



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 30, 2020 – 01:21 PM EST

PDB ID : 6V3B
EMDB ID: : EMD-21032
Title : Cryo-EM structure of the Acinetobacter baumannii Ribosome: 70S in Empty state
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2019-11-25
Resolution : 2.91 Å(reported)
Based on PDB ID : 5AFI

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

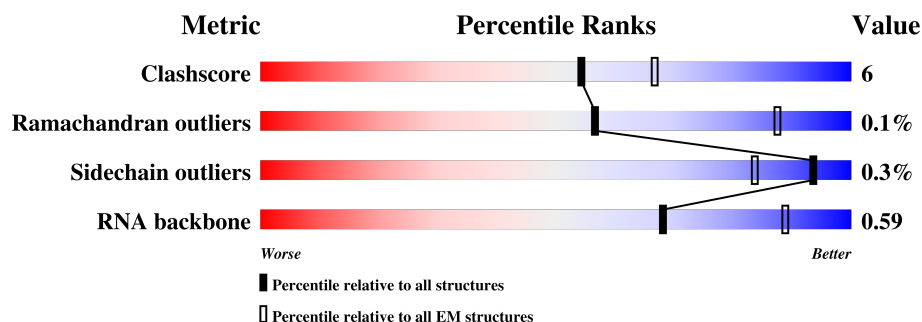
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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.








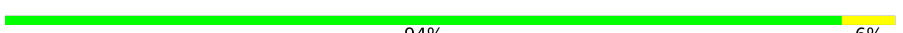



















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	0	51	92% 8%
2	1	44	86% 14%
3	2	64	77% 17% . . .
4	3	38	92% 8%
5	AN1	2918	64% 30% 5% .
6	B	115	53% 37% 9% .
7	C	274	89% 10% .
8	D	212	92% 8%





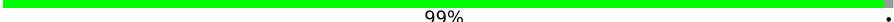
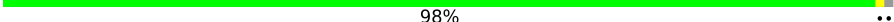
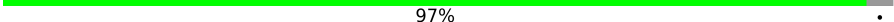

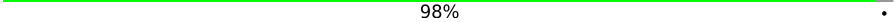
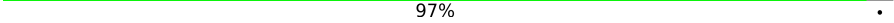
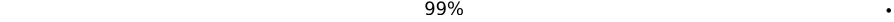
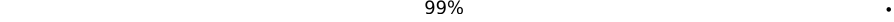

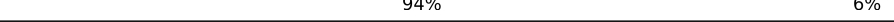


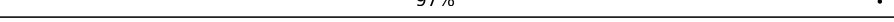

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	
31	sN1	1544	
32	b	250	
33	c	250	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	d	208	 100%
35	e	165	 94% 6%
36	f	127	 74% 26%
37	g	156	 89% 10%
38	h	131	 99%
39	i	128	 98%
40	j	103	 97%
41	k	128	 91% 9%
42	l	124	 98%
43	m	118	 97%
44	n	101	 99%
45	o	89	 99%
46	p	101	 81% 18%
47	q	85	 94% 6%
48	r	75	 71% 29%
49	s	91	 90% 10%
50	t	88	 97%
51	u	71	 28% 70%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 140290 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 protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN1	2892	Total	C	N	O	P	0	0
			62023	27689	11345	20098	2891		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	270	Total	C	N	O	S	0	0
			2096	1291	434	363	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	186	Total	C	N	O	S	0	0
			1419	893	265	257	4		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1381	877	247	249	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	146	Total	C	N	O	S	0	0
			1089	673	215	200	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O	S	0	0
			857	528	173	155	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	117	Total	C	N	O	0	0
			919	578	177	164		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	90	Total	C	N	O		0	0
			702	447	127	128			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	100	Total	C	N	O		0	0
			749	465	139	145			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	80	Total	C	N	O	S	0	0
			598	370	115	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	62	Total	C	N	O	S	0	0
			498	308	96	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	58	Total	C	N	O	S	0	0
			463	286	88	85	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	sN1	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	94	Total	C	N	O	S	0	0
			793	499	147	143	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	141	Total	C	N	O	S	0	0
			1111	696	210	199	6		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			995	621	198	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	83	Total	C	N	O	S	0	0
			649	406	129	113	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			630	396	118	115	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	53	Total	C	N	O	0	0
			438	282	75	81		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	85	Total	C	N	O	S	0	0
			658	406	138	112	2		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	u	21	Total	C	N	O	0	0
			182	115	37	30		

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total	Zn	0
			1	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	AN1	52	Total	Mg	0
			52	52	
53	sN1	41	Total	Mg	0
			41	41	

- Molecule 54 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
54	AN1	1	Total	Na	0
			1	1	

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	O	0
			1	1	
55	AN1	253	Total	O	0
			253	253	

Continued on next page...

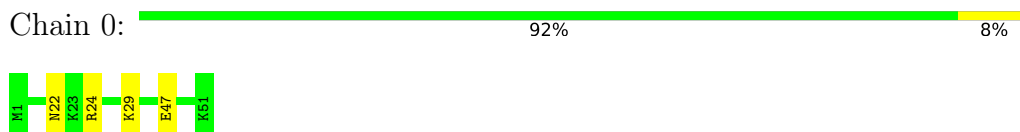
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
55	B	5	Total 5	O 5	0
55	C	3	Total 3	O 3	0
55	D	3	Total 3	O 3	0
55	E	2	Total 2	O 2	0
55	K	3	Total 3	O 3	0
55	M	1	Total 1	O 1	0
55	P	1	Total 1	O 1	0
55	Q	3	Total 3	O 3	0
55	R	1	Total 1	O 1	0
55	V	2	Total 2	O 2	0
55	Y	1	Total 1	O 1	0
55	Z	1	Total 1	O 1	0
55	sN1	107	Total 107	O 107	0
55	g	1	Total 1	O 1	0
55	h	1	Total 1	O 1	0
55	i	2	Total 2	O 2	0
55	m	2	Total 2	O 2	0
55	n	1	Total 1	O 1	0
55	s	3	Total 3	O 3	0
55	t	1	Total 1	O 1	0

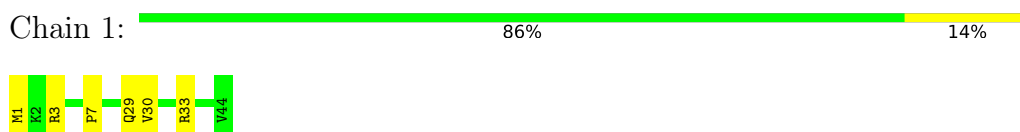
3 Residue-property plots

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.

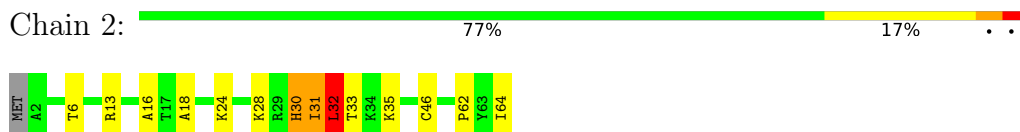
- Molecule 1: 50S ribosomal protein L33



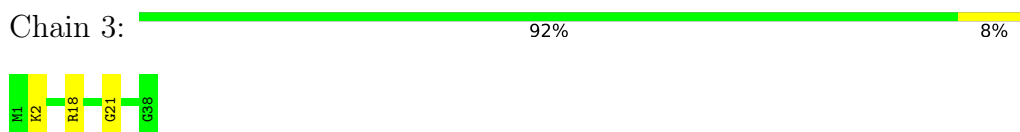
- Molecule 2: 50S ribosomal protein L34



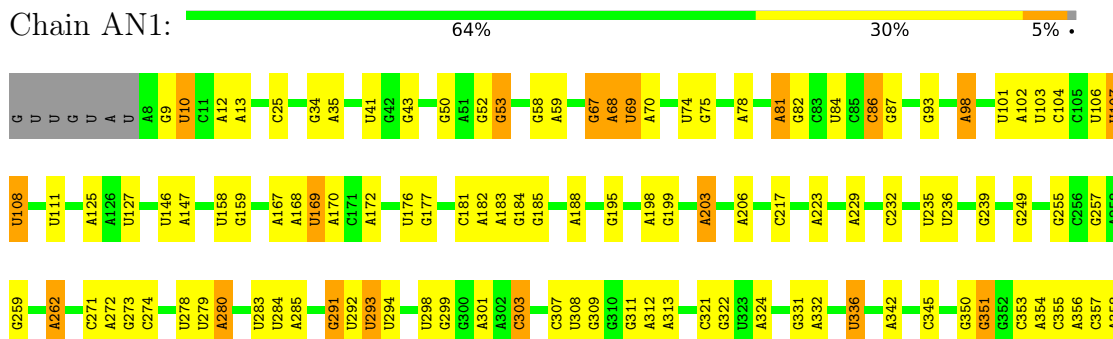
- Molecule 3: 50S ribosomal protein L35



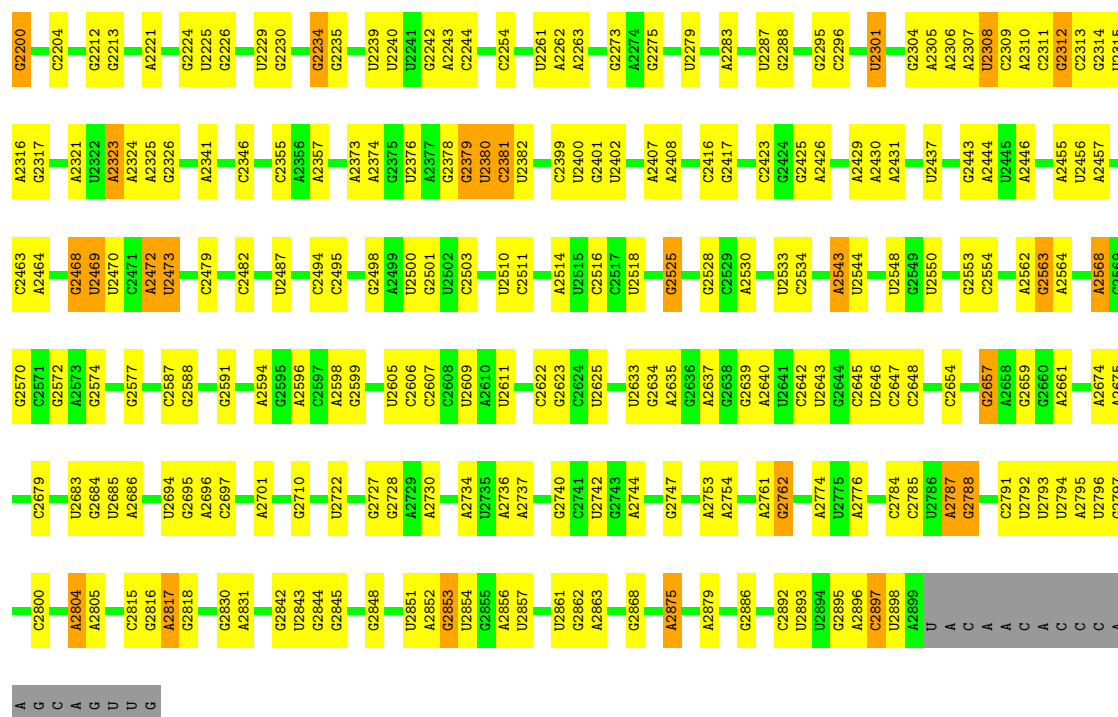
- Molecule 4: 50S ribosomal protein L36



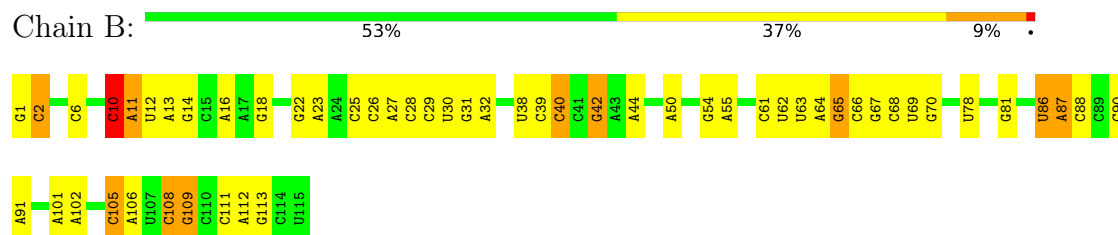
- Molecule 5: 23s ribosomal RNA



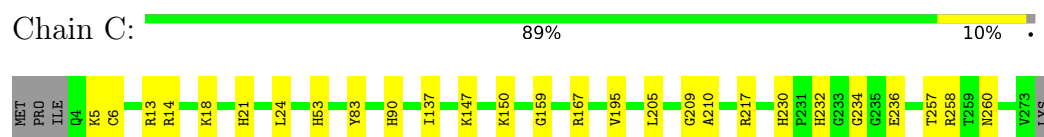
A2122	G2028	A1914	U1826	U1712	A1564	U1477	A1381		U1078	A976		A861	U745	A625	Q517	U359
G2123	A2029	A1915	G1827	U1713	A1567	G1478	U1382	A1242	U1079	A977	A978	G862	A750	G626	CS18	A364
G2124	U2030	C1916	C1828	G1714	A1568	U1479	A1387	G1245	A1080	A979	A1081	C963	A751	A627	A519	U365
	C2039	G1917	C1829		A1569	U1480	U1388	G1248	A1082	C979	A1083	C964	A752	A630	G521	G366
U2127	G2048	G1918	U1830	G1717	A1570	U1481	U1389	A1248	A1084	A980	A1085	C965	A753	A631	CS26	A367
G2129	G2049	U1919	G1831	G1718	U1574	U1485	U1390	G1251	A1085	A981	A1086	C966	A754	A632	A527	C368
A2130	A2050	C1920	G1835	U1719	U1577	G1486	U1407	G1257	A1087	A993	A1088	C967	A755	A633	A528	G369
A2131	G2051	U1921	U1836	C1726	A1577	U1487	A1408	A1287	A1088	A997	A1089	C968	A756	A634	G529	C371
G2132	G2052	A1923	G1842		U1582	C1488		A1288	G1088	A998	A1089	C969	A757	A635	CS30	U372
C2133	C2053	G1925	A1843	U1730	U1583	U1490	G1412	A1270	C1089	A999	A1090	C970	A758	A636	A531	A373
	G2054	U1926	G1844	C1731	A1584	A1491	G1413	A1273	C1090	A999	A1091	C971	A759	A637		
A2137	A2057	A1932	U1846	G1734	U1587		U1415	G1274	A1095	A1000	A1092	C972	A760	A638	U543	
A2138	G2058	A1933	U1847		C1588	G1498		G1275	G1096	A1001	A1093	C973	A761	A639	U544	G385
	C2059	U1934	U1855	G1739	A1588	U1499	G1421	U1276	A1097	A1002	A1094	C974	A762	A640	U545	U386
U2142	A2060	U1935	U1856		C1589	U1500	G1422	U1277	A1098	A1003	A1095	C975	A763	A641	Q546	G395
G2144	C2061	U1936	U1857	G1742	A1589	C1501	A1423	U1287	A1100	A1004	A1096	C976	A764	A642	U547	A403
U2146	G2065	C1937	U1860	U1743	C1590	U1502	C1424	G1288	C1101	G1023	A1097	C977	A765	A643	U552	
U2147	A2066	U1938	U1861	C1744	A1591	U1503	G1425	U1289	G1102	A1024	A1098	C978	A766	A644	G553	G410
C2148	A2067	U1939	U1862	U1745	C1592	U1504	G1426	U1290	A1103	A1025	A1099	C979	A767	A645	A554	C413
A2149	C2068	G1863	G1864	G1746	A1595	U1505	A1427	A1296	G1104	A1026	A1099	C980	A768	A646	A561	A414
G2150	G2069	U1942	C1865		A1596	G1510	G1428	A1303	A1108	C1027	A1099	C981	A769	A647	CS52	
U2070	U2071	C1943	U1866	G1749	C1603	G1517	A1429	G1304	G1109	G1028	A1099	C982	A770	A648	CS53	G423
U2072	U2072	G1950	U1867	C1750	C1604	U1518	G1430	G1305	U1110	A1029	A1099	C983	A771	A649	U564	G424
		U1951	U1875	G1752	A1606	U1519	C1432	U1307	G1112	G1031	A1099	C984	A772	A650	A571	C434
C2077	C2077	U1959	C1870	G1759	A1616	G1521	A1436	C1309	G1113	U1032	A1099	C985	A773	A651	U571	G449
A2078	A2078	G1960	U1871	G1760	G1617	C1522	U1437	C1310	G1121	A1036	A1099	C986	A774	A652	CS57	C455
G2089	G2089	C1961	U1872		G1617	C1523	U1438	C1311	U1129	A1037	A1099	C987	A775	A653	A573	G462
A2090	A2090	U1962	C1875	G1767	A1623	U1526	U1439	G1312	A1130	G1038	A1099	C988	A776	A654	U578	
C2091	C2091	C1963	U1876	A1768	A1624	U1527	C1441	G1316	G1131	G1039	A1099	C989	A777	A655	CS79	A465
U2163	U2093	U1966	U1877	G1769	A1624	U1528	C1442	A1316	C1131	C1040	A1099	C990	A778	A656	A570	
G2164	U2094	U1967	U1878	U1775	G1634	U1529	C1443	U1324	G1132	U1042	A1099	C991	A779	A657	A580	
A2165	U2095	G1968	G1880	A1776	A1635	U1530	C1444	U1325	C1133	U1043	A1099	C992	A780	A658	G551	C474
A2166	G2096	U1978	A1885		C1642	U1531	G1447	G1336	A1140	G1044	A1099	C993	A781	A659		G475
A2167	A2097		U1886	A1780	U1645	U1532	U1448	U1337	U1148	G1053	A1099	C994	A782	A660	U587	A478
U2168	C2098	U1987	C1888	U1792	U1646	G1533	U1453	C1340	G1149	A1054	A1099	C995	A783	A661	A588	A479
A2169	C2099	G1988	C1889	C1793	U1647	U1534	U1454	U1341	U1150	A1055	A1099	C996	A784	A662	A479	G480
C2171	U2104	U1989	A1895	G1796	G1647	C1537	U1455	A1348	U1167	U1057	A1099	C997	A785	A663	U591	
A2172	U2105	C1992	U1899	A1797	A1662	U1538	U1456	A1349	U1170	U1058	A1099	C998	A786	A664	U592	G493
G2173	G2106	C1993	G1899	A1798	G1665	G1539	G1462	G1356	U1171	U1059	A1099	C999	A787	A665	U596	U498
C2174	U2107	U1998	A1899	A1799	G1666	C1540	A1463	C1357	U1172	G1060	A1099	C1000	A788	A666	A597	G499
G2175	G2108	A2010	G1902		G1672	G1541	A1464	C1358	G1173	U1061	A1099	C1001	A789	A667	G598	
U2176	U2109	A2011	C1903	A1804	G1673	U1542	A1465	G1359	G1174	U1062	A1099	C1002	A790	A668	A601	A502
G2177	G2111	A2012	C1904	A1805	G1674	U1543	A1466	A1360	G1175	U1063	A1099	C1003	A791	A669	U603	
G2178	G2112	U2018	U1905	A1806	G1675	U1544	G1467	A1361	U1183	U1064	A1099	C1004	A792	A670	A504	
	A2113	G2020	G1906	G1807	U1679	U1545	A1468	A1362	U1184	U1065	A1099	C1005	A793	A671	A606	C508
U2184	U2185	G2021	U1907	U1808	G1680	U1546	A1469	G1363	U1185	U1066	A1099	C1006	A794	A672	A607	C509
G2186	G2186	C2022	U1908	G1812	U1681	U1547	A1470	G1364	U1186	U1067	A1099	C1007	A795	A673	U611	U510
A2187	A2187	G2116	A1909		U1682	U1548	G1471	U1373	A1199	A1068	A1099	C1008	A796	A674	A612	G511
G2188	G2188	G2117	U1910	A1817	U1683	U1549	G1472	U1374	A1200	A1069	A1099	C1009	A797	A675	A613	
		G2118	G1911	G1818	U1684	U1550	G1473	U1375	G1201	A1070	A1099	C1010	A798	A676	A614	C516
A2194	A2194	G2026	A1912	A1825	G1708	U1561	G1474	A1378	G1202	C1076	A1099	C1011	A799	A677		
		A2027	U1913			C1562	A1475		G1203	C1077	A1099	C1012	A800	A678		



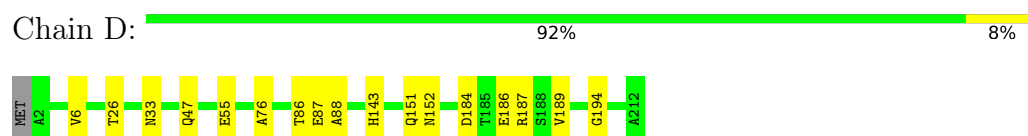
• Molecule 6: 5S ribosomal RNA



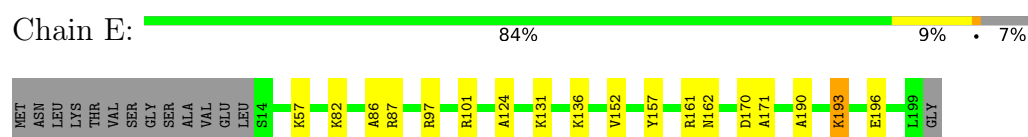
• Molecule 7: 50S ribosomal protein L2



• Molecule 8: 50S ribosomal protein L3



• Molecule 9: 50S ribosomal protein L4



- Chain L:  93% 7%



- Molecule 17: 50S ribosomal protein L17

Chain M: 90% 6% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N: 84% 14%



- Molecule 19: 50S ribosomal protein L19

Chain O: 84% 12%



- Molecule 20: 50S ribosomal protein L20

Chain P: 91% 8%



- Molecule 21: 50S ribosomal protein L21

Chain Q: 84% 16%



- Molecule 22: 50S ribosomal protein L22

Chain R: 93% 7%




- Molecule 23: 50S ribosomal protein L23

Chain S: 73% 12% 15%




- Molecule 24: 50S ribosomal protein L24

Chain T:  83% 12% 5%




- Molecule 25: 50S ribosomal protein L25

Chain U:  84% 15% .




- Molecule 26: 50S ribosomal protein L27

Chain V:  87% 7% 6%




- Molecule 27: 50S ribosomal protein L28

Chain W:  90% 9% .




- Molecule 28: 50S ribosomal protein L29

Chain X:  83% 12% 5%



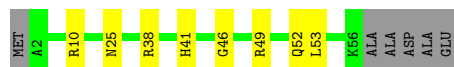
- Molecule 29: 50S ribosomal protein L30

Chain Y:  90% 10%




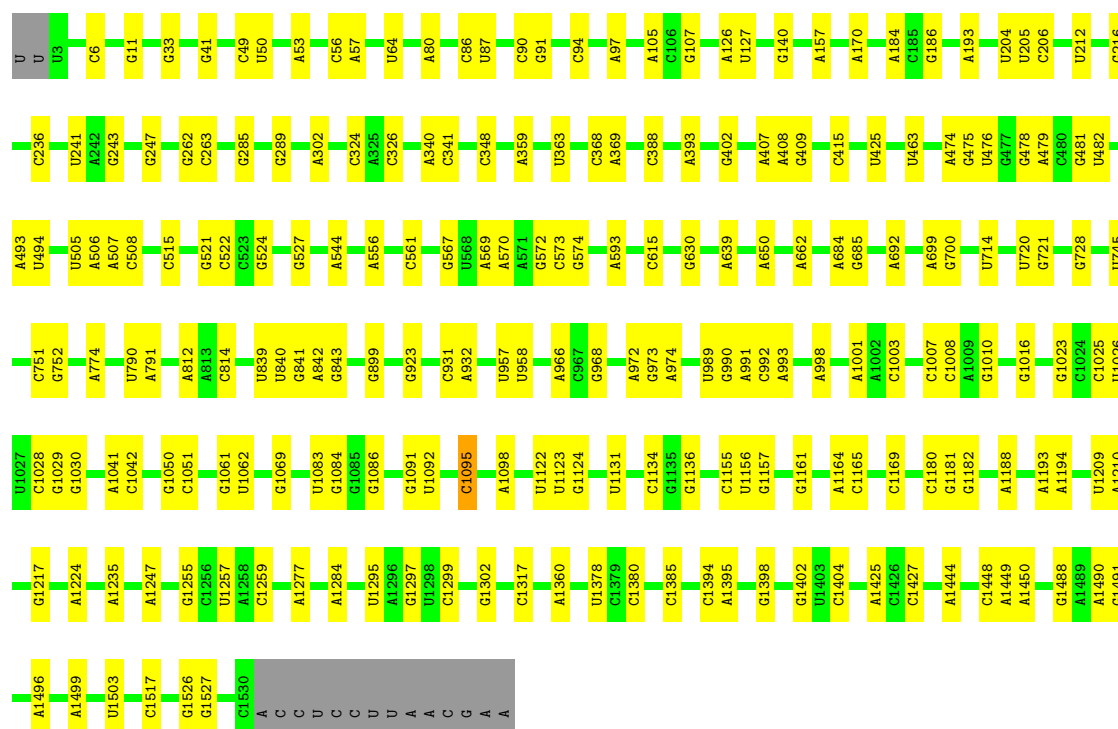
- Molecule 30: 50S ribosomal protein L32

Chain Z:  77% 13% 10%



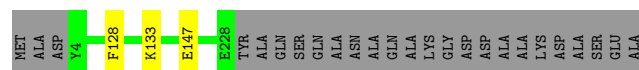
- Molecule 31: 16s Ribosomal RNA

Chain sN1:  85% 14% .



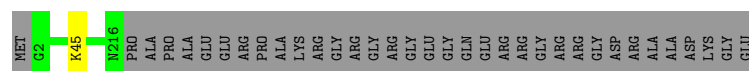
• Molecule 32: 30S ribosomal protein S2

Chain b: 89% 10%



• Molecule 33: 30S ribosomal protein S3

Chain c: 86% 14%



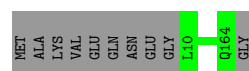
• Molecule 34: 30S ribosomal protein S4

Chain d: 100%



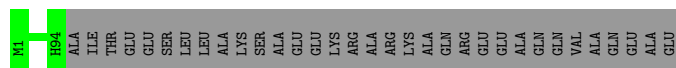
• Molecule 35: 30S ribosomal protein S5

Chain e: 94% 6%




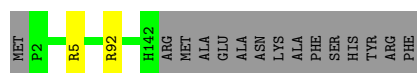
• Molecule 36: 30S ribosomal protein S6

Chain f:  74% 26%



- Molecule 37: 30S ribosomal protein S7

Chain g:  89% 10%



- Molecule 38: 30S ribosomal protein S8

Chain h:  99%



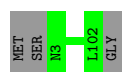
- Molecule 39: 30S ribosomal protein S9

Chain i:  98%



- Molecule 40: 30S ribosomal protein S10

Chain j:  97%



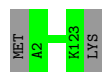
- Molecule 41: 30S ribosomal protein S11

Chain k:  91% 9%



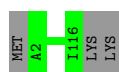
- Molecule 42: 30S ribosomal protein S12

Chain l:  98%



- Molecule 43: 30S ribosomal protein S13

Chain m:  97%



- Molecule 44: 30S ribosomal protein S14

Chain n: 99%



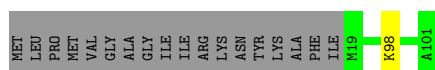
- Molecule 45: 30S ribosomal protein S15

Chain o: 99%



- Molecule 46: 30S ribosomal protein S16

Chain p: 81% 18%



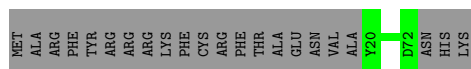
- Molecule 47: 30S ribosomal protein S17

Chain q: 94% 6%



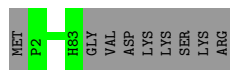
- Molecule 48: 30S ribosomal protein S18

Chain r: 71% 29%



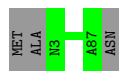
- Molecule 49: 30S ribosomal protein S19

Chain s: 90% 10%

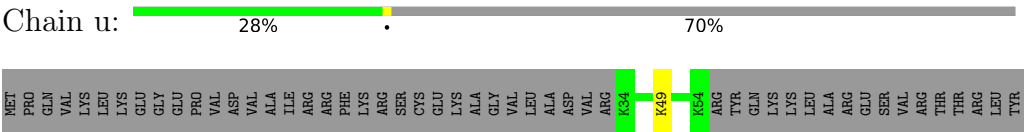


- Molecule 50: 30S ribosomal protein S20

Chain t: 97%



● Molecule 51: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66318	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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: 3TD, 5MU, ZN, OMG, OMU, MA6, NA, MG, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 7MG, PSU

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	O	0.24	0/434	0.42	0/573
10	F	0.26	0/1401	0.51	0/1877
11	G	0.26	0/1337	0.43	0/1807
12	H	0.26	0/461	0.51	0/616
13	I	0.25	0/1151	0.40	0/1551
14	J	0.24	0/956	0.45	0/1286
15	K	0.24	0/1097	0.44	0/1461
16	L	0.24	0/1104	0.43	0/1475
17	M	0.24	0/956	0.41	0/1282
18	N	0.24	0/865	0.43	0/1156
19	O	0.24	0/931	0.43	0/1249
2	1	0.23	0/367	0.38	0/481
20	P	0.25	0/947	0.34	0/1262
21	Q	0.23	0/818	0.45	0/1094
22	R	0.23	0/831	0.40	0/1113
23	S	0.25	0/708	0.42	0/947
24	T	0.24	0/753	0.48	0/1010
25	U	0.24	0/770	0.42	0/1036
26	V	0.25	0/606	0.46	0/810
27	W	0.23	0/642	0.43	0/856
28	X	0.23	0/499	0.37	0/662
29	Y	0.23	0/468	0.42	0/624
3	2	0.24	0/515	0.53	1/678 (0.1%)
30	Z	0.23	0/462	0.41	0/615
31	sN1	0.18	0/36476	0.75	6/56895 (0.0%)
32	b	0.26	0/1799	0.49	0/2429
33	c	0.24	0/1714	0.42	0/2304
34	d	0.24	0/1653	0.40	0/2213
35	e	0.24	0/1141	0.43	0/1537
36	f	0.24	0/808	0.48	0/1089
37	g	0.24	0/1127	0.39	0/1511
38	h	0.24	0/993	0.42	0/1331

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	i	0.24	0/1006	0.42	0/1346
4	3	0.23	0/296	0.47	0/389
40	j	0.23	0/811	0.42	0/1096
41	k	0.25	0/878	0.44	0/1189
42	l	0.25	0/958	0.47	0/1284
43	m	0.23	0/913	0.41	0/1226
44	n	0.24	0/803	0.38	0/1071
45	o	0.23	0/715	0.35	0/958
46	p	0.24	0/660	0.41	0/886
47	q	0.22	0/637	0.44	0/858
48	r	0.25	0/445	0.45	0/601
49	s	0.23	0/664	0.39	0/897
5	AN1	0.22	0/69101	0.77	20/107780 (0.0%)
50	t	0.25	0/664	0.36	0/885
51	u	0.30	0/184	0.54	0/240
6	B	0.20	0/2739	0.80	3/4266 (0.1%)
7	C	0.24	0/2136	0.43	0/2869
8	D	0.25	0/1590	0.45	0/2142
9	E	0.24	0/1440	0.41	0/1944
All	All	0.22	0/151430	0.69	30/226757 (0.0%)

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	H	0	1
3	2	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	415	C	N3-C2-O2	-7.48	116.66	121.90
31	sN1	1095	C	N1-C2-O2	6.81	122.99	118.90
31	sN1	1095	C	N3-C2-O2	-6.72	117.20	121.90
5	AN1	788	U	C2-N1-C1'	6.71	125.76	117.70
3	2	32	LEU	CA-CB-CG	6.66	130.62	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	HIS	Peptide
12	H	47	PHE	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	0	427	0	462	2	0
2	1	363	0	401	6	0
3	2	509	0	566	12	0
4	3	295	0	326	2	0
5	AN1	62023	0	31194	497	0
6	B	2450	0	1241	44	0
7	C	2096	0	2157	19	0
8	D	1572	0	1610	12	0
9	E	1419	0	1464	16	0
10	F	1381	0	1433	53	0
11	G	1318	0	1373	19	0
12	H	458	0	480	12	0
13	I	1125	0	1148	16	0
14	J	946	0	1007	5	0
15	K	1089	0	1159	17	0
16	L	1087	0	1162	6	0
17	M	942	0	987	5	0
18	N	857	0	899	10	0
19	O	919	0	973	9	0
20	P	934	0	997	7	0
21	Q	807	0	842	14	0
22	R	826	0	894	6	0
23	S	702	0	756	10	0
24	T	749	0	797	9	0
25	U	760	0	783	11	0
26	V	598	0	600	4	0
27	W	632	0	667	6	0
28	X	498	0	537	6	0
29	Y	463	0	488	3	0
30	Z	456	0	448	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	sN1	32782	0	16507	0	0
32	b	1769	0	1787	0	0
33	c	1690	0	1774	0	0
34	d	1631	0	1691	0	0
35	e	1129	0	1174	0	0
36	f	793	0	788	0	0
37	g	1111	0	1163	0	0
38	h	985	0	1047	0	0
39	i	995	0	1053	0	0
40	j	801	0	832	0	0
41	k	862	0	877	0	0
42	l	945	0	996	0	0
43	m	903	0	962	0	0
44	n	792	0	833	0	0
45	o	705	0	712	0	0
46	p	649	0	660	0	0
47	q	630	0	678	0	0
48	r	438	0	456	0	0
49	s	646	0	663	0	0
50	t	658	0	710	0	0
51	u	182	0	198	0	0
52	3	1	0	0	0	0
53	AN1	52	0	0	0	0
53	sN1	41	0	0	0	0
54	AN1	1	0	0	0	0
55	3	1	0	0	0	0
55	AN1	253	0	0	2	0
55	B	5	0	0	1	0
55	C	3	0	0	0	0
55	D	3	0	0	0	0
55	E	2	0	0	0	0
55	K	3	0	0	0	0
55	M	1	0	0	0	0
55	P	1	0	0	1	0
55	Q	3	0	0	0	0
55	R	1	0	0	0	0
55	V	2	0	0	0	0
55	Y	1	0	0	0	0
55	Z	1	0	0	0	0
55	g	1	0	0	0	0
55	h	1	0	0	0	0
55	i	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	m	2	0	0	0	0
55	n	1	0	0	0	0
55	s	3	0	0	0	0
55	sN1	107	0	0	0	0
55	t	1	0	0	0	0
All	All	140290	0	93412	768	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 6.

The worst 5 of 768 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)
5:AN1:1462:G:H1	5:AN1:1520:A:N6	1.43	1.16
5:AN1:2096:G:H1	5:AN1:2185:U:H3	0.91	0.90
6:B:70:G:H21	6:B:101:A:H62	1.11	0.89
6:B:2:C:O2	6:B:113:G:N2	2.08	0.86
10:F:146:ILE:HD12	10:F:149:ILE:HD11	1.59	0.84

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	
1	0	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	2	61/64 (95%)	58 (95%)	1 (2%)	2 (3%)	4	16
4	3	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	C	268/274 (98%)	260 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	209/212 (99%)	203 (97%)	6 (3%)	0	100	100
9	E	184/200 (92%)	184 (100%)	0	0	100	100
10	F	173/178 (97%)	151 (87%)	21 (12%)	1 (1%)	27	60
11	G	172/177 (97%)	166 (96%)	6 (4%)	0	100	100
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	J	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
15	K	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
16	L	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
17	M	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	111 (96%)	4 (4%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
22	R	107/109 (98%)	107 (100%)	0	0	100	100
23	S	88/106 (83%)	85 (97%)	3 (3%)	0	100	100
24	T	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
26	V	78/85 (92%)	78 (100%)	0	0	100	100
27	W	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
28	X	60/65 (92%)	58 (97%)	2 (3%)	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	53/61 (87%)	51 (96%)	2 (4%)	0	100	100
32	b	223/250 (89%)	211 (95%)	12 (5%)	0	100	100
33	c	213/250 (85%)	204 (96%)	9 (4%)	0	100	100
34	d	205/208 (99%)	204 (100%)	1 (0%)	0	100	100
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
36	f	92/127 (72%)	88 (96%)	4 (4%)	0	100	100
37	g	139/156 (89%)	137 (99%)	2 (1%)	0	100	100
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
39	i	125/128 (98%)	123 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	j	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
41	k	115/128 (90%)	109 (95%)	6 (5%)	0	100	100
42	l	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	81/101 (80%)	80 (99%)	1 (1%)	0	100	100
47	q	78/85 (92%)	77 (99%)	1 (1%)	0	100	100
48	r	51/75 (68%)	51 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	83/88 (94%)	83 (100%)	0	0	100	100
51	u	19/71 (27%)	16 (84%)	3 (16%)	0	100	100
All	All	5361/5872 (91%)	5203 (97%)	155 (3%)	3 (0%)	56	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
3	2	32	LEU
10	F	139	PRO

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	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	216/220 (98%)	216 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	144/155 (93%)	143 (99%)	1 (1%)	85	96
10	F	145/147 (99%)	144 (99%)	1 (1%)	85	96
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	108/108 (100%)	107 (99%)	1 (1%)	81	94
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	99/102 (97%)	99 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	76/87 (87%)	76 (100%)	0	100	100
24	T	82/85 (96%)	82 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	54/56 (96%)	54 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
32	b	185/200 (92%)	182 (98%)	3 (2%)	65	88
33	c	175/198 (88%)	174 (99%)	1 (1%)	87	96
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	86/111 (78%)	86 (100%)	0	100	100
37	g	116/128 (91%)	114 (98%)	2 (2%)	63	87
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	98 (99%)	1 (1%)	78	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	62 (98%)	1 (2%)	65	88
47	q	72/76 (95%)	72 (100%)	0	100	100
48	r	47/66 (71%)	47 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	18/62 (29%)	17 (94%)	1 (6%)	23	54
All	All	4436/4756 (93%)	4424 (100%)	12 (0%)	93	98

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	b	147	GLU
33	c	45	LYS
39	i	104	ARG
32	b	133	LYS
37	g	92	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
21	Q	87	GLN
27	W	36	HIS
45	o	37	ASN
22	R	37	ASN
25	U	16	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	sN1	1524/1544 (98%)	212 (13%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	AN1	2888/2918 (98%)	493 (17%)	10 (0%)
6	B	114/115 (99%)	18 (15%)	1 (0%)
All	All	4526/4577 (98%)	723 (15%)	11 (0%)

5 of 723 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AN1	10	U
5	AN1	41	U
5	AN1	50	G
5	AN1	53	G
5	AN1	58	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	AN1	782	G
5	AN1	893	U
5	AN1	2170	C
5	AN1	478	A
5	AN1	1538	A

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	AN1	1907	5	16,21,22	1.13	1 (6%)	20,30,33	3.12	6 (30%)
5	3TD	AN1	1911	5	16,22,23	3.24	6 (37%)	19,32,35	1.55	3 (15%)
5	PSU	AN1	1913	5	16,21,22	1.06	1 (6%)	20,30,33	3.21	7 (35%)
5	5MU	AN1	1935	5	13,22,23	1.61	2 (15%)	14,32,35	3.00	2 (14%)
5	6MZ	AN1	2026	5	17,25,26	1.99	3 (17%)	15,36,39	4.27	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	7MG	AN1	2065	5	20,26,27	4.45	10 (50%)	24,39,42	1.77	6 (25%)
5	OMG	AN1	2247	5	18,26,27	3.50	7 (38%)	22,38,41	1.81	4 (18%)
5	2MG	AN1	2441	5	18,26,27	4.57	7 (38%)	19,38,41	2.20	8 (42%)
5	PSU	AN1	2453	5	16,21,22	1.11	2 (12%)	20,30,33	3.05	6 (30%)
5	2MA	AN1	2499	5,53	16,25,26	4.15	5 (31%)	17,37,40	2.48	5 (29%)
5	PSU	AN1	2500	5	16,21,22	1.15	2 (12%)	20,30,33	3.15	6 (30%)
5	OMU	AN1	2548	5	14,22,23	3.51	5 (35%)	17,31,34	0.63	0
5	PSU	AN1	2576	5	16,21,22	1.13	2 (12%)	20,30,33	3.06	6 (30%)
5	PSU	AN1	2601	5	16,21,22	1.11	1 (6%)	20,30,33	3.15	6 (30%)
5	PSU	AN1	952	5	16,21,22	1.14	2 (12%)	20,30,33	3.07	6 (30%)
31	2MG	sN1	1204	31	18,26,27	4.60	7 (38%)	19,38,41	2.29	8 (42%)
31	4OC	sN1	1399	31	16,23,24	3.46	6 (37%)	20,32,35	1.09	1 (5%)
31	UR3	sN1	1495	31	13,22,23	3.21	3 (23%)	15,32,35	0.66	0
31	MA6	sN1	1515	31	16,26,27	1.07	2 (12%)	16,38,41	4.13	3 (18%)
31	MA6	sN1	1516	31	16,26,27	1.07	2 (12%)	16,38,41	4.24	3 (18%)
31	PSU	sN1	513	31	16,21,22	1.06	1 (6%)	20,30,33	3.34	6 (30%)
31	7MG	sN1	524	31	20,26,27	4.54	10 (50%)	24,39,42	1.77	6 (25%)
31	2MG	sN1	963	31	18,26,27	4.66	7 (38%)	19,38,41	2.28	8 (42%)
31	5MC	sN1	964	31	14,22,23	3.23	5 (35%)	17,32,35	1.34	3 (17%)

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
5	PSU	AN1	1907	5	-	1/7/25/26	0/2/2/2
5	3TD	AN1	1911	5	-	3/7/25/26	0/2/2/2
5	PSU	AN1	1913	5	-	4/7/25/26	0/2/2/2
5	5MU	AN1	1935	5	-	0/3/25/26	0/2/2/2
5	6MZ	AN1	2026	5	-	2/5/27/28	0/3/3/3
5	7MG	AN1	2065	5	-	3/7/37/38	0/3/3/3
5	OMG	AN1	2247	5	-	0/5/27/28	0/3/3/3
5	2MG	AN1	2441	5	-	1/5/27/28	0/3/3/3
5	PSU	AN1	2453	5	-	0/7/25/26	0/2/2/2
5	2MA	AN1	2499	5,53	-	2/3/25/26	0/3/3/3
5	PSU	AN1	2500	5	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMU	AN1	2548	5	-	2/5/27/28	0/2/2/2
5	PSU	AN1	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	AN1	2601	5	-	0/7/25/26	0/2/2/2
5	PSU	AN1	952	5	-	0/7/25/26	0/2/2/2
31	2MG	sN1	1204	31	-	0/5/27/28	0/3/3/3
31	4OC	sN1	1399	31	-	2/7/29/30	0/2/2/2
31	UR3	sN1	1495	31	-	2/3/25/26	0/2/2/2
31	MA6	sN1	1515	31	-	0/7/29/30	0/3/3/3
31	MA6	sN1	1516	31	-	3/7/29/30	0/3/3/3
31	PSU	sN1	513	31	-	0/7/25/26	0/2/2/2
31	7MG	sN1	524	31	-	3/7/37/38	0/3/3/3
31	2MG	sN1	963	31	-	0/5/27/28	0/3/3/3
31	5MC	sN1	964	31	-	0/3/25/26	0/2/2/2

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	sN1	963	2MG	C2-N2	13.83	1.45	1.34
31	sN1	1204	2MG	C2-N2	13.56	1.45	1.34
5	AN1	2441	2MG	C2-N2	13.47	1.45	1.34
31	sN1	524	7MG	C4-N3	10.59	1.47	1.34
5	AN1	2065	7MG	C4-N3	10.43	1.47	1.34

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	1516	MA6	N1-C6-N6	-14.29	102.02	117.06
31	sN1	1515	MA6	N1-C6-N6	-13.87	102.46	117.06
5	AN1	2026	6MZ	C1'-N9-C4	-13.25	103.75	126.64
31	sN1	513	PSU	N1-C2-N3	-11.39	119.38	128.43
5	AN1	1913	PSU	N1-C2-N3	-10.62	119.99	128.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AN1	1913	PSU	O4'-C1'-C5-C4
5	AN1	1913	PSU	O4'-C1'-C5-C6
5	AN1	2548	OMU	C3'-C4'-C5'-O5'
5	AN1	2548	OMU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	sN1	1516	MA6	C5-C6-N6-C9

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AN1	1911	3TD	2	0
5	AN1	1913	PSU	1	0
5	AN1	2026	6MZ	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 95 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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.