



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 07:13 pm BST

PDB ID : 5NCO / pdb_00005nco
EMDB ID : EMD-3617
Title : Quaternary complex between SRP, SR, and SecYEG bound to the translating ribosome
Authors : Jomaa, A.; Hwang Fu, Y.; Boerhinger, D.; Leibundgut, M.; Shan, S.O.; Ban, N.
Deposited on : 2017-03-06
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

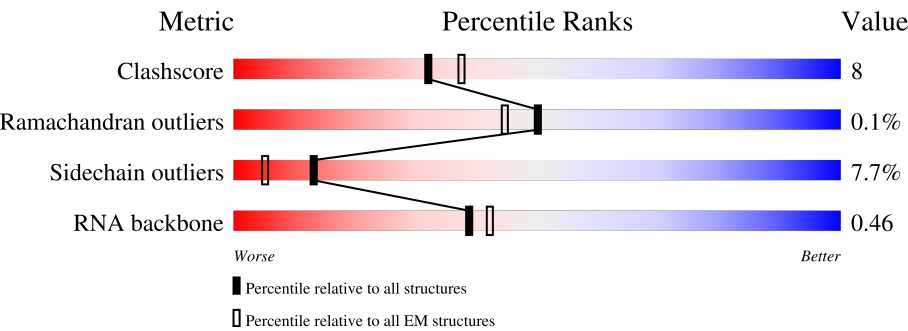
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 4.80 Å.

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








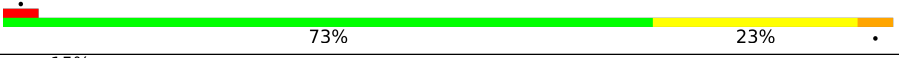

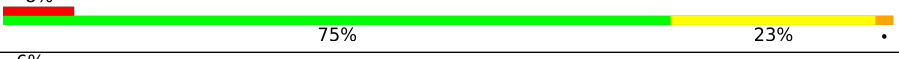
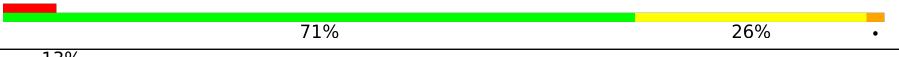


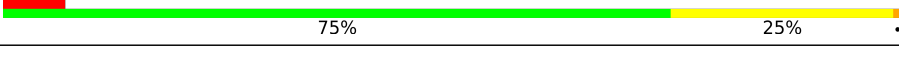







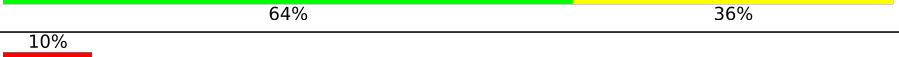
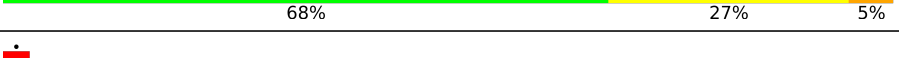
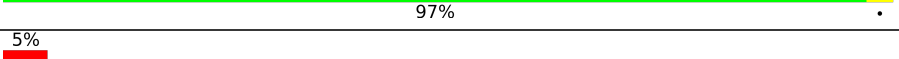

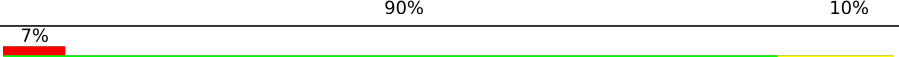

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	104	
2	2	3	
3	A	2903	
4	B	120	
5	C	271	
6	D	209	
7	E	201	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	F	177	
9	G	176	
10	H	149	
11	I	125	
12	J	134	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	125	
18	P	117	
19	Q	114	
20	R	117	
21	S	103	
22	T	110	
23	U	95	
24	V	102	
25	W	94	
26	X	76	
27	Y	77	
28	Z	62	
29	a	58	
30	b	56	
31	c	51	
32	d	46	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	e	64	
34	f	38	
35	g	416	
36	h	56	
37	i	450	
38	j	71	
39	k	23	
40	l	271	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 101694 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 4.5S SRP RNA (Ffs).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	104	Total	C	N	O	P	0	0
			2224	991	401	728	104		

- Molecule 2 is a RNA chain called P-site tRNA-CCA end.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	598	169	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	g	416	Total	C	N	O	0	0
			1664	832	416	416		

- Molecule 36 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	h	56	Total	C	N	O	0	0
			224	112	56	56		

- Molecule 37 is a protein called Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	450	Total	C	N	O	S	0	0
			3384	2129	609	628	18		

- Molecule 38 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	j	71	Total	C	N	O	0	0
			284	142	71	71		

- Molecule 39 is a protein called Signal sequence (1A9L).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	23	Total	C	N	O	0	0
			159	107	25	27		

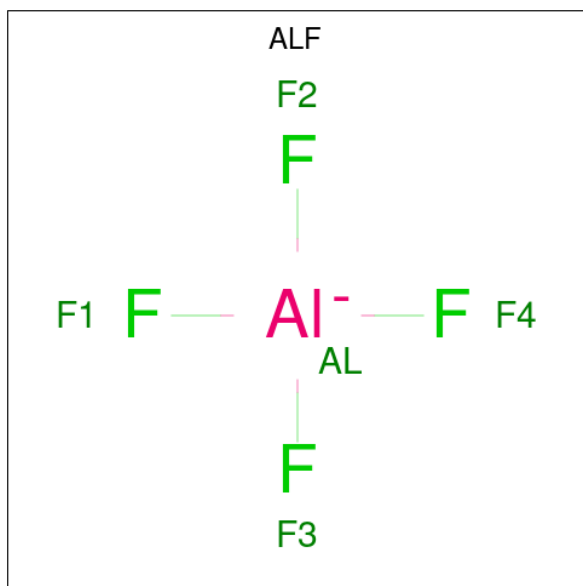
- Molecule 40 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	271	Total	C	N	O	S	0	0
			2067	1306	356	399	6		

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	f	1	Total	Zn	0
			1	1	

- Molecule 42 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

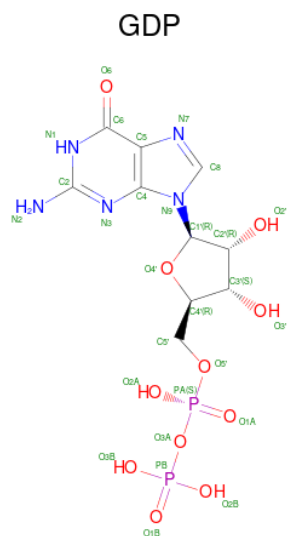


Mol	Chain	Residues	Atoms			AltConf
42	i	1	Total	Al	F	0
			5	1	4	
42	1	1	Total	Al	F	0
			5	1	4	

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	i	1	Total	Mg	0
			1	1	
43	1	1	Total	Mg	0
			1	1	

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

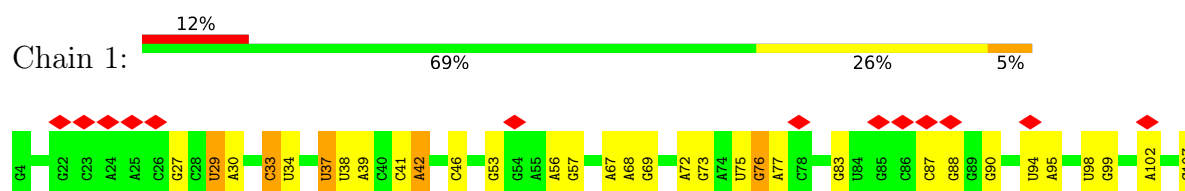


Mol	Chain	Residues	Atoms					AltConf
44	i	1	Total 28	C 10	N 5	O 11	P 2	0
44	l	1	Total 28	C 10	N 5	O 11	P 2	0

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.

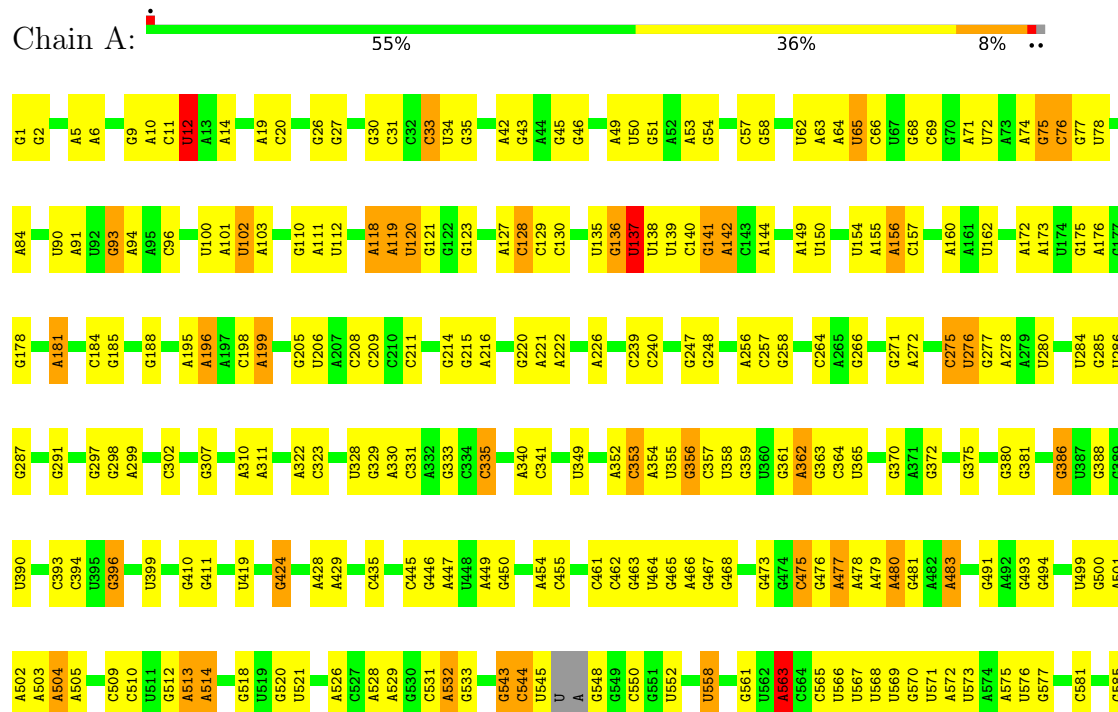
- Molecule 1: 4.5S SRP RNA (Ffs)



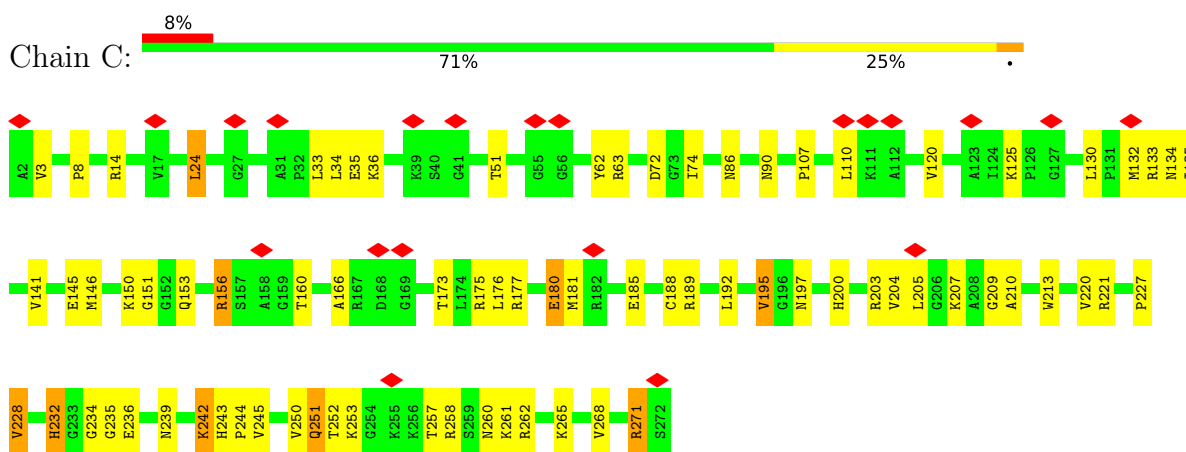
- Molecule 2: P-site tRNA-CCA end



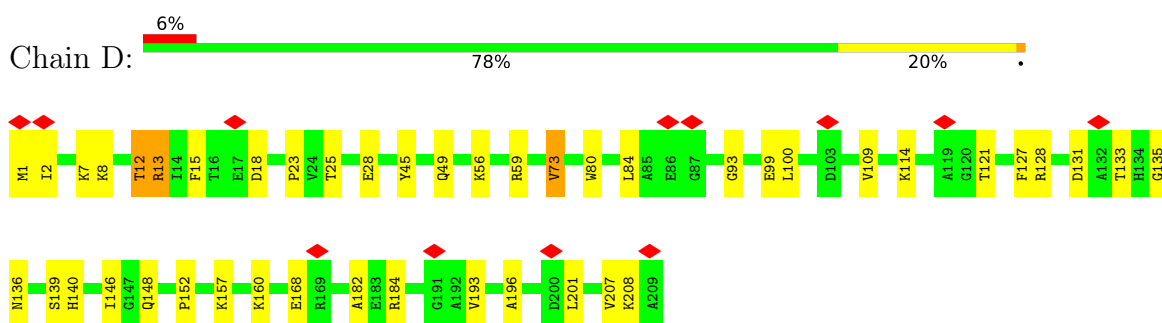
- Molecule 3: 23S rRNA



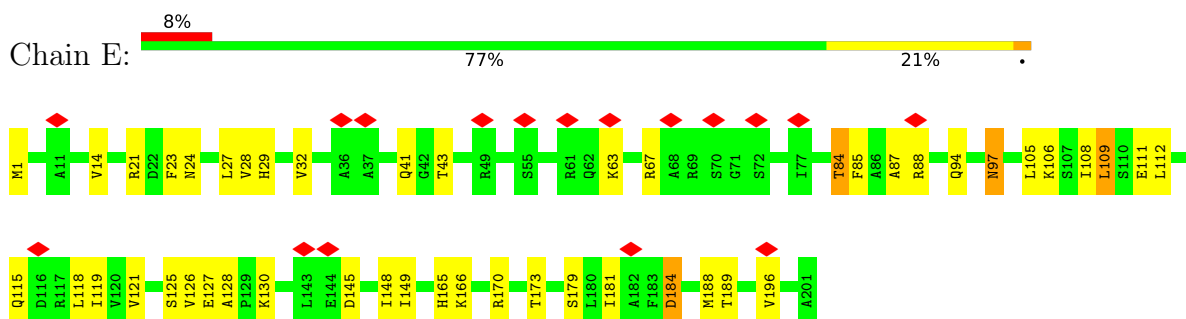
A588	A670	G776	C848	C946	A1028	U1105	G1212	A1327	A1419	U1497	U1584	A1677	A1785	C1807	G1807	A1808	G1816	C1822	U1825	G1826	U1827	A1829	C1837	C1838	G1846	A1847	A1848	G1849	G1850	A1853	A1858	U1859	G1869	C1870	A1871	A1872	C1873	C1874	G1875	A1876	A1877
A849	C671	G777	U850	C947	U1033	G1106	G1218	A1328	A1420	C1498	C1585	A1678	A1786	C1800	C1801	A1809	U1818	U1820	U1827	G1828	U1829	A1847	C1760	C1761	C1762	C1763	C1764	U1769	G1770	A1773	C1774	U1775	A1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881	
C672	C673	G778	U850	C948	U1033	G1110	G1218	A1329	A1421	C1499	C1586	A1679	A1787	C1802	C1803	A1808	U1819	U1821	U1828	G1829	U1830	A1848	C1761	C1762	C1763	C1764	U1770	G1771	A1774	C1775	U1776	A1781	U1782	A1877	A1878	A1879	A1880	A1881			
G674	G675	G779	U851	C949	U1034	G1111	A1230	G1332	G1422	G1500	A1590	G1681	C1789	A1790	A1791	G1797	U1798	U1820	U1827	G1828	U1829	A1848	C1760	C1761	C1762	C1763	C1764	U1769	G1770	A1773	C1774	U1775	A1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881	
A761	A762	A763	G857	G953	G1038	G1112	U1231	G1337	G1423	U1506	C1592	A1689	A1791	A1792	A1793	G1798	U1799	U1820	U1827	G1828	U1829	A1847	C1760	C1761	C1762	C1763	C1764	U1769	G1770	A1773	C1774	U1775	A1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881	
A764	A765	A766	C858	G954	A1039	G1115	U1231	G1337	G1423	U1506	C1592	A1689	A1791	A1792	A1793	G1798	U1799	U1820	U1827	G1828	U1829	A1847	C1760	C1761	C1762	C1763	C1764	U1769	G1770	A1773	C1774	U1775	A1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881	
A767	A768	A769	C859	G955	A1040	G1116	U1234	G1338	G1424	U1507	C1593	A1690	A1794	A1795	A1796	G1799	U1800	U1821	U1828	G1829	U1830	A1848	C1761	C1762	C1763	C1764	U1769	G1770	A1773	C1774	U1775	A1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881		
A770	A771	A772	C860	G956	A1041	G1117	U1235	G1339	G1425	U1508	C1594	A1691	A1796	A1797	A1798	G1800	U1801	U1822	U1829	G1830	U1831	A1849	C1762	C1763	C1764	U1770	G1771	A1774	C1775	U1776	A1781	U1782	A1877	A1878	A1879	A1880	A1881				
A773	A774	A775	C861	G957	A1042	G1118	U1236	G1340	G1426	U1509	C1595	A1692	A1797	A1798	A1799	G1801	U1802	U1823	U1830	G1831	U1832	A1849	C1762	C1763	C1764	U1770	G1771	A1774	C1775	U1776	A1781	U1782	A1877	A1878	A1879	A1880	A1881				
C679	C680	C681	C862	U958	A1043	G1119	U1237	G1341	G1427	U1510	C1596	A1693	A1799	A1800	A1801	G1802	U1803	U1824	U1831	U1832	A1850	C1763	C1764	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881	
G785	G786	G787	C863	U959	A1044	G1120	U1238	G1342	G1428	U1511	C1597	A1694	A1800	A1801	A1802	G1803	U1804	U1825	U1832	U1833	A1851	C1764	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881		
A788	A789	A790	C864	G960	A1048	G1125	U1239	G1343	G1432	U1512	C1598	A1695	A1801	A1802	A1803	G1804	U1805	U1826	U1833	U1834	A1852	C1765	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881			
A885	A886	A887	C865	G961	A1049	G1126	U1240	G1344	G1433	U1513	C1599	A1696	A1802	A1803	A1804	G1805	U1806	U1827	U1834	U1835	A1853	C1766	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881				
A888	A889	A890	C866	G962	A1050	G1127	U1241	G1345	G1434	U1514	C1600	A1697	A1803	A1804	A1805	G1806	U1807	U1828	U1835	U1836	A1854	C1767	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881					
A891	A892	A893	C867	G963	A1051	G1128	U1242	G1346	G1435	U1515	C1601	A1698	A1804	A1805	A1806	G1807	U1808	U1829	U1836	U1837	A1855	C1768	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881						
A894	A895	A896	C868	G964	A1052	G1129	U1243	G1347	G1436	U1516	C1602	A1699	A1805	A1806	A1807	G1808	U1809	U1830	U1837	U1838	A1856	C1769	U1776	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881							
A897	A898	A899	C869	G965	A1053	G1130	U1244	G1348	G1437	U1517	C1603	A1700	A1794	A1795	A1796	G1809	U1810	U1831	U1838	U1839	A1857	C1770	U1777	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881								
A899	A900	A901	C870	G966	A1054	G1131	U1245	G1349	G1438	U1518	C1604	A1701	A1795	A1796	A1797	G1810	U1811	U1832	U1839	U1840	A1858	C1771	U1778	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881									
A902	A903	A904	C871	G967	A1055	G1132	U1246	G1350	G1439	U1519	C1605	A1702	A1796	A1797	A1798	G1811	U1812	U1833	U1840	U1841	A1859	C1772	U1779	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881										
A905	A906	A907	C872	G968	A1056	G1133	U1247	G1351	G1440	U1520	C1606	A1703	A1797	A1798	A1799	G1812	U1813	U1834	U1841	U1842	A1860	C1773	U1780	U1781	U1782	A1877	A1878	A1879	A1880	A1881											
A908	A909	A910	C873	G969	A1057	G1134	U1248	G1352	G1441	U1521	C1607	A1704	A1798	A1799	A1800	G1813	U1814	U1835	U1842	U1843	A1861	C1774	U1781	U1782	A1877	A1878	A1879	A1880	A1881												
A911	A912	A913	C874	G970	A1058	G1135	U1249	G1353	G1442	U1522	C1608	A1705	A1799	A1800	A1801	G1814	U1815	U1836	U1843	U1844	A1862	C1775	U1782	A1877	A1878	A1879	A1880	A1881													
A914	A915	A916	C875	G971	A1059	G1136	U1250	G1354	G1443	U1523	C1609	A1706	A1800	A1801	A1802	G1815	U1816	U1837	U1844	U1845	A1863	C1776	U1783	A1877	A1878	A1879	A1880	A1881													
A917	A918	A919	C876	G972	A1060	G1137	U1251	G1355	G1444	U1524	C1610	A1707	A1801	A1802	A1803	G1816	U1817	U1838	U1845	U1846	A1864	C1777	U1784	A1877	A1878	A1879	A1880	A1881													
A920	A921	A922	C877	G973	A1061	G1138	U1252	G1356	G1445	U1525	C1611	A1708	A1802	A1803	A1804	G1817	U1818	U1839	U1846	U1847	A1865	C1778	U1785	A1877	A1878	A1879	A1880	A1881													
A923	A924	A925	C878	G974	A1062	G1139	U1253	G1357	G1446	U1526	C1612	A1709	A1803	A1804	A1805	G1818	U1819	U1840	U1847	U1848	A1866	C1779	U1786	A1877	A1878	A1879	A1880	A1881													
A926	A927	A928	C879	G975	A1063	G1140	U1254	G1358	G1447	U1527	C1613	A1710	A1804	A1805	A1806	G1819	U1820	U1841	U1848	U1849	A1867	C1780	U1787	A1877	A1878	A1879	A1880	A1881													
A929	A930	A931	C880	G976	A1064	G1141	U1255	G1359	G1448	U1528	C1614	A1711	A1805	A1806	A1807	G1820	U1821	U1842	U1849	U1850	A1868	C1781	U1788	A1877	A1878	A1879	A1880	A1881													
A932	A933	A934	C881	G977	A1065	G1142	U1256	G1360	G1449	U1529	C1615	A1712	A1806	A1807	A1808	G1821	U1822	U1843	U1850	U1851	A1869	C1782	U1789	A1877	A1878	A1879	A1880	A1881													
A935	A936	A937	C882	G978	A1066	G1143	U1257	G1361	G1450	U1530	C1616	A1713	A1807	A1808	A1809	G1822	U1823	U1844	U1851	U1852	A1870	C1783	U1790	A1877	A1878	A1879	A1880	A1881													
A938	A939	A940	C883	G979	A1067	G1144	U1258	G1362	G1451	U1531	C1617	A1714	A1808	A1809	A1810	G1823	U1824	U1845	U1852	U1853	A1871	C1784	U1791	A1877	A1878	A1879	A1880	A1881													
A941	A942	A943	C884	G980	A1068	G1145	U1259	G1363	G1452	U1532	C1618	A1715	A1809	A1810	A1811	G1824	U1825	U1846	U1853	U1854	A1872	C1785	U1792	A1877	A1878	A1879	A1880	A1881													
A944	A945	A946	C885	G981	A1069	G1146	U1260	G1364	G1453	U1533	C1619	A1716	A1810	A1811	A1812	G1825	U1826	U1847	U1854	U1855	A1873	C1786	U1793	A1877	A1878	A1879	A1880	A1881													
A947	A948	A949	C886	G982	A1070	G1147	U1261	G1365	G1454	U1534	C1620	A1717	A1811	A1812	A1813	G1826	U1827	U1848	U1855	U1856	A1874	C1787	U1794	A1877	A1878	A1879	A1880	A1881													
A950	A951	A952	C887	G983	A1071	G1148	U1262	G1366	G1455	U1535	C1621	A1718	A1812	A1813	A1814	G1827	U1828	U1849	U1856	U1857	A1875	C1788	U1795	A1877	A1878	A1879	A1880	A1881													
A953	A954	A955	C888	G984	A1072	G1149	U1263	G1367	G1456	U1536	C1622	A1719	A1813	A1814	A1815	G1828	U1829	U1850	U1857	U1858	A1876	C1789	U1796	A1877	A1878	A1879	A1880	A1881													
A956	A957	A958	C889	G985	A1073	G1150	U1264	G1368	G1457	U1537	C1623	A1720	A1814	A1815	A1816	G1829	U1830	U1851	U1858	U1859	A1877	C1790	U1797	A1877	A1878	A1879	A1880	A1881													
A959	A960	A961	C890	G986	A1074	G1151	U1265	G1369	G1458	U1538	C1624	A1721	A1815	A1816	A1817	G1830	U1831	U1852	U1859	U1860	A1878	C1791	U1798	A1877	A1878	A1879	A1880	A1881													
A962	A963	A964	C891	G987	A1075	G1152	U1266	G1370	G1459	U1539	C1625	A1722	A1816	A1817	A1818	G1831	U1832	U1853	U1860	U1861	A1879	C1792	U1799	A1877	A1878	A1879	A1880	A1881													
A965	A966	A967	C892	G988	A1076	G1153	U1267	G1371	G1460	U1540	C1626	A1723	A1817	A1818	A1819	G1832	U1833	U1854	U1861	U1862	A1880	C1793	U1800	A1877	A1878	A1879	A1880	A1881													



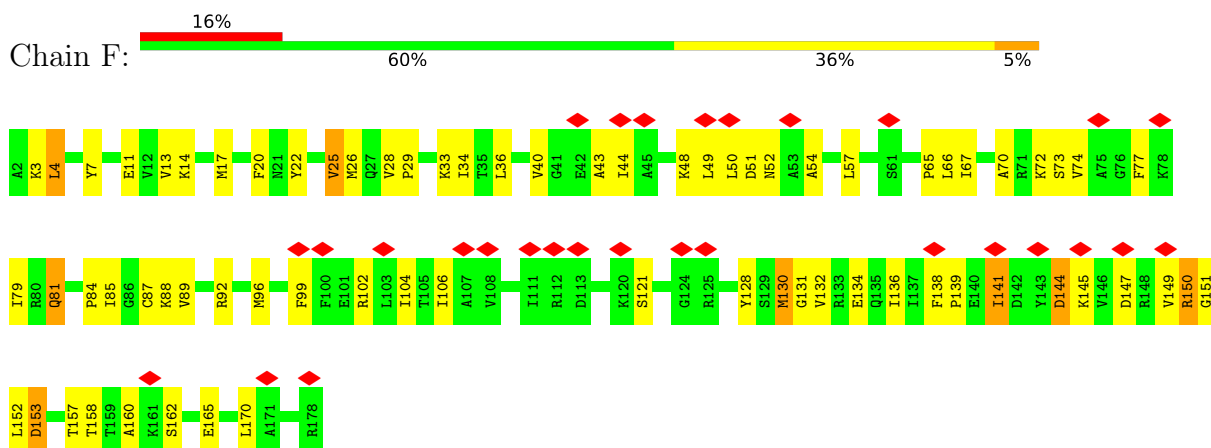
• Molecule 6: 50S ribosomal protein L3



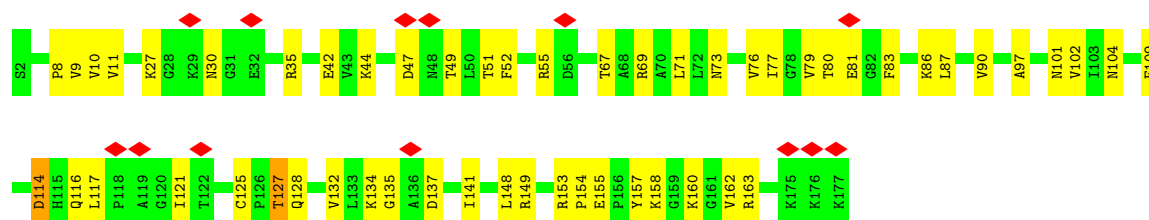
• Molecule 7: 50S ribosomal protein L4



• Molecule 8: 50S ribosomal protein L5



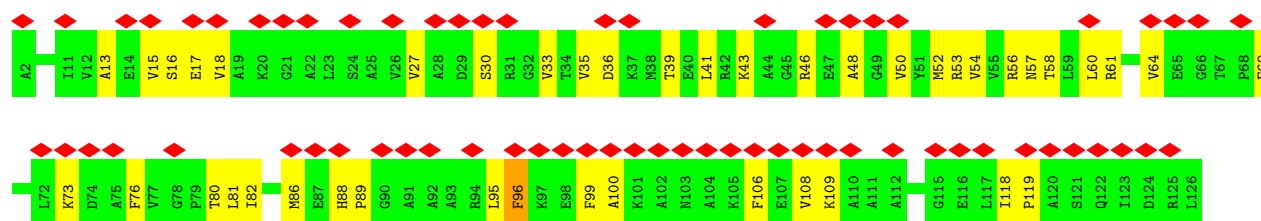
• Molecule 9: 50S ribosomal protein L6



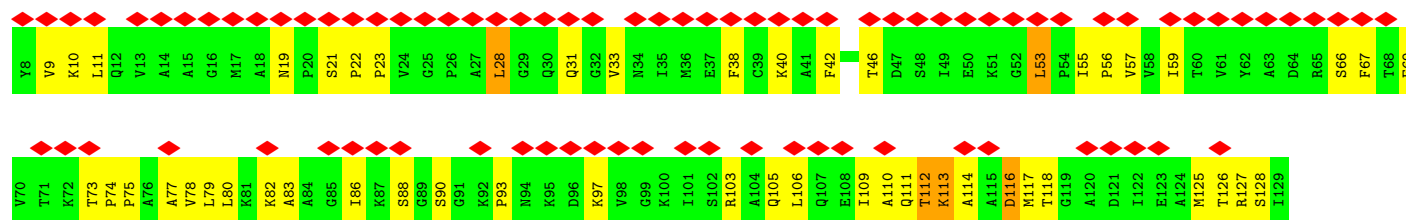
• Molecule 10: 50S ribosomal protein L9

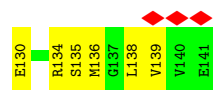


• Molecule 11: 50S ribosomal protein L10



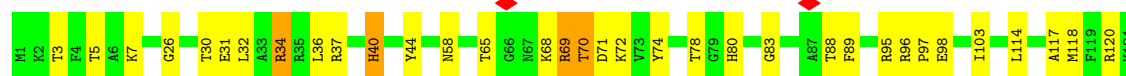
• Molecule 12: 50S ribosomal protein L11





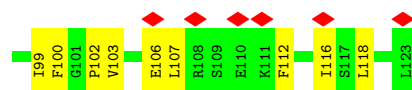
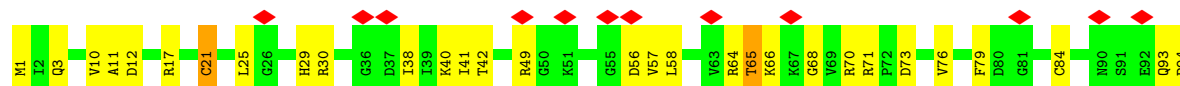
- Molecule 13: 50S ribosomal protein L13

Chain K: 73% 23%



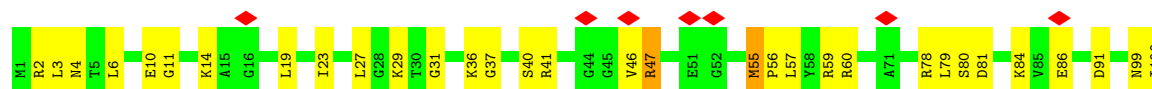
- Molecule 14: 50S ribosomal protein L14

Chain L: 15% 68% 30%



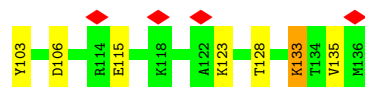
- Molecule 15: 50S ribosomal protein L15

Chain M: 8% 75% 23%

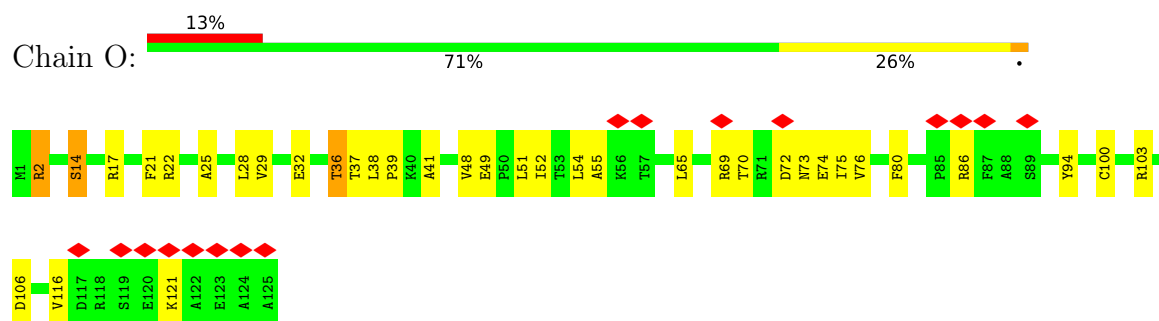


- Molecule 16: 50S ribosomal protein L16

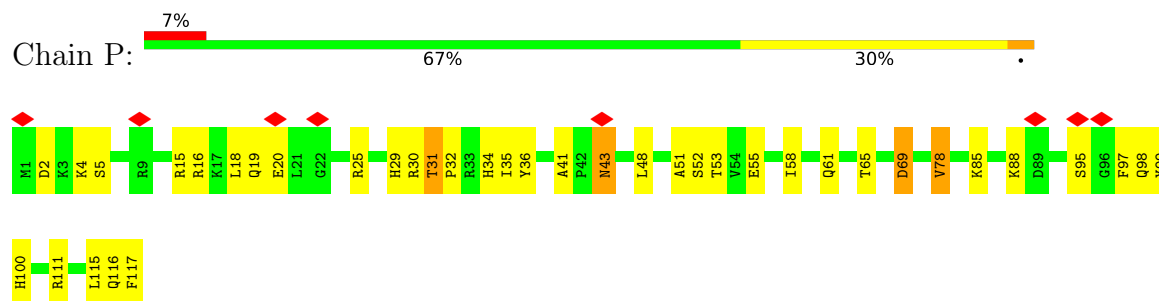
Chain N: 6% 71% 26%



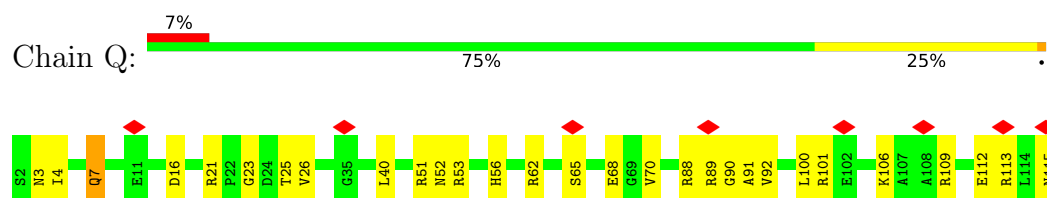
- Molecule 17: 50S ribosomal protein L17



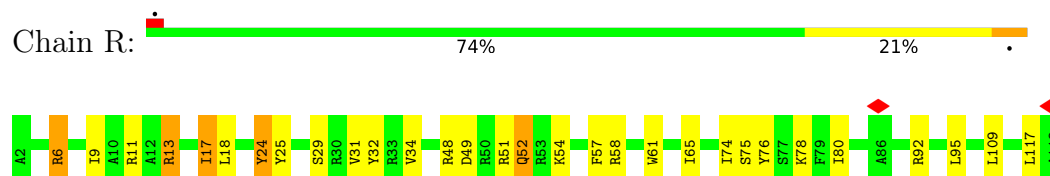
- Molecule 18: 50S ribosomal protein L18



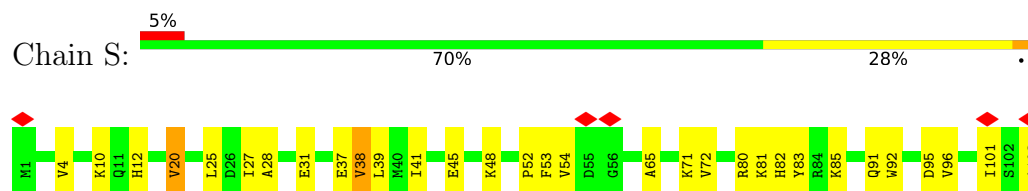
- Molecule 19: 50S ribosomal protein L19



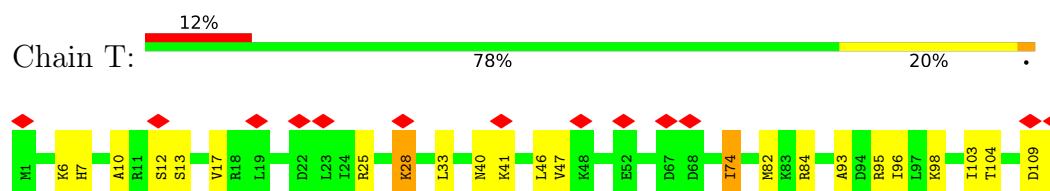
- Molecule 20: 50S ribosomal protein L20



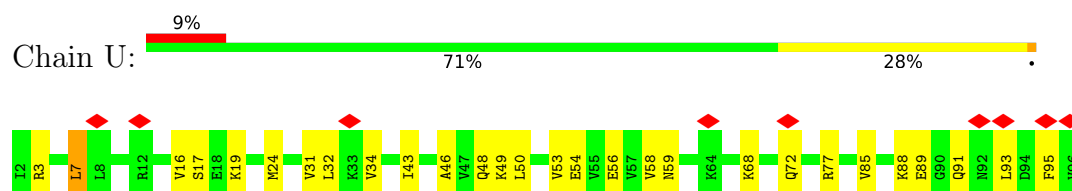
- Molecule 21: 50S ribosomal protein L21



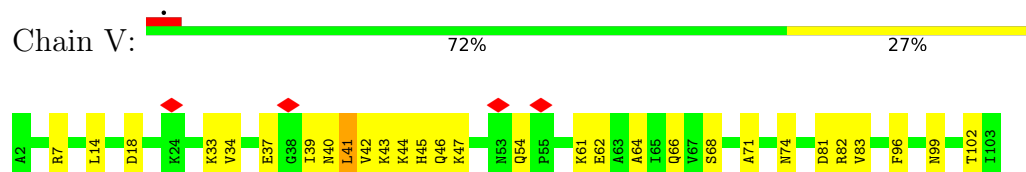
- Molecule 22: 50S ribosomal protein L22



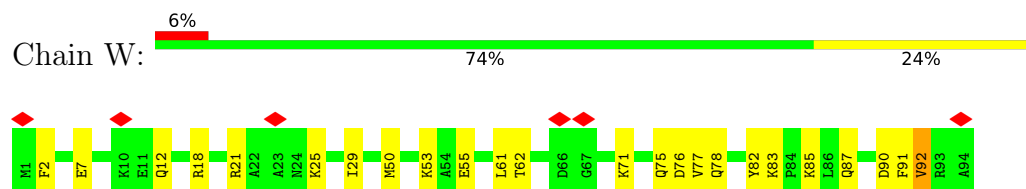
- Molecule 23: 50S ribosomal protein L23



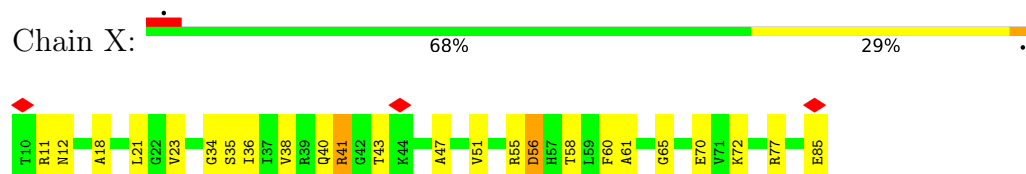
- Molecule 24: 50S ribosomal protein L24



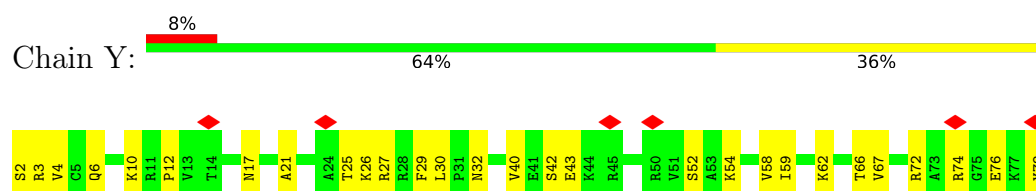
- Molecule 25: 50S ribosomal protein L25



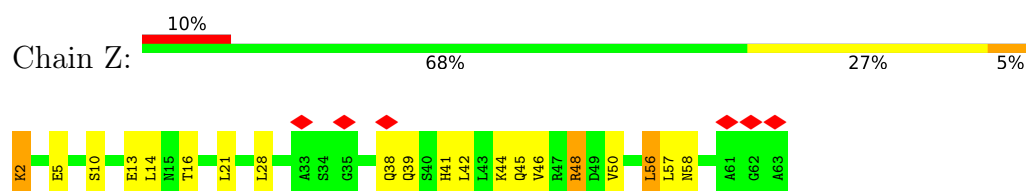
- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S ribosomal protein L28



- Molecule 28: 50S ribosomal protein L29

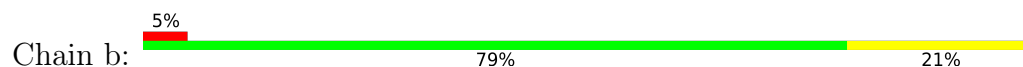


- Molecule 29: 50S ribosomal protein L30

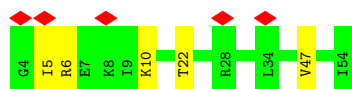




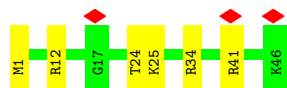
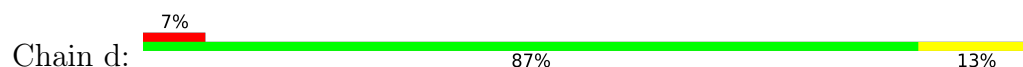
- Molecule 30: 50S ribosomal protein L32



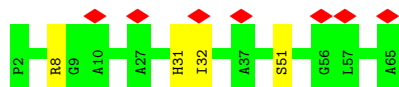
- Molecule 31: 50S ribosomal protein L33



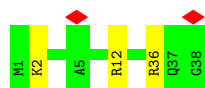
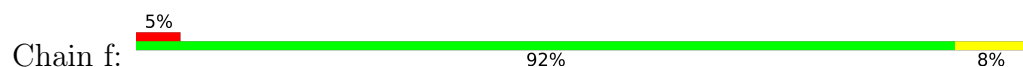
- Molecule 32: 50S ribosomal protein L34



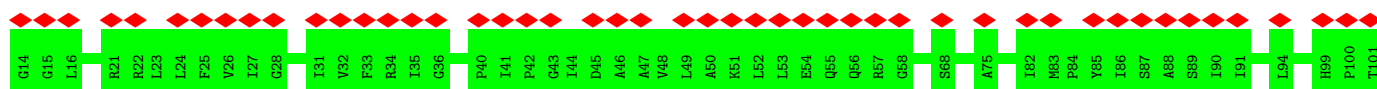
- Molecule 33: 50S ribosomal protein L35

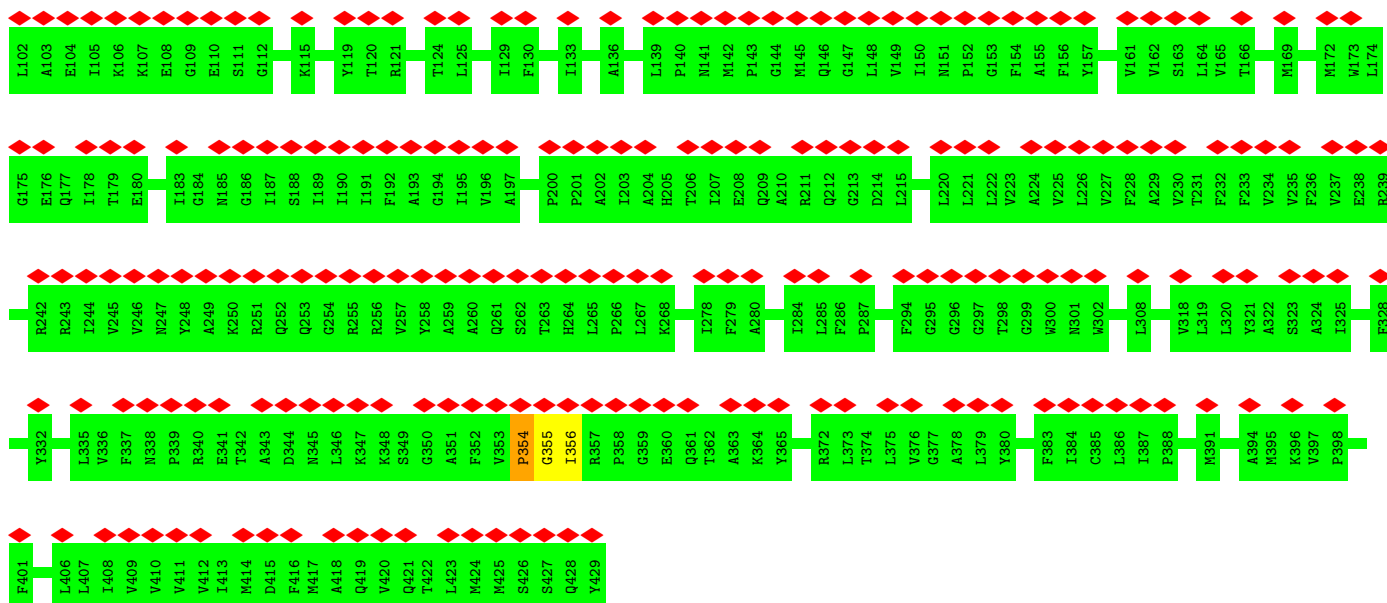


- Molecule 34: 50S ribosomal protein L36

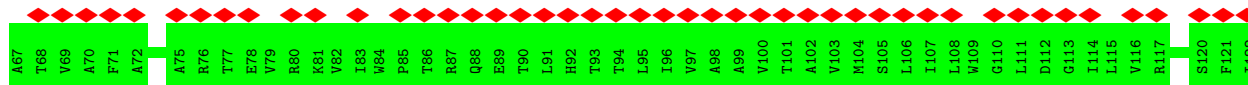
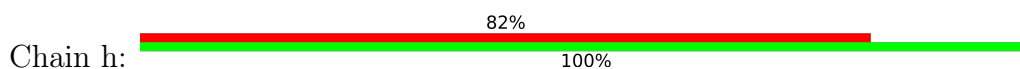


- Molecule 35: Protein translocase subunit SecY

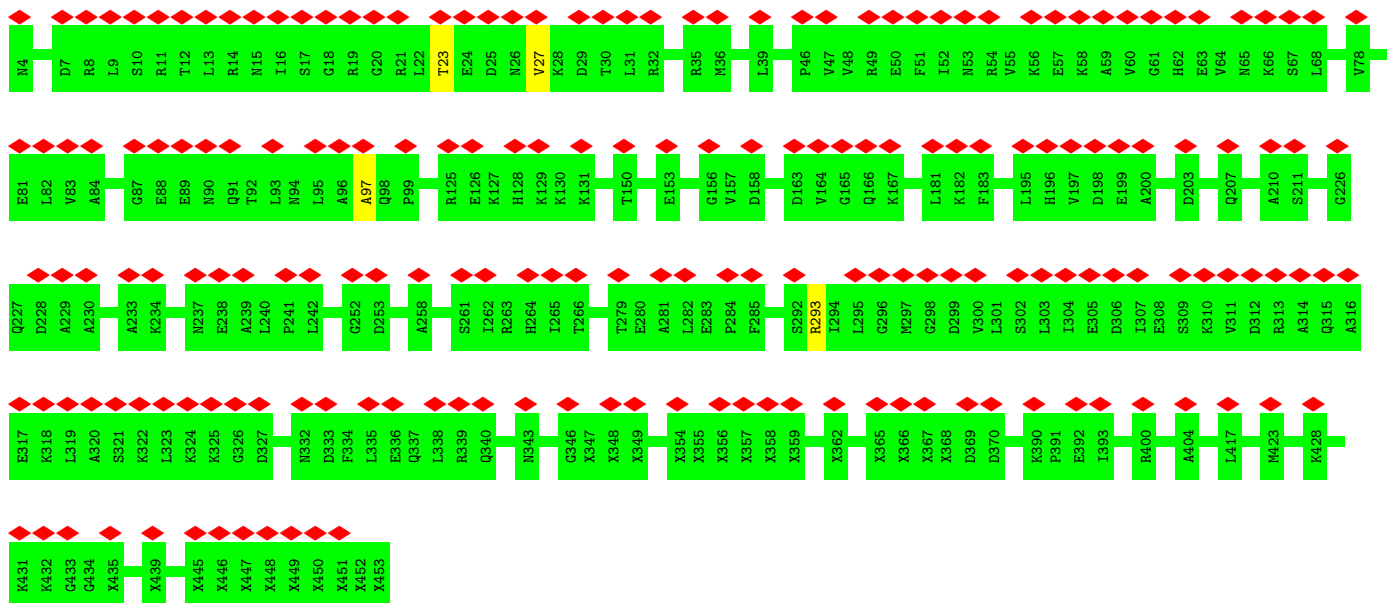
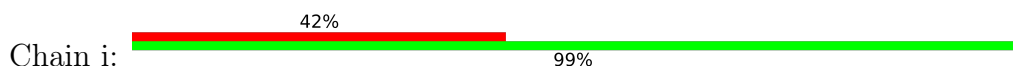




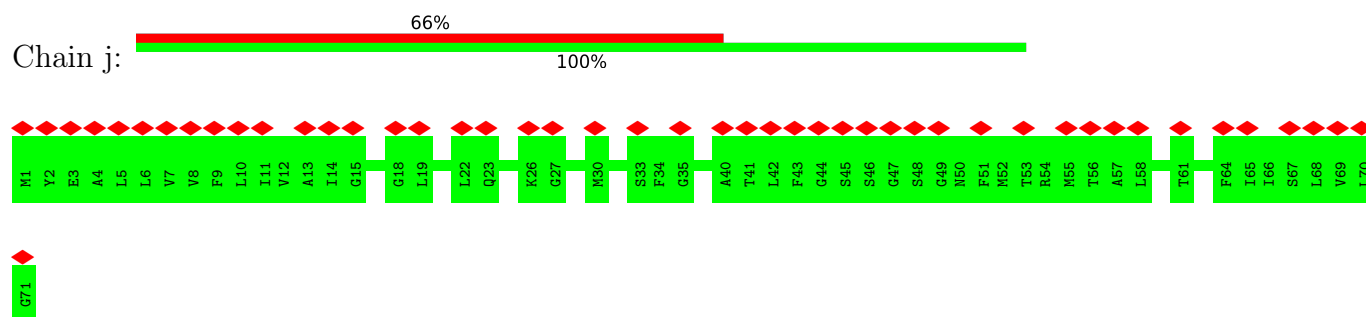
• Molecule 36: Protein translocase subunit SecE



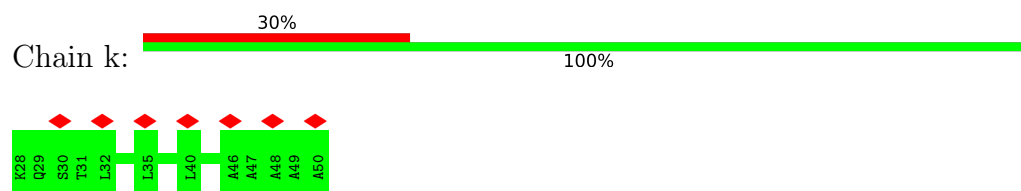
• Molecule 37: Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein



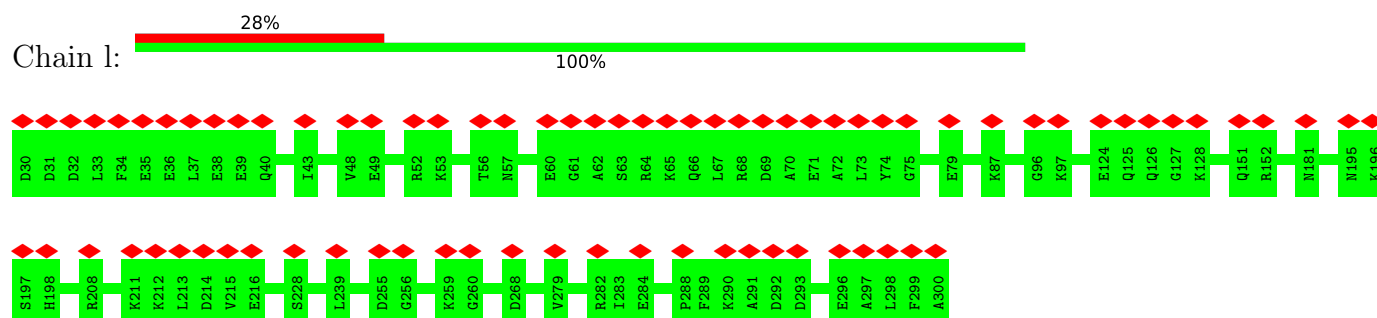
- Molecule 38: Protein-export membrane protein SecG



- Molecule 39: Signal sequence (1A9L)



- Molecule 40: Signal recognition particle receptor FtsY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; After 3D reconstruction 3D maps were sharpened	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GDP, ALF

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	1	0.15	0/2486	0.70	0/3874
2	2	0.57	0/68	1.27	1/103 (1.0%)
3	A	0.69	13/69329 (0.0%)	1.17	188/108152 (0.2%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2122	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1435	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
10	H	0.43	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1290 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.60	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.46	0/763	0.65	0/1021
24	V	0.38	0/788	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.42	0/502	0.54	0/667
29	a	0.38	0/453	0.56	0/605
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.47	0/513	0.63	0/676
34	f	0.49	0/303	0.58	0/397
35	g	0.27	0/1663	0.51	5/2077 (0.2%)
36	h	0.16	0/223	0.29	0/277
37	i	0.21	0/3170	0.39	0/4255
38	j	0.16	0/283	0.27	0/352
39	k	0.21	0/159	0.40	0/218
40	l	0.20	0/2091	0.36	0/2822
All	All	0.60	13/109794 (0.0%)	1.02	198/163369 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	C	0	1
9	G	0	1
12	J	0	1
35	g	0	1
37	i	0	1
All	All	0	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.93	1.33	1.37
3	A	1254	A	N9-C4	-6.48	1.33	1.37
3	A	1321	A	N9-C4	6.30	1.41	1.37
3	A	776	G	N9-C4	6.01	1.42	1.38
3	A	1490	A	N9-C4	5.92	1.41	1.37

The worst 5 of 198 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.21	113.67	121.00
3	A	2422	C	O4'-C1'-N1	9.37	115.69	108.20
3	A	1838	C	C6-N1-C2	9.15	123.96	120.30
35	g	354	PRO	C-N-CA	-8.94	103.53	122.30
3	A	2423	U	C5-C6-N1	8.77	127.08	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	g	354	PRO	Peptide
37	i	293	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2224	0	1124	11	0
2	2	62	0	34	1	0
3	A	61902	0	31134	679	0
4	B	2569	0	1301	19	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	33	0
7	E	1552	0	1619	27	0
8	F	1411	0	1444	44	0
9	G	1323	0	1371	33	0
10	H	1110	0	1148	24	0
11	I	946	0	976	30	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	23	0
14	L	946	0	1023	21	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	24	0
17	O	993	0	1034	24	0
18	P	900	0	935	22	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	20	0
24	V	780	0	831	16	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Z	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	g	1664	0	476	0	0
36	h	224	0	58	0	0
37	i	3384	0	3512	0	0
38	j	284	0	95	0	0
39	k	159	0	189	0	0
40	l	2067	0	2114	0	0
41	f	1	0	0	0	0
42	i	5	0	0	0	0
42	l	5	0	0	0	0
43	i	1	0	0	0	0
43	l	1	0	0	0	0
44	i	28	0	12	0	0
44	l	28	0	12	0	0
All	All	101694	0	68522	1166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
23:U:24:MET:SD	23:U:93:LEU:CD1	2.60	0.90
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:276:U:O2	3:A:278:A:N6	2.07	0.86

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	
5	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
9	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	19	56
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	53
12	J	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
20	R	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	12	46
24	V	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	b	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	c	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	g	414/416 (100%)	402 (97%)	12 (3%)	0	100	100
36	h	54/56 (96%)	54 (100%)	0	0	100	100
37	i	408/450 (91%)	397 (97%)	10 (2%)	1 (0%)	44	78
38	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
39	k	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
40	l	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
All	All	4667/4779 (98%)	4520 (97%)	143 (3%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	i	97	ALA
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

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	
5	C	216/216 (100%)	192 (89%)	24 (11%)	5	18
6	D	164/164 (100%)	154 (94%)	10 (6%)	15	37
7	E	165/165 (100%)	152 (92%)	13 (8%)	10	29
8	F	148/148 (100%)	130 (88%)	18 (12%)	4	16
9	G	137/137 (100%)	129 (94%)	8 (6%)	17	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	114/114 (100%)	100 (88%)	14 (12%)	4	16
11	I	95/95 (100%)	90 (95%)	5 (5%)	19	41
12	J	104/104 (100%)	93 (89%)	11 (11%)	5	20
13	K	116/116 (100%)	105 (90%)	11 (10%)	7	22
14	L	104/104 (100%)	94 (90%)	10 (10%)	7	22
15	M	103/103 (100%)	94 (91%)	9 (9%)	8	26
16	N	109/109 (100%)	100 (92%)	9 (8%)	9	28
17	O	102/102 (100%)	95 (93%)	7 (7%)	13	33
18	P	87/87 (100%)	75 (86%)	12 (14%)	3	14
19	Q	99/99 (100%)	90 (91%)	9 (9%)	7	24
20	R	89/89 (100%)	82 (92%)	7 (8%)	10	29
21	S	84/84 (100%)	76 (90%)	8 (10%)	7	22
22	T	93/93 (100%)	88 (95%)	5 (5%)	18	40
23	U	82/82 (100%)	77 (94%)	5 (6%)	15	37
24	V	83/83 (100%)	76 (92%)	7 (8%)	9	28
25	W	78/78 (100%)	72 (92%)	6 (8%)	10	30
26	X	57/58 (98%)	51 (90%)	6 (10%)	5	20
27	Y	67/67 (100%)	63 (94%)	4 (6%)	16	38
28	Z	54/54 (100%)	47 (87%)	7 (13%)	3	15
29	a	48/48 (100%)	46 (96%)	2 (4%)	25	47
30	b	47/47 (100%)	35 (74%)	12 (26%)	0	3
31	c	45/46 (98%)	40 (89%)	5 (11%)	5	18
32	d	38/38 (100%)	32 (84%)	6 (16%)	2	11
33	e	51/51 (100%)	47 (92%)	4 (8%)	10	29
34	f	34/34 (100%)	31 (91%)	3 (9%)	8	25
37	i	336/338 (99%)	334 (99%)	2 (1%)	84	88
39	k	16/16 (100%)	16 (100%)	0	100	100
40	l	217/217 (100%)	217 (100%)	0	100	100
All	All	3382/3386 (100%)	3123 (92%)	259 (8%)	13	30

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	b	25	VAL
30	b	52	ARG
12	J	66	SER
12	J	28	LEU
31	c	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	48	GLN
32	d	29	GLN
23	U	59	ASN
28	Z	39	GLN
40	l	161	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	103/104 (99%)	22 (21%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3102/3130 (99%)	554 (17%)	19 (0%)

5 of 554 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	G
1	1	29	U
1	1	30	A
1	1	33	C
1	1	34	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	2422	C
3	A	2602	A
3	A	2756	U
3	A	2430	A
3	A	1344	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
42	ALF	i	1001	-	0,4,4	-	-	-		
44	GDP	l	1003	43	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
44	GDP	i	1003	43	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
42	ALF	l	1001	-	0,4,4	-	-	-		

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
44	GDP	i	1003	43	-	4/12/32/32	0/3/3/3
44	GDP	l	1003	43	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	l	1003	GDP	C6-N1	-2.44	1.34	1.37
44	i	1003	GDP	C6-N1	-2.35	1.34	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	i	1003	GDP	PA-O3A-PB	-3.78	119.86	132.83
44	l	1003	GDP	PA-O3A-PB	-3.67	120.23	132.83
44	i	1003	GDP	C3'-C2'-C1'	3.00	105.49	100.98
44	l	1003	GDP	C3'-C2'-C1'	2.94	105.40	100.98
44	l	1003	GDP	C8-N7-C5	2.37	107.50	102.99

There are no chirality outliers.

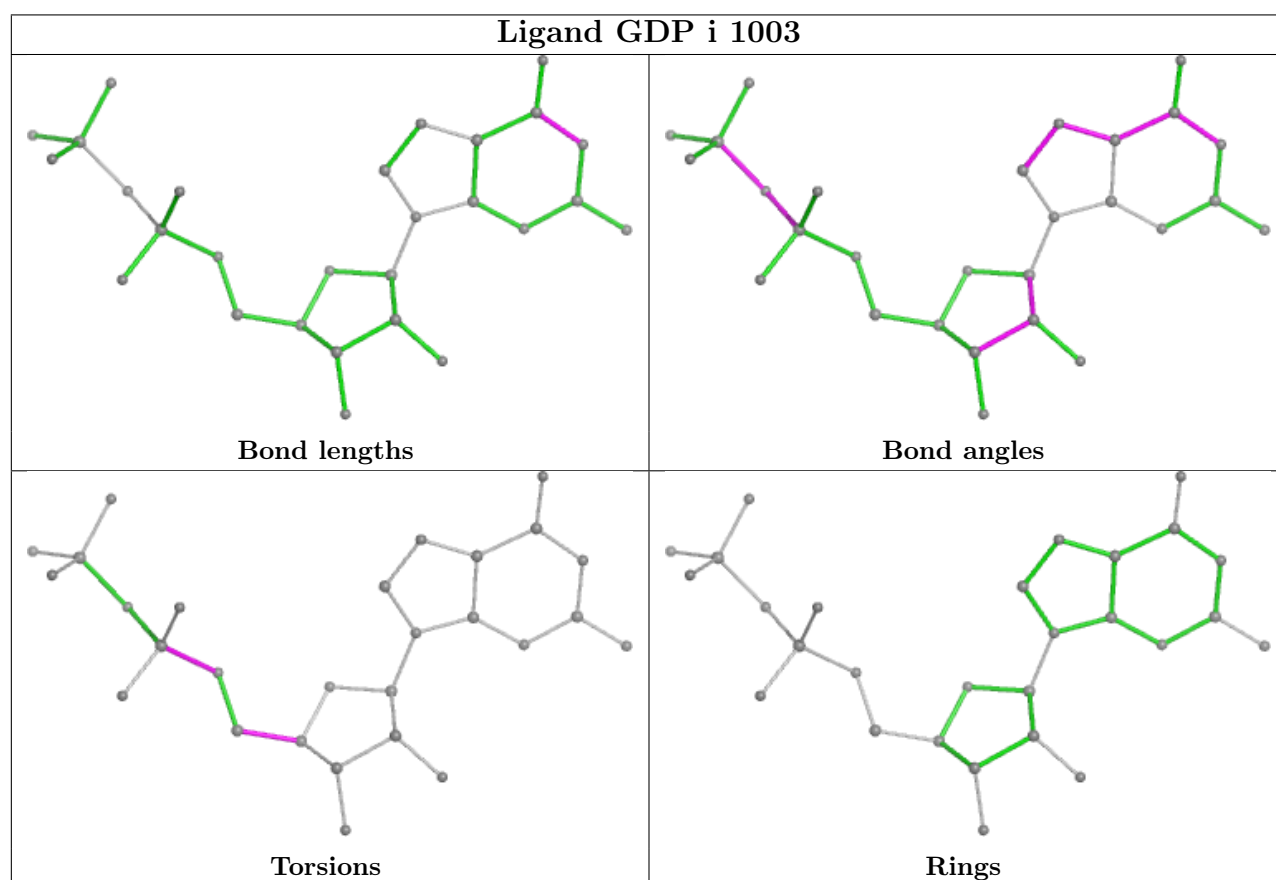
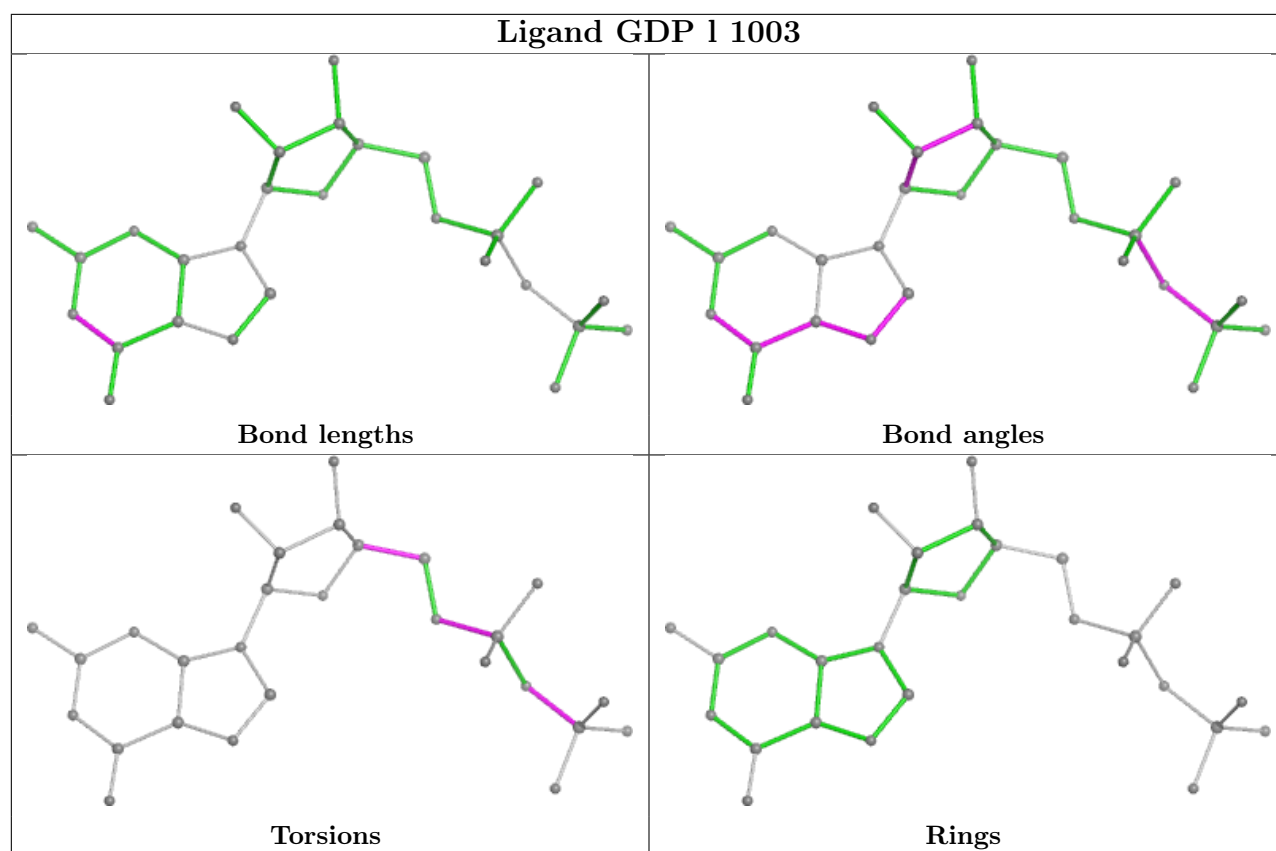
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	i	1003	GDP	C5'-O5'-PA-O3A
44	i	1003	GDP	O4'-C4'-C5'-O5'
44	i	1003	GDP	C3'-C4'-C5'-O5'
44	l	1003	GDP	PA-O3A-PB-O2B
44	l	1003	GDP	C5'-O5'-PA-O1A

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.

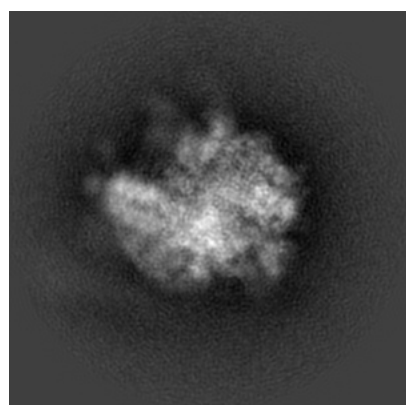
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3617. These allow visual inspection of the internal detail of the map and identification of artifacts.

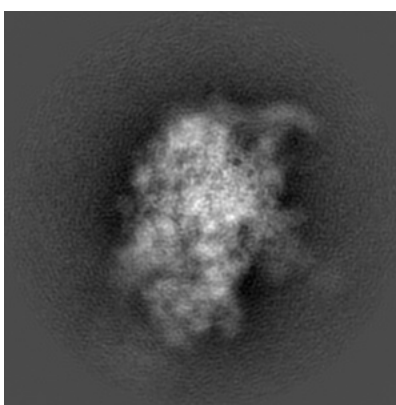
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

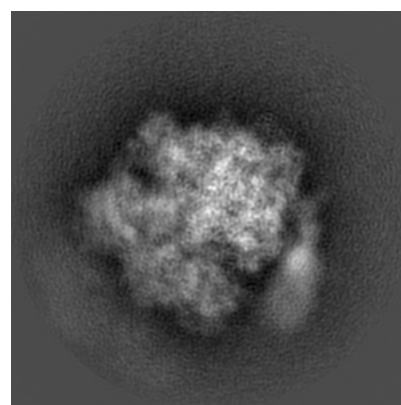
6.1.1 Primary map



X



Y

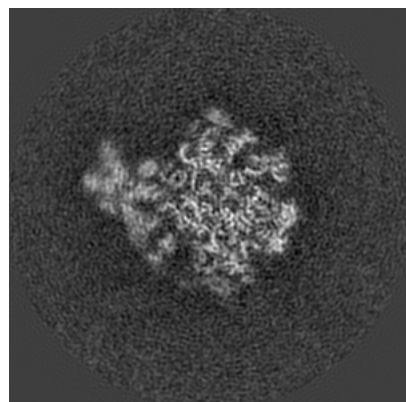


Z

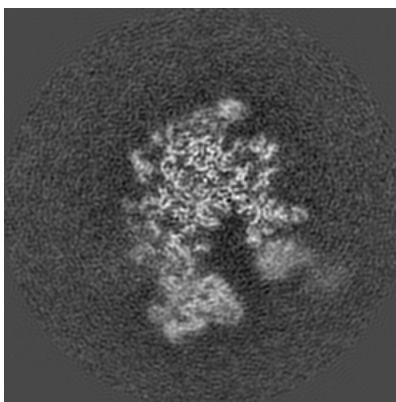
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

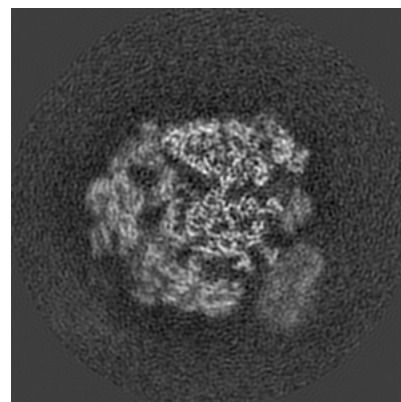
6.2.1 Primary map



X Index: 160



Y Index: 160

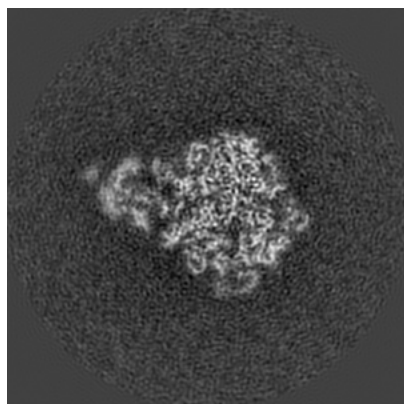


Z Index: 160

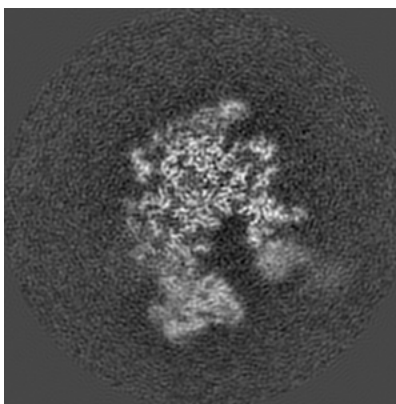
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

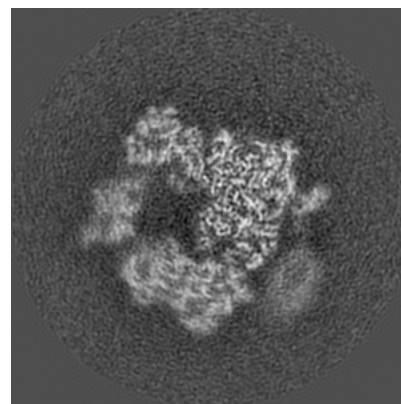
6.3.1 Primary map



X Index: 170



Y Index: 159

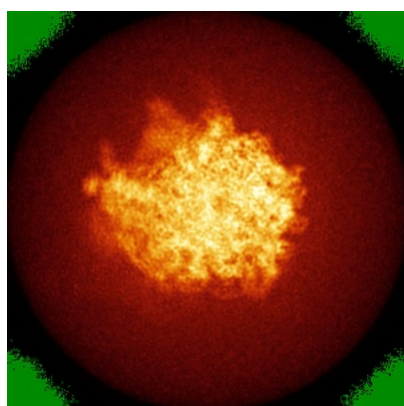


Z Index: 175

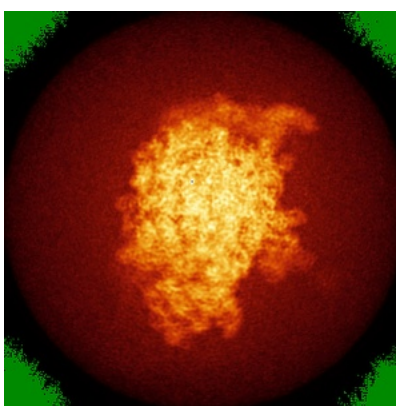
The images above show the largest variance slices of the map in three orthogonal directions.

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

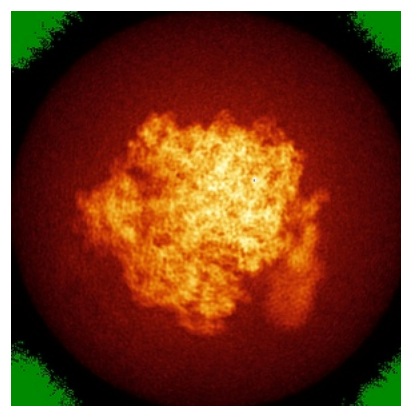
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

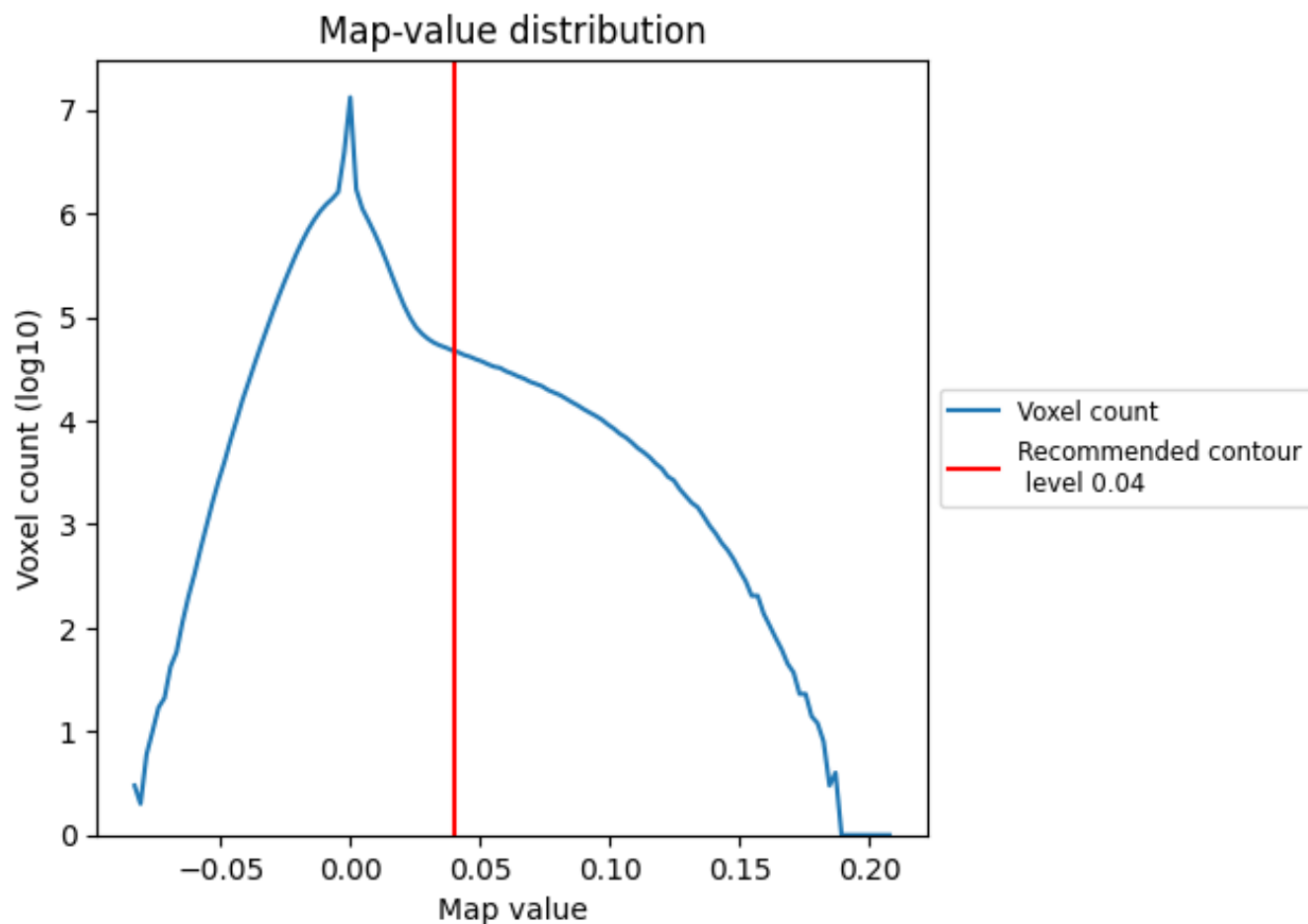
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

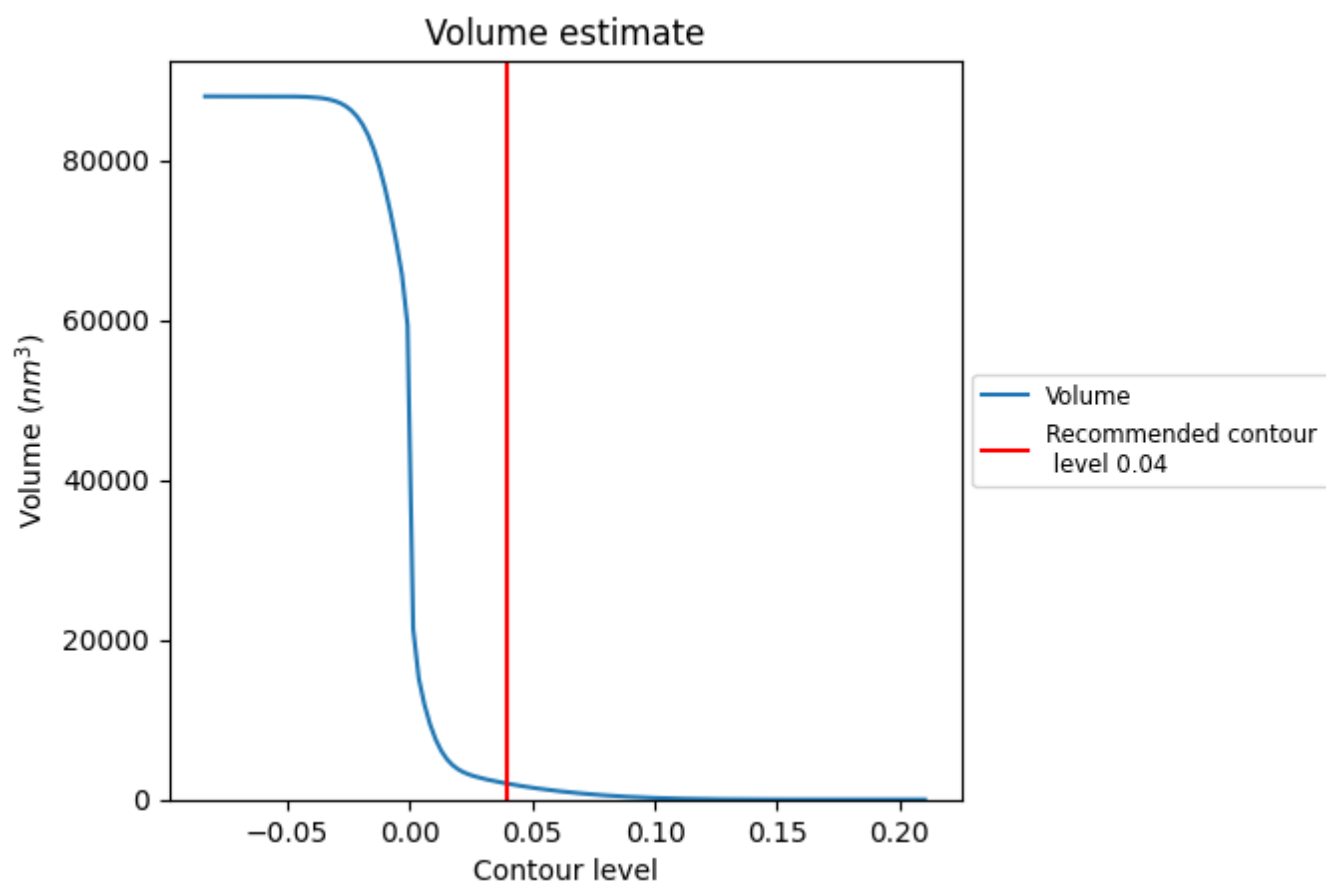
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

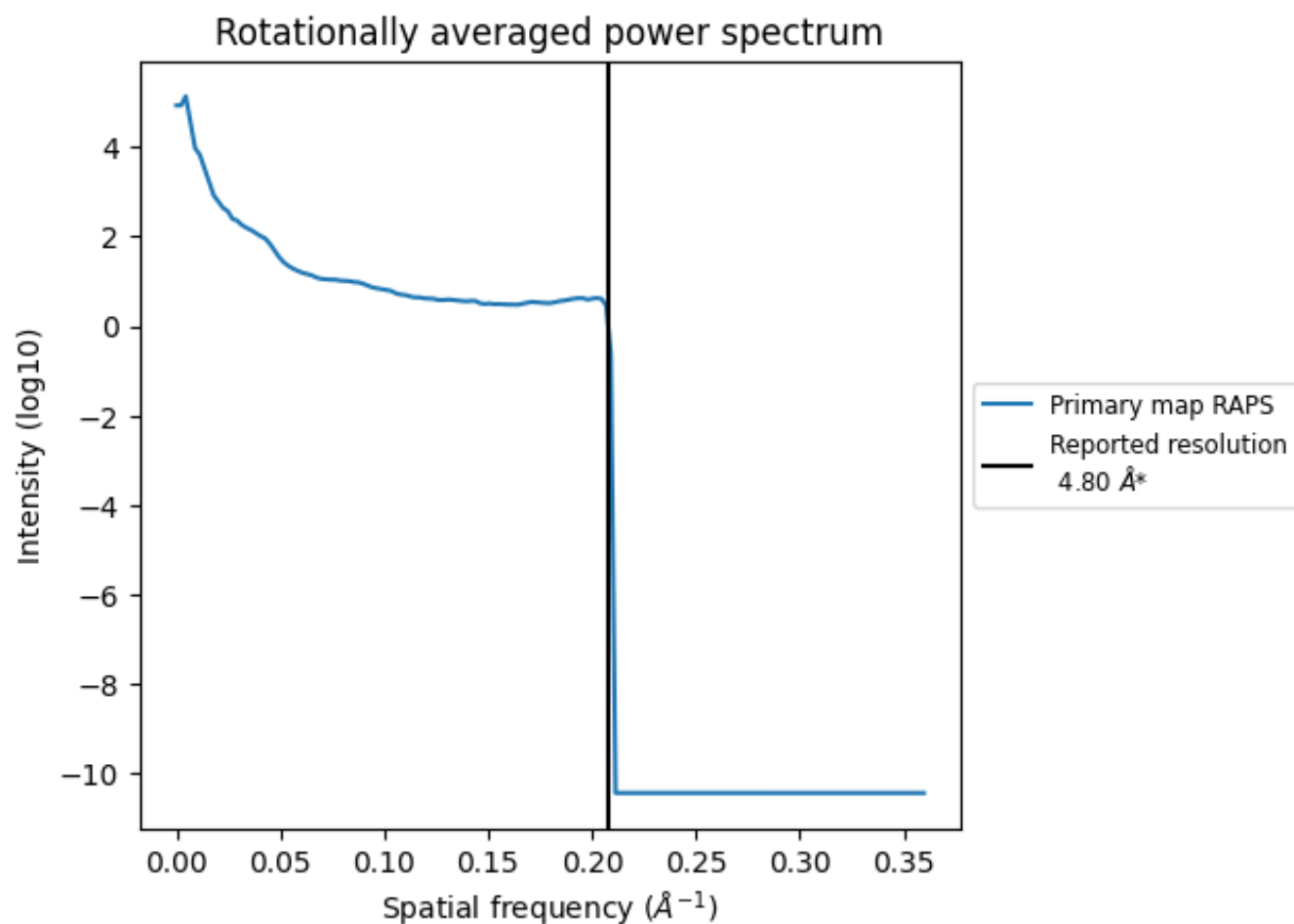
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1992 nm³; this corresponds to an approximate mass of 1799 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 0.208 Å⁻¹

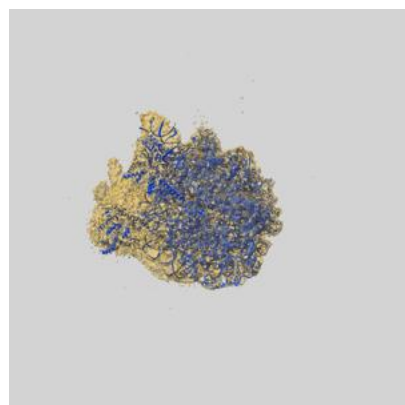
8 Fourier-Shell correlation

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

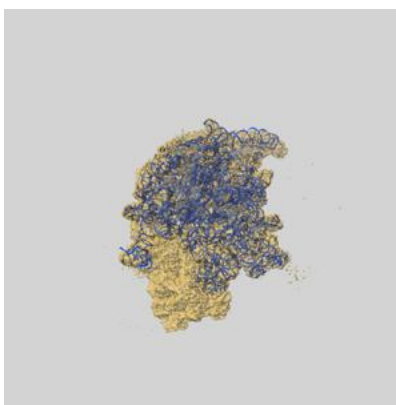
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3617 and PDB model 5NCO. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

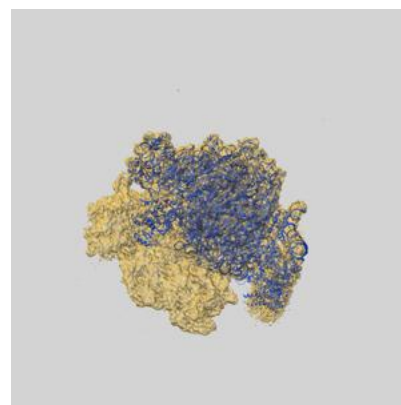
9.1 Map-model overlay [i](#)



X



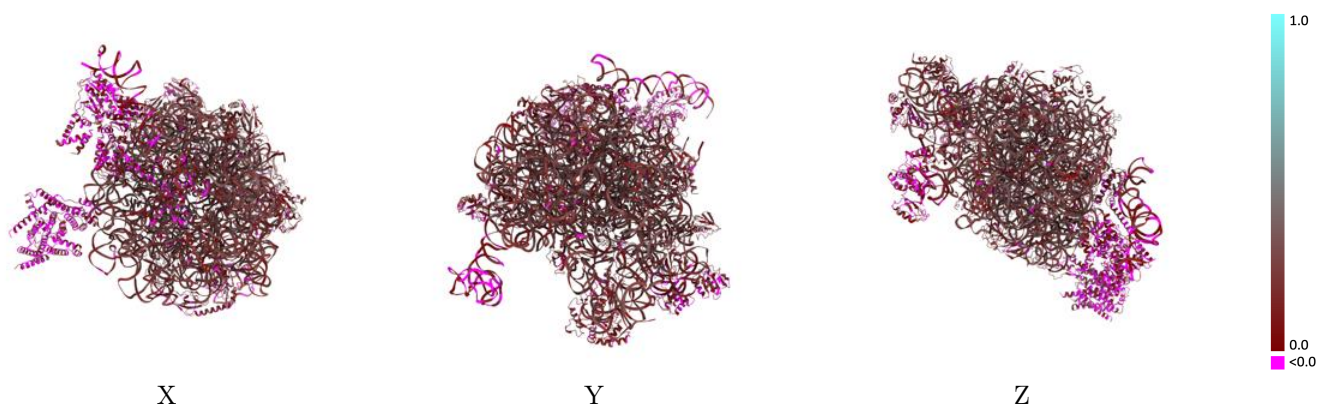
Y



Z

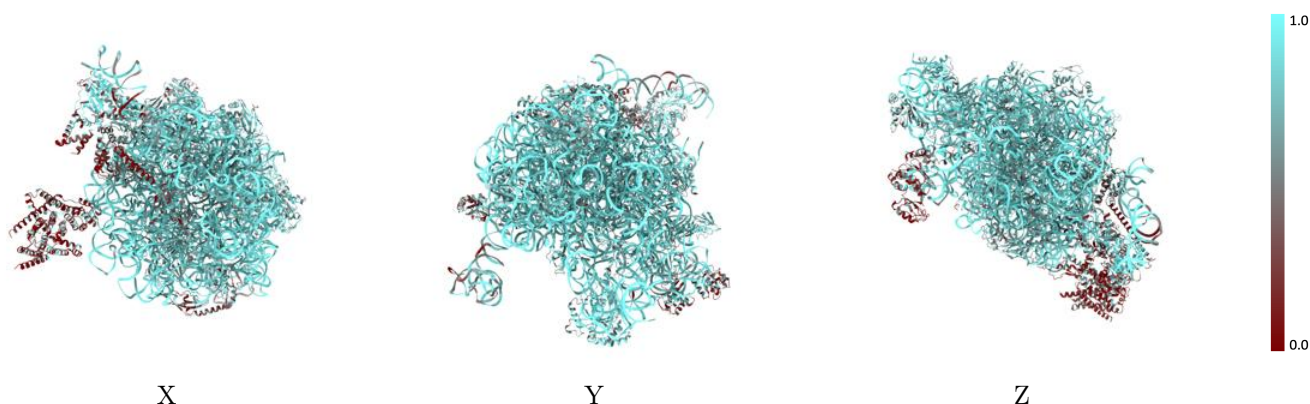
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



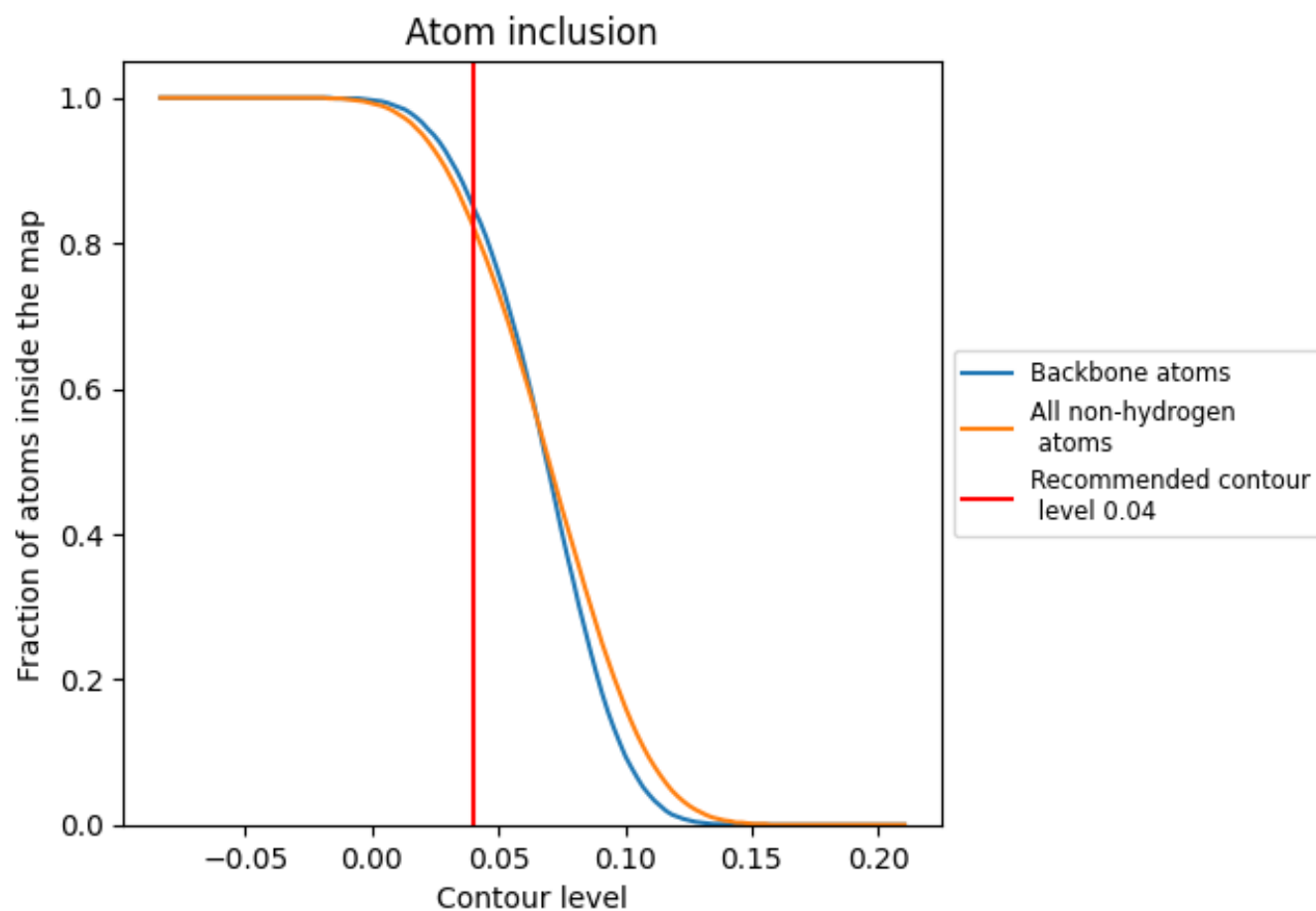
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.2180
1	 0.7470	 0.0820
2	 0.9030	 0.2780
A	 0.9270	 0.2540
B	 0.9510	 0.2450
C	 0.7000	 0.2090
D	 0.7160	 0.2310
E	 0.7210	 0.2080
F	 0.6910	 0.1350
G	 0.7310	 0.2130
H	 0.4340	 0.1410
I	 0.4080	 0.0570
J	 0.3230	 0.0500
K	 0.7270	 0.2280
L	 0.6250	 0.2120
M	 0.7440	 0.2090
N	 0.7420	 0.2390
O	 0.6560	 0.2170
P	 0.7800	 0.1880
Q	 0.6840	 0.2320
R	 0.7880	 0.2280
S	 0.7340	 0.2260
T	 0.6670	 0.2230
U	 0.6860	 0.2060
V	 0.7080	 0.2070
W	 0.7130	 0.2120
X	 0.7500	 0.1850
Y	 0.7010	 0.2080
Z	 0.6910	 0.1640
a	 0.7730	 0.2340
b	 0.7240	 0.2260
c	 0.6670	 0.1380
d	 0.7160	 0.2070
e	 0.6930	 0.2100
f	 0.7750	 0.1990



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.2910	 0.0050
h	 0.1560	 -0.0410
i	 0.5010	 0.0590
j	 0.2820	 0.0170
k	 0.6670	 0.1140
l	 0.6440	 0.0390