



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

Oct 23, 2019 – 01:40 PM EDT

PDB ID : 6GXM  
EMDB ID: : EMD-0080  
Title : Cryo-EM structure of an E. coli 70S ribosome in complex with RF3-GDPCP, RF1(GAQ) and Pint-tRNA (State II)  
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.  
Deposited on : 2018-06-27  
Resolution : 3.80 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 : 1.8.0 (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

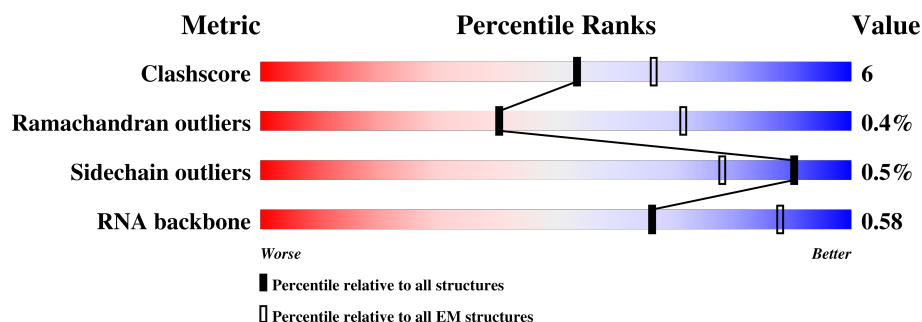
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.






















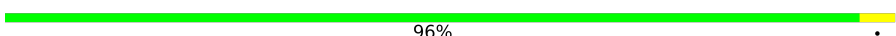





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	58% 36% 6%
3	C	271	80% 20%
4	D	209	85% 15%
5	E	201	86% 14%
6	F	177	84% 16%
7	G	176	93% 6% .
8	H	149	84% 16%

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Mol	Chain	Length	Quality of chain
9	I	141	 88% 12%
10	J	142	 89% 11%
11	K	122	 84% 16%
12	L	143	 85% 15%
13	M	136	 86% 13% .
14	N	120	 86% 14%
15	O	116	 89% 11%
16	P	114	 87% 13%
17	Q	117	 87% 13%
18	R	103	 85% 15%
19	S	110	 89% 11%
20	T	93	 77% 23%
21	U	102	 86% 13% .
22	V	94	 86% 14%
23	W	75	 93% 7%
24	X	77	 86% 14%
25	Y	63	 86% 14%
26	Z	58	 88% 12%
27	0	56	 82% 18%
28	1	50	 96% .
29	2	46	 80% 20%
30	3	64	 88% 9% . .
31	4	38	 84% 16%
32	5	131	 80% 20%
33	7	7	 14% 43% 43%

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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	98% ..
39	f	100	96% .
40	g	151	100%
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	95% 5%
51	r	65	100%
52	s	79	100%
53	t	85	100%
54	u	65	98% .
55	v	248	96% .
56	w	529	91% . 6%
57	x	77	71% 23% 5%
58	z	14	93% 7%

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 151394 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 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	U	conflict	GB 1402434313

- 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	248	Total	C	N	O	S	0	0
			1932	1180	368	375	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	167	CYS	SER	conflict	UNP P0A7I0
v	234	ALA	GLY	conflict	UNP P0A7I0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	498	Total	C	N	O	S	0	0
			3938	2495	679	744	20		

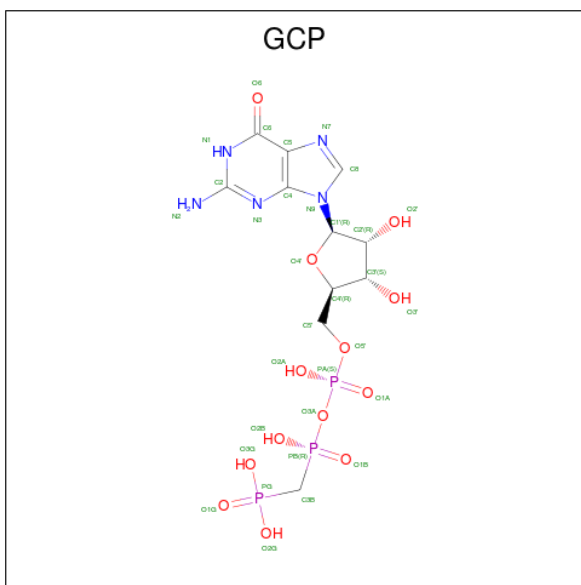
- Molecule 57 is a RNA chain called fMet-tRNA.

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		

- 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>).

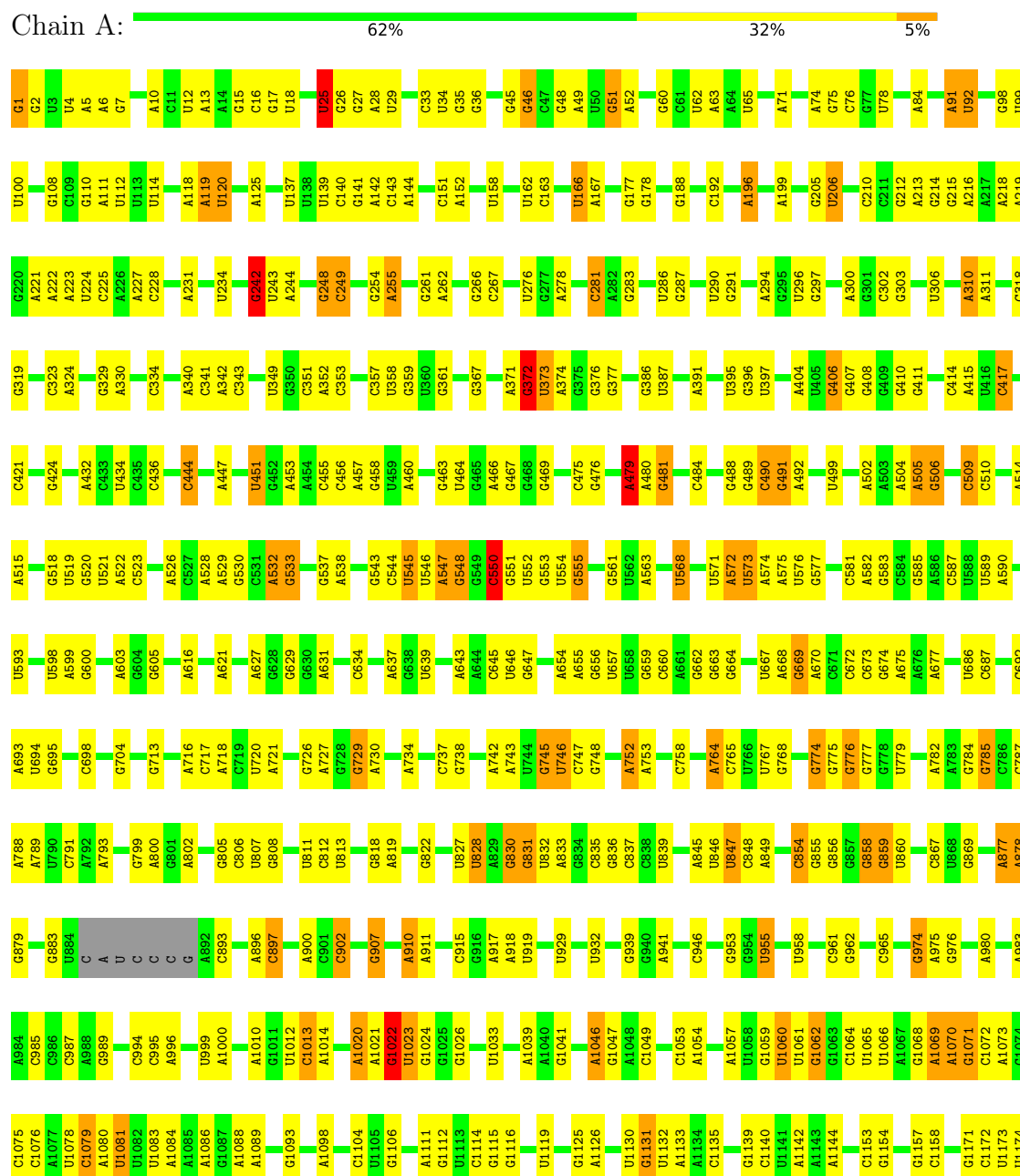


Mol	Chain	Residues	Atoms					AltConf
59	w	1	Total	C	N	O	P	0
			31	11	4	13	3	

### 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

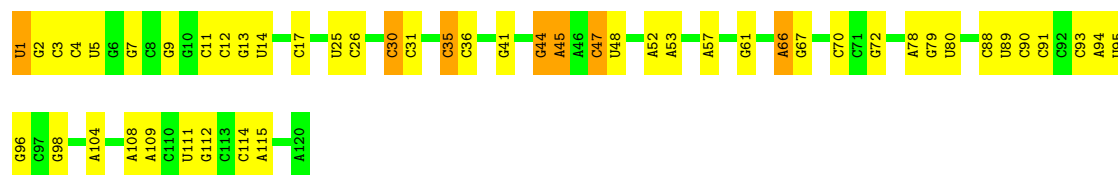


A2820	G2722	C2621	C2520	A2430	A2322	G2229	G2118	C2021	A1912	A1801	G1682	C1536	G1416	G1295	A1175
A2821	A2726	G2629	G2523	U2431	G2325	G2230	G2119	U2022	A1913	A1802	G1687	C1537	C1417	G1296	U1176
A2822	G2731	G2630	G2524	A2432	C2326	U2231	G2120	C2023	C1914	C1806	G1694	A1544	C1418	G1300	C1178
C2824	G2732	G2631	G2525	A2435	A2327	C2232	G2121	C2024	U1917	G1807	C1695	G1555	A1419	A1301	C1179
G2825	A2733	G2634	G2526	U2441	U2329	G2233	G2122	C2025	U1918	A1808	G1699	G1559	A1420	U1180	U1181
U2832	G2734	A2635	G2527	C2442	G2330	G2234	U2123	U2028	G1921	A1809	G1700	U1560	G1421	C1306	G1182
U2833	U2739	A2636	A2528	C2443	G2331	G2235	U2124	G2029	G1922	G1810	A1700	G1561	C1422	U1313	G1183
G2834	U2743	G2637	G2529	C2444	U2332	G2236	G2125	A2030	A1927	G1811	A1701	C1562	C1423	C1314	U1188
A2835	G2744	C2646	G2530	G2445	A2333	U2237	G2126	A2031	U1928	U1812	G1702	C1563	G1424	G1190	U1189
U2836	C2745	U2647	G2531	U2446	A2334	U2238	G2127	A2032	G1929	G1813	G1703	C1564	A1430	A1321	A1204
A2837	U2746	G2648	G2532	U2447	A2335	U2239	U2128	U2033	G1930	G1814	G1704	A1569	A1431	G1323	A1205
G2846	G2747	G2649	A2533	U2448	A2336	U2240	G2129	G2034	U1931	U1815	G1705	U1578	A1432	G1324	G1206
U2847	A2748	A2654	U2534	U2449	A2337	U2241	G2130	G2035	U1932	G1816	G1706	A1579	A1433	U1326	U1209
G2848	G2749	G2655	G2535	U2450	A2338	U2242	G2131	C2036	A1933	G1817	G1707	C1585	A1434	U1327	C1210
U2849	C2752	U2656	U2536	U2451	A2339	U2243	G2132	C2037	U1934	G1818	G1708	U1592	A1435	C1330	C1211
A2850	G2753	G2657	G2537	U2452	A2340	U2244	G2133	C2038	U1935	G1819	G1709	C1593	A1436	G1331	G1212
U2851	U2755	G2658	C2538	U2453	A2341	U2245	G2134	U2039	U1936	G1820	G1710	C1594	C1437	U1329	U1215
G2861	A2757	A2662	A2539	U2454	A2342	U2246	G2135	G2040	A1937	G1821	G1711	C1595	C1438	G1332	G1216
C2862	U2758	G2663	G2540	U2455	A2343	U2247	G2136	G2041	U1938	G1822	G1712	C1596	A1439	G1333	G1217
G2864	C2762	C2664	A2541	U2456	A2344	U2248	G2137	C2042	U1939	G1823	G1713	C1597	A1440	G1334	G1218
A2867	A2765	G2665	G2542	U2457	A2345	U2249	G2138	C2043	U1940	G1824	G1714	C1598	A1441	G1335	G1219
U2868	G2766	G2666	U2543	U2458	A2346	U2250	G2139	A2052	U1941	G1825	G1715	C1603	A1442	U1336	U1220
A2872	U2767	C2667	G2544	U2459	A2347	U2251	G2140	G2053	U1942	G1826	G1716	C1604	A1443	G1337	G1221
U2873	G2770	G2668	C2545	U2460	A2348	U2252	G2141	C2054	U1943	G1827	G1717	C1605	A1444	G1338	G1222
C2880	C2771	U2669	U2546	U2461	A2349	U2253	G2142	U2055	U1944	G1828	G1718	C1606	A1445	G1339	G1223
A2883	A2776	G2670	G2547	U2462	A2350	U2254	G2143	G2056	U1945	G1829	G1719	C1607	A1446	G1340	G1224
U2884	G2777	C2671	A2548	U2463	A2351	U2255	G2144	A2057	U1946	G1830	G1720	C1608	A1447	G1341	G1225
A2893	U2778	U2672	G2549	U2464	A2352	U2256	G2145	G2058	A1947	G1831	G1721	C1609	C1448	G1342	A1237
G2894	G2779	C2673	U2550	U2465	A2353	U2257	G2146	C2059	U1948	G1832	G1722	C1610	A1449	U1242	U1247
U2898	U2780	G2674	G2551	U2466	A2354	U2258	G2147	A2060	A1949	G1833	G1723	C1611	A1450	A1248	A1249
A2900	A2781	G2675	U2552	U2467	A2355	U2259	G2148	G2061	U1950	G1834	G1724	C1612	A1451	G1250	G1251
C2901	G2782	U2676	G2553	U2468	A2356	U2260	G2149	A2062	U1951	G1835	G1725	C1613	A1452	G1252	A1253
U2902	C2788	G2677	U2554	U2469	A2357	U2261	G2150	C2063	U1952	G1836	G1726	C1614	A1453	A1254	U1255
G2903	U2791	C2703	G2555	U2470	A2358	U2262	G2151	U2064	U1953	G1837	G1727	C1615	A1454	G1256	G1257
A2904	C2794	C2704	A2556	U2471	A2359	U2263	G2152	A2065	U1954	G1838	G1728	C1616	A1455	G1258	G1259
U2905	G2795	G2705	U2557	U2472	A2360	U2264	G2153	C2066	U1955	G1839	G1729	C1617	A1456	C1260	C1261
A2906	U2796	U2706	G2558	U2473	A2361	U2265	G2154	G2067	U1956	G1840	G1730	C1618	A1457	G1262	G1263
C2907	G2797	G2707	U2559	U2474	A2362	U2266	G2155	A2068	U1957	G1841	G1731	C1619	A1458	U1264	U1265
U2908	U2798	U2708	G2560	U2475	A2363	U2267	G2156	C2069	U1958	G1842	G1732	C1620	A1459	G1266	G1267
A2909	C2799	C2709	U2561	U2476	A2364	U2268	G2157	A2070	U1959	G1843	G1733	C1621	A1460	G1268	G1269
G2910	U2800	G2710	G2562	U2477	A2365	U2269	G2158	C2071	U1960	G1844	G1734	C1622	A1461	G1269	G1270
C2911	A2801	U2711	U2563	U2478	A2366	U2270	G2159	C2072	U1961	G1845	G1735	C1623	A1462	A1376	G1271
U2912	G2802	C2712	G2564	U2479	A2367	U2271	G2160	U2073	U1962	G1846	G1736	C1624	A1463	A1377	A1272
A2913	U2803	U2713	U2565	U2480	A2368	U2272	G2161	A2074	U1963	G1847	G1737	C1625	A1464	A1378	A1273
G2914	C2804	G2714	G2566	U2481	A2369	U2273	G2162	C2075	U1964	G1848	G1738	C1626	A1465	G1380	G1274
U2915	U2805	C2715	U2567	U2482	A2370	U2274	G2163	U2076	U1965	G1849	G1739	C1627	A1466	G1381	A1275
A2916	G2806	U2716	G2568	U2483	A2371	U2275	G2164	C2077	U1966	G1850	G1740	C1628	A1467	G1382	G1276
C2917	C2807	G2717	U2569	U2484	A2372	U2276	G2165	A2078	U1967	G1851	G1741	C1629	A1468	G1383	G1277
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G2921	C2811	C2721	U2573	U2488	A2376	U2280	G2169	C2082	U1971	G1855	G1745	C1633	A1472	C1290	C1291
C2922	U2812	U2722	G2574	U2489	A2377	U2281	G2170	U2083	U1972	G1856	G1746	C1634	A1473	G1292	G1293
U2923	A2813	G2723	U2575	U2490	A2378	U2282	G2171	A2084	U1973	G1857	G1747	C1635	A1474	U1400	U1294
A2924	G2814	U2724	G2576	U2491	A2379	U2283	G2172	C2085	U1974	G1858	G1748	C1636	A1475	G1401	G1295
G2925	U2815	C2725	U2577	U2492	A2380	U2284	G2173	U2086	U1975	G1859	G1749	C1637	A1476	G1296	G1296
U2926	C2816	G2726	G2578	U2493	A2381	U2285	G2174	C2087	U1976	G1860	G1750	C1638	A1477	G1297	G1297
A2927	U2817	U2727	U2579	U2494	A2382	U2286	G2175	A2088	U1977	G1861	G1751	C1639	A1478	G1298	G1298
C2928	C2818	C2728	G2580	U2495	A2383	U2287	G2176	C2089	U1978	G1862	G1752	C1640	A1479	G1299	G1299
U2929	A2819	G2729	U2581	U2496	A2384	U2288	G2177	U2090	U1979	G1863	G1753	C1641	A1480	C1291	G1291
G2930	U2820	U2730	G2582	U2497	A2385	U2289	G2178	C2091	U1980	G1864	G1754	C1642	A1481	G1292	G1292
A2931	C2821	C2731	U2583	U2498	A2386	U2290	G2179	A2092	U1981	G1865	G1755	C1643	A1482	G1293	G1293
U2932	U2822	G2732	U2584	U2499	A2387	U2291	G2180	C2093	U1982	G1866	G1756	C1644	A1483	G1294	G1294
C2933	A2823	U2733	G2585	U2500	A2388	U2292	G2181	U2094	U1983	G1867	G1757	C1645	A1484	C1295	C1295
U2934	G2824	U2734	U2586	U2501	A2389	U2293	G2182	A2095	U1984	G1868	G1758	C1646	A1485	G1296	G1296
A2935	U2825	C2735	G2587	U2502	A2390	U2294	G2183	C2096	U1985	G1869	G1759	C1647	A1486	G1297	G1297
G2936	C2826	G2736	U2588	U2503	A2391	U2295	G2184	U2097	U1986	G1870	G1760	C1648	A1487	C1298	G1298
U2937	A2827	U2737	U2589	U2504	A2392	U2296	G2185	A2098	U1987	G1871	G1761	C1649	A1488	G1299	G1299
C2938	U2828	C2738	G2590	U2505	A2393	U2297	G2186	C2099	U1988	G1872	G1762	C1650	A1489	G1300	G1300
U2939	G2829	U2739	U2591	U2506	A2394	U2298	G2187	U2100	U1989	G1873	G1763	C1651	A1490	G1301	G1301
A2940	C2830	G2740	G2592	U2507	A2395	U2299	G2188	U2101	U1990	G1874	G1764	C1652	A1491	C1291	G1302
G2941	U2831	U2741	U2593	U2508	A2396	U2300	G2189	A2102	U1991	G1875	G1765	C1653	A1492	G1292	G1303
U2942	A2832	C2742	G2594	U2509	A2397	U2301	G2190	C2103	U1992	G1876	G1766	C1654	A1493	G1293	G1304
C2943	C2833	G2743	U2595	U2510	A2398	U2302	G2191	U2104	U1993	G1877	G1767	C1655	A1494	G1294	G1305
U2944	U2834	U2744	U2596	U2511	A2399	U2303	G2192	A2105	U1994	G1878	G1768	C1656	A1495	C1295	G1306
A2945	G2835	C2745	G2597	U2512	A2400	U2304	G2193	C2106	U1995	G1879	G1769	C1657	A1496	G1296	G1307
G2946	C2836	G2746	U2598	U2513	A2401	U2305	G2194	U2107	U1996	G1880	G1770	C1658	A1497	G1297	G1308
U2947	U2837	U2747	U2599	U2514	A2402	U2306	G2195	A2108	U1997	G1881	G1771	C1659	A1498	G1298	G1309
A2948	A2838	C2748	G2600	U2515	A2403	U2307	G2196	C2109	U1998	G1882	G1772	C1660	A1499	G1299	G1310
G2949	C2839	G2749	U2601	U2516	A2404	U2308	G2197	U2110	U1999	G1883	G1773	C1661	A1500	G1300	G1311
U2950	U2840	U2750	U2602												




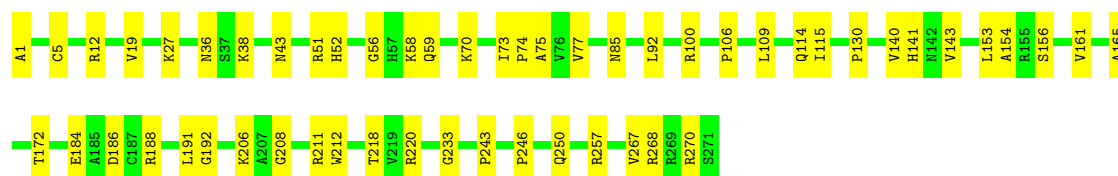
- Molecule 2: 5S ribosomal RNA

Chain B: 




- Molecule 3: 50S ribosomal protein L2

Chain C: 




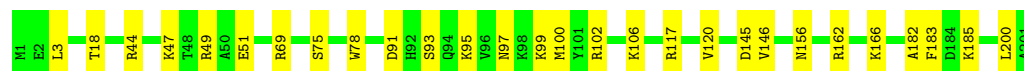
- Molecule 4: 50S ribosomal protein L3

Chain D: 




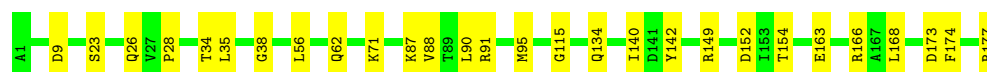
- Molecule 5: 50S ribosomal protein L4

Chain E: 

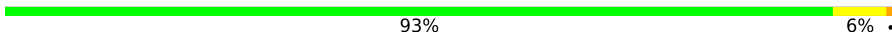


- Molecule 6: 50S ribosomal protein L5

Chain F: 




- Molecule 7: 50S ribosomal protein L6

Chain G: 



- Molecule 8: 50S ribosomal protein L9

Chain H: 



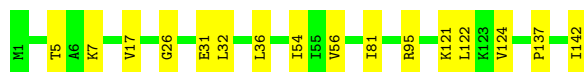
- Molecule 9: 50S ribosomal protein L11

Chain I: 88% 12%



- Molecule 10: 50S ribosomal protein L13

Chain J: 89% 11%



- Molecule 11: 50S ribosomal protein L14

Chain K: 84% 16%



- Molecule 12: 50S ribosomal protein L15

Chain L: 85% 15%



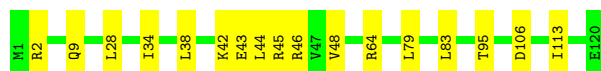
- Molecule 13: 50S ribosomal protein L16

Chain M: 86% 13%



- Molecule 14: 50S ribosomal protein L17

Chain N: 86% 14%

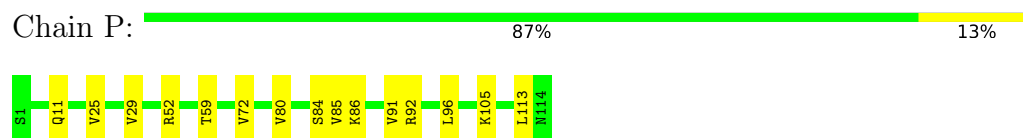


- Molecule 15: 50S ribosomal protein L18

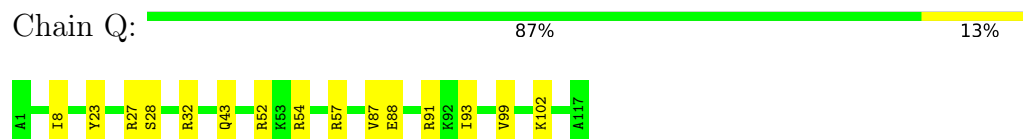
Chain O: 89% 11%



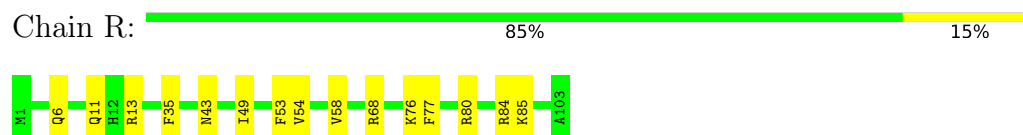
- Molecule 16: 50S ribosomal protein L19



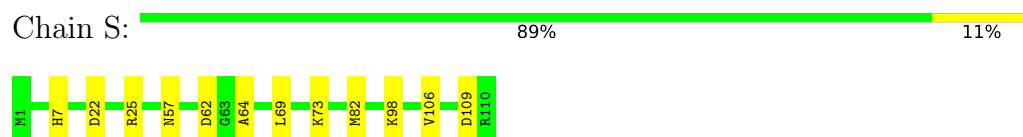
- Molecule 17: 50S ribosomal protein L20



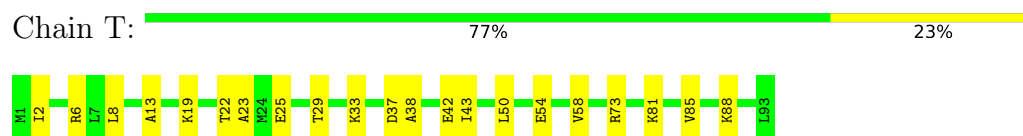
- Molecule 18: 50S ribosomal protein L21



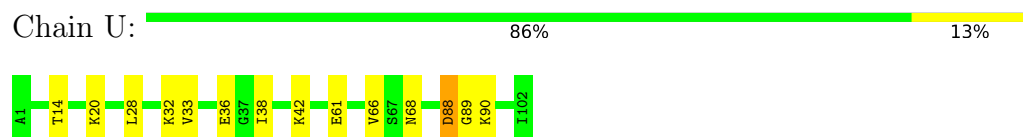
- Molecule 19: 50S ribosomal protein L22



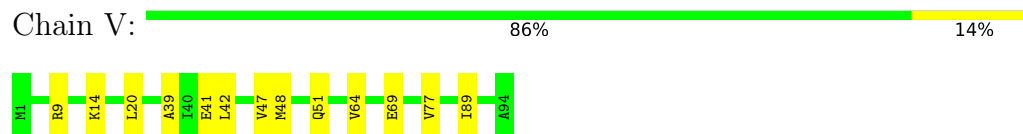
- Molecule 20: 50S ribosomal protein L23



- 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%




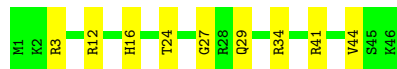
- Molecule 28: 50S ribosomal protein L33

Chain 1:  96%




- Molecule 29: 50S ribosomal protein L34

Chain 2:  80% 20%

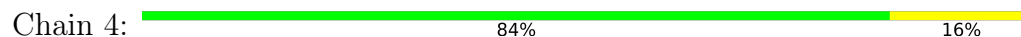


- Molecule 30: 50S ribosomal protein L35

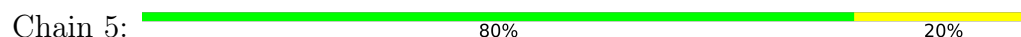
Chain 3:  88% 9%



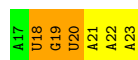
- Molecule 31: 50S ribosomal protein L36



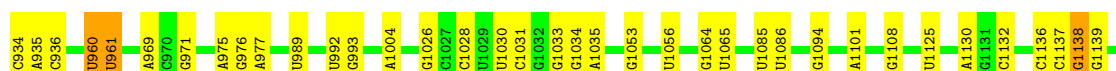
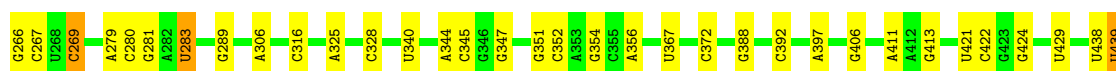
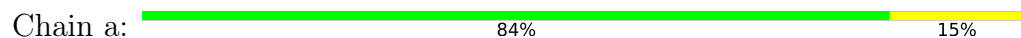
- Molecule 32: 50S ribosomal protein L10



- Molecule 33: mRNA



- Molecule 34: 16S ribosomal RNA



- 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:  98% ..



- Molecule 39: 30S ribosomal protein S6

Chain f:  96% .



- Molecule 40: 30S ribosomal protein S7

Chain g:  100%

There are no outlier residues recorded for this chain.

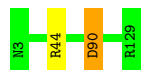
- Molecule 41: 30S ribosomal protein S8

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%



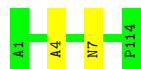
- Molecule 45: 30S ribosomal protein S12

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:  95% 5%



- 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%



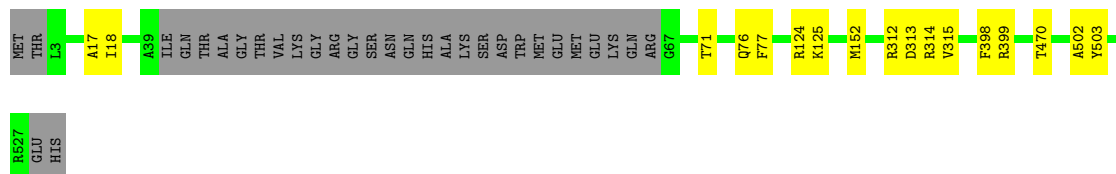
- Molecule 55: Peptide chain release factor RF1

Chain v:  96%



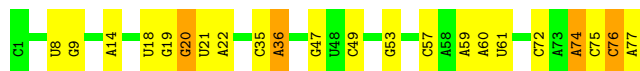
- Molecule 56: Peptide chain release factor RF3

Chain w:  91% 6%



- Molecule 57: fMet-tRNA

Chain x:  71% 23% 5%



- 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	49415	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	0.32	3/69639 (0.0%)	1.01	234/108640 (0.2%)
10	J	0.25	0/1152	0.46	0/1551
11	K	0.28	0/947	0.53	0/1268
12	L	0.27	0/1054	0.53	0/1403
13	M	0.28	0/1093	0.58	2/1460 (0.1%)
14	N	0.27	0/973	0.52	0/1301
15	O	0.25	0/902	0.46	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	0.49	0/1156
2	B	0.39	1/2876 (0.0%)	1.16	32/4483 (0.7%)
20	T	0.26	0/744	0.54	0/994
21	U	0.29	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	0.25	0/453	0.50	0/605
27	0	0.24	0/450	0.46	0/599
28	1	0.26	0/416	0.50	0/554
29	2	0.23	0/380	0.44	0/498
3	C	0.26	0/2121	0.51	0/2852
30	3	0.26	0/513	0.64	1/676 (0.1%)
31	4	0.25	0/303	0.50	0/397
32	5	0.30	0/1001	0.64	0/1350
33	7	0.32	0/169	0.79	0/261
34	a	0.29	1/36967 (0.0%)	0.98	79/57666 (0.1%)
35	b	0.28	0/1735	0.55	0/2338
36	c	0.25	0/1651	0.46	0/2225
37	d	0.26	0/1665	0.55	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	0.50	0/2134
40	g	0.28	0/1195	0.51	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	0.26	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	0.28	0/657	0.58	0/881
51	r	0.24	0/511	0.47	0/689
52	s	0.26	0/652	0.49	0/877
53	t	0.28	0/671	0.48	0/888
54	u	0.32	0/500	0.65	0/668
55	v	0.61	2/1963 (0.1%)	0.78	6/2646 (0.2%)
56	w	0.28	0/4011	0.60	1/5421 (0.0%)
57	x	0.44	1/1832 (0.1%)	1.14	14/2855 (0.5%)
58	z	0.26	0/127	0.49	0/175
6	F	0.29	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	0.31	8/164033 (0.0%)	0.90	373/244403 (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
13	M	0	1
18	R	0	1
21	U	0	1
30	3	0	1
32	5	0	1
35	b	0	3
38	e	0	1
39	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	i	0	1
43	j	0	1
45	l	0	1
46	m	0	1
50	q	0	2
56	w	0	7
6	F	0	2
7	G	0	3
All	All	0	29

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1913	A	O3'-P	-33.11	1.21	1.61
55	v	191	GLU	C-N	17.65	1.74	1.34
55	v	329	LEU	C-N	16.65	1.72	1.34
57	x	36	A	O3'-P	-11.81	1.47	1.61
1	A	1	G	OP3-P	-10.60	1.48	1.61

The worst 5 of 373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1913	A	P-O3'-C3'	28.62	154.05	119.70
55	v	191	GLU	O-C-N	17.70	151.02	122.70
1	A	1912	A	OP1-P-O3'	15.73	139.80	105.20
1	A	1913	A	OP1-P-O3'	15.48	139.26	105.20
1	A	1912	A	P-O3'-C3'	14.49	137.09	119.70

There are no chirality outliers.

5 of 29 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 ⓘ

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	461	0
2	B	2572	0	1302	20	0
3	C	2082	0	2157	34	0
4	D	1565	0	1616	20	0
5	E	1552	0	1619	18	0
6	F	1410	0	1447	17	0
7	G	1323	0	1374	5	0
8	H	1111	0	1148	13	0
9	I	1032	0	1088	10	0
10	J	1129	0	1162	11	0
11	K	938	0	1012	12	0
12	L	1045	0	1117	15	0
13	M	1074	0	1157	11	0
14	N	960	0	1000	12	0
15	O	892	0	923	10	0
16	P	917	0	965	11	0
17	Q	947	0	1022	13	0
18	R	816	0	839	11	0
19	S	857	0	922	7	0
20	T	738	0	807	15	0
21	U	779	0	834	7	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	7	0
28	1	409	0	440	1	0
29	2	377	0	418	7	0
30	3	504	0	574	6	0
31	4	302	0	343	3	0
32	5	988	0	1025	14	0
33	7	151	0	76	6	0
34	a	33016	0	16615	0	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	0	0
37	d	1643	0	1710	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1932	0	1881	0	0
56	w	3938	0	3932	0	0
57	x	1640	0	837	0	0
58	z	120	0	128	0	0
59	w	31	0	12	0	0
All	All	151394	0	104019	694	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 694 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:N3	1.91	1.19
1:A:593:U:H3	1:A:664:G:H1	1.06	1.01
1:A:306:U:H3	1:A:310:A:H62	0.99	0.95
1:A:1476:U:H3	1:A:1515:A:H62	1.00	0.95
1:A:545:U:H3	1:A:548:G:H1	1.01	0.92

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%)	259 (96%)	10 (4%)	0	100	100
4	D	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
5	E	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
6	F	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
7	G	174/176 (99%)	162 (93%)	10 (6%)	2 (1%)	16	57
8	H	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
9	I	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
12	L	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	24	65
13	M	134/136 (98%)	123 (92%)	10 (8%)	1 (1%)	24	65
14	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
15	O	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
16	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	17	58
19	S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	19	60
20	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
21	U	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	17	58
22	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	W	73/75 (97%)	70 (96%)	3 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	54 (87%)	6 (10%)	2 (3%)	4	38
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
32	5	129/131 (98%)	103 (80%)	26 (20%)	0	100	100
35	b	216/218 (99%)	195 (90%)	21 (10%)	0	100	100
36	c	204/206 (99%)	195 (96%)	7 (3%)	2 (1%)	17	58
37	d	203/205 (99%)	183 (90%)	20 (10%)	0	100	100
38	e	155/157 (99%)	136 (88%)	17 (11%)	2 (1%)	13	54
39	f	98/100 (98%)	80 (82%)	16 (16%)	2 (2%)	8	47
40	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
41	h	127/129 (98%)	121 (95%)	6 (5%)	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%)	101 (89%)	13 (11%)	0	100	100
45	l	121/123 (98%)	99 (82%)	21 (17%)	1 (1%)	21	62
46	m	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
47	n	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
48	o	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
49	p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
50	q	78/80 (98%)	66 (85%)	11 (14%)	1 (1%)	13	54
51	r	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
52	s	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
53	t	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
54	u	63/65 (97%)	50 (79%)	12 (19%)	1 (2%)	11	50
55	v	246/248 (99%)	226 (92%)	17 (7%)	3 (1%)	14	56
56	w	494/529 (93%)	427 (86%)	63 (13%)	4 (1%)	21	62
58	z	12/14 (86%)	11 (92%)	0	1 (8%)	1	16
All	All	6535/6674 (98%)	5961 (91%)	547 (8%)	27 (0%)	40	75

5 of 27 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	91
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%)	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	88
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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
32	5	100/100 (100%)	100 (100%)	0	100	100
35	b	180/180 (100%)	177 (98%)	3 (2%)	63	84
36	c	170/170 (100%)	170 (100%)	0	100	100
37	d	172/172 (100%)	170 (99%)	2 (1%)	74	88
38	e	114/119 (96%)	113 (99%)	1 (1%)	81	91
39	f	87/87 (100%)	87 (100%)	0	100	100
40	g	124/124 (100%)	124 (100%)	0	100	100
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	201/201 (100%)	198 (98%)	3 (2%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	w	427/453 (94%)	422 (99%)	5 (1%)	74	88
58	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5406/5460 (99%)	5379 (100%)	27 (0%)	90	96

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	d	80	ARG
42	i	44	ARG
56	w	125	LYS
37	d	177	MET
14	N	2	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
32	5	4	ASN
39	f	58	HIS
56	w	311	HIS
35	b	23	ASN
37	d	115	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2894/2903 (99%)	537 (18%)	29 (1%)
2	B	119/120 (99%)	14 (11%)	2 (1%)
33	7	6/7 (85%)	6 (100%)	2 (33%)
34	a	1538/1539 (99%)	219 (14%)	0
57	x	76/77 (98%)	20 (26%)	0
All	All	4633/4646 (99%)	796 (17%)	33 (0%)

5 of 796 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	25	U
1	A	27	G

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Mol	Chain	Res	Type
1	A	34	U

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1300	G
1	A	1913	A
2	B	88	C
1	A	1378	A
1	A	1399	C

## 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	-	25,33,34	2.66	9 (36%)	33,52,54	1.95	5 (15%)

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	-	-	8/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	601	GCP	C4-N9	-7.36	1.37	1.47
59	w	601	GCP	C2-N1	-5.98	1.37	1.45
59	w	601	GCP	PB-O3A	5.60	1.64	1.58
59	w	601	GCP	C5-C6	-4.56	1.44	1.52
59	w	601	GCP	C6-N1	2.58	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	w	601	GCP	C4-C5-N7	6.10	110.55	102.46
59	w	601	GCP	N3-C2-N1	5.40	123.54	112.00
59	w	601	GCP	C5-C6-N1	-5.29	111.97	118.27
59	w	601	GCP	O6-C6-C5	3.68	127.40	119.82
59	w	601	GCP	PA-O3A-PB	-2.36	124.83	132.49

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

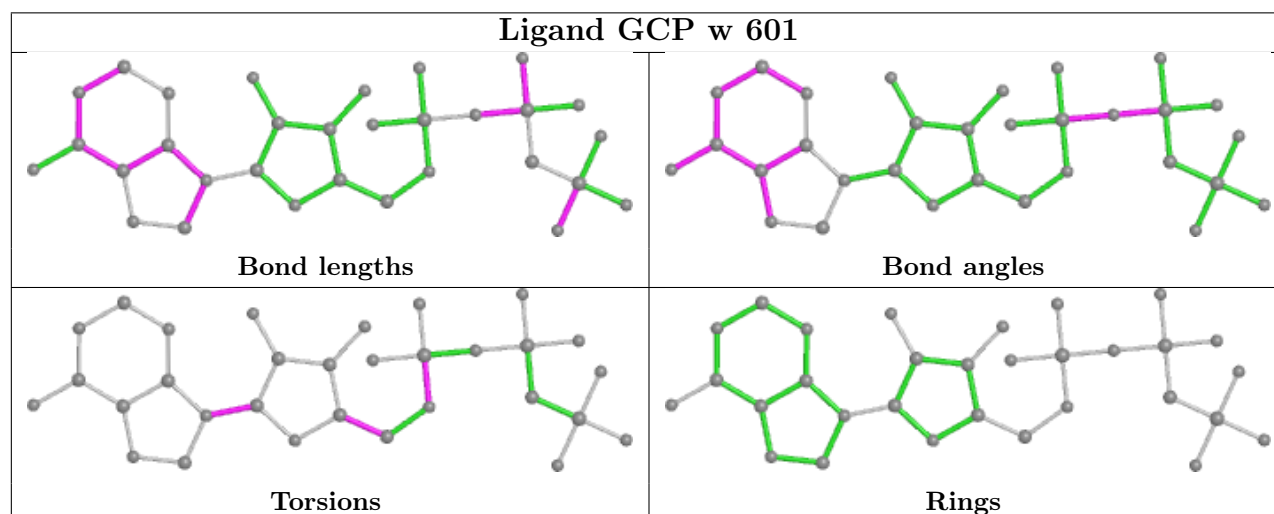
Mol	Chain	Res	Type	Atoms
59	w	601	GCP	C5'-O5'-PA-O3A
59	w	601	GCP	O4'-C1'-N9-C4
59	w	601	GCP	C2'-C1'-N9-C8
59	w	601	GCP	C2'-C1'-N9-C4
59	w	601	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	v	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	191:GLU	C	192:SER	N	1.74
1	v	329:LEU	C	330:ASP	N	1.72
1	A	1913:A	O3'	1914:C	P	1.21