



# wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 30, 2020 – 01:22 PM EST

PDB ID : 6V3A  
EMDB ID: : EMD-21031  
Title : Cryo-EM structure of the Acinetobacter baumannii Ribosome: 70S with E-site tRNA  
Authors : Morgan, C.E.; Yu, E.W.  
Deposited on : 2019-11-25  
Resolution : 2.82 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

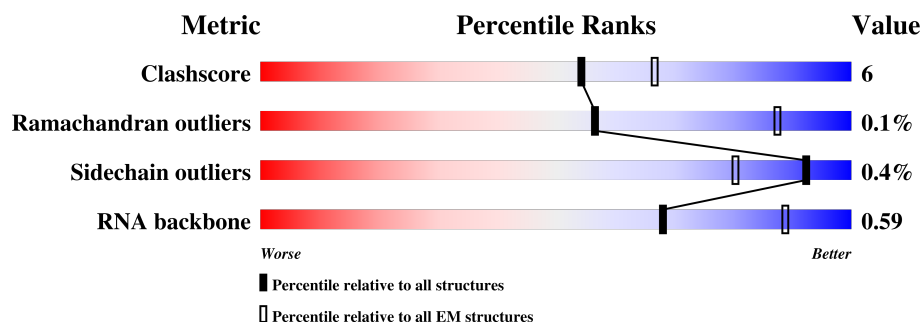
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.82 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  $\geq 3$ , 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	88% 12%
2	1	44	84% 16%
3	2	64	81% 13% . . .
4	3	38	82% 18%
5	AN1	2918	65% 29% 5% .
6	B	115	61% 32% 7%
7	C	274	82% 17% .
8	D	212	86% 14%

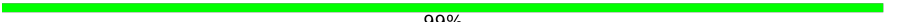
















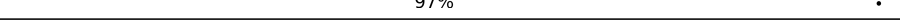


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Mol	Chain	Length	Quality of chain
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	
31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

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Mol	Chain	Length	Quality of chain
34	d	208	 99%
35	e	165	 94% 6%
36	f	127	 74% 26%
37	g	156	 90% 10%
38	h	131	 99% .
39	i	128	 98% ..
40	j	103	 97% .
41	k	128	 91% . 9%
42	l	124	 97% . .
43	m	118	 97% .
44	n	101	 98% ..
45	o	89	 99% .
46	p	101	 82% 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%
52	v	77	 65% 35%
53	w	3	 67% 33%

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 142113 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 a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	77	Total	C	N	O	P	S	0	0
			1636	733	291	535	76	1		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	AN1	49	Total	Mg	0
			49	49	
55	sN1	44	Total	Mg	0
			44	44	

- Molecule 56 is SODIUM ION (three-letter code: NA) (formula: Na).

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

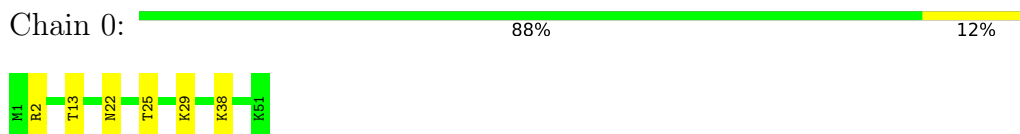
- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	AN1	319	Total	O	0
			319	319	
57	B	4	Total	O	0
			4	4	
57	C	5	Total	O	0
			5	5	
57	D	3	Total	O	0
			3	3	
57	E	3	Total	O	0
			3	3	
57	K	3	Total	O	0
			3	3	
57	O	1	Total	O	0
			1	1	
57	P	3	Total	O	0
			3	3	
57	Q	1	Total	O	0
			1	1	
57	U	1	Total	O	0
			1	1	
57	sN1	163	Total	O	0
			163	163	
57	i	5	Total	O	0
			5	5	
57	j	2	Total	O	0
			2	2	
57	m	1	Total	O	0
			1	1	
57	o	1	Total	O	0
			1	1	
57	p	1	Total	O	0
			1	1	
57	q	2	Total	O	0
			2	2	
57	t	2	Total	O	0
			2	2	

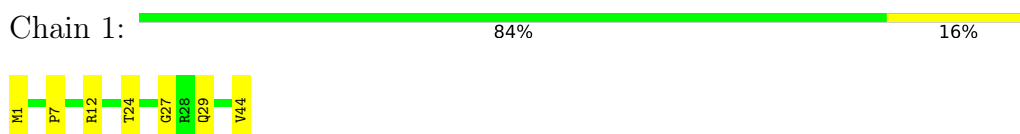
### 3 Residue-property plots

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.

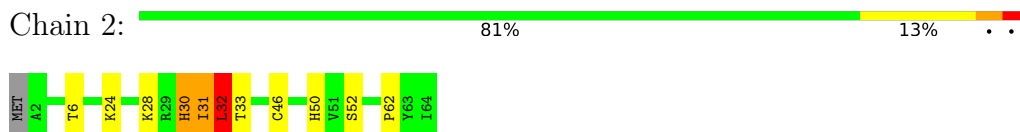
- Molecule 1: 50S ribosomal protein L33



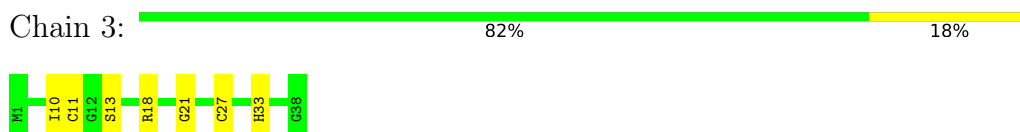
- Molecule 2: 50S ribosomal protein L34



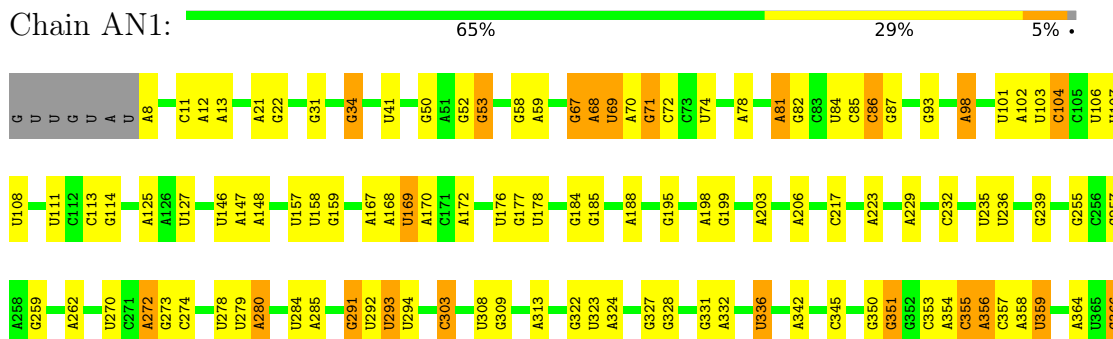
- Molecule 3: 50S ribosomal protein L35



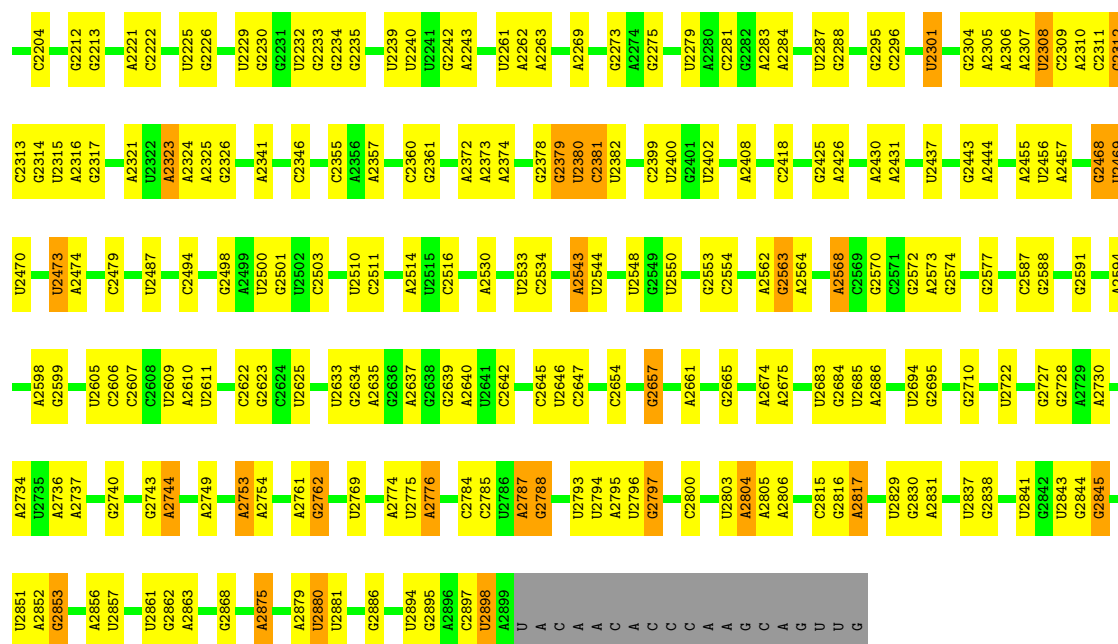
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 23S ribosomal RNA

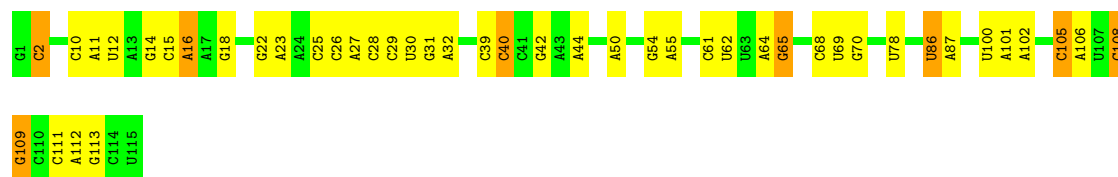


A2122	G2028	A1912	G1679	C1537	U1453	G1356	U1176	A1064	C958	C849	G711	A594	U503	A367
G2123	A2029	U1913	G1680	A1538	G1494	C1357	A1177	G1065	C961	A950	U712	G595	A504	C368
C2125	U2030	A1914	U1681	G1539	C1455	A1360	C1178	A1066	C961	G854	A713	U596	C508	A370
C2039	C2039	C1916	U1691	G1541	A1361	A1361	U1183	G1068	A970	G855	A714	C509	C511	G371
A2048	G2048	G1917	U1825	A1542	G1462	G1363	U1193	A1069	G971	G856	C715	U510	G511	U372
G2128	G2049	U1918	U1826	A1543	A1463	G1363	U1194	A1070	A976	G857	A716	C516	C516	A373
G2130	A2050	G1920	G1711	G1544	A1464	G1364	U1194	C1076	A977	G862	U717	G517	U386	
A2139	C2051	U1921	G1712	U1545	A1465	G1366	U1199	C1077	A978	C963	A719	C518	A519	
C2133	G2052	U1922	U1713	U1549	G1470	G1366	A1200	U1078	A980	G610	C721	U520	U520	G395
U2142	A2056	G1925	G1714	G1550	U1471	A1373	A1201	U1080	A981	G873	G724	A612	G521	A403
A2143	G2057	A1843	G1717	A1564	U1472	U1374	G1227	A1081	G990	A876	G727	A625	C526	G410
G2144	A2058	U1718	U1844	G1565	G1473	G1375	U1226	A1082	C991	G877	A728	G826	A527	A411
G2145	C2059	G1927	U1719	G1566	C1475	A1378	G1227	G1084	A993	G878	U745	A627	A528	C412
U2146	C2060	U1928	U1725	A1567	U1476	A1381	G1230	G1085	A997	G879	C753	A630	G529	C413
G2147	C2061	G1929	C1726	A1569	U1478	U1382	G1231	A1086	A998	G880	A754	C530	C530	A414
C2148	A1932	U1855	U1731	A1570	U1479	A1387	A1242	A1087	U1004	G881	G761	A631	A531	U415
A2149	U1860	U1855	G1734	U1576	U1483	U1388	G1245	U1091	C1004	C983	A762	G633	A537	C416
U2151	A1861	A1862	A1735	A1577	U1484	A1390	G1245	A1092	U1009	A884	G763	A634	C541	U418
G2152	U1935	G1863	G1742	G1582	G1485	A1393	A1248	A1095	C1010	C887	C763	A635	G542	C419
G2153	U1936	G1864	C1743	G1583	G1487	G1393	G1251	G1096	G1023	C988	G773	G636	U543	G423
C2068	A1937	A1865	C1744	U1584	A1488	A1408	G1259	A1100	A1025	G889	G774	U637	U544	G424
C2069	G1938	A1866	U1745	G1585	A1489	A1409	G1260	G1101	A1026	A890	U780	U643	C545	C425
C2070	C1938	A1867	G1746	U1586	A1490	G1411	G1261	A1102	G1027	A894	A781	U644	G546	U426
U2071	U1939	A1868	G1749	U1587	A1491	G1412	A1267	A1103	G1028	C995	G782	A644	U547	A427
C2077	G1940	G1870	C1750	C1589	G1496	G1413	G1276	G1104	G1029	U651	G783	U652	U552	A428
A2078	C1961	A1871	A1751	C1590	U1500	U1415	U1277	A1108	U1030	A653	A787	A654	A554	C434
U2082	U1962	A1872	G1752	G1591	U1502	U1415	G1278	G1109	G1031	A898	U788	U655	A561	G437
G2083	C1963	C1875	G1759	G1593	C1503	G1423	A1296	U1110	U1032	C900	G803	U656	A561	A438
G2089	A1966	U1879	G1760	U1595	U1504	G1424	G1304	C1111	A1036	U904	G804	G657	U564	C455
C2096	U1967	G1880	C1767	A1596	U1506	G1425	G1305	G1112	A1037	A908	U805	U663	U569	A456
A2097	G1968	A1881	U1769	C1603	U1507	G1427	G1306	G1113	G1038	A664	C810	A664	A570	G462
C2098	U1978	A1885	A1769	G1604	C1508	A1428	G1307	U1129	G1039	A909	C810	U665	U571	G462
U2104	U1987	A1886	U1775	G1605	U1509	A1429	U1307	A1130	C1040	C912	A817	G666	A572	A465
U2105	G1988	C1888	A1776	A1606	G1510	G1430	U1308	A1131	U1041	A916	U825	A668	A573	A469
G2106	U1989	G1889	A1776	A1606	G1510	G1431	U1309	C1132	U1042	A916	U825	A668	U574	A469
U2107	C1993	A1895	A1780	A1616	A1520	C1432	C1309	A1140	G1044	C929	U825	A673	G575	C474
G2108	U2018	G1902	U1792	G1617	C1522	U1433	G1311	G1149	A1045	U930	G828	A674	G577	A478
U2109	A2010	A1899	C1793	A1624	A1523	A1435	G1312	G1154	G1052	A675	G829	A675	U578	A478
G2111	G1903	G1902	U1794	A1624	A1524	U1436	U1324	U1165	G1053	A938	U830	A678	C579	A479
G2112	C1904	G1903	G1795	C1642	G1528	U1437	U1336	A1166	A1054	A942	A831	G679	G581	G480
A2113	U1905	C1905	A1797	U1645	U1529	C1441	G1336	U1167	U1057	G943	G832	A678	U567	G493
G2114	G2020	C1905	A1797	U1646	C1531	C1442	U1340	A1170	G1059	A944	G843	U684	A588	C494
A2115	C2021	G1906	A1798	U1646	C1531	C1442	U1340	U1171	G1060	A844	G843	U684	U567	G493
G2116	U2022	U1907	A1799	G1647	U1532	C1442	U1340	U1172	G1061	A845	A844	U684	A588	C494
U2119	A1908	A1908	A1799	G1647	U1532	C1442	U1340	U1172	G1061	A845	A844	U684	A588	C494
A2120	G2025	C1909	A1805	G1672	U1533	G1447	A1348	U1171	G1061	U955	A845	U684	A588	C494
G2120	A1909	A1909	A1806	C1673	U1534	U1448	A1349	U1172	U1062	U955	A845	U684	A588	C494
G2121	C1673	C1673	G1807	C1673	U1535	U1449	A1349	U1172	U1062	U955	A845	U684	A588	C494
					U1536	U1449	A1349	U1172	U1062	U955	A845	U684	A588	C494
					A1536	U1449	A1349	U1172	U1062	U955	A845	U684	A588	C494



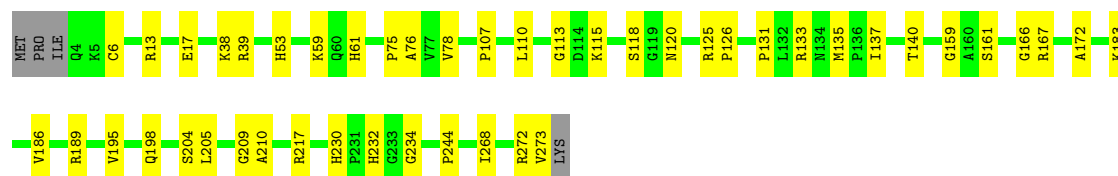
- Molecule 6: 5s ribosomal RNA

Chain B: 61% 32% 7%



- Molecule 7: 50S ribosomal protein L2

Chain C: 82% 17%



- Molecule 8: 50S ribosomal protein L3

Chain D: 86% 14%



- Molecule 9: 50S ribosomal protein L4

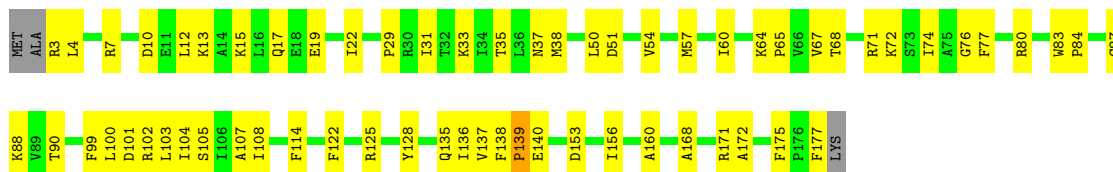
Chain E: 83% 11% 7%





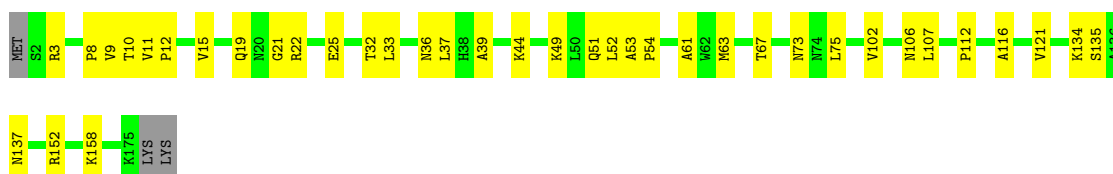
• Molecule 10: 50S ribosomal protein L5

Chain F: 63% 35% ..



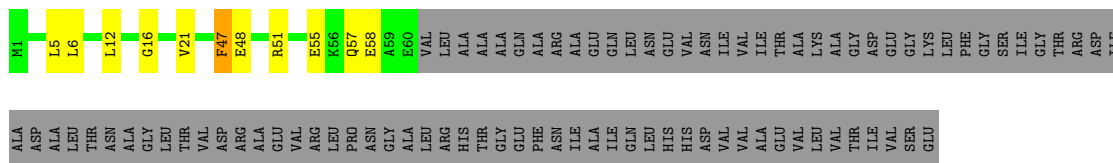
• Molecule 11: 50S ribosomal protein L6

Chain G: 77% 21% .



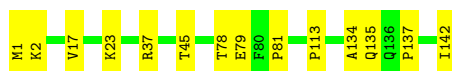
• Molecule 12: 50S ribosomal protein L9

Chain H: 33% 7% . 59%



• Molecule 13: 50S ribosomal protein L13

Chain I: 90% 10%



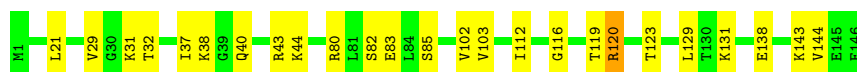
• Molecule 14: 50S ribosomal protein L14

Chain J: 91% 9%



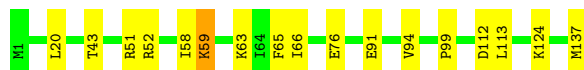
• Molecule 15: 50S ribosomal protein L15

Chain K: 83% 16% .



- Molecule 16: 50S ribosomal protein L16

Chain L: 88% 12% .



- Molecule 17: 50S ribosomal protein L17

Chain M: 85% 10% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N: 84% 14% .



- Molecule 19: 50S ribosomal protein L19

Chain O: 80% 16% .



- Molecule 20: 50S ribosomal protein L20

Chain P: 92% 6% .



- Molecule 21: 50S ribosomal protein L21

Chain Q: 83% 17%

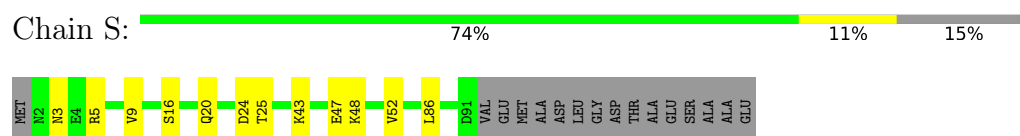


- Molecule 22: 50S ribosomal protein L22

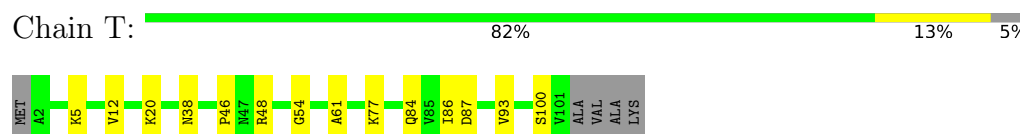
Chain R: 93% 7%



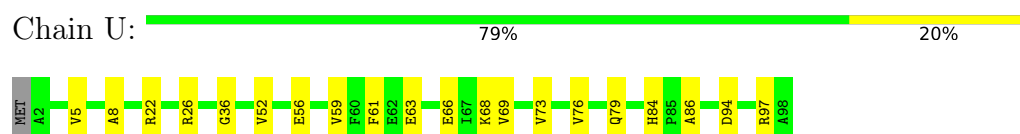
- Molecule 23: 50S ribosomal protein L23



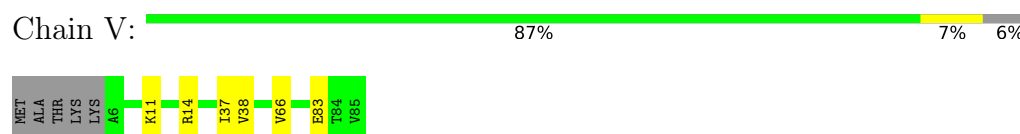
- Molecule 24: 50S ribosomal protein L24



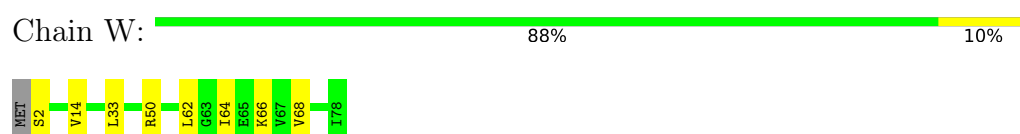
- Molecule 25: 50S ribosomal protein L25



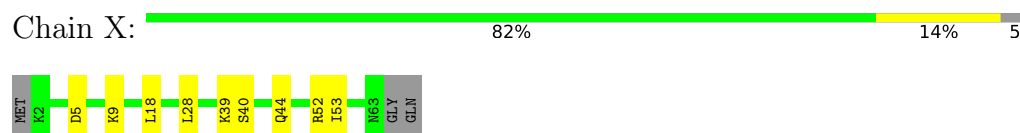
- Molecule 26: 50S ribosomal protein L27



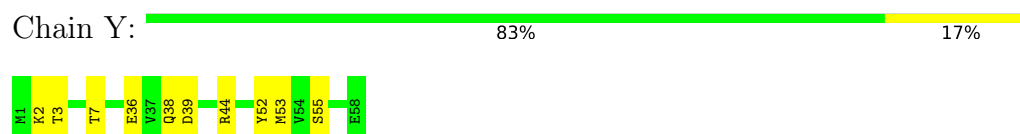
- Molecule 27: 50S ribosomal protein L28



- Molecule 28: 50S ribosomal protein L29



- Molecule 29: 50S ribosomal protein L30



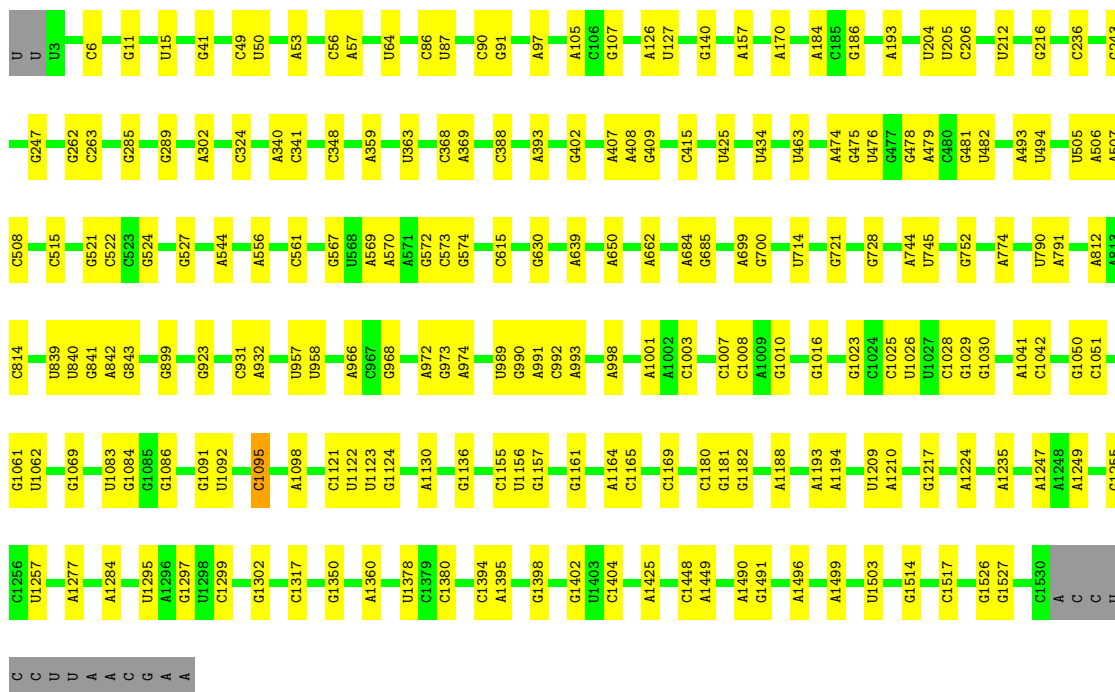
- Molecule 30: 50S ribosomal protein L32





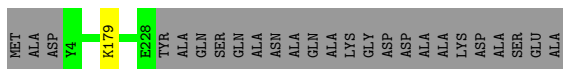
- Molecule 31: 16s Ribosomal RNA

Chain sN1:  86% 13%



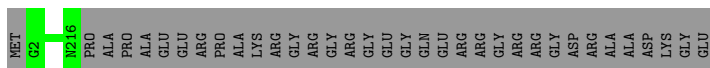
- Molecule 32: 30S ribosomal protein S2

Chain b:  90% 10%



- Molecule 33: 30S ribosomal protein S3

Chain c:  86% 14%



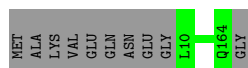
- Molecule 34: 30S ribosomal protein S4

Chain d:  99%



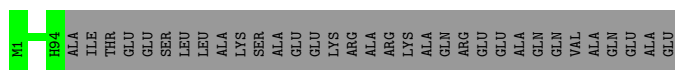
- Molecule 35: 30S ribosomal protein S5

Chain e:  94% 6%




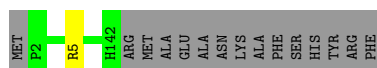
- Molecule 36: 30S ribosomal protein S6

Chain f:  74% 26%



- Molecule 37: 30S ribosomal protein S7

Chain g:  90% 10%



- Molecule 38: 30S ribosomal protein S8

Chain h:  99% .



- Molecule 39: 30S ribosomal protein S9

Chain i:  98% ..



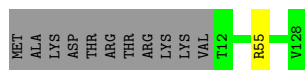
- Molecule 40: 30S ribosomal protein S10

Chain j:  97% .



- Molecule 41: 30S ribosomal protein S11

Chain k:  91% . 9%



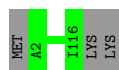
- Molecule 42: 30S ribosomal protein S12

Chain l:  97% ..



- Molecule 43: 30S ribosomal protein S13

Chain m: 97%



- Molecule 44: 30S ribosomal protein S14

Chain n: 98%



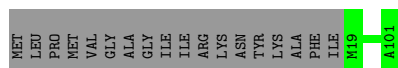
- Molecule 45: 30S ribosomal protein S15

Chain o: 99%



- Molecule 46: 30S ribosomal protein S16

Chain p: 82% 18%



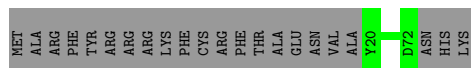
- Molecule 47: 30S ribosomal protein S17

Chain q: 94% 6%



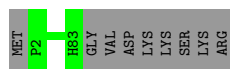
- Molecule 48: 30S ribosomal protein S18

Chain r: 71% 29%

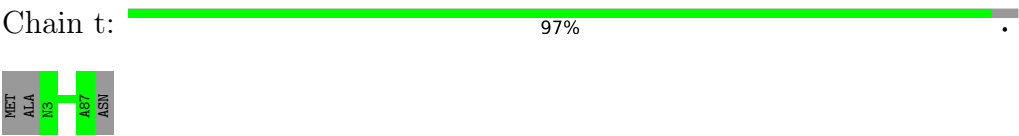


- Molecule 49: 30S ribosomal protein S19

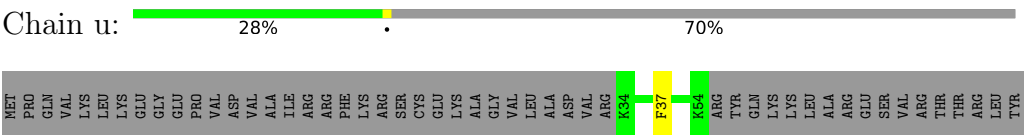
Chain s: 90% 10%



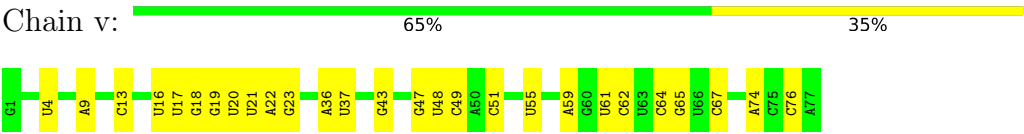
● Molecule 50: 30S ribosomal protein S20



● Molecule 51: 30S ribosomal protein S21



● Molecule 52: tRNA-met



● Molecule 53: mRNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	90845	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, H2U, NA, MG, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 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	0	0.24	0/434	0.40	0/573
10	F	0.26	0/1401	0.49	0/1877
11	G	0.25	0/1337	0.43	0/1807
12	H	0.25	0/461	0.51	0/616
13	I	0.25	0/1151	0.41	0/1551
14	J	0.24	0/956	0.44	0/1286
15	K	0.25	0/1097	0.44	0/1461
16	L	0.24	0/1104	0.44	0/1475
17	M	0.24	0/956	0.41	0/1282
18	N	0.24	0/865	0.46	0/1156
19	O	0.24	0/931	0.43	0/1249
2	1	0.23	0/367	0.39	0/481
20	P	0.25	0/947	0.34	0/1262
21	Q	0.23	0/818	0.45	0/1094
22	R	0.24	0/831	0.40	0/1113
23	S	0.25	0/708	0.41	0/947
24	T	0.24	0/753	0.48	0/1010
25	U	0.24	0/770	0.41	0/1036
26	V	0.25	0/606	0.44	0/810
27	W	0.22	0/642	0.41	0/856
28	X	0.24	0/499	0.39	0/662
29	Y	0.23	0/468	0.41	0/624
3	2	0.24	0/515	0.55	1/678 (0.1%)
30	Z	0.22	0/462	0.41	0/615
31	sN1	0.19	0/36476	0.75	5/56895 (0.0%)
32	b	0.26	0/1799	0.49	0/2429
33	c	0.23	0/1714	0.42	0/2304
34	d	0.24	0/1653	0.41	0/2213
35	e	0.24	0/1141	0.43	0/1537
36	f	0.24	0/808	0.47	0/1089
37	g	0.23	0/1127	0.40	0/1511

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	h	0.24	0/993	0.41	0/1331
39	i	0.24	0/1006	0.41	0/1346
4	3	0.23	0/296	0.48	0/389
40	j	0.23	0/811	0.42	0/1096
41	k	0.24	0/878	0.43	0/1189
42	l	0.23	0/958	0.46	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	0.43	0/858
48	r	0.24	0/445	0.39	0/601
49	s	0.23	0/664	0.40	0/897
5	AN1	0.22	0/69101	0.77	19/107780 (0.0%)
50	t	0.24	0/664	0.34	0/885
51	u	0.30	0/184	0.51	0/240
52	v	0.18	0/1739	0.76	0/2709
53	w	0.23	0/72	0.94	0/110
6	B	0.19	0/2739	0.77	0/4266
7	C	0.24	0/2136	0.43	0/2869
8	D	0.24	0/1590	0.45	0/2142
9	E	0.24	0/1440	0.40	0/1944
All	All	0.22	0/153241	0.69	25/229576 (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
51	u	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	1308	U	C2-N1-C1'	7.42	126.61	117.70
31	sN1	415	C	N3-C2-O2	-7.38	116.73	121.90
31	sN1	1095	C	N1-C2-O2	7.08	123.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	32	LEU	CA-CB-CG	6.96	131.31	115.30
31	sN1	1095	C	N3-C2-O2	-6.58	117.29	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	HIS	Peptide
12	H	47	PHE	Peptide
51	u	37	PHE	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	3	0
2	1	363	0	401	5	0
3	2	509	0	566	9	0
4	3	295	0	327	5	0
5	AN1	62023	0	31193	492	0
6	B	2450	0	1241	34	0
7	C	2096	0	2157	32	0
8	D	1572	0	1610	22	0
9	E	1419	0	1464	17	0
10	F	1381	0	1433	53	0
11	G	1318	0	1373	26	0
12	H	458	0	480	9	0
13	I	1125	0	1148	12	0
14	J	946	0	1007	6	0
15	K	1089	0	1159	15	0
16	L	1087	0	1162	10	0
17	M	942	0	987	8	0
18	N	857	0	899	12	0
19	O	919	0	973	14	0
20	P	934	0	997	6	0
21	Q	807	0	842	13	0
22	R	826	0	894	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	S	702	0	756	6	0
24	T	749	0	797	8	0
25	U	760	0	783	13	0
26	V	598	0	600	3	0
27	W	632	0	667	5	0
28	X	498	0	537	5	0
29	Y	463	0	488	7	0
30	Z	456	0	448	10	0
31	sN1	32782	0	16506	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	v	1636	0	832	0	0
53	w	65	0	33	0	0
54	3	1	0	0	0	0
55	AN1	49	0	0	0	0
55	sN1	44	0	0	0	0
56	AN1	1	0	0	0	0
57	AN1	319	0	0	1	0
57	B	4	0	0	0	0
57	C	5	0	0	0	0
57	D	3	0	0	0	0
57	E	3	0	0	0	0
57	K	3	0	0	0	0
57	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	P	3	0	0	0	0
57	Q	1	0	0	0	0
57	U	1	0	0	0	0
57	i	5	0	0	0	0
57	j	2	0	0	0	0
57	m	1	0	0	0	0
57	o	1	0	0	0	0
57	p	1	0	0	0	0
57	q	2	0	0	0	0
57	sN1	163	0	0	0	0
57	t	2	0	0	0	0
All	All	142113	0	94276	786	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 786 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	1.45	1.15
5:AN1:1463:A:N7	5:AN1:1544:G:O6	1.99	0.96
6:B:70:G:H21	6:B:101:A:H62	1.00	0.93
6:B:70:G:N2	6:B:101:A:H62	1.70	0.89
6:B:2:C:O2	6:B:113:G:N2	2.06	0.89

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
1	0	49/51 (96%)	48 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	2	61/64 (95%)	58 (95%)	1 (2%)	2 (3%)	4	14
4	3	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	C	268/274 (98%)	260 (97%)	8 (3%)	0	100	100
8	D	209/212 (99%)	204 (98%)	5 (2%)	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	58
11	G	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
12	H	58/148 (39%)	56 (97%)	1 (2%)	1 (2%)	10	30
13	I	140/142 (99%)	138 (99%)	2 (1%)	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%)	133 (98%)	2 (2%)	0	100	100
17	M	117/125 (94%)	117 (100%)	0	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	112 (97%)	3 (3%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	94 (93%)	7 (7%)	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%)	94 (96%)	4 (4%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	78/85 (92%)	78 (100%)	0	0	100	100
27	W	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
28	X	60/65 (92%)	60 (100%)	0	0	100	100
29	Y	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	Z	53/61 (87%)	52 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	207 (93%)	16 (7%)	0	100	100
33	c	213/250 (85%)	207 (97%)	6 (3%)	0	100	100
34	d	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	f	92/127 (72%)	89 (97%)	3 (3%)	0	100	100
37	g	139/156 (89%)	138 (99%)	1 (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
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
42	l	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
43	m	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	p	81/101 (80%)	80 (99%)	1 (1%)	0	100	100
47	q	78/85 (92%)	78 (100%)	0	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%)	5209 (97%)	148 (3%)	4 (0%)	56	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
3	2	32	LEU
10	F	139	PRO
12	H	48	GLU

### 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%)	46 (98%)	1 (2%)	56	85
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%)	215 (100%)	1 (0%)	90	96
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	144/155 (93%)	144 (100%)	0	100	100
10	F	145/147 (99%)	144 (99%)	1 (1%)	85	96
11	G	139/142 (98%)	138 (99%)	1 (1%)	85	96
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%)	106 (98%)	2 (2%)	60	86
16	L	113/113 (100%)	112 (99%)	1 (1%)	81	94
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%)	80 (98%)	2 (2%)	52	82
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%)	184 (100%)	1 (0%)	90	96
33	c	175/198 (88%)	175 (100%)	0	100	100
34	d	170/171 (99%)	169 (99%)	1 (1%)	87	96
35	e	113/120 (94%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	86/111 (78%)	86 (100%)	0	100	100
37	g	116/128 (91%)	115 (99%)	1 (1%)	81	94
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	98 (99%)	1 (1%)	78	93
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	87 (99%)	1 (1%)	76	93
42	l	104/106 (98%)	102 (98%)	2 (2%)	60	86
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	80 (99%)	1 (1%)	74	92
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
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%)	18 (100%)	0	100	100
All	All	4436/4756 (93%)	4419 (100%)	17 (0%)	92	97

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	T	48	ARG
24	T	77	LYS
41	k	55	ARG
16	L	59	LYS
42	l	44	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
25	U	16	GLN
32	b	80	ASN
45	o	40	GLN
25	U	79	GLN
29	Y	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	sN1	1524/1544 (98%)	204 (13%)	0
5	AN1	2888/2918 (98%)	494 (17%)	10 (0%)
52	v	76/77 (98%)	27 (35%)	0
53	w	2/3 (66%)	1 (50%)	0
6	B	114/115 (99%)	21 (18%)	1 (0%)
All	All	4604/4657 (98%)	747 (16%)	11 (0%)

5 of 747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AN1	21	A
5	AN1	22	G
5	AN1	34	G
5	AN1	41	U
5	AN1	50	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 ⓘ

28 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	1.11	1 (6%)	20,30,33	3.12	6 (30%)
5	3TD	AN1	1911	5	16,22,23	3.23	6 (37%)	19,32,35	1.52	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PSU	AN1	1913	5	16,21,22	1.05	1 (6%)	20,30,33	3.20	7 (35%)
5	5MU	AN1	1935	5	13,22,23	1.62	2 (15%)	14,32,35	2.99	2 (14%)
5	6MZ	AN1	2026	5	17,25,26	2.00	3 (17%)	15,36,39	4.31	4 (26%)
5	7MG	AN1	2065	5	20,26,27	4.46	10 (50%)	24,39,42	1.76	6 (25%)
5	OMG	AN1	2247	5	18,26,27	3.52	7 (38%)	22,38,41	1.77	5 (22%)
5	2MG	AN1	2441	5	18,26,27	4.57	7 (38%)	19,38,41	2.23	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	55,5	16,25,26	4.14	5 (31%)	17,37,40	2.44	5 (29%)
5	PSU	AN1	2500	5	16,21,22	1.14	1 (6%)	20,30,33	3.14	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	1.12	2 (12%)	20,30,33	3.04	6 (30%)
5	PSU	AN1	2601	5	16,21,22	1.10	1 (6%)	20,30,33	3.17	6 (30%)
5	PSU	AN1	952	5	16,21,22	1.11	1 (6%)	20,30,33	3.12	6 (30%)
31	2MG	sN1	1204	31	18,26,27	4.62	7 (38%)	19,38,41	2.24	8 (42%)
31	4OC	sN1	1399	31	16,23,24	3.47	6 (37%)	20,32,35	1.09	1 (5%)
31	UR3	sN1	1495	31	13,22,23	3.21	3 (23%)	15,32,35	0.67	0
31	MA6	sN1	1515	31	16,26,27	1.08	2 (12%)	16,38,41	4.18	3 (18%)
31	MA6	sN1	1516	31	16,26,27	1.07	2 (12%)	16,38,41	4.42	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	4.61	7 (38%)	19,38,41	2.27	8 (42%)
31	5MC	sN1	964	31	14,22,23	3.22	5 (35%)	17,32,35	1.35	2 (11%)
52	H2U	v	20	52	17,21,22	3.24	4 (23%)	20,30,33	2.74	5 (25%)
52	5MU	v	55	52	13,22,23	1.67	2 (15%)	14,32,35	2.94	2 (14%)
52	PSU	v	56	52	16,21,22	1.03	1 (6%)	20,30,33	3.23	7 (35%)
52	4SU	v	8	52	13,21,22	4.42	5 (38%)	14,30,33	1.40	2 (14%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	55,5	-	2/3/25/26	0/3/3/3
5	PSU	AN1	2500	5	-	0/7/25/26	0/2/2/2
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	-	0/3/25/26	0/2/2/2
31	MA6	sN1	1515	31	-	3/7/29/30	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
52	H2U	v	20	52	-	3/7/38/39	0/2/2/2
52	5MU	v	55	52	-	2/3/25/26	0/2/2/2
52	PSU	v	56	52	-	3/7/25/26	0/2/2/2
52	4SU	v	8	52	-	2/3/25/26	0/2/2/2

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	sN1	1204	2MG	C2-N2	13.65	1.45	1.34
31	sN1	963	2MG	C2-N2	13.62	1.45	1.34
5	AN1	2441	2MG	C2-N2	13.49	1.45	1.34
52	v	8	4SU	C5-C4	10.81	1.51	1.38
31	sN1	524	7MG	C4-N3	10.59	1.47	1.34

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	1516	MA6	N1-C6-N6	-14.99	101.28	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	1515	MA6	N1-C6-N6	-14.13	102.19	117.06
5	AN1	2026	6MZ	C1'-N9-C4	-13.40	103.48	126.64
31	sN1	513	PSU	N1-C2-N3	-11.28	119.46	128.43
52	v	56	PSU	N1-C2-N3	-10.89	119.77	128.43

There are no chirality outliers.

5 of 39 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'
31	sN1	1515	MA6	C5-C6-N6-C9

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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