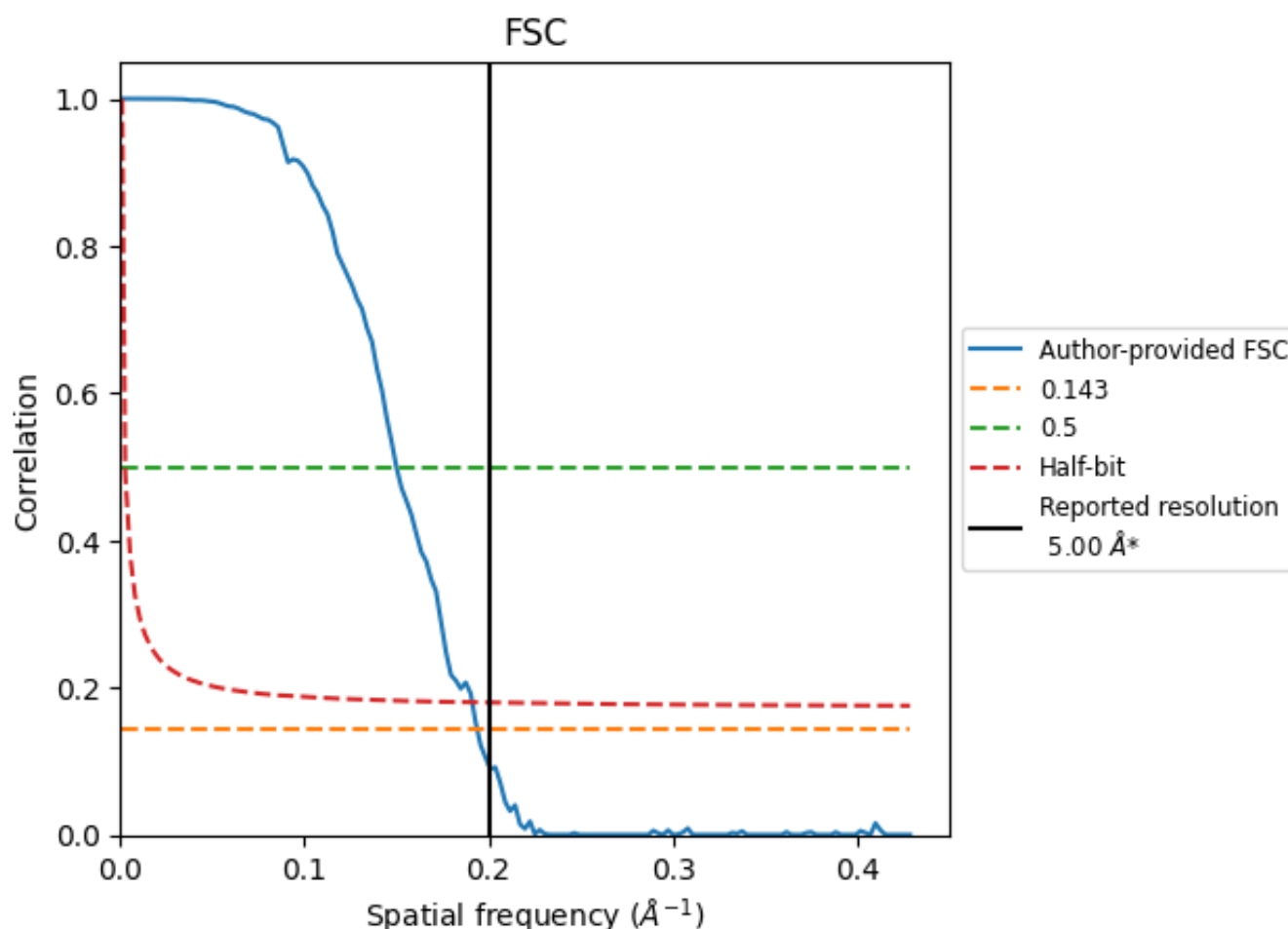


\*Reported resolution corresponds to spatial frequency of 0.200 Å<sup>-1</sup>

## 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 0.200 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

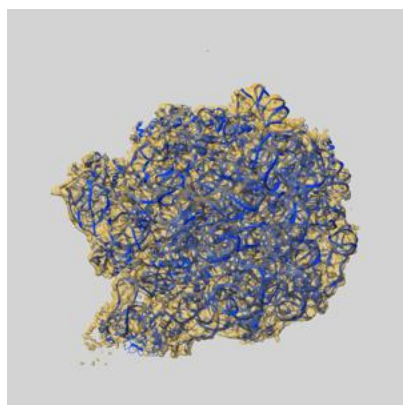
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	5.16	6.67	5.23
Unmasked-calculated*	-	-	-

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

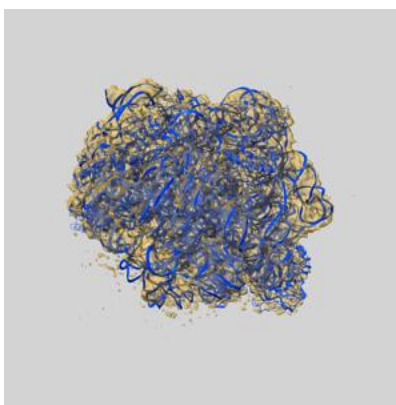
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6149 and PDB model 3J8G. Per-residue inclusion information can be found in section [3](#) on page [9](#).

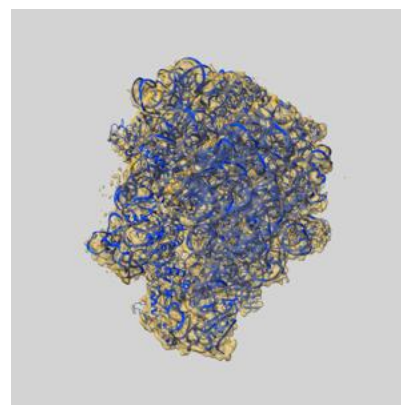
### 9.1 Map-model overlay [i](#)



X



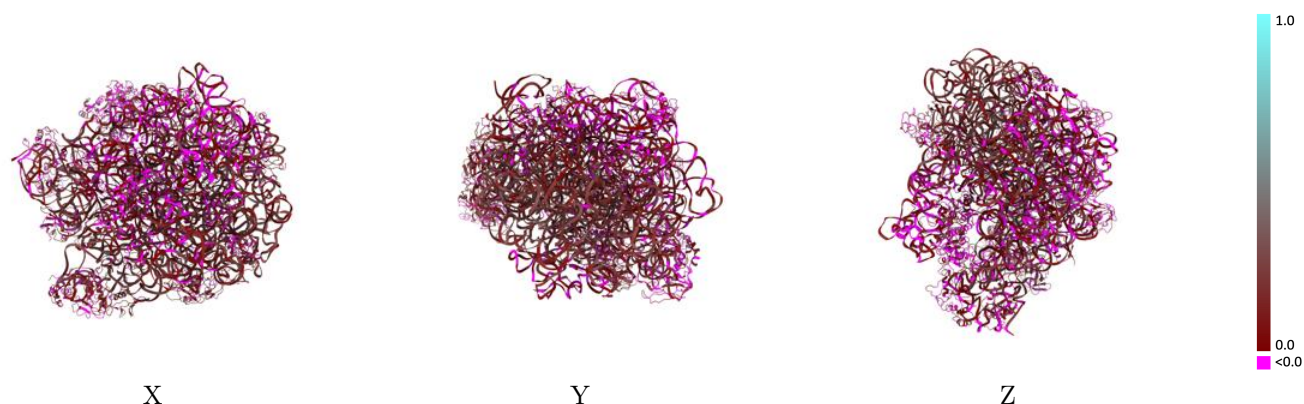
Y



Z

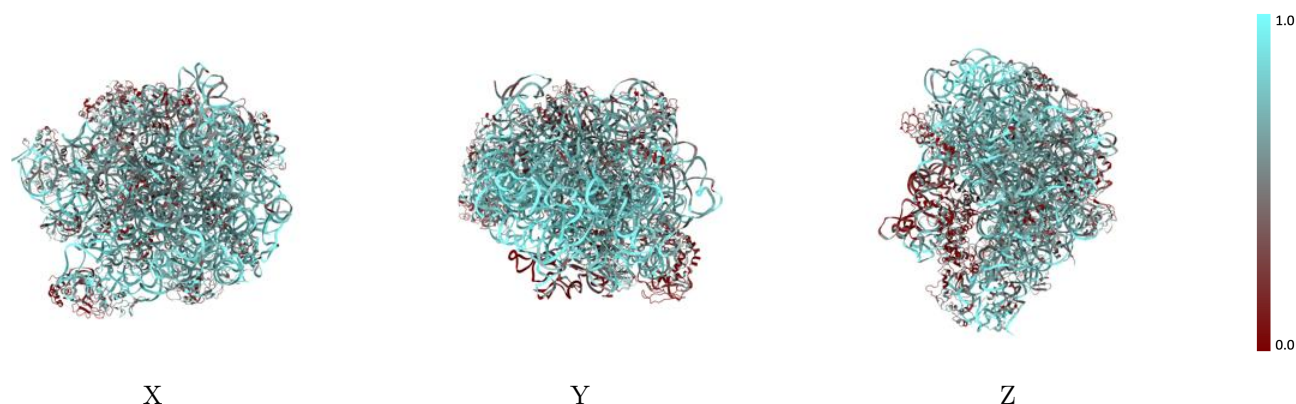
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

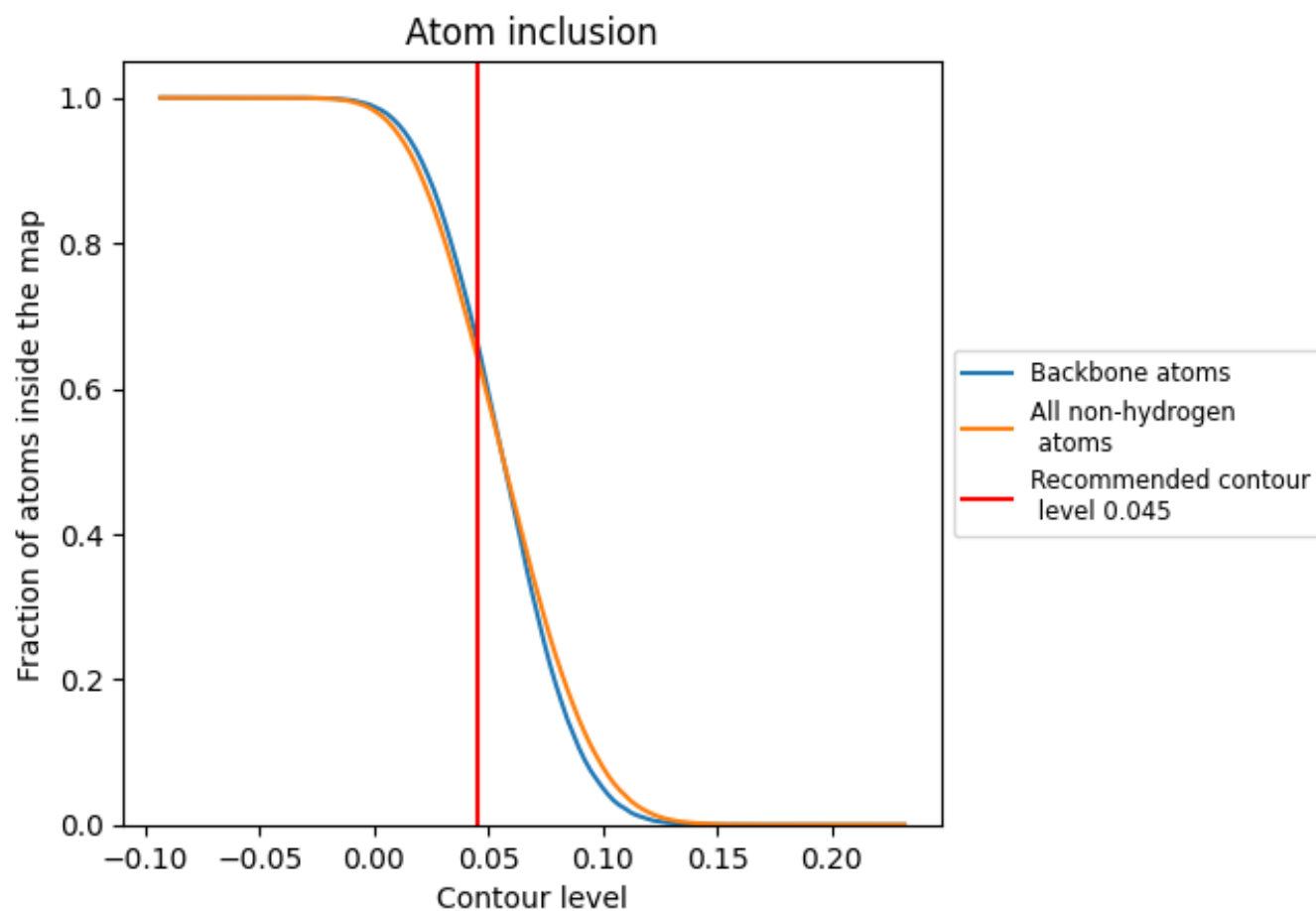
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.045).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 65% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6458	 0.1310
0	 0.4326	 0.0960
1	 0.4366	 0.0650
2	 0.4600	 0.0490
3	 0.5187	 0.1010
5	 0.2172	 0.0350
6	 0.5324	 0.1150
7	 0.4440	 0.0540
8	 0.6370	 0.1510
A	 0.7772	 0.1370
B	 0.7329	 0.1480
C	 0.5888	 0.1510
D	 0.6001	 0.1610
E	 0.4217	 0.0490
F	 0.4555	 0.0680
G	 0.6016	 0.1610
H	 0.1651	 0.0600
I	 0.0460	 0.0270
J	 0.5009	 0.1070
K	 0.6060	 0.1510
L	 0.4459	 0.0560
M	 0.6142	 0.1780
N	 0.6193	 0.1280
O	 0.5284	 0.0920
P	 0.5608	 0.1610
Q	 0.5000	 0.0650
R	 0.4555	 0.0500
S	 0.4402	 0.0580
T	 0.5249	 0.1040
U	 0.4282	 0.0400
W	 0.5583	 0.1540
X	 0.3427	 0.0850
Y	 0.4845	 0.0580

