



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 03:35 PM EDT

PDB ID : 5GAF
EMDB ID: : EMD-8002
Title : RNC in complex with SRP
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : unknown
Resolution : 4.30 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.

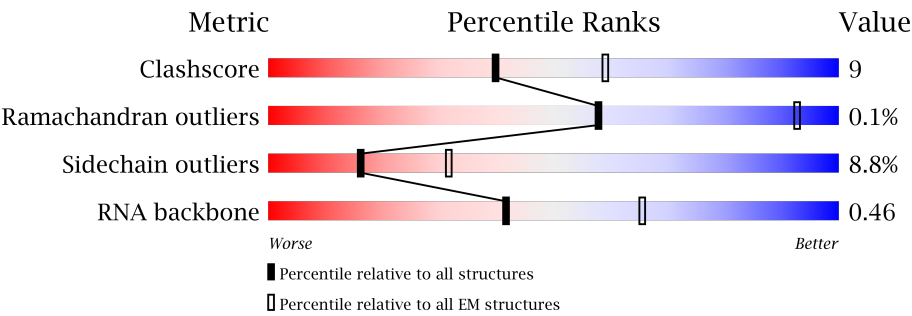
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.























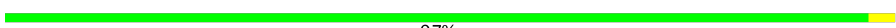




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	113	<div><div>10%19%8%•62%</div></div>
2	2	3	<div><div>33%33%33%</div></div>
3	A	2883	<div><div>55%36%8%•</div></div>
4	B	120	<div><div>74%23%•</div></div>
5	C	271	<div><div>71%26%•</div></div>
6	D	209	<div><div>78%20%•</div></div>
7	E	201	<div><div>77%21%•</div></div>
8	F	177	<div><div>60%35%5%</div></div>




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Mol	Chain	Length	Quality of chain
9	G	176	 69% 29% .
10	H	149	 66% 32% .
11	I	125	 66% 33% .
12	J	134	 57% 39% .
13	K	142	 73% 23% .
14	L	123	 67% 31% .
15	M	144	 75% 23% .
16	N	136	 72% 26% .
17	O	125	 71% 26% .
18	P	117	 65% 32% .
19	Q	114	 75% 25% .
20	R	117	 74% 21% .
21	S	103	 70% 28% .
22	T	110	 78% 20% .
23	U	95	 78% 20% .
24	V	102	 70% 29% .
25	W	94	 74% 24% .
26	X	76	 66% 32% .
27	Y	77	 65% 34% .
28	Z	62	 65% 31% 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	i	398	 95%••
36	k	18	 89%11%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 96182 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 SRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 2 is a RNA chain called tRNA CCAend.

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 ribosomal RNA.

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 ribosomal RNA.

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	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- 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 Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	398	Total	C	N	O	S	0	0
			3036	1910	548	560	18		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

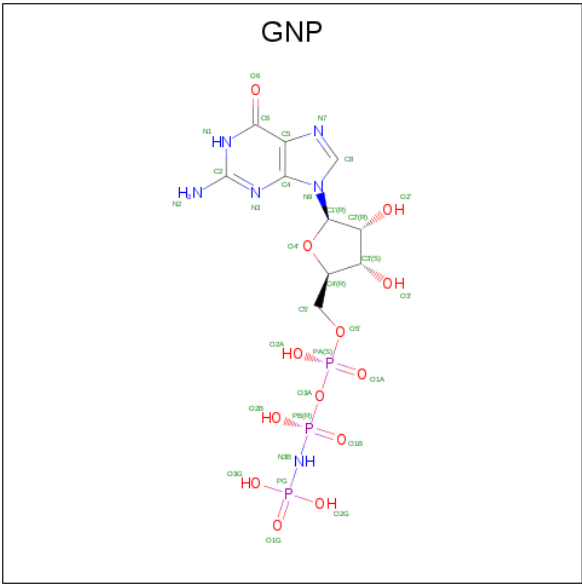
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	P	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	
37	B	11	Total	Mg	0
			11	11	
37	b	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	A	412	Total	Mg	0
			412	412	
37	2	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

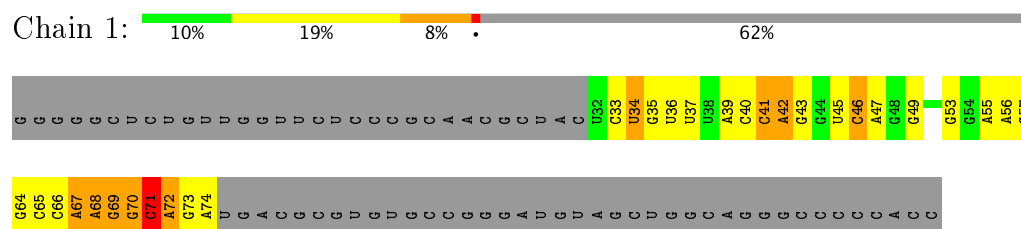
- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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.

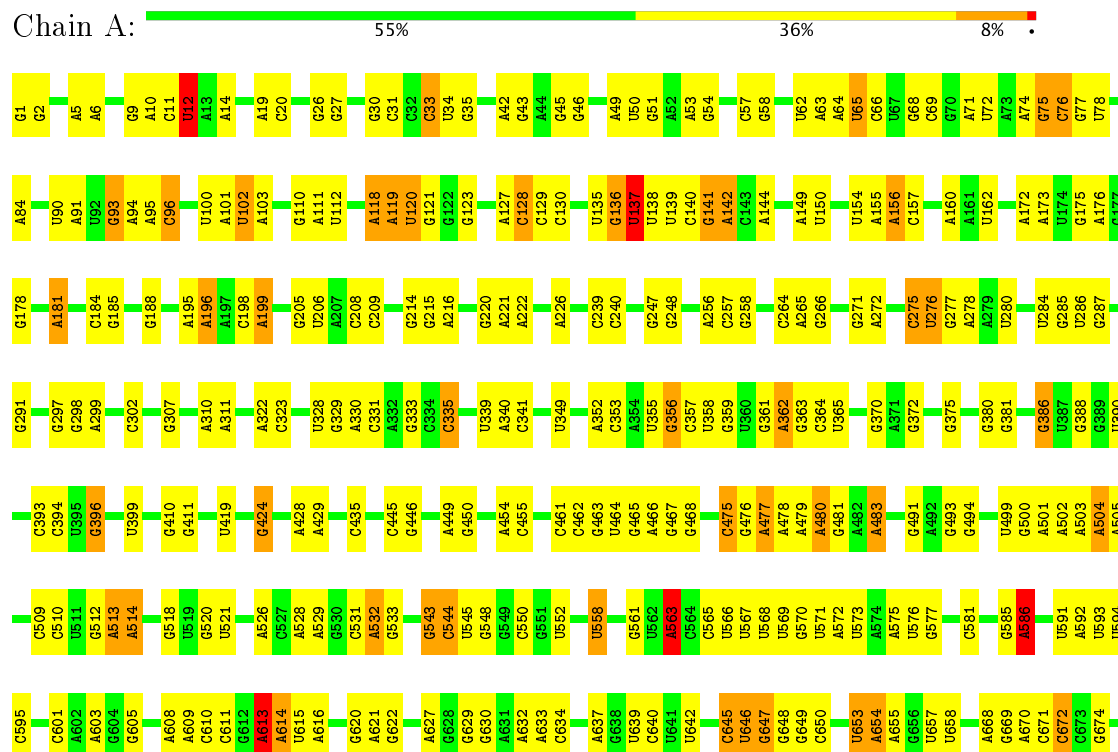
• Molecule 1: SRP 4.5S RNA



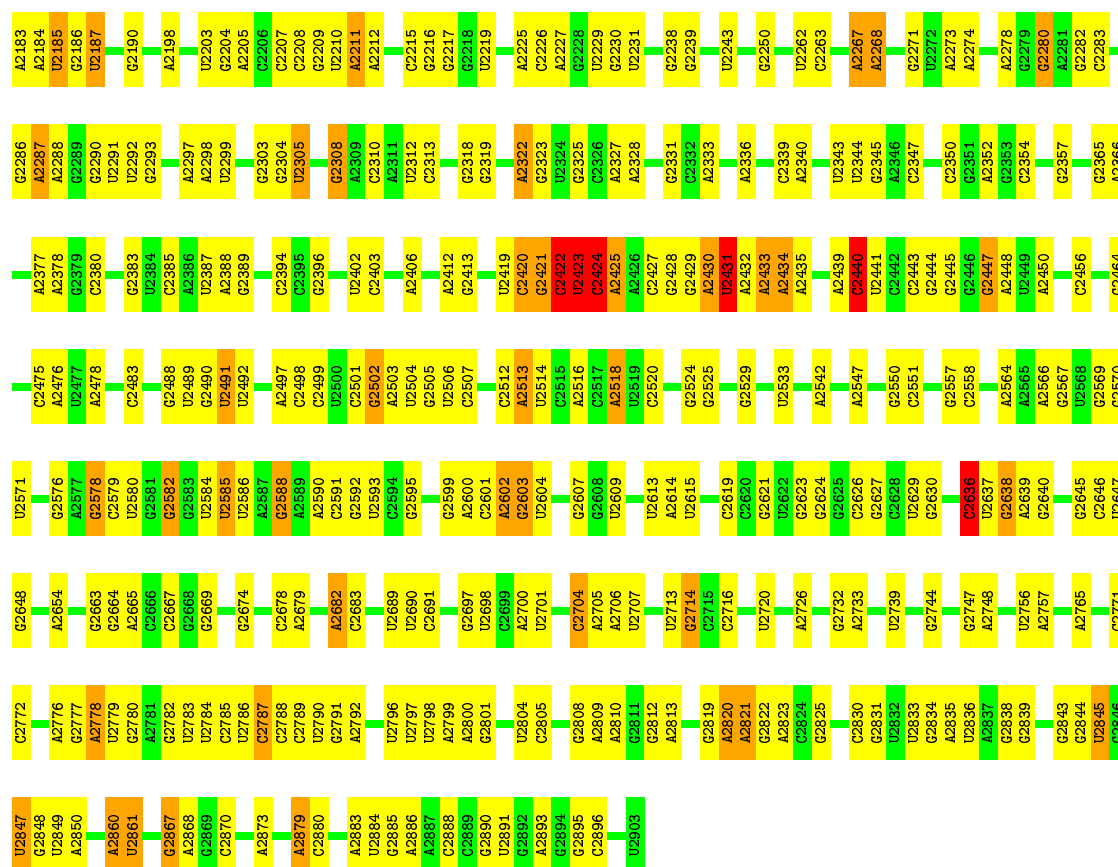
• Molecule 2: tRNA CCAend



• Molecule 3: 23S ribosomal RNA

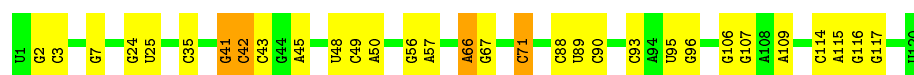


A2114	U2026	U1923	C1816	U1729	G1627	G1529	U1442	G1355	G1252	U1130	U1060	U970	G858	G784	A677
G2115	G2027	C1924	G1817	C1730	G1628	G1530	U1443	C1362	A1263	G1131	U1061	G971	G859	G785	C678
A2116	A2030	A1927	U1818	G1731	G1628	C1631	C1446	C1363	U1254	A1132	G1061	A972	U860		C679
U2118	A2031	A1928	U1820	C1732	G1631	A1532	C1446	G1364	U1255	A1133	U1062	A788	A861	A788	C680
A2119	G2032	G1929	A1821	U1735	G1634	U1534	G1448	A1365	G1256	G1135	C1063	G974	A862	A789	C681
C2120	A2033	G1930	C1822	A1736	A1634	A1535	G1449	A1366	C1261	G1136	U1065	A975	A863	U790	
G2121		U1931		U1736		C1536	G1450	A1367	A1262		U1066	G976	C864	C791	A685
U2122	G2038		U1825	G1737	A1637	G1537	C1451	G1374	U1267	G1139	A1067	A981	C865	A792	U686
G2123	U2039	C1934	U1826	G1738	C1638	U1542	A1452	U1379	U1268	C1140	A1068	G982	G869	A793	A706
	G2040	G1935	U1827	C1639	C1639	A1543	A1453	U1379	U1267	U1141	A1069	A983	U870	C795	G707
A2126	U2041	A1936	G1828	G1743	G1642	A1544	C1463	U1379	U1268	A1142	A1070	A984	U871	C796	
C2127	A2042	A1937	A1829	U1761	G1643	A1545	G1464	A1383	A1269	A1143	G1071	G987	U872	C797	G711
G2128	C2043	A1938		C1752	C1644	G1546	G1465	U1383	G1270		C1072			G798	G712
C2129		U1939	C1837	G1756	C1645	U1554	U1467	C1386	G1271	G1149	A1073	A990	G876	G799	G713
U2130	C2047		G1838	A1757	C1646	U1554	U1468	A1387	A1272	C1150	G1074	A990	A877	A800	U714
U2131	U1946	C1947	G1839	G1758	U1648	G1560	A1469	U1388	A1275	G1154	C1075	C994	A878	G801	
C2132	C2050		G1846	U1759	G1649	U1563	A1470	U1394	A1287	A1155	U1077	C995	A879	A718	A718
G2133	A2051	U1955	A1847	C1760	G1652	C1564	U1473	A1395	G1288		U1078	A996	G880	C719	C719
A2134	U1956	U1956	A1848	A1761	G1652	C1564	U1473	U1396	U1289	G1179	A1086	C997	G882	G805	U720
A2135	C2054	C1957	G1849	A1762	G1653	C1565	U1474	U1397	C1290	U1181	A1088	C998	G881	A721	A721
	C2055	C1958	G1850	G1763	A1654	A1566	U1474	C1398	U1294	G1172	U1082	U999	U895	G808	A722
G2138	G2056	G1959	A1853	C1764	A1655	U1569	G1482	C1399	U1294	U1173	U1083	A1000	A896	G809	G729
		A1960				A1570	G1483	U1400	U1294	G1173	A1084	A1001	C897	U810	A730
C2143	A2060	C1961	A1858	U1769	G1659	A1570	U1484	U1401	G1300	C1178	A1085	A1002	C898	U811	
G2144	G2061	U1962	U1859	G1770	G1660	A1571	U1485	U1402	A1301	U1180	A1087	C1005	U906	C812	G733
C2146	A2062	U1963	G1871	C1774	G1667	U1572	U1490	U1403	A1302	G1181	A1088	C1006	U907	C815	G738
A2147			G1872	U1775		U1576	G1491	U1406	G1303	G1182	A1090	C1007	G907	C816	
G2148	G2069	A1966	G1869	A1773	A1664	U1577	G1492	G1410	A1308	G1187	G1093	A1009	A909	A742	U741
	A2070	C1967	C1870	C1774	G1667	U1578	G1493	C1414	U1313	U1188	U1094	A910	A911	A743	A742
U2151	A2071	A1970	A1871	U1775		U1578	G1494	U1415	U1314	U1198	A1095	G1012	A911	U747	
G2152	C2072	U1971	G1873	U1781	A1672	G1581	A1495	U1416	A1321	U1199	A1096	C1013	G914	G822	U747
A2153	C2073	U1972	C1874	U1782	G1674	G1582	A1496	G1417	G1324	A1205	U1097	A1021	C915	U824	A753
U2155	G1974	G1973	G1875	A1785	A1677	U1584	U1497	G1418	G1324	G1206	G1099	A1022	G916	A825	A754
G2156		G1974	A1876	A1786	G1681	C1585	C1498	G1419	G1324	G1206	G1099	A1023	A917	U826	U755
C2157	U2086	G1980	G1877	A1786	G1681	C1585	C1499	A1419	A1327	G1210	C1100	G1024	G930	U827	A756
A2158	G2087	A1981	G1878	A1786	G1681	C1585	C1499	A1419	A1327	G1210	C1100	G1024	G930	A829	G757
G2159		U1982	U1880	A1789	A1689	A1590	G1500	A1420	A1328	G1211	G1101	G1025	U931	U828	C758
C2160	C2161	G1983	C1881	C1790	A1689	A1591	G1501	G1421	U1329	G1212	A1103	G1026	U932	G830	G759
G2162		A1791		A1791	G1695	C1592	A1502	G1422	G1332	G1218	G1104	A1028	A933	G831	
	G2093	U1991	G1888			A1597	U1506	G1423	G1332	G1218	U1105	A1028	U832	U832	G763
C2164		G1992		A1794	A1700	A1598	C1507	G1424	G1337	A1230	G1110	U1033	C946	A833	G764
G2165	A2097	U1993	G1896	C1795	A1700	A1598	C1507	G1424	G1337	A1230	G1110	U1033	C946	A833	C765
U2166				U1796	C1706	A1603	A1508	G1425	G1338	U1231	A1111	G1038	C948	C835	
G2167	A2101	C1997	A1899	G1797	G1707	C1604	A1509	G1426	G1338	U1231	A1111	G1038	C948	U839	G772
G2168	C2102			U1798	G1707	C1604	A1509	G1426	G1338	U1231	A1111	G1038	C948	C840	G773
C2169	C2103	C2000	C1902	G1799	C1708	C1605	G1511	A1427	U1340	G1236	G1113	A1039	G949	G774	
A2170	C2104		G1903	C1800	U1709	C1606	G1511	A1428	G1341	G1237	G1113	A1040	G953	G775	
	U2105	G2012	G1904	C1801	G1710	C1607	A1515	G1432	G1342	A1238	G1114	C1044	C957	A845	G776
C2171	U2106		C1905	A1802	A1711	A1608	G1516	A1433	U1342	G1238	G1115	C1045	U958	U846	G777
A2173	G2107	G2018	G1906	A1802	A1711	A1608	G1516	A1434	U1342	G1238	G1115	C1045	U958	U847	G778
C2174	A2108			G1807	G1715	A1610	G1517	G1435	U1344	C1243	G1116	A1046	A959	G779	
	U2109	C2021	A1918	A1808	G1721	A1614	G1524	G1436	G1346	A1247	G1125	A1047	A960	G780	
G2177	G2110	U2022	A1919	A1809	G1721	A1614	G1525	C1437	G1361	A1248	A1126	G1047	A961	A781	A781
C2178	U2111	C2023	G1920	A1722	A1722	C1615	G1526	U1439	C1361	U1249	A1127	A1048	A849	U850	G782
	G2112	G2024	G1921	G1811	U1725	C1617	A1528	A1439	A1364	G1251	G1129	G1056	C968	A782	A782
U2182	C2025		G1922									A1057	G969	G657	A783



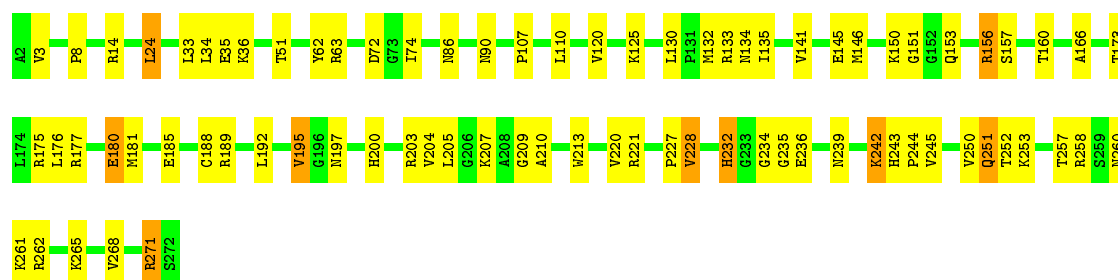
• Molecule 4: 5S ribosomal RNA

Chain B: 74% 23%



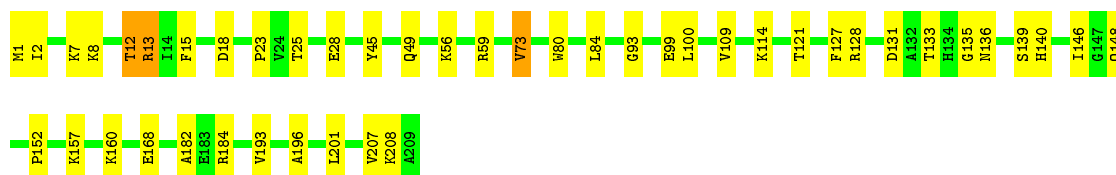
• Molecule 5: 50S ribosomal protein L2

Chain C: 71% 26%



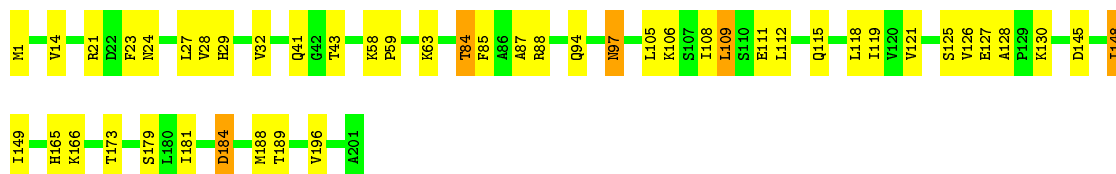
• Molecule 6: 50S ribosomal protein L3

Chain D: 78% 20%



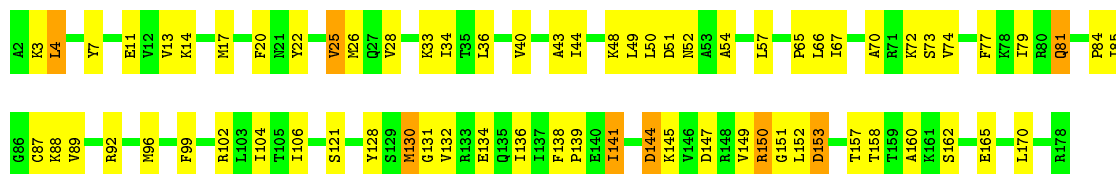
• Molecule 7: 50S ribosomal protein L4

Chain E: 77% 21% .



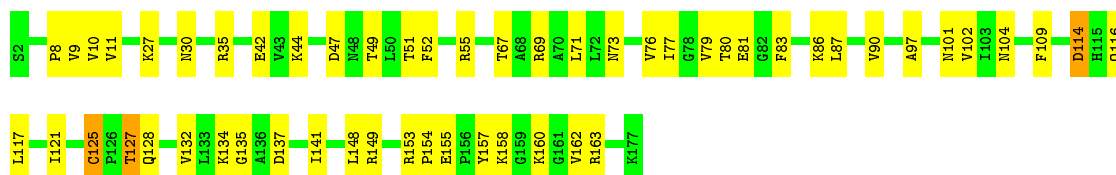
• Molecule 8: 50S ribosomal protein L5

Chain F: 60% 35% 5% .



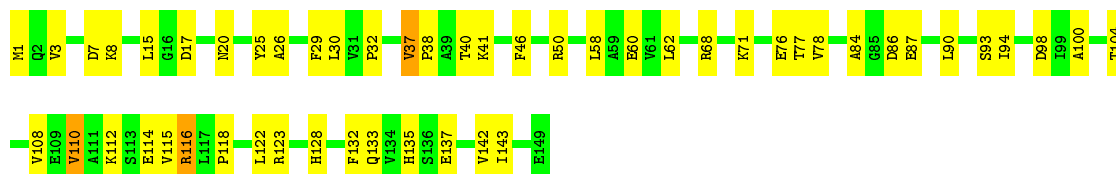
• Molecule 9: 50S ribosomal protein L6

Chain G: 69% 29% .



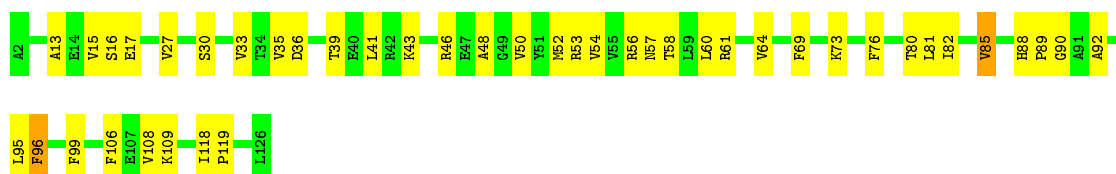
• Molecule 10: 50S ribosomal protein L9

Chain H: 66% 32% .

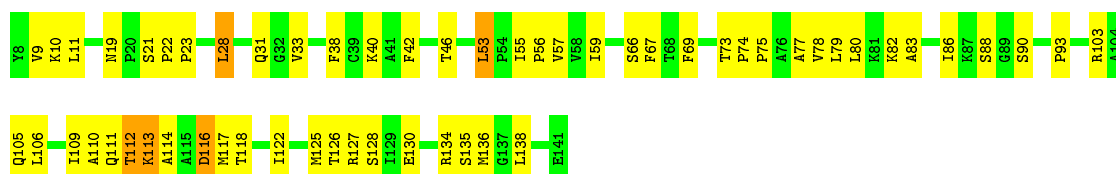


• Molecule 11: 50S ribosomal protein L10

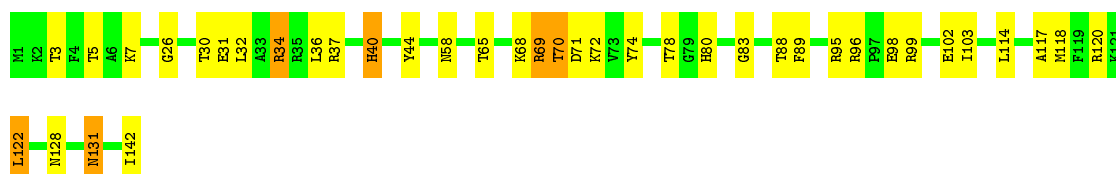
Chain I: 66% 33% .



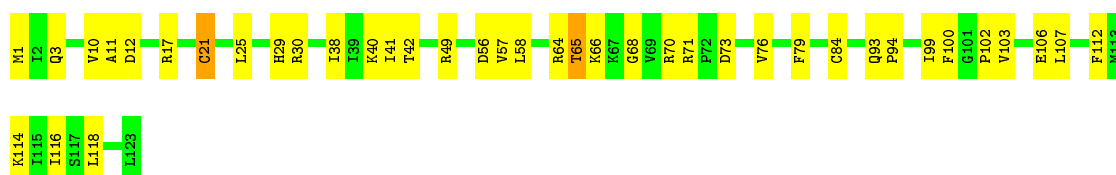
- Molecule 12: 50S ribosomal protein L11



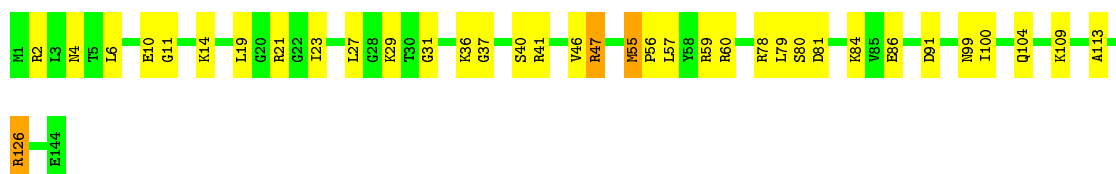
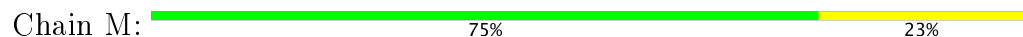
- Molecule 13: 50S ribosomal protein L13



- Molecule 14: 50S ribosomal protein L14

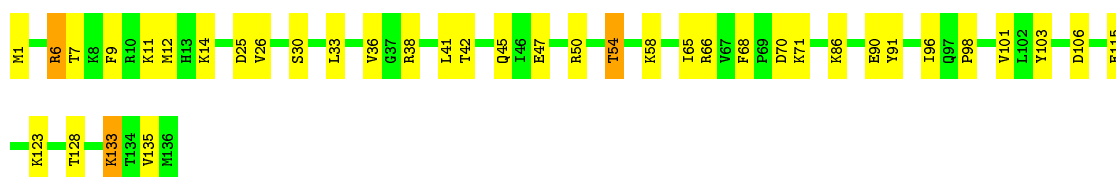


- Molecule 15: 50S ribosomal protein L15



- Molecule 16: 50S ribosomal protein L16





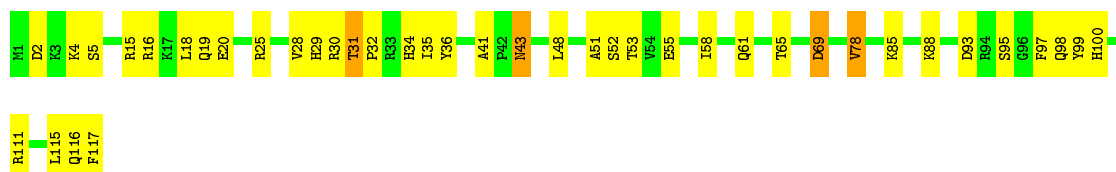
- Molecule 17: 50S ribosomal protein L17

Chain O: 71% 26% .



- Molecule 18: 50S ribosomal protein L18

Chain P: 65% 32% .



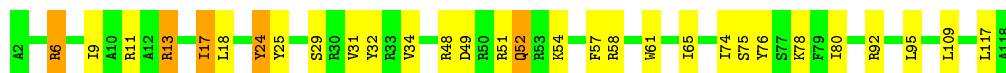
- Molecule 19: 50S ribosomal protein L19

Chain Q: 75% 25% .



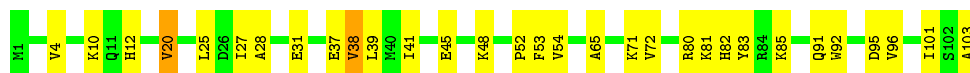
- Molecule 20: 50S ribosomal protein L20

Chain R: 74% 21% .



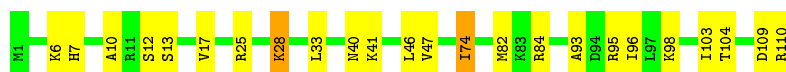
- Molecule 21: 50S ribosomal protein L21

Chain S: 70% 28% .



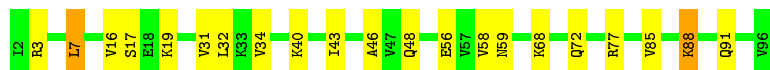
- Molecule 22: 50S ribosomal protein L22

Chain T: 78% 20% .



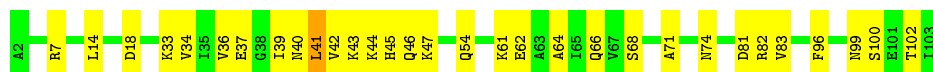
- Molecule 23: 50S ribosomal protein L23

Chain U: 78% 20%



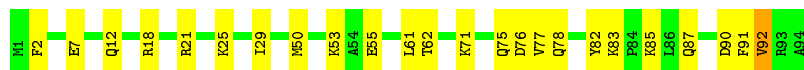
- Molecule 24: 50S ribosomal protein L24

Chain V: 70% 29%



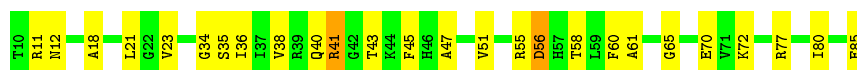
- Molecule 25: 50S ribosomal protein L25

Chain W: 74% 24%



- Molecule 26: 50S ribosomal protein L27

Chain X: 66% 32%



- Molecule 27: 50S ribosomal protein L28

Chain Y: 65% 34%



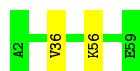
- Molecule 28: 50S ribosomal protein L29

Chain Z: 65% 31% 5%

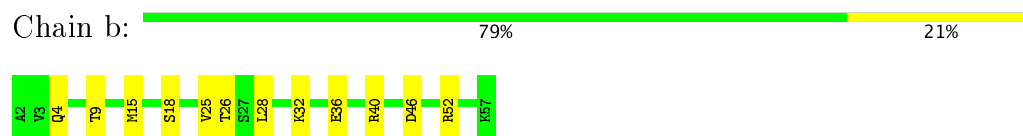


- Molecule 29: 50S ribosomal protein L30

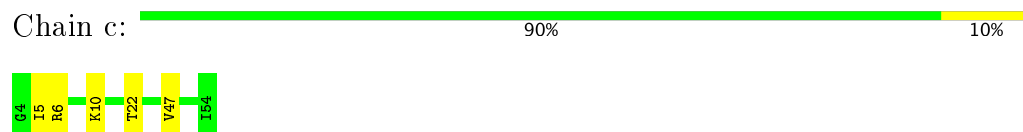
Chain a: 97%



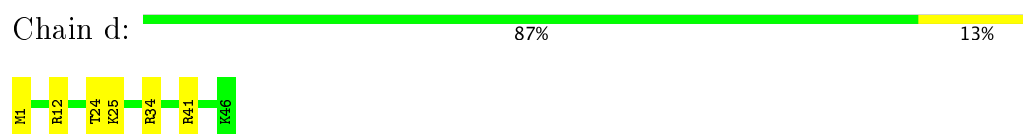
- Molecule 30: 50S ribosomal protein L32



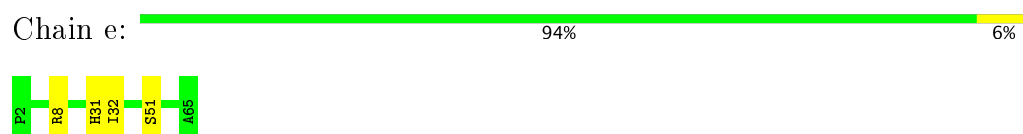
- Molecule 31: 50S ribosomal protein L33



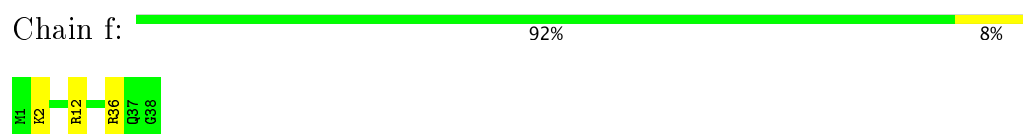
- Molecule 32: 50S ribosomal protein L34



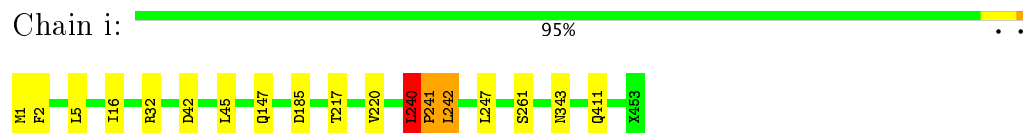
- Molecule 33: 50S ribosomal protein L35



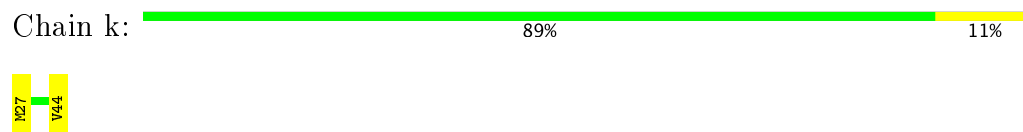
- Molecule 34: 50S ribosomal protein L36



- Molecule 35: Signal recognition particle protein



- Molecule 36: 1A9L SS



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	16407	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: ZN, MG, GNP

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	0.26	0/1037	0.93	1/1616 (0.1%)
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (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	0.58	0/68	1.26	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	0.63	2/763 (0.3%)	0.76	2/1021 (0.2%)
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	0.45	0/502	0.61	0/667
29	a	0.38	0/453	0.56	0/605
3	A	0.68	14/69329 (0.0%)	1.17	181/108152 (0.2%)
30	b	0.43	0/450	0.62	0/599
31	c	0.43	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.26	0/2954	0.48	1/3967 (0.0%)
36	k	0.30	0/137	0.60	0/186
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2122	0.65	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
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	0.62	16/103847 (0.0%)	1.04	190/155265 (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	i	0	2
5	C	0	1
9	G	0	1
All	All	0	5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	U	88	LYS	CA-C	8.36	1.74	1.52
3	A	2542	A	N9-C4	-6.90	1.33	1.37
3	A	1254	A	N9-C4	-6.35	1.34	1.37
3	A	1321	A	N9-C4	6.05	1.41	1.37
3	A	776	G	N9-C4	5.94	1.42	1.38

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.31	113.62	121.00
3	A	1838	C	C6-N1-C2	9.36	124.05	120.30
3	A	2422	C	O4'-C1'-N1	9.24	115.59	108.20
23	U	88	LYS	CB-CA-C	8.84	128.07	110.40
3	A	2423	U	C5-C6-N1	8.78	127.09	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide

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Mol	Chain	Res	Type	Group
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	i	240	LEU	Peptide
35	i	241	PRO	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	926	0	467	25	0
2	2	62	0	34	1	0
3	A	61902	0	31132	683	0
4	B	2569	0	1301	19	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	32	0
7	E	1552	0	1619	27	0
8	F	1411	0	1444	42	0
9	G	1323	0	1371	35	0
10	H	1110	0	1148	23	0
11	I	946	0	978	31	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	22	0
15	M	1053	0	1129	25	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	23	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	15	0
24	V	780	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0
28	Z	501	0	531	31	0
29	a	449	0	488	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	i	3036	0	3154	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	A	412	0	0	0	0
37	B	11	0	0	0	0
37	C	2	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
39	i	32	0	13	0	0
All	All	96182	0	64732	1193	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1193 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)
23:U:88:LYS:CA	23:U:88:LYS:C	1.74	1.53
28:Z:9:LYS:NZ	28:Z:17:GLU:HG3	1.61	1.15
3:A:96:C:OP1	28:Z:39:GLN:NE2	1.92	1.02
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	106 (98%)	2 (2%)	0	100	100
23	U	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
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%)	57 (95%)	3 (5%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	i	374/398 (94%)	357 (96%)	15 (4%)	2 (0%)	32	74
36	k	16/18 (89%)	11 (69%)	5 (31%)	0	100	100
All	All	3822/3908 (98%)	3685 (96%)	133 (4%)	4 (0%)	58	89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	i	240	LEU
35	i	241	PRO
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	33
6	D	164/164 (100%)	154 (94%)	10 (6%)	22	57
7	E	165/165 (100%)	152 (92%)	13 (8%)	14	48
8	F	148/148 (100%)	130 (88%)	18 (12%)	6	29
9	G	137/137 (100%)	129 (94%)	8 (6%)	23	58
10	H	114/114 (100%)	100 (88%)	14 (12%)	5	29
11	I	95/95 (100%)	89 (94%)	6 (6%)	21	55
12	J	104/104 (100%)	93 (89%)	11 (11%)	8	34
13	K	116/116 (100%)	105 (90%)	11 (10%)	10	39
14	L	104/104 (100%)	94 (90%)	10 (10%)	10	38
15	M	103/103 (100%)	94 (91%)	9 (9%)	12	43
16	N	109/109 (100%)	100 (92%)	9 (8%)	13	46
17	O	102/102 (100%)	95 (93%)	7 (7%)	18	53
18	P	87/87 (100%)	75 (86%)	12 (14%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Q	99/99 (100%)	90 (91%)	9 (9%)	11	41
20	R	89/89 (100%)	82 (92%)	7 (8%)	14	48
21	S	84/84 (100%)	76 (90%)	8 (10%)	10	39
22	T	93/93 (100%)	88 (95%)	5 (5%)	26	60
23	U	82/82 (100%)	76 (93%)	6 (7%)	16	51
24	V	83/83 (100%)	76 (92%)	7 (8%)	13	46
25	W	78/78 (100%)	72 (92%)	6 (8%)	15	49
26	X	57/58 (98%)	51 (90%)	6 (10%)	8	35
27	Y	67/67 (100%)	63 (94%)	4 (6%)	22	57
28	Z	54/54 (100%)	49 (91%)	5 (9%)	10	40
29	a	48/48 (100%)	46 (96%)	2 (4%)	34	66
30	b	47/47 (100%)	35 (74%)	12 (26%)	0	6
31	c	45/46 (98%)	40 (89%)	5 (11%)	7	33
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	43
35	i	313/315 (99%)	296 (95%)	17 (5%)	26	60
36	k	17/17 (100%)	15 (88%)	2 (12%)	6	30
All	All	3143/3147 (100%)	2867 (91%)	276 (9%)	16	43

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	L	116	ILE
18	P	31	THR
34	f	12	ARG
15	M	47	ARG
16	N	115	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	3	GLN
20	R	81	ASN
35	i	147	GLN

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Mol	Chain	Res	Type
17	O	18	GLN
19	Q	52	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	16 (38%)	1 (2%)
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2883 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3119 (97%)	548 (18%)	20 (0%)

5 of 548 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	37	U
1	1	39	A
1	1	41	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	1344	U
3	A	1494	A
3	A	2424	C
3	A	830	G
3	A	1110	G

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 433 ligands modelled in this entry, 432 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GNP	i	1400	-	27,34,34	2.40	11 (40%)	26,54,54	1.68	5 (19%)

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
39	GNP	i	1400	-	-	0/16/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	i	1400	GNP	C4-N9	-6.28	1.39	1.47
39	i	1400	GNP	C5-C6	-3.35	1.46	1.53
39	i	1400	GNP	PB-O2B	-2.44	1.50	1.56
39	i	1400	GNP	PG-O2G	-2.22	1.50	1.56
39	i	1400	GNP	C8-N9	-2.21	1.40	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	i	1400	GNP	O6-C6-N1	-3.06	118.61	122.70
39	i	1400	GNP	O1G-PG-N3B	-2.82	107.58	111.79
39	i	1400	GNP	O3A-PB-N3B	-2.29	100.23	106.59
39	i	1400	GNP	O2B-PB-O1B	4.18	118.56	109.87
39	i	1400	GNP	O6-C6-C5	4.79	128.85	119.69

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	4
35	i	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	297:MET	C	328:GLY	N	35.34
1	A	882:G	O3'	894:U	P	17.07
1	A	545:U	O3'	548:G	P	16.33
1	A	1912:A	O3'	1917:U	P	16.01
1	i	343:ASN	C	369:ASP	N	12.86