



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

Feb 13, 2019 – 02:47 PM EST

PDB ID : 6GXN  
EMDB ID: : EMD-0081  
Title : Cryo-EM structure of an E. coli 70S ribosome in complex with RF3-GDPCP, RF1(GAQ) and Pint-tRNA (State III)  
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.  
Deposited on : 2018-06-27  
Resolution : 3.90 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-20031633

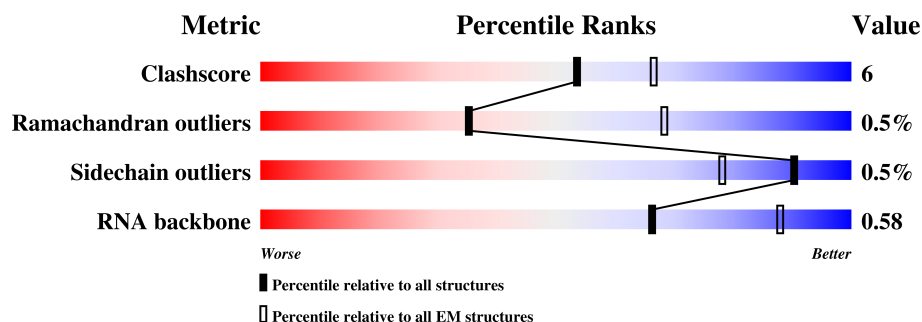
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.
















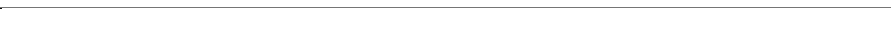

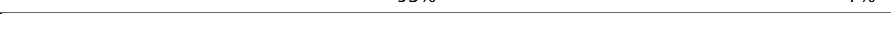
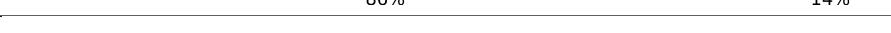
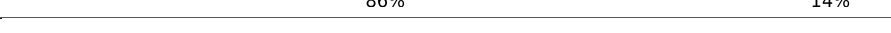







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	I	141	
10	J	142	
11	K	122	
12	L	143	
13	M	136	
14	N	120	
15	O	116	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	93	
21	U	102	
22	V	94	
23	W	75	
24	X	77	
25	Y	63	
26	Z	58	
27	0	56	
28	1	50	
29	2	46	
30	3	64	
31	4	38	
32	5	131	
33	7	7	

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Mol	Chain	Length	Quality of chain
34	a	1539	84% 15% .
35	b	218	97% .
36	c	206	99% .
37	d	205	98% .
38	e	157	97% ..
39	f	100	97% ..
40	g	151	99% .
41	h	129	100%
42	i	127	98% ..
43	j	98	99% .
44	k	116	99% .
45	l	123	98% .
46	m	114	98% .
47	n	101	100%
48	o	88	100%
49	p	82	100%
50	q	80	96% .
51	r	65	100%
52	s	79	100%
53	t	85	100%
54	u	65	98% .
55	v	350	98% ..
56	w	529	91% . 6%
57	x	77	68% 30% .
58	z	14	93% 7%

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 151860 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	2895	Total	C	N	O	P	0	0
			62153	27726	11439	20093	2895		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1036415628
A	1847	G	A	conflict	GB 1036415628

- 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	-	expression tag	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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	7	Total	C	N	O	P	0	0
			151	68	29	47	7		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	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 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

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

- Molecule 52 is a protein called 30S ribosomal protein S19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

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

- Molecule 55 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	348	Total	C	N	O	S	0	0
			2436	1483	469	475	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	167	CYS	SER	conflict	UNP P0A7I0

- Molecule 56 is a protein called Peptide chain release factor RF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	496	Total	C	N	O	S	0	0
			3923	2487	674	742	20		

- Molecule 57 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

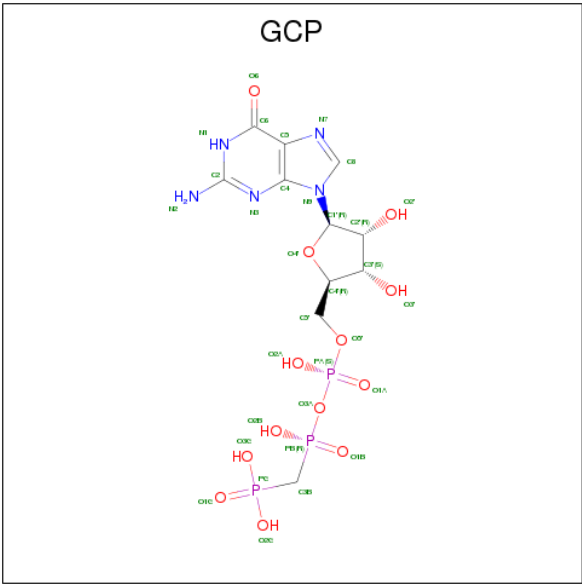
- Molecule 58 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	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 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

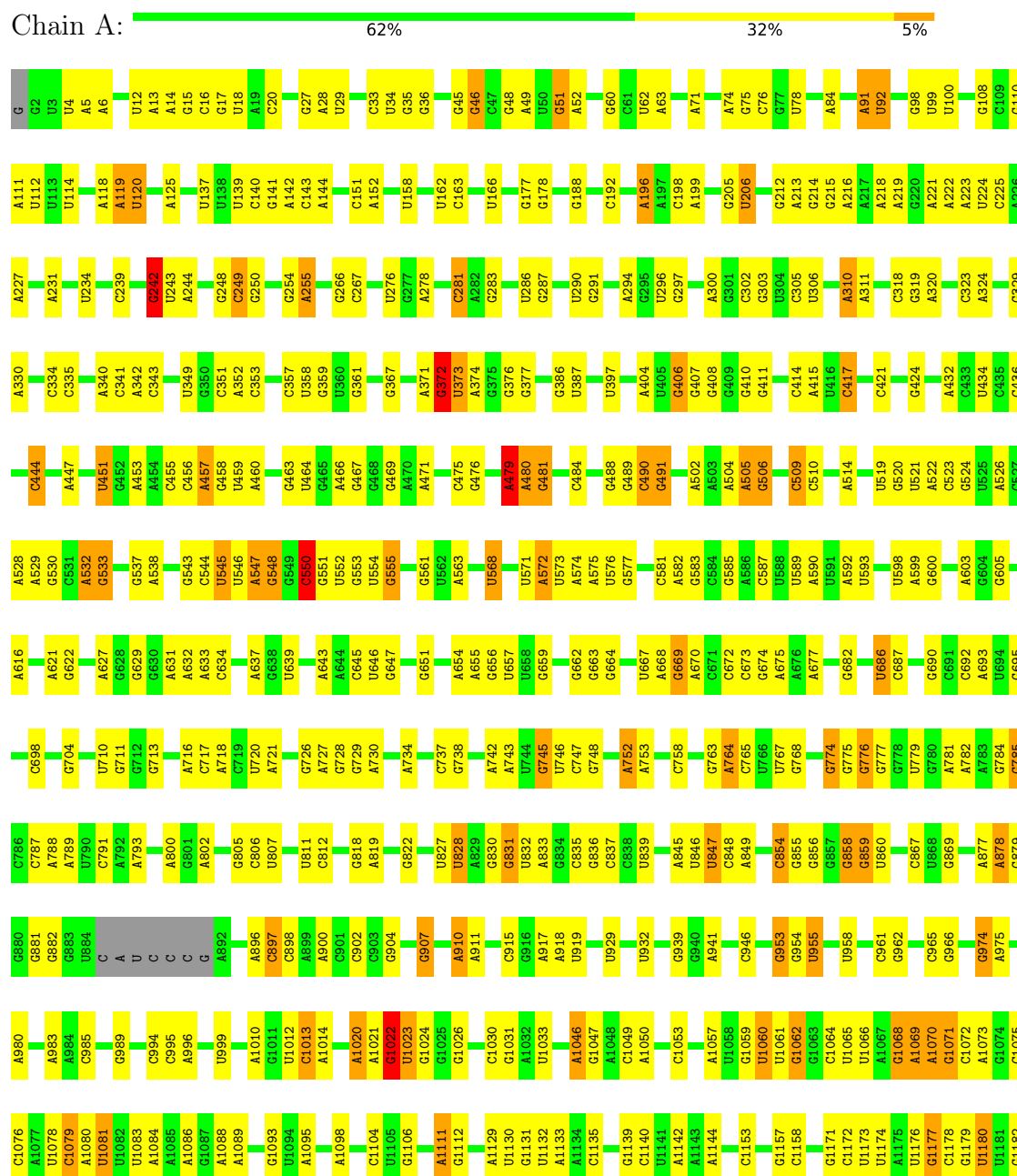


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	w	1	32	11	5	13	3	0

### 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.

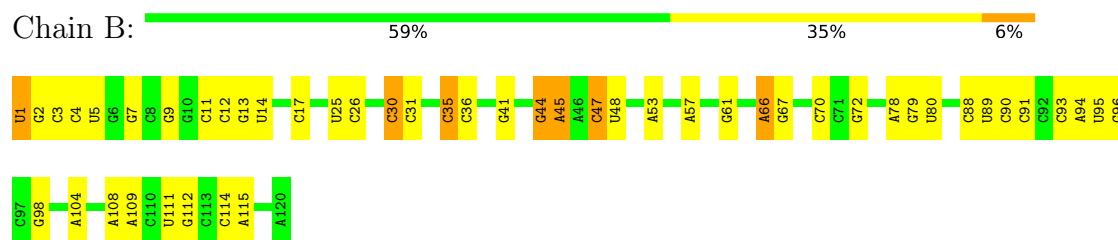
#### • Molecule 1: 23S ribosomal RNA



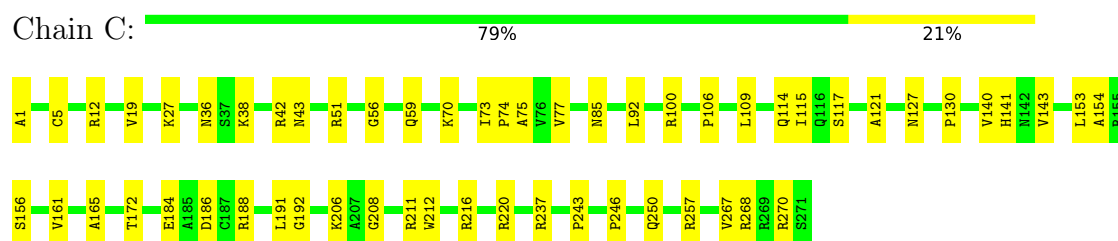
A2835	U2743	G2633	G2523	A2426	A2322	U2229	G2112	A2020	U1911	A1801	G1682	C1536	C1399	G1300	U1188
U2836	G2744	A2634	G2529	G2427	G2325	G2230	U2113	C2021	A1912	A1802	G1687	G1537	G1416	A1301	A1189
A2837	G2745	A2635	A2530	G2428	C2326	G2231	U2118	C2022	A1913	C1806	G1687	A1544	C1417	C1306	G1190
G2847	U2746	C2636	A2531	A2430	A2327	G2233	A2119	G2024	U1915	A1807	C1694	G1555	A1418	G1309	G1202
G2848	G2747	C2646	G2535	A2435	A2328	G2234	G2120	U2028	A1916	A1809	G1695	U1559	A1419	U1203	U1203
U2849	A2748	U2647	G2536	U2441	G2329	G2238	G2127	G2029	U1917	A1810	G1699	U1560	G1420	A1204	A1204
U2861	G2751	G2648	C2539	G2442	A2333	G2239	U2131	A2030	G1921	G1811	A1700	C1565	G1422	A1205	G1206
G2862	C2752	A2654	A2547	C2443	A2334	U2240	U2132	A2031	G1922	U1812	A1701	C1566	C1428	U1209	U1209
G2863	C2755	U2656	U2552	G2444	A2335	G2242	G2133	G2032	A1928	G1816	G1704	C1567	C1429	G1210	G1210
G2864	C2762	G2659	G2555	G2447	A2336	U2244	G2136	U2034	A1929	G1817	A1705	A1569	G1430	C1211	C1211
U2872	G2763	A2662	U2554	A2448	C2342	U2245	G2140	A2037	G1929	U1818	G1715	U1578	A1431	G1212	G1212
A2873	A2765	C2665	C2559	A2450	G2345	G2246	G2141	A2037	G1930	U1818	G1716	A1579	A1432	G1215	G1215
U2880	U2768	A2665	A2560	G2456	G2346	U2247	G2144	C2043	A1936	G1827	G1724	C1585	G1435	U1326	C1221
G2880	U2769	C2666	A2564	U2457	C2347	G2248	C2145	C2047	A1937	G1828	U1729	C1592	G1436	U1222	U1222
U2884	G2770	G2673	A2565	G2458	U2348	G2250	C2146	G2048	U1938	A1829	C1730	A1593	C1447	U1224	U1224
U2893	C2771	U2676	A2566	A2459	C2350	G2251	A2147	C2049	U1940	G1831	G1731	A1597	C1447	G1225	G1225
G2894	G2776	C2676	G2567	U2460	C2354	C2254	G2157	C2050	U1944	G1833	C1732	A1598	G1450	G1226	A1226
A2899	U2777	A2682	G2570	A2468	G2357	C2258	G2162	A2052	G1945	U1834	G1733	A1603	G1452	G1227	G1227
G2894	G2778	C2683	U2571	U2473	G2357	A2268	A2163	C2055	A1953	G1839	G1737	C1607	C1453	A1237	A1237
U2898	U2779	A2687	A2572	U2474	G2360	G2271	C2164	G2056	G1954	G1840	G1738	C1607	C1454	U1242	U1242
A2900	G2780	G2688	A2573	G2475	G2361	G2271	A2170	A2060	U1955	U1841	A1744	A1610	C1461	C1243	C1243
G2901	A2781	U2689	U2580	A2476	G2361	G2271	A2171	G2061	U1956	G1842	A1745	C1611	C1461	A1244	A1244
C2902	G2782	C2690	G2581	U2476	G2370	G2279	U2172	A2062	A1960	G1847	A1746	C1612	A1469	C1348	C1348
U2903	C2788	G2691	G2582	C2483	G2371	C2283	A2173	C2063	G1961	U1848	A1753	A1634	C1349	A1247	A1247
U2911	G2791	C2692	U2585	G2484	U2372	G2286	C2175	U2068	U1962	A1848	G1753	A1635	A1353	U1248	U1248
C2794	C2794	G2693	U2586	U2491	G2373	A2287	C2176	G2069	U1963	G1858	A1754	U1636	G1355	U1249	U1249
G2795	U2796	U2694	A2590	G2494	G2383	A2288	C2177	A2070	G1967	G1862	A1757	U1637	G1356	C1251	C1251
U2796	G2797	C2695	A2598	G2495	U2384	G2289	C2178	A2071	U1970	U1870	U1758	C1638	A1490	G1252	G1252
U2798	U2798	C2696	A2599	A2497	C2385	G2290	C2179	C2073	A1971	A1871	G1760	C1646	G1491	A1253	A1253
A2800	A2800	C2712	G2602	G2498	G2391	U2291	U2185	C2073	U1972	A1872	C1764	U1647	G1492	U1254	U1254
G2801	G2801	U2713	G2603	G2502	A2392	G2292	G2186	U2076	G1986	G1873	C1764	U1648	C1493	U1255	U1255
G2802	G2802	G2714	U2604	A2503	C2394	G2293	U2186	U2076	U1987	G1873	C1764	U1648	C1493	G1256	G1256
U2808	C2715	C2715	U2605	U2504	C2395	G2296	U2189	U2081	A1987	U1880	A1773	G1651	G1500	G1266	G1266
A2809	G2716	G2716	U2609	G2505	G2396	A2297	U2192	A2082	U1991	G1884	C1774	G1660	A1504	G1269	A1269
G2818	U2818	C2717	U2613	G2506	U2402	C2300	A2198	U2086	G1992	G1884	U1779	G1661	A1504	C1270	C1270
A2820	A2820	U2720	A2614	G2507	C2403	G2306	A2211	G2087	U1996	U1884	U1780	G1662	A1509	G1271	G1271
G2822	G2822	G2721	U2615	G2508	U2404	G2307	U2212	G2087	G1997	C1892	U1781	G1663	G1510	A1272	A1272
A2823	A2823	U2722	G2618	G2509	C2405	G2308	U2213	G2096	U1998	C1893	U1782	A1664	G1510	G1380	G1380
G2824	G2824	C2723	U2619	G2510	U2406	G2309	U2214	A2094	A1998	G1896	A1783	A1665	A1515	A1287	A1287
G2825	G2825	U2724	G2621	C2511	C2416	G2313	U2215	G2100	G2002	A1899	A1787	G1667	A1522	C1289	C1289
U2832	U2832	G2731	U2629	C2512	C2417	A2314	U2216	A2108	U2007	A1901	U1796	G1668	G1524	C1290	C1290
U2833	G2732	G2732	G2630	A2513	U2423	A2314	U2216	U2109	C2008	A1901	G1797	A1669	G1524	C1291	C1291
G2834	U2833	A2733	G2631	U2514	C2424	U2320	A2225	G2110	G2009	G1907	U1797	U1675	A1533	U1394	G1293
U2739	U2739	A2632	A2632	U2520	A2425	U2321	C2226	U2111	G2010	G1907	G1799	C1674	A1535	A1395	C1294
														C1398	G1296



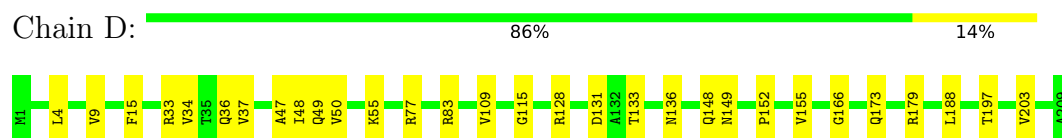
- Molecule 2: 5S ribosomal RNA



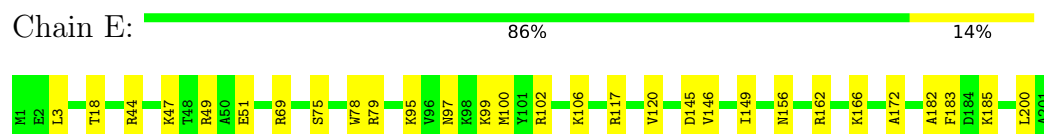
- Molecule 3: 50S ribosomal protein L2



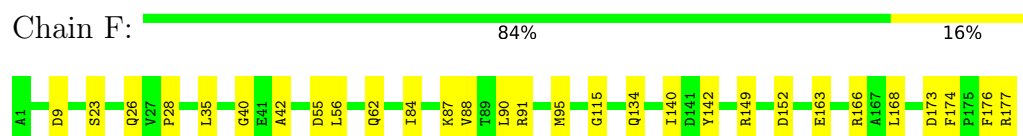
- Molecule 4: 50S ribosomal protein L3



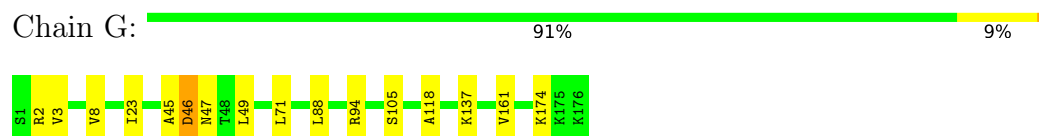
- Molecule 5: 50S ribosomal protein L4



- 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%



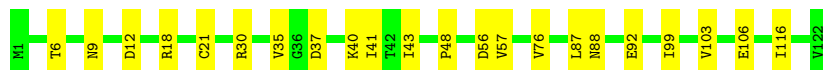
- Molecule 10: 50S ribosomal protein L13

Chain J: 87% 13%



- Molecule 11: 50S ribosomal protein L14

Chain K: 82% 18%



- Molecule 12: 50S ribosomal protein L15

Chain L: 87% 13%



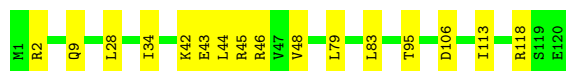
- Molecule 13: 50S ribosomal protein L16

Chain M: 85% 14%



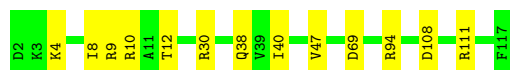
- Molecule 14: 50S ribosomal protein L17

Chain N: 87% 13%

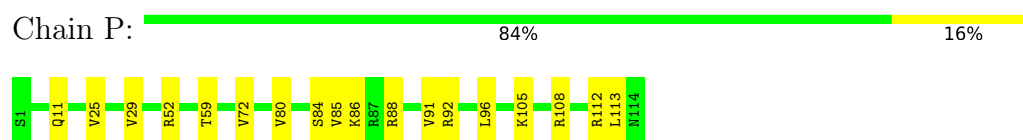


- Molecule 15: 50S ribosomal protein L18

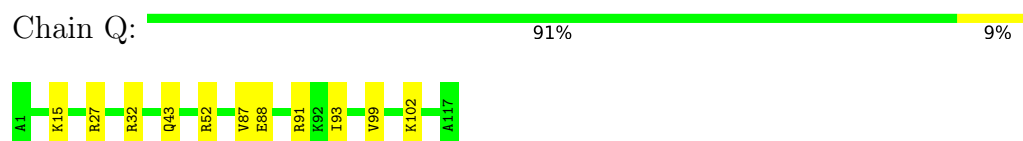
Chain O: 89% 11%



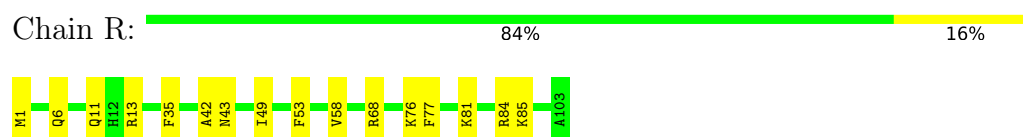
- Molecule 16: 50S ribosomal protein L19



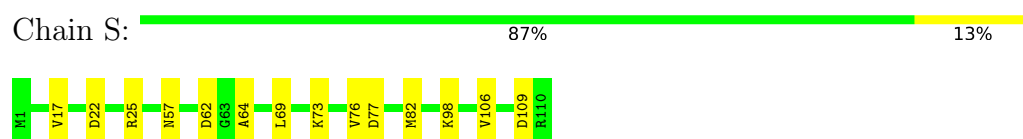
- Molecule 17: 50S ribosomal protein L20



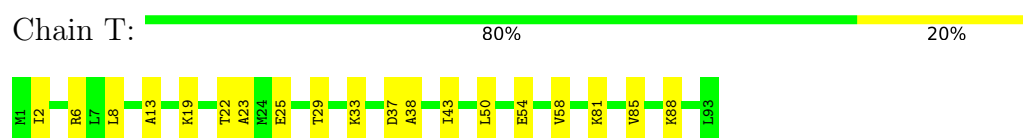
- Molecule 18: 50S ribosomal protein L21



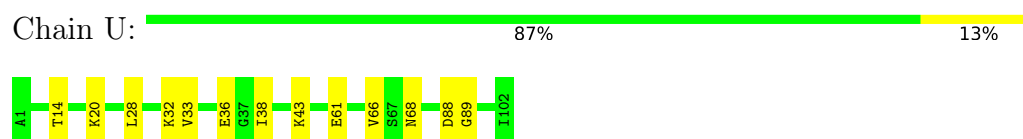
- Molecule 19: 50S ribosomal protein L22



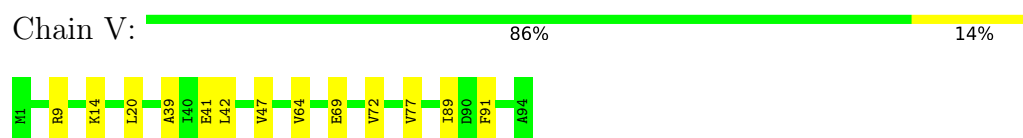
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25




- Molecule 23: 50S ribosomal protein L27

Chain W:  93% 7%



- Molecule 24: 50S ribosomal protein L28

Chain X:  86% 14%




- Molecule 25: 50S ribosomal protein L29

Chain Y:  86% 14%




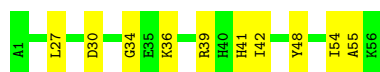
- Molecule 26: 50S ribosomal protein L30

Chain Z:  88% 12%




- Molecule 27: 50S ribosomal protein L32

Chain 0:  82% 18%



- Molecule 28: 50S ribosomal protein L33

Chain 1:  90% 10%



- Molecule 29: 50S ribosomal protein L34

Chain 2:  72% 28%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  73% 25% .



- Molecule 31: 50S ribosomal protein L36

Chain 4: 82% 16% .



- Molecule 32: 50S ribosomal protein L10

Chain 5: 80% 20%



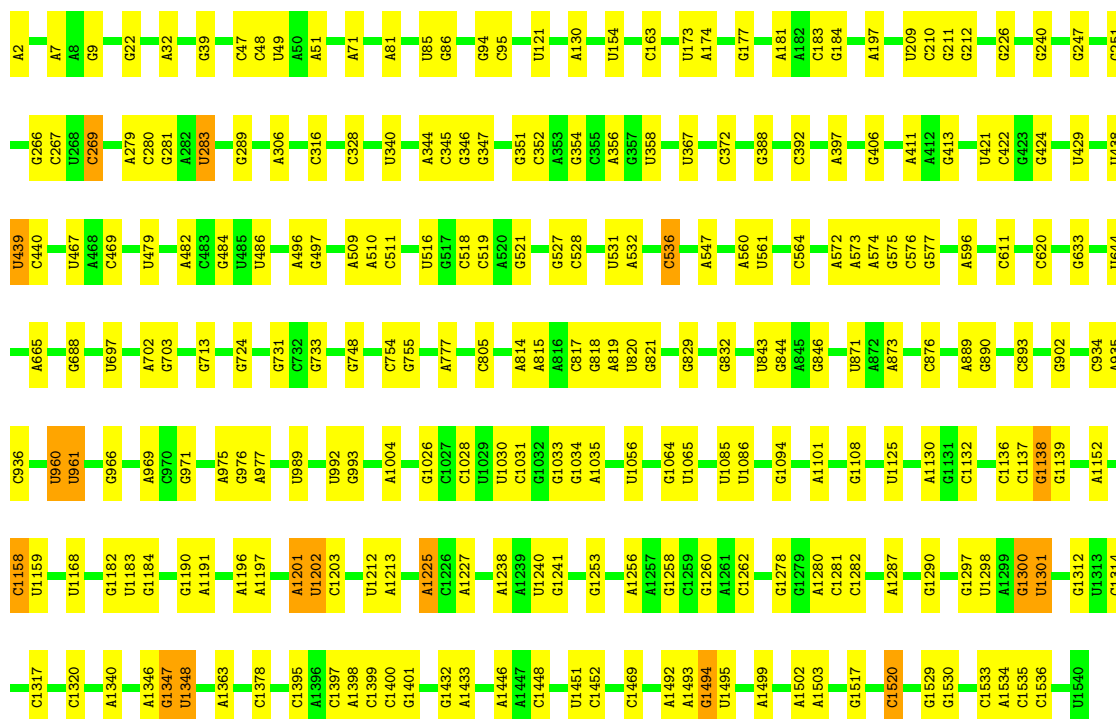
- Molecule 33: mRNA

Chain 7: 86% 14%



- Molecule 34: 16S ribosomal RNA

Chain a: 84% 15% .



- Molecule 35: 30S ribosomal protein S2

Chain b:  97% .



- Molecule 36: 30S ribosomal protein S3

Chain c:  99% .



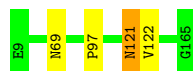
- Molecule 37: 30S ribosomal protein S4

Chain d:  98% .



- Molecule 38: 30S ribosomal protein S5

Chain e:  97% ..



- Molecule 39: 30S ribosomal protein S6

Chain f:  97% ..



- Molecule 40: 30S ribosomal protein S7

Chain g:  99% .



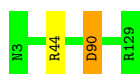
- Molecule 41: 30S ribosomal protein S8

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 30S ribosomal protein S9

Chain i:  98% ..



- Molecule 43: 30S ribosomal protein S10

Chain j:  99%



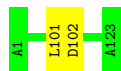
- Molecule 44: 30S ribosomal protein S11

Chain k:  99%



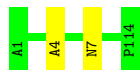
- Molecule 45: 30S ribosomal protein S12

Chain l:  98%



- Molecule 46: 30S ribosomal protein S13

Chain m:  98%



- Molecule 47: 30S ribosomal protein S14

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S15

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S16

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S17

Chain q:  96%



- Molecule 51: 30S ribosomal protein S18

Chain r: 100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S19

Chain s: 100%

There are no outlier residues recorded for this chain.

- Molecule 53: 30S ribosomal protein S20

Chain t: 100%

There are no outlier residues recorded for this chain.

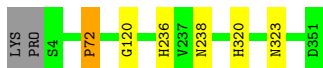
- Molecule 54: 30S ribosomal protein S21

Chain u: 98%



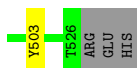
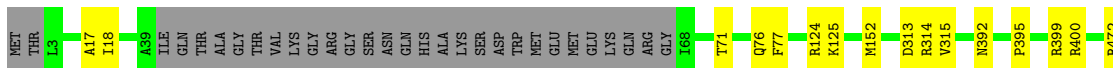
- Molecule 55: Peptide chain release factor RF1

Chain v: 98%



- Molecule 56: Peptide chain release factor RF3

Chain w: 91% 6%



- Molecule 57: fMet-tRNA

Chain x: 68% 30%



- Molecule 58: Apidaecin



Chain z:

93%

7%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54142	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	0/69612	1.00	222/108599 (0.2%)
10	J	0.25	0/1152	0.46	0/1551
11	K	0.28	0/947	0.53	0/1268
12	L	0.28	0/1054	0.54	0/1403
13	M	0.27	0/1093	0.58	1/1460 (0.1%)
14	N	0.27	0/973	0.52	0/1301
15	O	0.25	0/902	0.47	0/1209
16	P	0.25	0/929	0.52	1/1242 (0.1%)
17	Q	0.26	0/960	0.45	0/1278
18	R	0.26	0/829	0.51	0/1107
19	S	0.24	0/864	0.50	0/1156
2	B	0.39	1/2876 (0.0%)	1.16	32/4483 (0.7%)
20	T	0.26	0/744	0.50	0/994
21	U	0.29	0/787	0.56	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	0.46	0/605
27	0	0.24	0/450	0.46	0/599
28	1	0.26	0/416	0.50	0/554
29	2	0.25	0/380	0.50	0/498
3	C	0.26	0/2121	0.51	0/2852
30	3	0.25	0/513	0.64	1/676 (0.1%)
31	4	0.26	0/303	0.52	0/397
32	5	0.31	0/1001	0.63	0/1350
33	7	0.33	0/169	0.87	0/261
34	a	0.29	1/36967 (0.0%)	0.98	84/57666 (0.1%)
35	b	0.28	0/1735	0.55	0/2338
36	c	0.26	0/1651	0.48	0/2225
37	d	0.27	0/1665	0.54	2/2227 (0.1%)
38	e	0.28	0/1154	0.58	0/1554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	f	0.31	0/835	0.62	0/1128
4	D	0.26	0/1586	0.51	0/2134
40	g	0.27	0/1195	0.52	0/1602
41	h	0.26	0/989	0.55	0/1326
42	i	0.27	0/1034	0.56	0/1375
43	j	0.27	0/796	0.60	0/1077
44	k	0.27	0/885	0.51	0/1195
45	l	0.28	0/969	0.59	0/1300
46	m	0.26	0/892	0.55	0/1193
47	n	0.24	0/811	0.50	0/1081
48	o	0.24	0/722	0.53	0/964
49	p	0.26	0/659	0.50	0/884
5	E	0.25	0/1571	0.47	0/2113
50	q	0.27	0/657	0.58	0/881
51	r	0.24	0/511	0.48	0/689
52	s	0.26	0/652	0.49	0/877
53	t	0.29	0/671	0.49	0/888
54	u	0.32	0/500	0.65	0/668
55	v	0.27	0/2468	0.53	1/3351 (0.0%)
56	w	0.29	0/3996	0.63	2/5402 (0.0%)
57	x	0.32	0/1832	1.16	18/2855 (0.6%)
58	z	0.25	0/127	0.50	0/175
6	F	0.32	0/1434	0.55	0/1926
7	G	0.26	0/1343	0.52	0/1816
8	H	0.26	0/1122	0.47	0/1515
9	I	0.29	0/1046	0.55	0/1410
All	All	0.29	2/164496 (0.0%)	0.89	364/245048 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
13	M	0	1
18	R	0	1
21	U	0	1
30	3	0	2
32	5	0	1
35	b	0	3
38	e	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	f	0	2
42	i	0	1
43	j	0	1
45	l	0	1
46	m	0	1
50	q	0	1
55	v	0	1
56	w	0	3
6	F	0	2
7	G	0	3
All	All	0	27

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	2	A	OP3-P	-10.54	1.48	1.61
2	B	1	U	OP3-P	-10.53	1.48	1.61

The worst 5 of 364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2604	U	C2-N1-C1'	10.47	130.26	117.70
1	A	2063	C	N1-C2-O2	9.84	124.80	118.90
1	A	2506	U	C2-N1-C1'	9.62	129.25	117.70
2	B	36	C	N1-C2-O2	9.44	124.56	118.90
1	A	2506	U	N1-C2-O2	9.31	129.31	122.80

There are no chirality outliers.

5 of 27 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	62153	0	31259	451	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	37	0
4	D	1565	0	1616	19	0
5	E	1552	0	1619	20	0
6	F	1410	0	1447	17	0
7	G	1323	0	1374	7	0
8	H	1111	0	1148	13	0
9	I	1032	0	1088	11	0
10	J	1129	0	1162	13	0
11	K	938	0	1012	12	0
12	L	1045	0	1117	14	0
13	M	1074	0	1157	12	0
14	N	960	0	1000	11	0
15	O	892	0	923	10	0
16	P	917	0	965	13	0
17	Q	947	0	1022	10	0
18	R	816	0	839	11	0
19	S	857	0	922	8	0
20	T	738	0	807	13	0
21	U	779	0	834	6	0
22	V	753	0	780	7	0
23	W	575	0	592	3	0
24	X	625	0	655	9	0
25	Y	509	0	543	7	0
26	Z	449	0	491	4	0
27	0	444	0	461	6	0
28	1	409	0	440	3	0
29	2	377	0	418	12	0
30	3	504	0	574	13	0
31	4	302	0	343	5	0
32	5	988	0	1025	14	0
33	7	151	0	76	3	0
34	a	33016	0	16616	0	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	0	0
37	d	1643	0	1710	0	0
38	e	1141	0	1170	0	0
39	f	817	0	808	0	0
40	g	1181	0	1240	0	0
41	h	979	0	1034	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	i	1022	0	1070	0	0
43	j	786	0	828	0	0
44	k	869	0	878	0	0
45	l	955	0	1019	0	0
46	m	883	0	944	0	0
47	n	799	0	841	0	0
48	o	714	0	737	0	0
49	p	649	0	666	0	0
50	q	648	0	691	0	0
51	r	504	0	502	0	0
52	s	637	0	665	0	0
53	t	665	0	714	0	0
54	u	495	0	486	0	0
55	v	2436	0	2125	0	0
56	w	3923	0	3916	0	0
57	x	1640	0	837	0	0
58	z	120	0	128	0	0
59	w	32	0	14	0	0
All	All	151860	0	104238	696	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 696 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:745:G:N7	1:A:746:U:C5	2.25	1.04
1:A:1476:U:H3	1:A:1515:A:H62	0.99	0.96
1:A:545:U:H3	1:A:548:G:H1	1.00	0.93
1:A:2475:C:H42	1:A:2529:G:N2	1.66	0.93
1:A:306:U:H3	1:A:310:A:H62	0.95	0.91

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	
3	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
4	D	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
6	F	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
7	G	174/176 (99%)	161 (92%)	10 (6%)	3 (2%)	10	48
8	H	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
9	I	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
12	L	141/143 (99%)	124 (88%)	16 (11%)	1 (1%)	24	64
13	M	134/136 (98%)	124 (92%)	8 (6%)	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%)	100 (93%)	7 (6%)	1 (1%)	19	59
20	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
21	U	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	17	57
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
24	X	75/77 (97%)	72 (96%)	3 (4%)	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%)	56 (90%)	4 (6%)	2 (3%)	4	36
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	102 (79%)	27 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	b	216/218 (99%)	196 (91%)	19 (9%)	1 (0%)	31	71
36	c	204/206 (99%)	196 (96%)	6 (3%)	2 (1%)	17	57
37	d	203/205 (99%)	183 (90%)	20 (10%)	0	100	100
38	e	155/157 (99%)	137 (88%)	15 (10%)	3 (2%)	9	46
39	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	8	45
40	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
41	h	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
42	i	125/127 (98%)	109 (87%)	15 (12%)	1 (1%)	21	62
43	j	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
44	k	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
45	l	121/123 (98%)	97 (80%)	23 (19%)	1 (1%)	21	62
46	m	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
47	n	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
48	o	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
49	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
50	q	78/80 (98%)	66 (85%)	11 (14%)	1 (1%)	13	53
51	r	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
52	s	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
53	t	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
54	u	63/65 (97%)	51 (81%)	11 (18%)	1 (2%)	11	49
55	v	346/350 (99%)	322 (93%)	21 (6%)	3 (1%)	19	59
56	w	492/529 (93%)	429 (87%)	55 (11%)	8 (2%)	11	49
58	z	12/14 (86%)	11 (92%)	0	1 (8%)	1	15
All	All	6633/6776 (98%)	6065 (91%)	534 (8%)	34 (0%)	35	71

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	46	ASP
13	M	58	LYS
30	3	31	ILE
36	c	96	VAL
50	q	69	THR

### 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%)	214 (99%)	2 (1%)	81	90
4	D	164/164 (100%)	163 (99%)	1 (1%)	87	94
5	E	165/165 (100%)	164 (99%)	1 (1%)	87	94
6	F	148/148 (100%)	147 (99%)	1 (1%)	85	93
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	88
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	83
24	X	67/67 (100%)	66 (98%)	1 (2%)	67	85
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	33 (97%)	1 (3%)	45	72
32	5	100/100 (100%)	100 (100%)	0	100	100
35	b	180/180 (100%)	177 (98%)	3 (2%)	63	83
36	c	170/170 (100%)	170 (100%)	0	100	100
37	d	172/172 (100%)	170 (99%)	2 (1%)	74	87
38	e	114/119 (96%)	113 (99%)	1 (1%)	81	90
39	f	87/87 (100%)	87 (100%)	0	100	100
40	g	124/124 (100%)	123 (99%)	1 (1%)	83	91
41	h	104/104 (100%)	104 (100%)	0	100	100
42	i	105/105 (100%)	104 (99%)	1 (1%)	78	89
43	j	86/86 (100%)	86 (100%)	0	100	100
44	k	89/89 (100%)	88 (99%)	1 (1%)	76	88
45	l	103/103 (100%)	103 (100%)	0	100	100
46	m	92/92 (100%)	91 (99%)	1 (1%)	76	88
47	n	79/83 (95%)	79 (100%)	0	100	100
48	o	76/76 (100%)	76 (100%)	0	100	100
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/74 (100%)	73 (99%)	1 (1%)	69	86
51	r	48/56 (86%)	48 (100%)	0	100	100
52	s	70/70 (100%)	70 (100%)	0	100	100
53	t	65/65 (100%)	65 (100%)	0	100	100
54	u	44/55 (80%)	44 (100%)	0	100	100
55	v	203/292 (70%)	201 (99%)	2 (1%)	78	89
56	w	426/453 (94%)	422 (99%)	4 (1%)	81	90
58	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5407/5551 (97%)	5379 (100%)	28 (0%)	90	95

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	b	35	ASN

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Mol	Chain	Res	Type
37	d	177	MET
56	w	124	ARG
35	b	202	ASN
37	d	80	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
38	e	69	ASN
42	i	36	GLN
56	w	445	GLN
39	f	11	HIS
41	h	3	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	533 (18%)	30 (1%)
2	B	119/120 (99%)	14 (11%)	2 (1%)
33	7	6/7 (85%)	5 (83%)	0
34	a	1538/1539 (99%)	219 (14%)	0
57	x	76/77 (98%)	21 (27%)	0
All	All	4632/4646 (99%)	792 (17%)	32 (0%)

5 of 792 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	14	A
1	A	27	G
1	A	34	U
1	A	35	G

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	U
1	A	1300	G
1	A	2808	G
1	A	1190	G

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Mol	Chain	Res	Type
1	A	1378	A

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

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	$\# Z  > 2$
59	GCP	w	601	-	25,34,34	2.38	7 (28%)	31,54,54	1.76	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
59	GCP	w	601	-	-	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)
59	w	601	GCP	C4-N9	-7.39	1.37	1.47
59	w	601	GCP	C5-C6	-4.55	1.44	1.52
59	w	601	GCP	C8-N9	-3.20	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	601	GCP	C5-C4	-2.31	1.38	1.52
59	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(°)
59	w	601	GCP	C5-C6-N1	-5.35	111.90	118.27
59	w	601	GCP	PA-O3A-PB	-2.48	124.35	132.42
59	w	601	GCP	O6-C6-C5	3.72	127.50	119.82
59	w	601	GCP	C4-C5-N7	6.11	110.56	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.