



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 23, 2017 – 12:52 AM EDT

PDB ID : 5NCO
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 : unknown
Resolution : 4.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

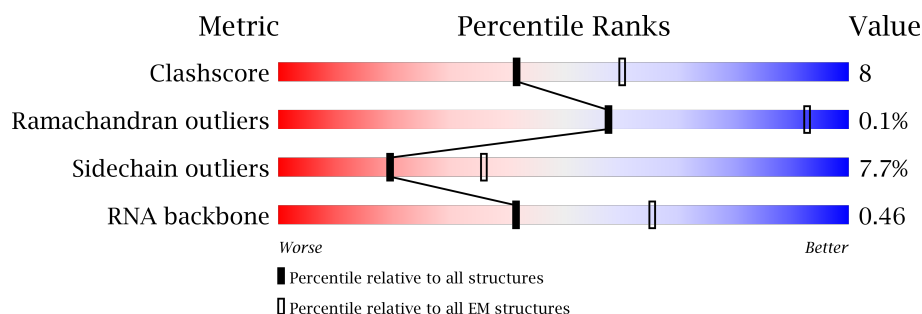
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.























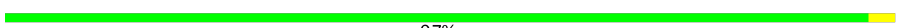




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	104	69% 26% 5%
2	2	3	33% 33% 33%
3	A	2903	55% 36% 8% ..
4	B	120	73% 24% .
5	C	271	71% 25% .
6	D	209	78% 20% .
7	E	201	77% 21% .
8	F	177	60% 36% 5%

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Mol	Chain	Length	Quality of chain
9	G	176	 69% 30% .
10	H	149	 65% 32% .
11	I	125	 66% 34% .
12	J	134	 57% 40% .
13	K	142	 73% 23% .
14	L	123	 68% 30% .
15	M	144	 75% 23% .
16	N	136	 71% 26% .
17	O	125	 71% 26% .
18	P	117	 67% 30% .
19	Q	114	 75% 25% .
20	R	117	 74% 21% .
21	S	103	 70% 28% .
22	T	110	 78% 20% .
23	U	95	 71% 28% .
24	V	102	 72% 27% .
25	W	94	 74% 24% .
26	X	76	 68% 29% .
27	Y	77	 64% 36% .
28	Z	62	 68% 27% 5%
29	a	58	 97% .
30	b	56	 79% 21%
31	c	51	 90% 10%
32	d	46	 87% 13%
33	e	64	 94% 6%

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Mol	Chain	Length	Quality of chain
34	f	38	 92%8%
35	g	416	 99%
36	h	56	 100%
37	i	450	 99%
38	j	71	 100%
39	k	23	 100%
40	l	271	 100%

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		

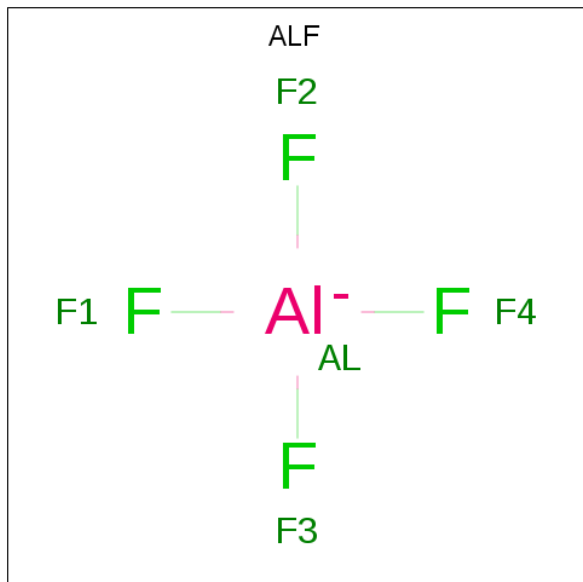
- Molecule 40 is a protein called Signal recognition particle receptor FtsY.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 42 is TETRAFLUOROALUMINATE ION (three-letter code: 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 (three-letter code: 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 (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

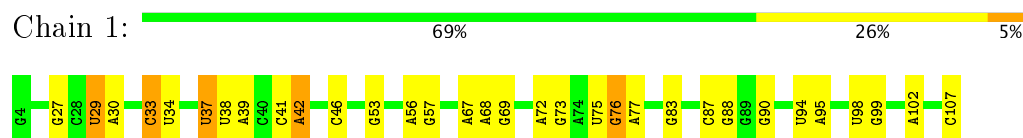


Mol	Chain	Residues	Atoms					AltConf
44	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
44	l	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

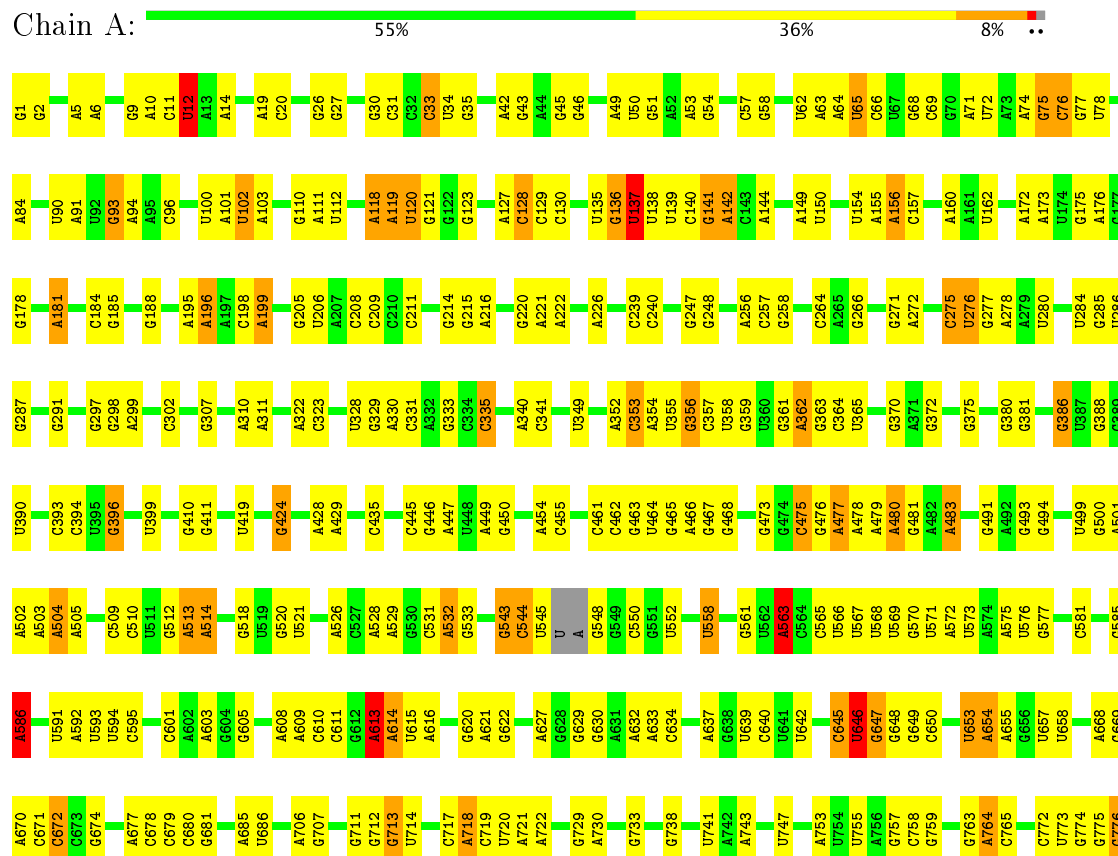
- Molecule 1: 4.5S SRP RNA (Ffs)



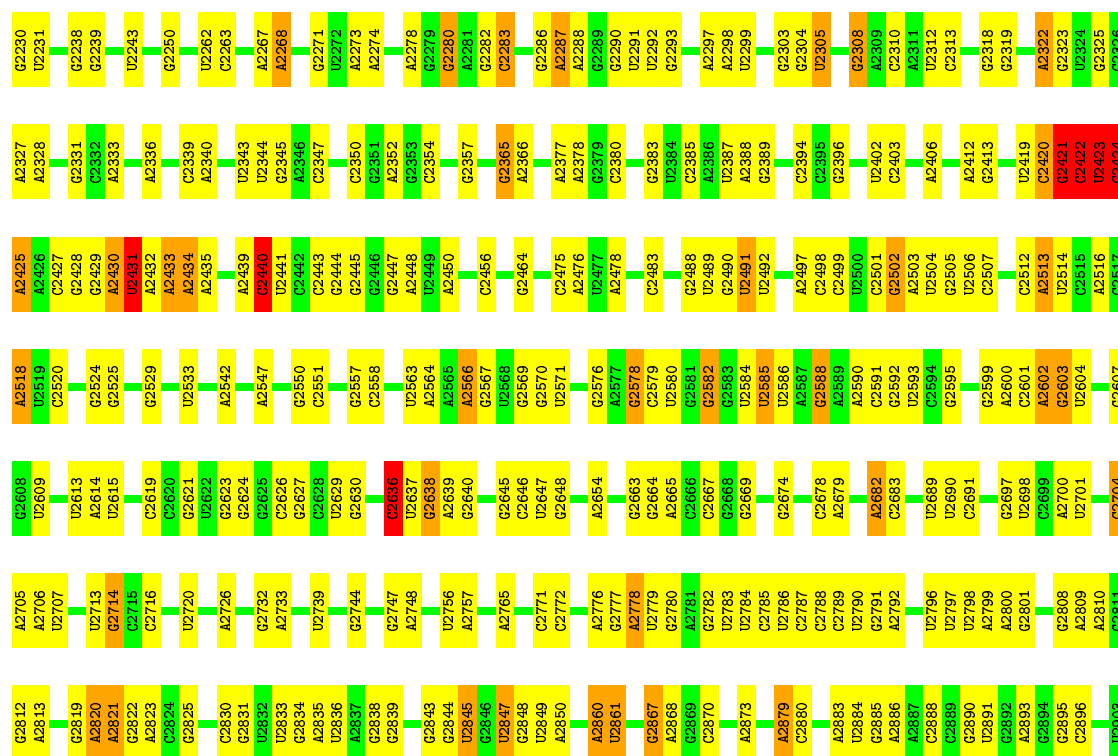
- Molecule 2: P-site tRNA-CCA end



- Molecule 3: 23S rRNA



G2152	C2072	G1972	C1881	A1789	G1681	A1590	G1500	A1420	A1328	G1106	C946	A849	G777
C2153	C2073	G1973	G1888	C1790	A1689	A1591	G1501	G1421	U1329	G1110	A947	U850	G778
A2154	U2074	C1974	A1791	A1794	A1689	C1592	A1502	G1422	G1332	G1111	C948	U851	U779
A2077	A2077	G1980	G1896	C1795	G1695	A1597	U1506	G1423	U1231	G1112	C949	G857	G780
U2086	U2086	U1982	A1899	U1796	A1700	A1598	C1507	G1424	U1232	G1115	G953	G858	A781
G2087	G2087	G1983	A1899	U1797	C1706	A1603	A1509	G1425	G1338	G1116	C957	G859	A782
A2090	A2090	U1991	C1902	U1798	C1706	C1604	A1509	A1427	U1339	G1125	U958	G861	A783
G2093	G2093	G1992	G1903	C1799	U1709	C1605	A1510	C1428	G1340	G1126	A959	G862	G784
A2161	A2161	U1993	G1904	C1800	U1710	C1606	A1511	A1429	G1341	A1127	A960	G863	G785
A2163	A2163	U1993	C1905	A1801	G1711	C1607	A1515	G1432	G1342	G1128	A961	G864	A788
C2164	C2164	G1996	G1906	A1802	A1711	A1608	A1516	A1433	G1343	A1129	C961	C865	A789
C2165	A2097	C1997	A1912	G1807	G1715	A1610	A1517	G1436	U1344	G1130	C968	G869	U790
U2166	A2101	C2000	A	A1808	G1715	A1610	G1524	C1437	G1346	U1130	G969	U870	C791
U2167	C2102	G2000	C	A1809	A1721	A1614	A1525	G1438	U1247	U1131	U770	U871	A792
A2168	C2103	G2012	U	A1810	A1722	C1615	A1526	U1438	G1248	G1132	U772	U872	A793
A2170	C2104	G2018	A	G1811	U1725	A1616	G1527	A1439	G1249	A1133	A972	A876	A794
A2171	U2105	G2018	U1917	G1816	U1725	C1617	A1528	U1442	G1251	G1134	A973	A877	C795
U2172	U2106	C2021	A1918	C1817	U1729	G1627	A1529	C1447	G1252	G1135	A974	A878	C796
A2173	A2107	U2022	A1919	U1818	C1730	G1628	G1530	C1362	A1254	G1136	A975	A879	G797
C2174	U2108	C2023	C1920	A1819	C1731	A1628	C1531	G1363	U1255	G1137	A976	G879	G798
A2175	U2109	G2024	G1921	U1820	C1732	G1631	C1532	C1448	G1364	G1139	A981	G880	A800
C2176	C2024	C2025	G1922	A1821	C1732	G1631	C1533	G1449	G1365	U1141	C982	G881	G801
C2177	C2025	U2026	U1923	C1822	A1735	A1634	U1534	G1450	A1366	U1142	C983	G882	A804
C2178	G2027	G2027	C1924	A1822	U1736	A1634	A1535	C1451	A1367	A1143	A984	G	G805
U2182	U2111	U2028	A1927	U1825	U1736	A1637	A1536	G1452	G1374	G1149	C987	U	C806
U2183	U2112	A2030	A1928	G1826	G1737	A1638	C1537	G1453	U1267	C1150	A989	A	U807
A2184	G2115	G2031	C1929	U1827	G1738	C1639	U1542	A1463	G1268	G1154	A990	C	G808
U2185	A2116	G2033	G1930	U1828	G1743	G1642	A1543	G1464	A1269	A1155	C994	C	G809
A2186	A2117	U2033	U1931	A1829	A1744	C1643	A1545	G1465	C1270	G1156	C995	C	U810
U2187	U2118	A2033	G1931	C1837	U1751	C1644	G1546	G1466	A1272	G1168	A996	A	U811
A2188	A2119	G2038	C1934	C1838	C1752	G1645	U1554	U1467	G1275	G1172	C997	C	U812
G2190	G2120	U2039	G1935	G1839	A1757	U1647	U1554	U1468	A1275	U1173	C998	U834	C814
A2198	U2122	G2040	A1936	A1840	U1758	U1648	G1560	A1469	A1287	U	U999	U835	C815
A2199	G2123	U2041	U1938	A1841	A1759	G1649	U1561	G1470	G1288	A	A1000	U836	C816
U2203	A2126	A2042	U1939	A1842	C1760	G1652	U1563	G1471	C1289	U	A1001	A819	A825
G2204	G2127	C2043	G1939	G1843	C1761	A1653	A1564	C1472	G1290	G1177	C1005	U826	A826
C2206	G2128	C2047	G1945	G1850	U1762	G1654	C1565	G1473	U1294	G1178	C1006	U827	U827
C2207	U2129	C2050	U1946	A1853	G1763	A1655	A1566	U1474	G1300	G1179	C1007	U828	U828
C2208	U2130	A2051	C1947	A1854	C1764	A1655	U1567	U1482	A1301	U1180	C1008	U829	A829
G2209	U2131	A2052	U1955	U1858	U1769	G1659	A1569	G1483	G1401	U1181	A1009	G830	G830
U2210	G2132	G2053	U1956	U1859	G1770	G1660	A1570	U1484	A1302	G1182	A1010	G831	A831
A2211	A2134	A2054	C1957	G1875	C1770	G1664	A1571	U1485	G1303	G1187	A1011	A911	U832
A2212	A2135	C2055	U1958	G1876	A1773	A1664	A1572	U1486	U1308	U1188	A1012	A833	U833
C2215	G2138	G2056	G1959	C1870	A1773	A1664	A1572	C1489	A1308	U1188	G914	G834	G834
G2216	C2143	A2060	C1961	A1872	U1775	G1667	U1576	A1490	U1308	U1188	C915	G835	C835
G2217	G2144	C2061	C1962	G1873	U1775	G1667	C1577	G1491	U1313	U1198	A1021	U839	U839
U2219	A2145	A2062	U1963	C1874	A1780	A1672	U1578	G1492	C1314	U1199	G1022	A917	C840
C2225	C2146	C2063	G1963	G1875	U1781	G1673	G1581	A1493	A1321	A1205	U1023	G830	G830
C2226	A2147	C2064	A1966	A1876	U1782	G1674	C1582	A1494	U1415	G1206	G1100	U931	A845
A2227	G2148	G2069	C1967	A1877	U1785	A1677	A1583	A1495	G1416	U1101	G1024	U932	U846
G2228	U2151	A2070	A1970	C1878	A1786	A1678	U1584	U1497	G1324	G1210	G1025	A933	U847
U2229	U2151	A2071	U1971	A1880	A1786	A1678	C1585	C1498	A1327	G1212	A1027	U848	C848



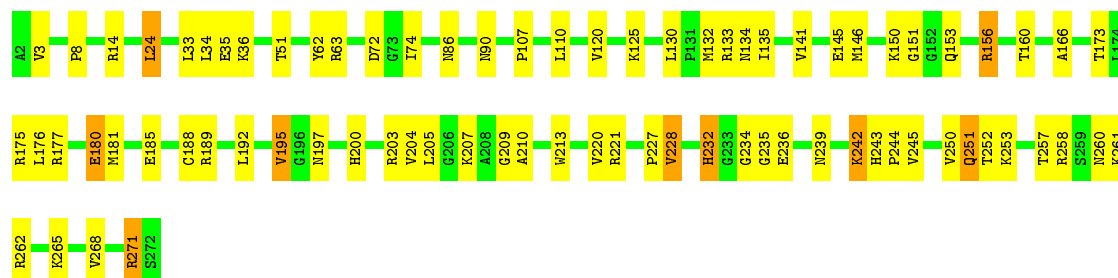
- Molecule 4: 5S rRNA

Chain B: 73% 24%

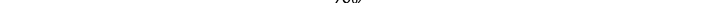


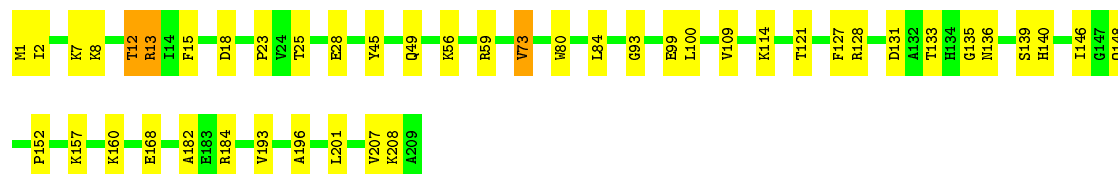
- Molecule 5: 50S ribosomal protein L2

Chain C: 71% 25% 4%

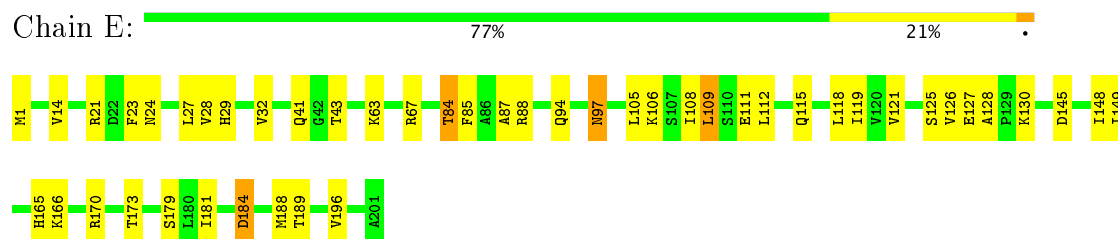


- Molecule 6: 50S ribosomal protein L3

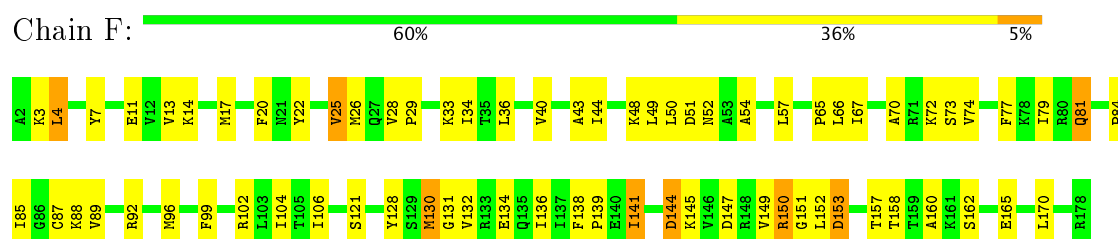
Chain D:  78% 20%



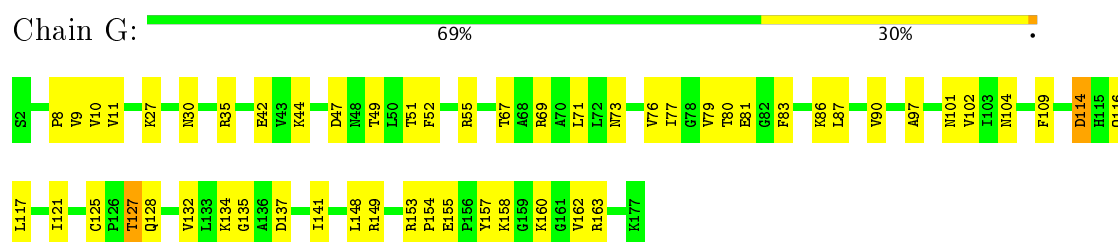
- Molecule 7: 50S ribosomal protein L4



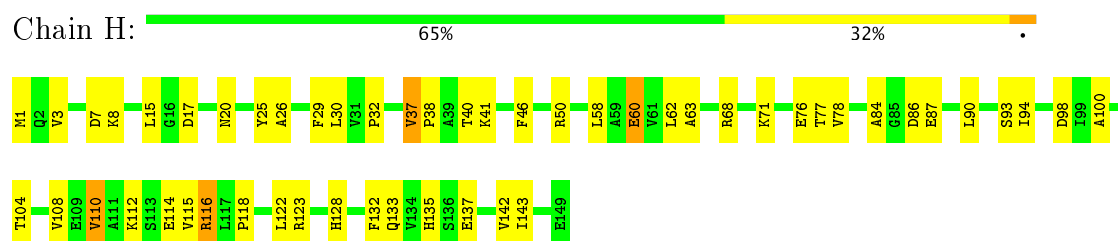
- Molecule 8: 50S ribosomal protein L5



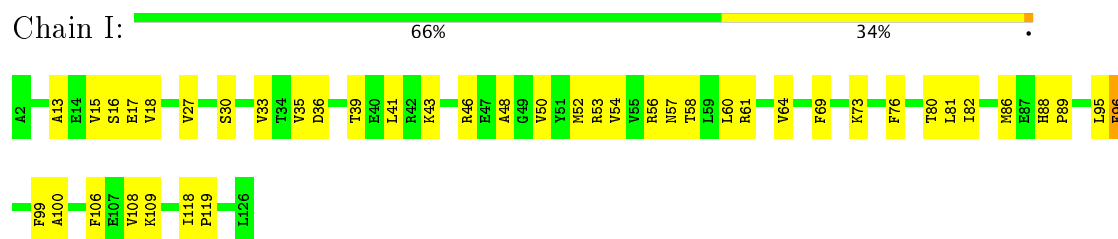
- Molecule 9: 50S ribosomal protein L6



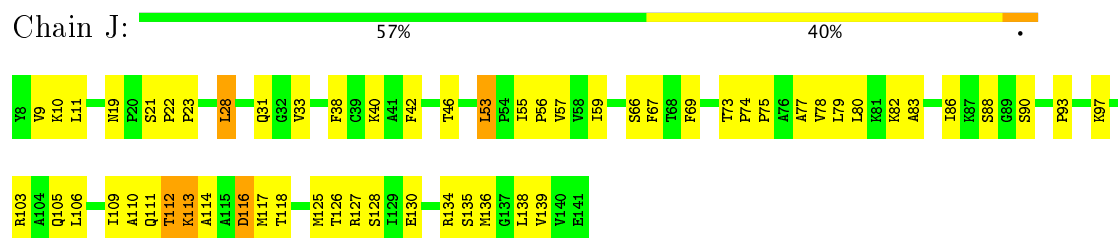
- Molecule 10: 50S ribosomal protein L9



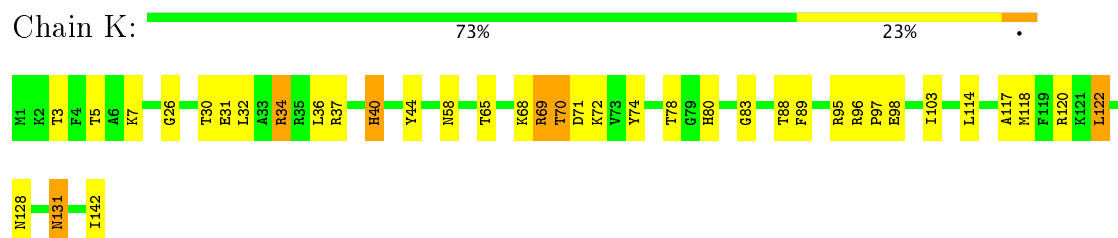
- Molecule 11: 50S ribosomal protein L10



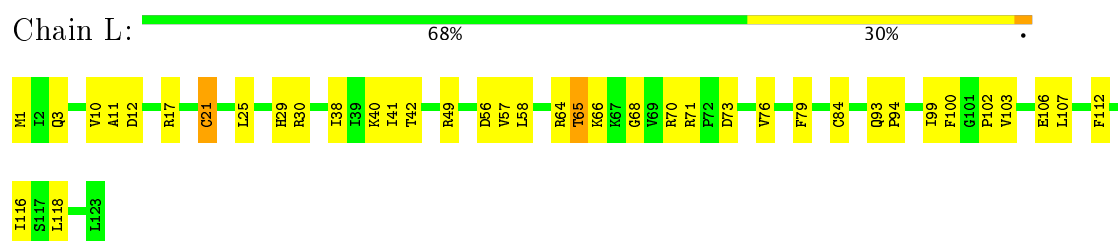
- Molecule 12: 50S ribosomal protein L11



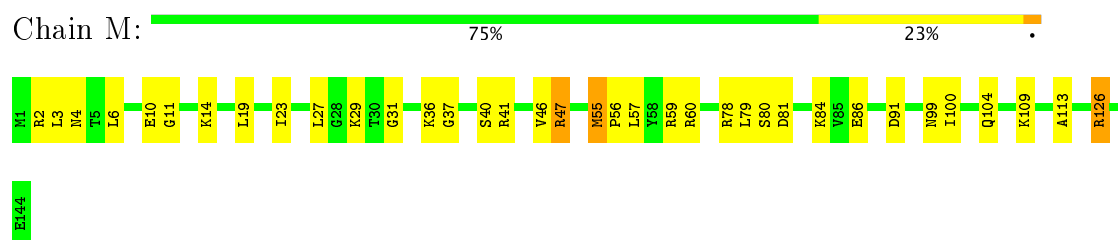
- Molecule 13: 50S ribosomal protein L13



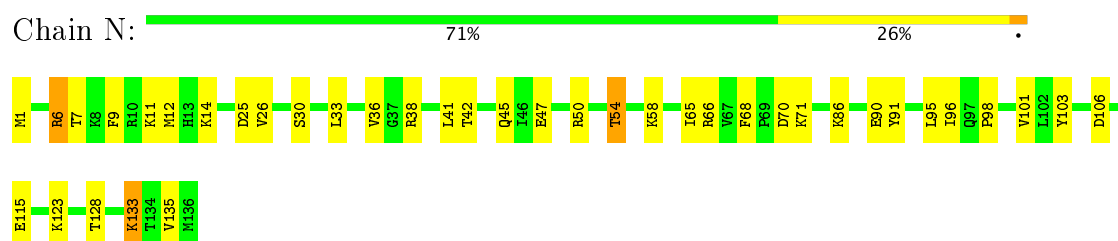
- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15

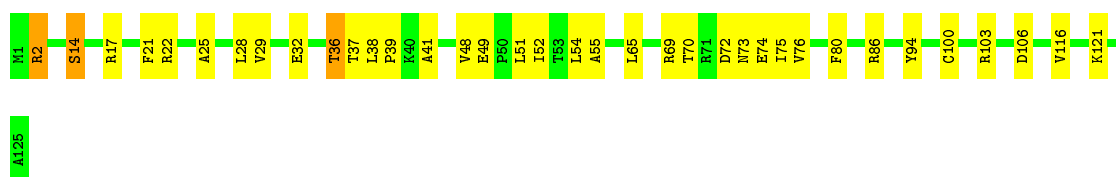


- Molecule 16: 50S ribosomal protein L16



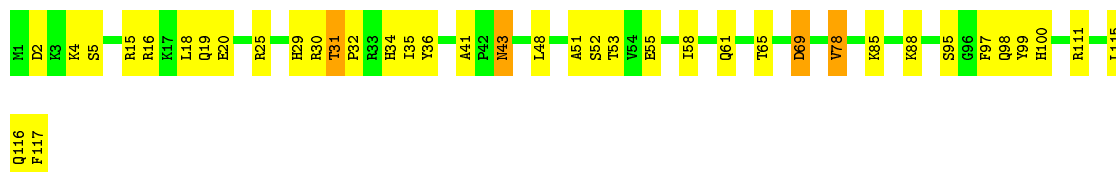
- Molecule 17: 50S ribosomal protein L17





- Molecule 18: 50S ribosomal protein L18

Chain P: 67% 30%



- Molecule 19: 50S ribosomal protein L19

Chain Q: 75% 25%



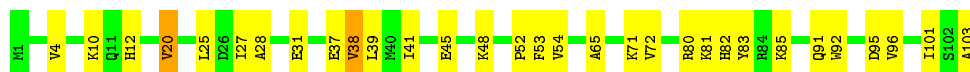
- Molecule 20: 50S ribosomal protein L20

Chain R: 74% 21%



- Molecule 21: 50S ribosomal protein L21

Chain S: 70% 28%



- Molecule 22: 50S ribosomal protein L22

Chain T: 78% 20%

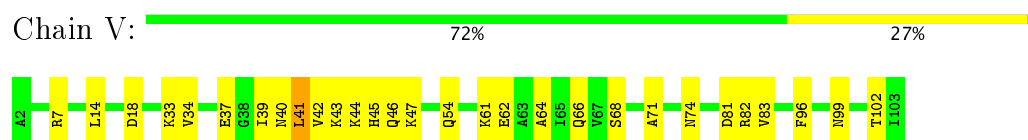


- Molecule 23: 50S ribosomal protein L23

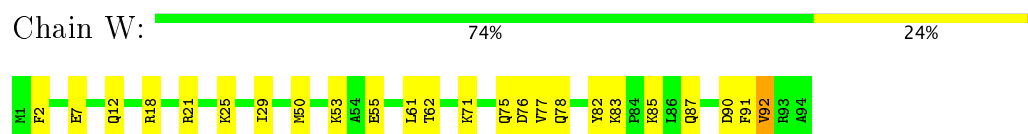
Chain U: 71% 28%



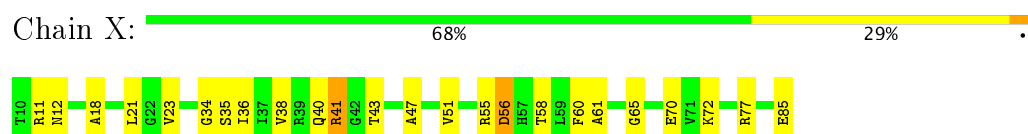
- Molecule 24: 50S ribosomal protein L24



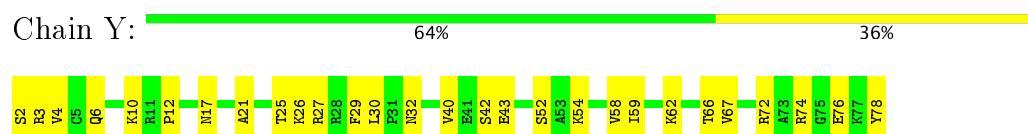
- Molecule 25: 50S ribosomal protein L25



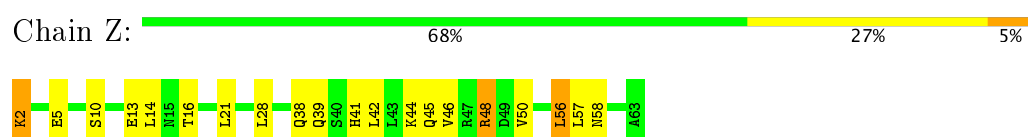
- Molecule 26: 50S ribosomal protein L27



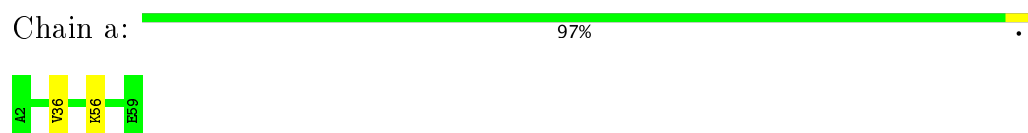
- Molecule 27: 50S ribosomal protein L28



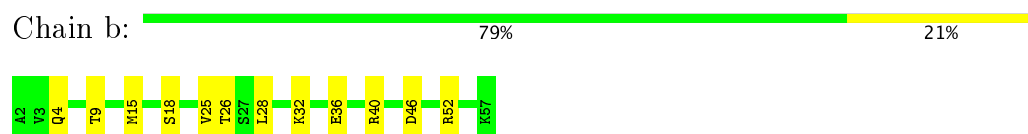
- Molecule 28: 50S ribosomal protein L29



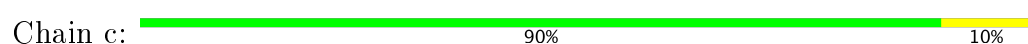
- Molecule 29: 50S ribosomal protein L30

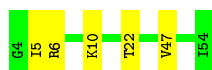


- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33





- Molecule 32: 50S ribosomal protein L34

Chain d: 87% 13%



- Molecule 33: 50S ribosomal protein L35

Chain e: 94% 6%



- Molecule 34: 50S ribosomal protein L36

Chain f: 92% 8%



- Molecule 35: Protein translocase subunit SecY

Chain g: 99%



- Molecule 36: Protein translocase subunit SecE

Chain h: 100%

There are no outlier residues recorded for this chain.

- 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

Chain i: 99%



- Molecule 38: Protein-export membrane protein SecG

Chain j: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: Signal sequence (1A9L)

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: Signal recognition particle receptor FtsY

Chain l:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 > 2$	RMSZ	# $ Z > 2$
1	1	0.15	0/2486	0.70	0/3874
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
2	2	0.57	0/68	1.27	1/103 (1.0%)
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
3	A	0.69	13/69329 (0.0%)	1.17	188/108152 (0.2%)
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
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	k	0.21	0/159	0.40	0/218
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
40	l	0.20	0/2091	0.36	0/2822
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
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
12	J	0	1
35	g	0	1
37	i	0	1
5	C	0	1
9	G	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

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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%)	25	68
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	22	66
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%)	17	60
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

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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%)	51	84
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%)	58	88

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%)	7	32
6	D	164/164 (100%)	154 (94%)	10 (6%)	22	56
7	E	165/165 (100%)	152 (92%)	13 (8%)	14	47
8	F	148/148 (100%)	130 (88%)	18 (12%)	6	28
9	G	137/137 (100%)	129 (94%)	8 (6%)	23	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	114/114 (100%)	100 (88%)	14 (12%)	5	28
11	I	95/95 (100%)	90 (95%)	5 (5%)	26	60
12	J	104/104 (100%)	93 (89%)	11 (11%)	8	33
13	K	116/116 (100%)	105 (90%)	11 (10%)	10	38
14	L	104/104 (100%)	94 (90%)	10 (10%)	10	38
15	M	103/103 (100%)	94 (91%)	9 (9%)	12	42
16	N	109/109 (100%)	100 (92%)	9 (8%)	13	45
17	O	102/102 (100%)	95 (93%)	7 (7%)	18	52
18	P	87/87 (100%)	75 (86%)	12 (14%)	4	25
19	Q	99/99 (100%)	90 (91%)	9 (9%)	11	41
20	R	89/89 (100%)	82 (92%)	7 (8%)	14	47
21	S	84/84 (100%)	76 (90%)	8 (10%)	10	38
22	T	93/93 (100%)	88 (95%)	5 (5%)	26	59
23	U	82/82 (100%)	77 (94%)	5 (6%)	22	56
24	V	83/83 (100%)	76 (92%)	7 (8%)	13	45
25	W	78/78 (100%)	72 (92%)	6 (8%)	15	48
26	X	57/58 (98%)	51 (90%)	6 (10%)	8	34
27	Y	67/67 (100%)	63 (94%)	4 (6%)	22	56
28	Z	54/54 (100%)	47 (87%)	7 (13%)	5	26
29	a	48/48 (100%)	46 (96%)	2 (4%)	34	65
30	b	47/47 (100%)	35 (74%)	12 (26%)	0	6
31	c	45/46 (98%)	40 (89%)	5 (11%)	7	32
32	d	38/38 (100%)	32 (84%)	6 (16%)	3	20
33	e	51/51 (100%)	47 (92%)	4 (8%)	15	48
34	f	34/34 (100%)	31 (91%)	3 (9%)	12	42
37	i	336/338 (99%)	334 (99%)	2 (1%)	89	94
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%)	19	48

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

Mol	Chain	Res	Type
14	L	49	ARG
17	O	36	THR
31	c	5	ILE
14	L	65	THR
15	M	91	ASP

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

Mol	Chain	Res	Type
14	L	3	GLN
17	O	18	GLN
32	d	29	GLN
15	M	104	GLN
18	P	100	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	1344	U
3	A	1721	G
3	A	2424	C
3	A	1110	G
3	A	2430	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.00	-	0,6,6	0.00	-
44	GDP	i	1003	43	25,30,30	1.16	2 (8%)	26,47,47	1.96	6 (23%)
42	ALF	l	1001	-	0,4,4	0.00	-	0,6,6	0.00	-
44	GDP	l	1003	43	25,30,30	1.17	2 (8%)	26,47,47	1.98	6 (23%)

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
42	ALF	i	1001	-	-	0/0/0/0	0/0/0/0
44	GDP	i	1003	43	-	0/12/32/32	0/3/3/3
42	ALF	l	1001	-	-	0/0/0/0	0/0/0/0
44	GDP	l	1003	43	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	l	1003	GDP	C5-C4	3.05	1.47	1.40
44	i	1003	GDP	C5-C4	3.08	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	i	1003	GDP	C6-C5	3.81	1.48	1.41
44	l	1003	GDP	C6-C5	3.92	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	i	1003	GDP	C5-C6-N1	-3.80	118.07	123.48
44	l	1003	GDP	C5-C6-N1	-3.78	118.11	123.48
44	l	1003	GDP	C6-C5-C4	-3.72	117.14	120.84
44	i	1003	GDP	C6-C5-C4	-3.58	117.29	120.84
44	l	1003	GDP	N3-C2-N1	-3.21	122.78	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.