



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

Aug 8, 2018 – 01:39 AM EDT

PDB ID : 6GXP  
EMDB ID: : EMD-0083  
Title : Cryo-EM structure of a rotated E. coli 70S ribosome in complex with RF3-GDPCP(RF3-only)  
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.  
Deposited on : 2018-06-27  
Resolution : 4.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 1.7.3 (157068), CSD as539be (2018)  
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) : rb-20031172

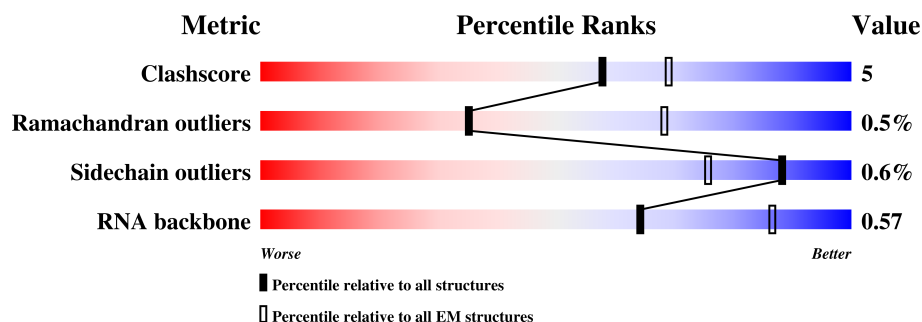
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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.
















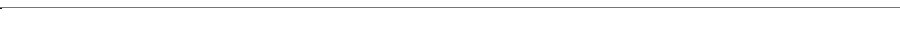


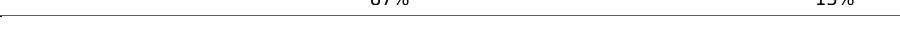
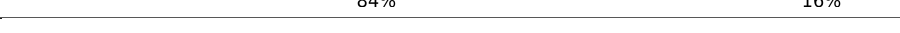







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	A	2903	62% 32% 5%
2	B	120	56% 39% 5%
3	C	271	82% 18%
4	D	209	85% 15%
5	E	201	86% 14%
6	F	177	82% 18%
7	G	176	91% 8% .
8	H	149	83% 17%

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Mol	Chain	Length	Quality of chain
9	I	141	 87% 13%
10	J	142	 88% 12%
11	K	122	 81% 19%
12	L	143	 87% 13%
13	M	136	 87% 13%
14	N	120	 88% 12%
15	O	116	 89% 11%
16	P	114	 86% 14%
17	Q	117	 91% 9%
18	R	103	 85% 15%
19	S	110	 87% 13%
20	T	93	 80% 20%
21	U	102	 90% 10%
22	V	94	 84% 16%
23	W	75	 92% 8%
24	X	77	 87% 13%
25	Y	63	 84% 16%
26	Z	58	 84% 16%
27	0	56	 88% 13%
28	1	50	 92% 8%
29	2	46	 80% 20%
30	3	64	 86% 11%
31	4	38	 92% 8%
32	5	131	 79% 21%
33	a	1539	 81% 17%

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Mol	Chain	Length	Quality of chain
34	b	218	97% .
35	c	206	99% .
36	d	205	99% .
37	e	157	98% ..
38	f	100	96% .
39	g	151	99% .
40	h	129	100% .
41	i	127	98% ..
42	j	98	100% .
43	k	112	96% . ..
44	l	123	98% .
45	m	114	98% ..
46	n	101	100% .
47	o	88	100% .
48	p	82	99% .
49	q	80	96% .
50	r	65	100% .
51	s	79	99% .
52	t	85	100% .
53	u	65	98% .
54	w	529	92% . 6%
55	z	14	93% . 7%

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 147637 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2896	Total	C	N	O	P	0	0
			62177	27736	11444	20101	2896		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1063812051
A	1847	G	A	conflict	GB 1063812051

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1373146531

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.



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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	112	Total	C	N	O	S	0	0
			829	511	161	154	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 54 is a protein called Peptide chain release factor RF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	499	Total	C	N	O	S	0	0
			3943	2498	680	745	20		

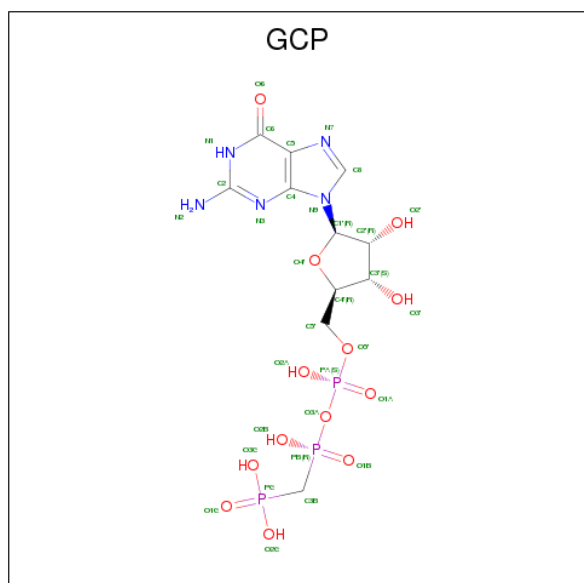
- Molecule 55 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	z	14	Total	C	N	O	0	0
			120	80	25	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP Q8WSY8

- Molecule 56 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).

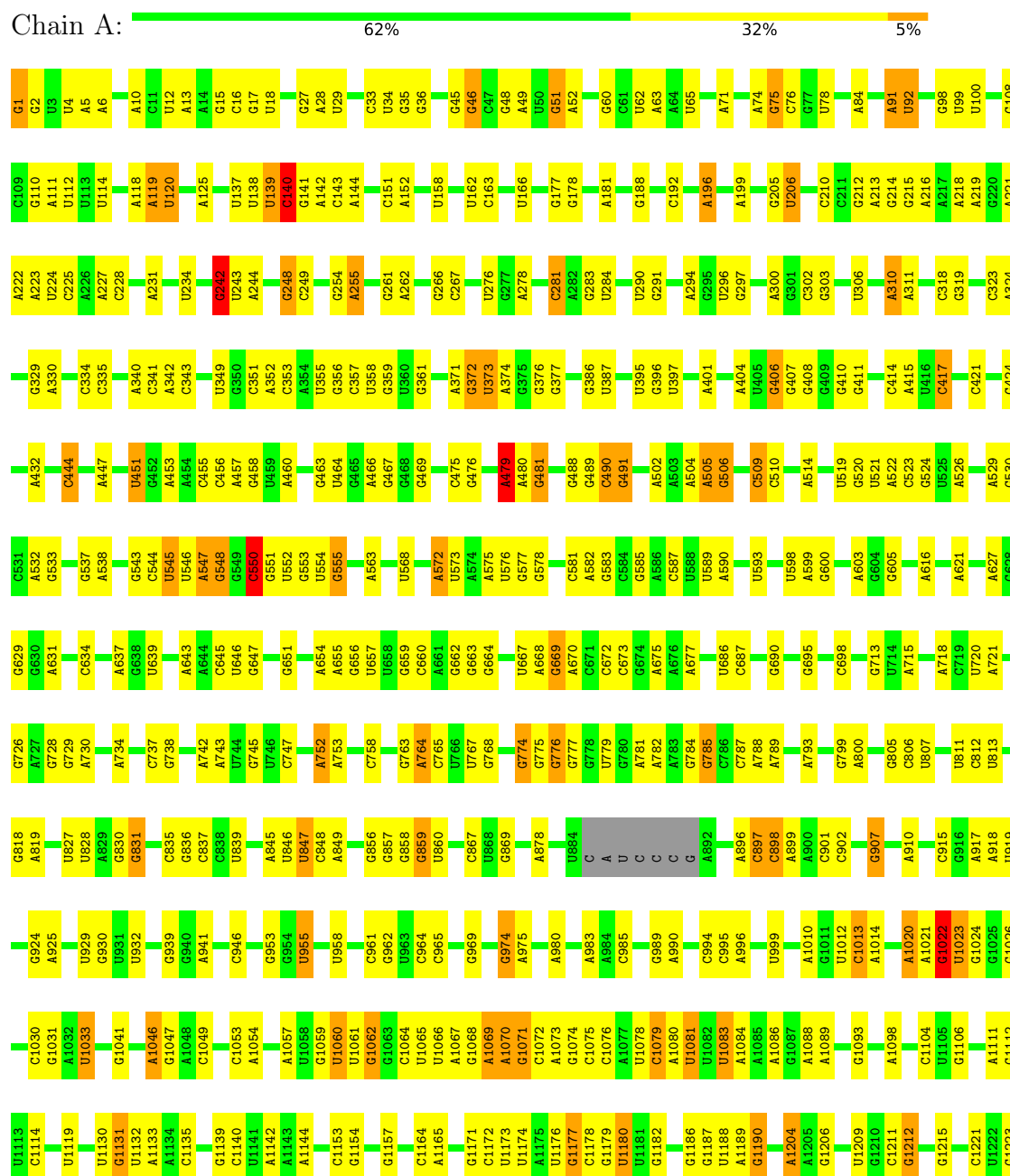


Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			32	11	5	13	3	

### 3 Residue-property plots

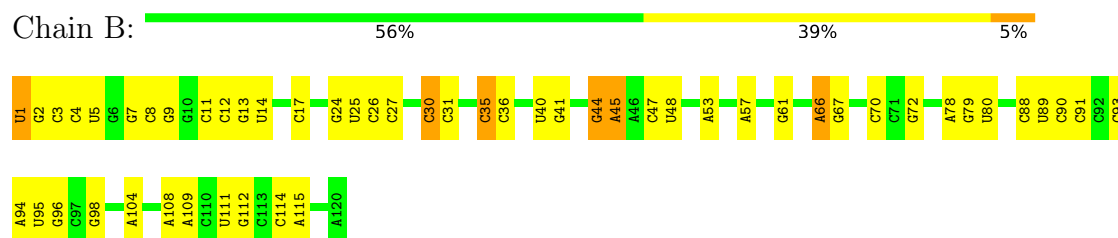
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 23S ribosomal RNA

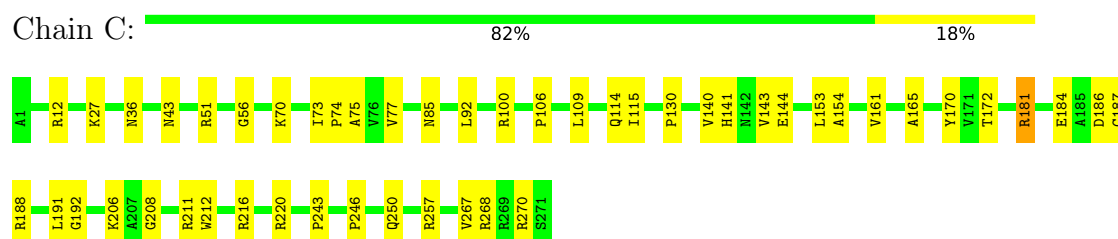


G2834	G2835	G2836	G2837	G2846	G2847	G2848	G2849	G2850	G2851	G2861	G2862	G2863	G2864	G2867	G2868	G2872	G2873	G2880	G2883	G2884	G2893	G2894	G2898	G2899	G2900	G2901	G2902	G2903
G2732	A2733	U2739	U2739	U2743	G2744	G2746	G2747	G2748	G2749	G2750	G2751	C2752	C2755	C2762	G2763	A2764	A2765	U2768	U2769	G2770	C2771	A2778	U2779	G2780	A2781	G2782	C2788	G2791
G2621	G2629	G2630	G2631	A2634	A2635	G2636	C2646	G2647	G2648	A2654	G2655	G2656	C2659	A2660	A2664	A2665	G2667	A2665	C2666	C2676	A2682	C2683	U2689	U2690	C2691	G2692	G2693	G2694
G2529	A2530	A2531	G2535	A2547	U2552	G2553	U2554	U2555	U2556	C2559	U2560	A2564	A2565	A2566	A2567	G2570	U2571	A2572	C2573	G2576	U2580	G2581	G2582	U2585	U2586	A2590	C2591	G2592
A2435	U2441	A2442	C2443	G2444	G2447	A2448	U2449	U2457	G2458	A2459	U2460	A2468	U2473	U2474	C2475	A2476	U2477	A2478	G2484	G2487	U2491	G2494	A2497	C2498	G2502	A2503	U2504	U2505
G2325	C2326	A2327	A2328	U2329	G2330	A2333	U2334	A2335	A2336	C2342	G2345	A2346	C2350	C2354	G2357	G2361	U2372	G2373	C2374	C2380	A2381	G2382	G2383	U2384	C2385	G2391	A2392	U2393
G2234	G2238	G2239	U2240	A2241	U2245	G2246	A2247	G2248	U2249	G2250	G2251	G2252	G2253	C2254	C2258	A2266	G2267	A2268	C2273	G2279	C2283	G2286	A2287	G2289	G2290	U2291	U2292	G2293
G2133	G2136	U2137	G2140	G2141	G2144	C2145	A2146	G2149	G2157	G2162	A2163	C2164	A2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	A2183	A2184	U2185	G2186	U2189	G2190	A2191
G2033	A2033	U2034	G2035	U2036	A2037	G2043	C2047	G2048	G2049	A2051	A2052	C2055	A2060	G2061	A2062	C2063	U2068	G2069	A2070	A2071	C2072	U2076	U2081	A2082	U2086	G2087	A2088	G2093
G1930	A1936	A1937	U1938	U1939	U1940	C1941	U1944	G1945	A1953	G1954	U1955	U1956	A1960	C1961	U1963	A1966	C1967	A1970	U1971	U1972	G1986	A1987	U1991	G1992	C1996	C1997	A1998	G2002
U1827	G1828	A1829	U1830	G1831	G1832	C1833	U1834	U1835	G1839	G1840	U1841	G1842	U1847	A1848	A1858	G1862	C1870	C1871	U1880	G1884	C1892	C1893	G1896	A1899	A1900	A1901	G1906	G1907
U1729	C1730	G1731	G1732	G1733	G1737	G1738	A1744	A1745	A1746	G1753	A1757	U1758	U1759	C1760	G1761	A1762	C1764	U1769	U1770	A1773	C1774	U1779	A1780	U1781	U1782	A1783	A1784	U1796
U1607	A1610	C1611	G1612	G1613	A1634	A1635	U1636	A1637	C1638	C1646	U1647	U1648	G1651	A1652	G1653	A1656	A1657	A1664	A1665	U1667	G1668	A1669	U1673	C1670	G1674	C1675	G1681	G1682
G1475	U1476	G1482	A1490	A1491	G1492	C1493	G1500	G1501	A1502	A1503	A1504	A1509	G1510	A1515	A1516	A1517	A1522	U1523	G1524	A1532	C1533	U1534	A1535	C1536	G1537	A1544	G1555	G1428
G1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1395	C1399	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1428	G1429	G1430	U1431
U1224	G1225	A1237	U1242	A1247	G1248	U1249	C1250	C1251	C1252	A1253	U1254	U1255	G1256	G1270	G1271	A1272	A1287	G1288	C1289	G1290	C1291	C1292	C1293	C1417	C1295	G1296	A1321	A1322
U1324	G1325	U1326	U1329	C1330	G1333	G1334	G1341	C1345	G1346	A1347	C1348	G1428	G1429	G1430	G1431	G1432	A1433	G1434	G1435	G1436	G1437	C1447	G1450	G1451	G1452	G1453	G1454	G1461
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U1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1395	C1399	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1428	G1429	G1430	U1431
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U1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1395	C1399	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1428	G1429	G1430	U1431
U1324	G1325	U1326	U1329	C1330	G1333	G1334	G1341	C1345	G1346	A1347	C1348	G1428	G1429	G1430	G1431	G1432	A1433	G1434	G1435	G1436	G1437	C1447	G1450	G1451	G1452	G1453	G1454	G1461
U1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1395	C1399	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1428	G1429	G1430	U1431
U1324	G1325	U1326	U1329	C1330	G1333	G1334	G1341	C1345	G1346	A1347	C1348	G1428	G1429	G1430	G1431	G1432	A1433	G1434	G1435	G1436	G1437	C1447	G1450	G1451	G1452	G1453	G1454	G1461
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U1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1395	C1399	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1428	G1429	G1430	U1431
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U1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1395	C1399	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1428	G1429	G1430	U1431
U1324	G1325	U1326	U1329	C1330	G1333	G1334	G1341	C1345	G1346	A1347	C1348	G1428	G1429	G1430	G1431	G1432	A1433	G1434	G1435	G1436	G1437	C1447	G1450	G1451	G1452	G1453	G1454	G1461
U1349	C1350	C1351	G1355	G1356	A1365	G1368	G1369	C1376	G1377	A1378	G1380	A1383	C1386	A1387	A1394	A1												

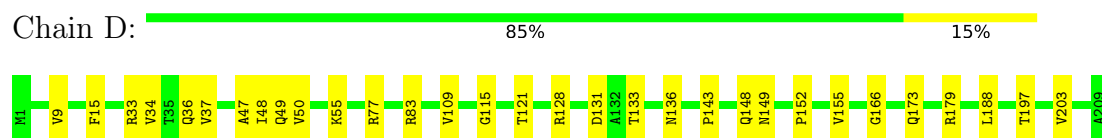
- Molecule 2: 5S ribosomal RNA



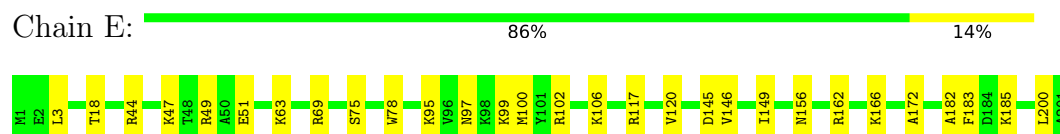
- Molecule 3: 50S ribosomal protein L2



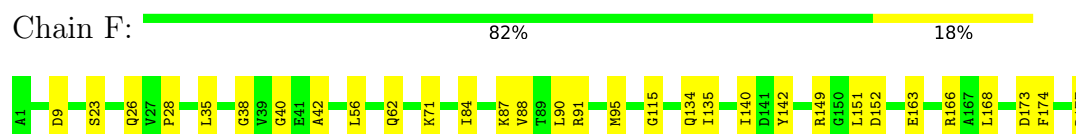
- Molecule 4: 50S ribosomal protein L3



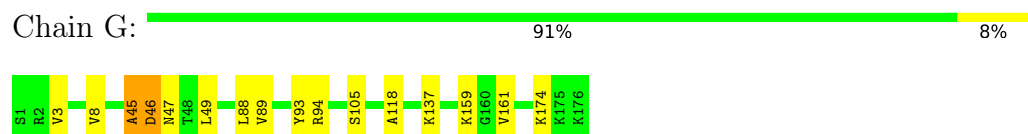
- Molecule 5: 50S ribosomal protein L4



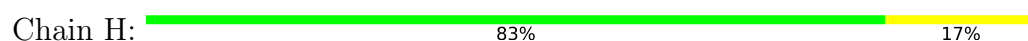
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9







• Molecule 9: 50S ribosomal protein L11

Chain I: 87% 13%



• Molecule 10: 50S ribosomal protein L13

Chain J: 88% 12%



• Molecule 11: 50S ribosomal protein L14

Chain K: 81% 19%



• Molecule 12: 50S ribosomal protein L15

Chain L: 87% 13%



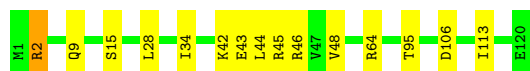
• Molecule 13: 50S ribosomal protein L16

Chain M: 87% 13%



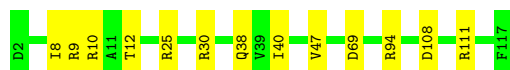
• Molecule 14: 50S ribosomal protein L17

Chain N: 88% 12%



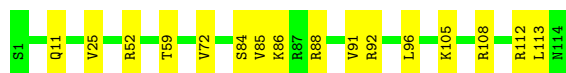
• Molecule 15: 50S ribosomal protein L18

Chain O: 89% 11%



- Molecule 16: 50S ribosomal protein L19

Chain P:  86% 14%




- Molecule 17: 50S ribosomal protein L20

Chain Q:  91% 9%




- Molecule 18: 50S ribosomal protein L21

Chain R:  85% 15%




- Molecule 19: 50S ribosomal protein L22

Chain S:  87% 13%




- Molecule 20: 50S ribosomal protein L23

Chain T:  80% 20%




- Molecule 21: 50S ribosomal protein L24

Chain U:  90% 10%




- Molecule 22: 50S ribosomal protein L25

Chain V:  84% 16%




- Molecule 23: 50S ribosomal protein L27

Chain W:  92% 8%




- Molecule 24: 50S ribosomal protein L28

Chain X:  87% 13%




- Molecule 25: 50S ribosomal protein L29

Chain Y:  84% 16%




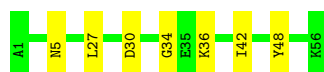
- Molecule 26: 50S ribosomal protein L30

Chain Z:  84% 16%



- Molecule 27: 50S ribosomal protein L32

Chain 0:  88% 13%




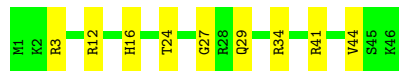
- Molecule 28: 50S ribosomal protein L33

Chain 1:  92% 8%




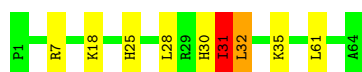
- Molecule 29: 50S ribosomal protein L34

Chain 2:  80% 20%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  86% 11% ..



- Molecule 31: 50S ribosomal protein L36

Chain 4: 92% 8%



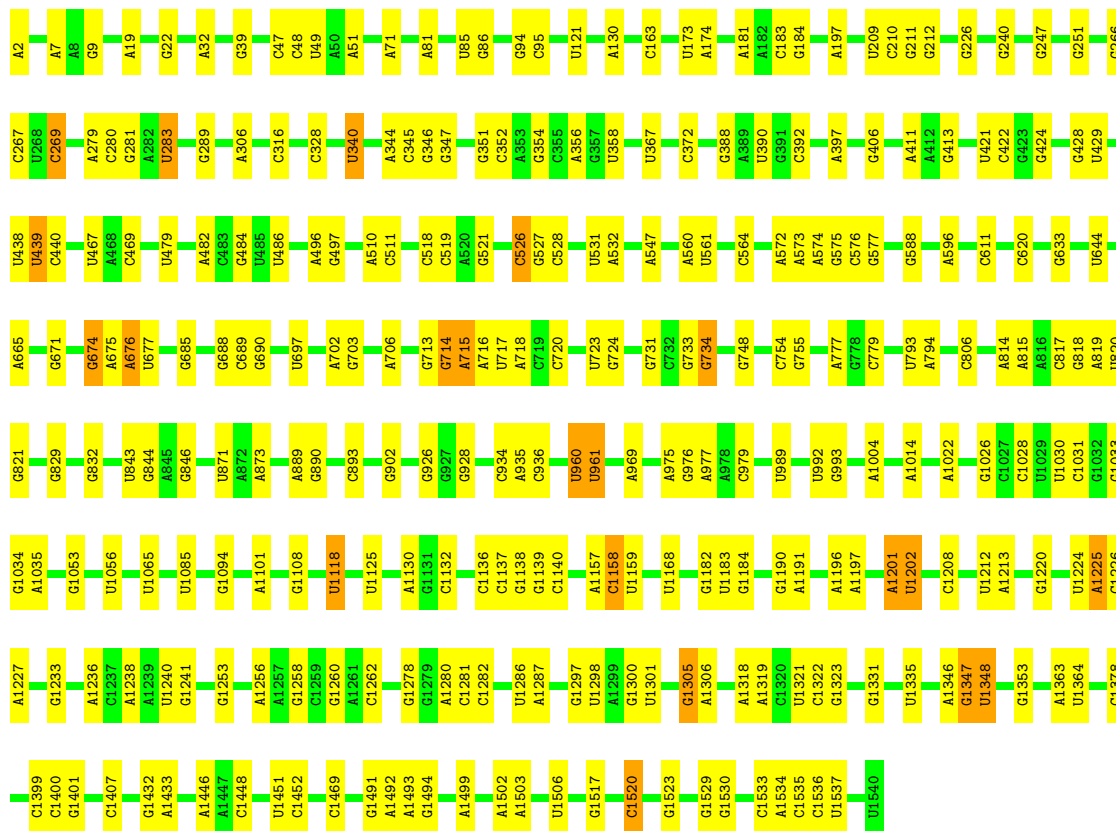
- Molecule 32: 50S ribosomal protein L10

Chain 5: 79% 21%



- Molecule 33: 16S ribosomal RNA

Chain a: 81% 17%



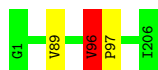
- Molecule 34: 30S ribosomal protein S2

Chain b: 97%



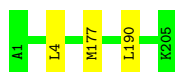
- Molecule 35: 30S ribosomal protein S3

Chain c:  99%



- Molecule 36: 30S ribosomal protein S4

Chain d:  99%



- Molecule 37: 30S ribosomal protein S5

Chain e:  98%



- Molecule 38: 30S ribosomal protein S6

Chain f:  96%



- Molecule 39: 30S ribosomal protein S7

Chain g:  99%



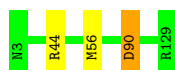
- Molecule 40: 30S ribosomal protein S8

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: 30S ribosomal protein S9

Chain i:  98%



- Molecule 42: 30S ribosomal protein S10

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 30S ribosomal protein S11

Chain k:  96% ..



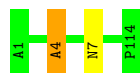
- Molecule 44: 30S ribosomal protein S12

Chain l:  98% .



- Molecule 45: 30S ribosomal protein S13

Chain m:  98% ..



- Molecule 46: 30S ribosomal protein S14

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S15

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S16

Chain p:  99% .



- Molecule 49: 30S ribosomal protein S17

Chain q:  96% .



- Molecule 50: 30S ribosomal protein S18

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 30S ribosomal protein S19

Chain s:  99%



- Molecule 52: 30S ribosomal protein S20

Chain t:  100%

There are no outlier residues recorded for this chain.

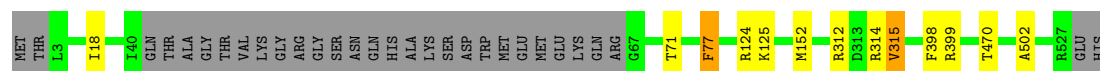
- Molecule 53: 30S ribosomal protein S21

Chain u:  98%



- Molecule 54: Peptide chain release factor RF3

Chain w:  92%



- Molecule 55: Apidaecin

Chain z:  93%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30535	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 ( $e^-/\text{\AA}^2$ )	45.9	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	A	0.29	1/69638 (0.0%)	1.00	229/108636 (0.2%)
10	J	0.25	0/1152	0.46	0/1551
11	K	0.28	0/947	0.54	0/1268
12	L	0.27	0/1054	0.53	0/1403
13	M	0.28	0/1093	0.58	1/1460 (0.1%)
14	N	0.26	0/973	0.52	0/1301
15	O	0.26	0/902	0.46	0/1209
16	P	0.25	0/929	0.51	1/1242 (0.1%)
17	Q	0.26	0/960	0.46	0/1278
18	R	0.26	0/829	0.51	0/1107
19	S	0.24	0/864	0.49	0/1156
2	B	0.38	1/2876 (0.0%)	1.16	31/4483 (0.7%)
20	T	0.26	0/744	0.53	0/994
21	U	0.30	0/787	0.55	0/1051
22	V	0.25	0/766	0.48	0/1025
23	W	0.26	0/582	0.42	0/769
24	X	0.24	0/635	0.46	0/848
25	Y	0.23	0/510	0.47	0/677
26	Z	0.24	0/453	0.50	0/605
27	0	0.23	0/450	0.46	0/599
28	1	0.26	0/416	0.50	0/554
29	2	0.24	0/380	0.44	0/498
3	C	0.25	0/2121	0.51	0/2852
30	3	0.25	0/513	0.64	2/676 (0.3%)
31	4	0.30	0/303	0.75	2/397 (0.5%)
32	5	0.30	0/1001	0.63	0/1350
33	a	0.31	5/36965 (0.0%)	1.01	101/57658 (0.2%)
34	b	0.28	0/1735	0.55	0/2338
35	c	0.26	0/1651	0.51	1/2225 (0.0%)
36	d	0.26	0/1665	0.54	2/2227 (0.1%)
37	e	0.27	0/1154	0.58	0/1554
38	f	0.31	0/835	0.62	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	g	0.27	0/1195	0.54	0/1602
4	D	0.26	0/1586	0.50	0/2134
40	h	0.27	0/989	0.56	0/1326
41	i	0.27	0/1034	0.58	0/1375
42	j	0.27	0/796	0.61	0/1077
43	k	0.48	3/845 (0.4%)	0.71	3/1145 (0.3%)
44	l	0.28	0/969	0.59	0/1300
45	m	0.28	0/892	0.57	0/1193
46	n	0.24	0/811	0.50	0/1081
47	o	0.24	0/722	0.52	0/964
48	p	0.26	0/659	0.51	0/884
49	q	0.28	0/657	0.58	0/881
5	E	0.25	0/1571	0.46	0/2113
50	r	0.25	0/511	0.52	0/689
51	s	0.27	0/652	0.51	0/877
52	t	0.28	0/671	0.48	0/888
53	u	0.31	0/500	0.62	0/668
54	w	0.29	0/4016	0.61	3/5428 (0.1%)
55	z	0.26	0/127	0.48	0/175
6	F	0.28	0/1434	0.55	0/1926
7	G	0.26	0/1343	0.52	1/1816 (0.1%)
8	H	0.26	0/1122	0.47	0/1515
9	I	0.29	0/1046	0.55	0/1410
All	All	0.29	10/160031 (0.0%)	0.90	377/238586 (0.2%)

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
11	K	0	1
13	M	0	1
18	R	0	1
21	U	0	1
30	3	0	1
32	5	0	1
34	b	0	2
37	e	0	1
38	f	0	2
39	g	0	1
41	i	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	l	0	1
45	m	0	1
48	p	0	1
49	q	0	1
54	w	0	3
6	F	0	2
7	G	0	3
All	All	0	26

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-10.61	1.48	1.61
2	B	1	U	OP3-P	-10.57	1.48	1.61
33	a	2	A	OP3-P	-10.56	1.48	1.61
33	a	716	A	C1'-N9	7.29	1.59	1.48
33	a	715	A	C5-C6	-6.55	1.35	1.41

The worst 5 of 377 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	715	A	N1-C6-N6	16.59	128.55	118.60
33	a	715	A	C5-C6-N6	-12.93	113.36	123.70
33	a	715	A	C5-N7-C8	-12.41	97.69	103.90
33	a	715	A	C4-C5-N7	12.12	116.76	110.70
33	a	715	A	N7-C8-N9	11.91	119.76	113.80

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	173	ASP	Peptide
6	F	174	PHE	Peptide
7	G	118	ALA	Peptide
7	G	45	ALA	Peptide
7	G	46	ASP	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	A	62177	0	31271	431	0
2	B	2572	0	1302	22	0
3	C	2082	0	2157	31	0
4	D	1565	0	1616	18	0
5	E	1552	0	1619	20	0
6	F	1410	0	1447	20	0
7	G	1323	0	1374	7	0
8	H	1111	0	1148	14	0
9	I	1032	0	1088	11	0
10	J	1129	0	1162	12	0
11	K	938	0	1012	15	0
12	L	1045	0	1117	12	0
13	M	1074	0	1157	9	0
14	N	960	0	1000	11	0
15	O	892	0	923	10	0
16	P	917	0	965	10	0
17	Q	947	0	1022	9	0
18	R	816	0	839	10	0
19	S	857	0	922	8	0
20	T	738	0	807	14	0
21	U	779	0	834	4	0
22	V	753	0	780	8	0
23	W	575	0	592	3	0
24	X	625	0	655	8	0
25	Y	509	0	543	9	0
26	Z	449	0	491	5	0
27	0	444	0	461	5	0
28	1	409	0	440	2	0
29	2	377	0	418	7	0
30	3	504	0	574	6	0
31	4	302	0	343	1	0
32	5	988	0	1025	14	0
33	a	33016	0	16619	0	0
34	b	1704	0	1732	0	0
35	c	1624	0	1699	0	0
36	d	1643	0	1710	0	0
37	e	1141	0	1170	0	0
38	f	817	0	808	0	0
39	g	1181	0	1240	0	0
40	h	979	0	1034	0	0
41	i	1022	0	1070	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	j	786	0	828	0	0
43	k	829	0	826	0	0
44	l	955	0	1019	0	0
45	m	883	0	944	0	0
46	n	799	0	841	0	0
47	o	714	0	737	0	0
48	p	649	0	666	0	0
49	q	648	0	691	0	0
50	r	504	0	502	0	0
51	s	637	0	665	0	0
52	t	665	0	714	0	0
53	u	495	0	486	0	0
54	w	3943	0	3934	0	0
55	z	120	0	128	0	0
56	w	32	0	13	0	0
All	All	147637	0	101180	661	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 5.

The worst 5 of 661 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)
1:A:593:U:H3	1:A:664:G:H1	1.12	0.97
1:A:1476:U:H3	1:A:1515:A:H62	0.99	0.94
1:A:545:U:H3	1:A:548:G:H1	1.02	0.94
1:A:2475:C:H42	1:A:2529:G:N2	1.67	0.92
1:A:306:U:H3	1:A:310:A:H62	0.96	0.91

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	
3	C	269/271 (99%)	260 (97%)	9 (3%)	0	100	100
4	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
6	F	175/177 (99%)	162 (93%)	13 (7%)	0	100	100
7	G	174/176 (99%)	162 (93%)	9 (5%)	3 (2%)	10	48
8	H	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
9	I	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
12	L	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	24	66
13	M	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	11	51
14	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
15	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
19	S	108/110 (98%)	99 (92%)	8 (7%)	1 (1%)	19	60
20	T	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
21	U	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	17	58
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
24	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
25	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
26	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
28	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
29	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	55 (89%)	5 (8%)	2 (3%)	4	35
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	101 (78%)	27 (21%)	1 (1%)	21	64
34	b	216/218 (99%)	194 (90%)	21 (10%)	1 (0%)	31	73
35	c	204/206 (99%)	196 (96%)	6 (3%)	2 (1%)	17	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	d	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
37	e	155/157 (99%)	142 (92%)	11 (7%)	2 (1%)	13	53
38	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	8	45
39	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
40	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
41	i	125/127 (98%)	109 (87%)	15 (12%)	1 (1%)	21	64
42	j	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
43	k	110/112 (98%)	96 (87%)	12 (11%)	2 (2%)	9	47
44	l	121/123 (98%)	96 (79%)	23 (19%)	2 (2%)	10	48
45	m	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	19	60
46	n	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
47	o	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
48	p	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
49	q	78/80 (98%)	65 (83%)	12 (15%)	1 (1%)	13	53
50	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
51	s	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
52	t	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
53	u	63/65 (97%)	49 (78%)	13 (21%)	1 (2%)	11	50
54	w	495/529 (94%)	432 (87%)	59 (12%)	4 (1%)	21	64
55	z	12/14 (86%)	11 (92%)	0	1 (8%)	1	15
All	All	6286/6422 (98%)	5731 (91%)	524 (8%)	31 (0%)	35	73

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	46	ASP
13	M	58	LYS
30	3	31	ILE
35	c	96	VAL
38	f	53	LYS

### 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	
3	C	216/216 (100%)	213 (99%)	3 (1%)	69	85
4	D	164/164 (100%)	163 (99%)	1 (1%)	87	93
5	E	165/165 (100%)	164 (99%)	1 (1%)	87	93
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	137 (100%)	0	100	100
8	H	114/114 (100%)	114 (100%)	0	100	100
9	I	109/109 (100%)	109 (100%)	0	100	100
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/103 (100%)	103 (100%)	0	100	100
12	L	102/102 (100%)	102 (100%)	0	100	100
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	100/100 (100%)	99 (99%)	1 (1%)	78	89
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	99 (100%)	0	100	100
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	83 (99%)	1 (1%)	74	87
19	S	93/93 (100%)	92 (99%)	1 (1%)	76	87
20	T	80/80 (100%)	80 (100%)	0	100	100
21	U	83/83 (100%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/57 (100%)	56 (98%)	1 (2%)	62	82
24	X	67/67 (100%)	66 (98%)	1 (2%)	67	84
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/48 (100%)	48 (100%)	0	100	100
27	0	47/47 (100%)	47 (100%)	0	100	100
28	1	45/45 (100%)	45 (100%)	0	100	100
29	2	38/38 (100%)	38 (100%)	0	100	100
30	3	51/51 (100%)	51 (100%)	0	100	100
31	4	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	5	100/100 (100%)	100 (100%)	0	100	100
34	b	180/180 (100%)	177 (98%)	3 (2%)	63	83
35	c	170/170 (100%)	168 (99%)	2 (1%)	74	87
36	d	172/172 (100%)	171 (99%)	1 (1%)	87	93
37	e	114/119 (96%)	113 (99%)	1 (1%)	81	90
38	f	87/87 (100%)	87 (100%)	0	100	100
39	g	124/124 (100%)	123 (99%)	1 (1%)	83	91
40	h	104/104 (100%)	104 (100%)	0	100	100
41	i	105/105 (100%)	104 (99%)	1 (1%)	78	89
42	j	86/86 (100%)	86 (100%)	0	100	100
43	k	85/85 (100%)	82 (96%)	3 (4%)	39	67
44	l	103/103 (100%)	103 (100%)	0	100	100
45	m	92/92 (100%)	91 (99%)	1 (1%)	76	87
46	n	79/83 (95%)	79 (100%)	0	100	100
47	o	76/76 (100%)	76 (100%)	0	100	100
48	p	65/65 (100%)	65 (100%)	0	100	100
49	q	74/74 (100%)	73 (99%)	1 (1%)	69	85
50	r	48/56 (86%)	48 (100%)	0	100	100
51	s	70/70 (100%)	69 (99%)	1 (1%)	69	85
52	t	65/65 (100%)	65 (100%)	0	100	100
53	u	44/55 (80%)	44 (100%)	0	100	100
54	w	427/453 (94%)	422 (99%)	5 (1%)	74	87
55	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5201/5255 (99%)	5171 (99%)	30 (1%)	88	93

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	c	89	VAL
37	e	69	ASN
54	w	125	LYS
36	d	177	MET
39	g	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
31	4	37	GLN
37	e	134	ASN
54	w	445	GLN
32	5	4	ASN
36	d	70	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	538 (18%)	29 (1%)
2	B	119/120 (99%)	15 (12%)	2 (1%)
33	a	1536/1539 (99%)	251 (16%)	0
All	All	4548/4562 (99%)	804 (17%)	31 (0%)

5 of 804 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	U
1	A	1378	A
1	A	2808	G
1	A	1182	G
1	A	1399	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
56	GCP	w	601	54	25,34,34	2.37	7 (28%)	31,54,54	1.75	4 (12%)

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
56	GCP	w	601	54	-	0/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	601	GCP	C4-N9	-7.33	1.38	1.47
56	w	601	GCP	C5-C6	-4.59	1.44	1.52
56	w	601	GCP	C8-N9	-3.18	1.37	1.46
56	w	601	GCP	C5-C4	-2.30	1.38	1.52
56	w	601	GCP	PB-O2B	-2.14	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	601	GCP	C5-C6-N1	-5.32	111.93	118.27
56	w	601	GCP	PA-O3A-PB	-2.55	124.14	132.42
56	w	601	GCP	O6-C6-C5	3.70	127.44	119.82
56	w	601	GCP	C4-C5-N7	6.09	110.53	102.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	a	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2179:C	O3'	2180:U	P	3.63
1	a	917:G	O3'	918:A	P	3.57
1	a	1394:A	O3'	1395:C	P	3.30