



# Full wwPDB/EMDatabank EM Map/Model Validation 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 Full wwPDB/EMDatabank EM Map/Model Validation 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

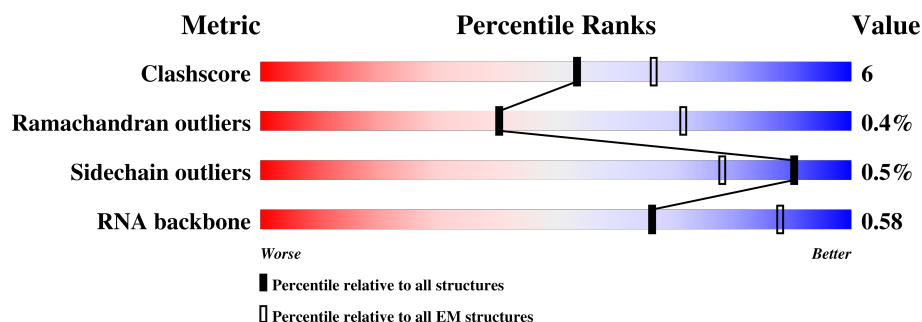
# 1 Overall quality at a glance

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.














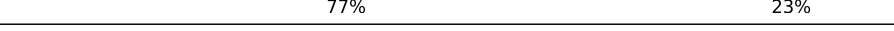


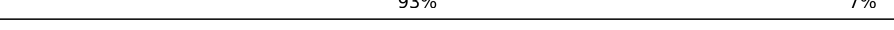




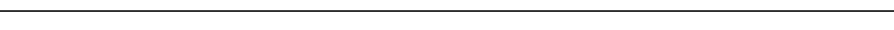

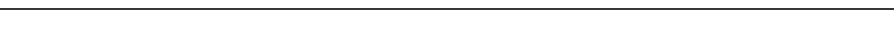
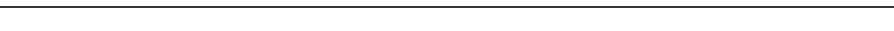


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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		

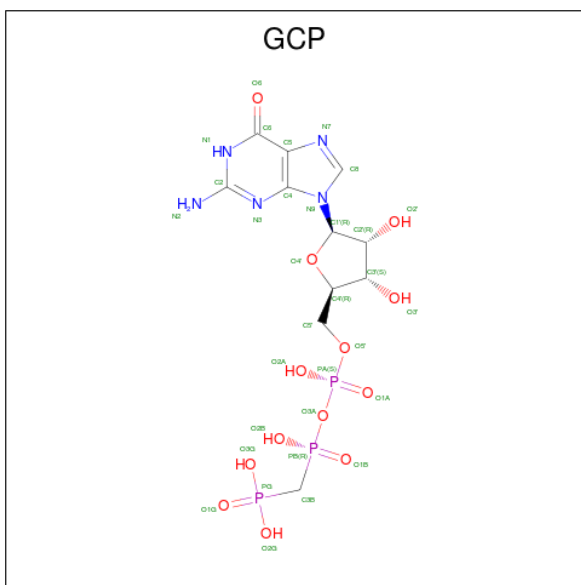
- Molecule 57 is a RNA chain called fMet-tRNA.

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:  $C_{11}H_{18}N_5O_{13}P_3$ ).

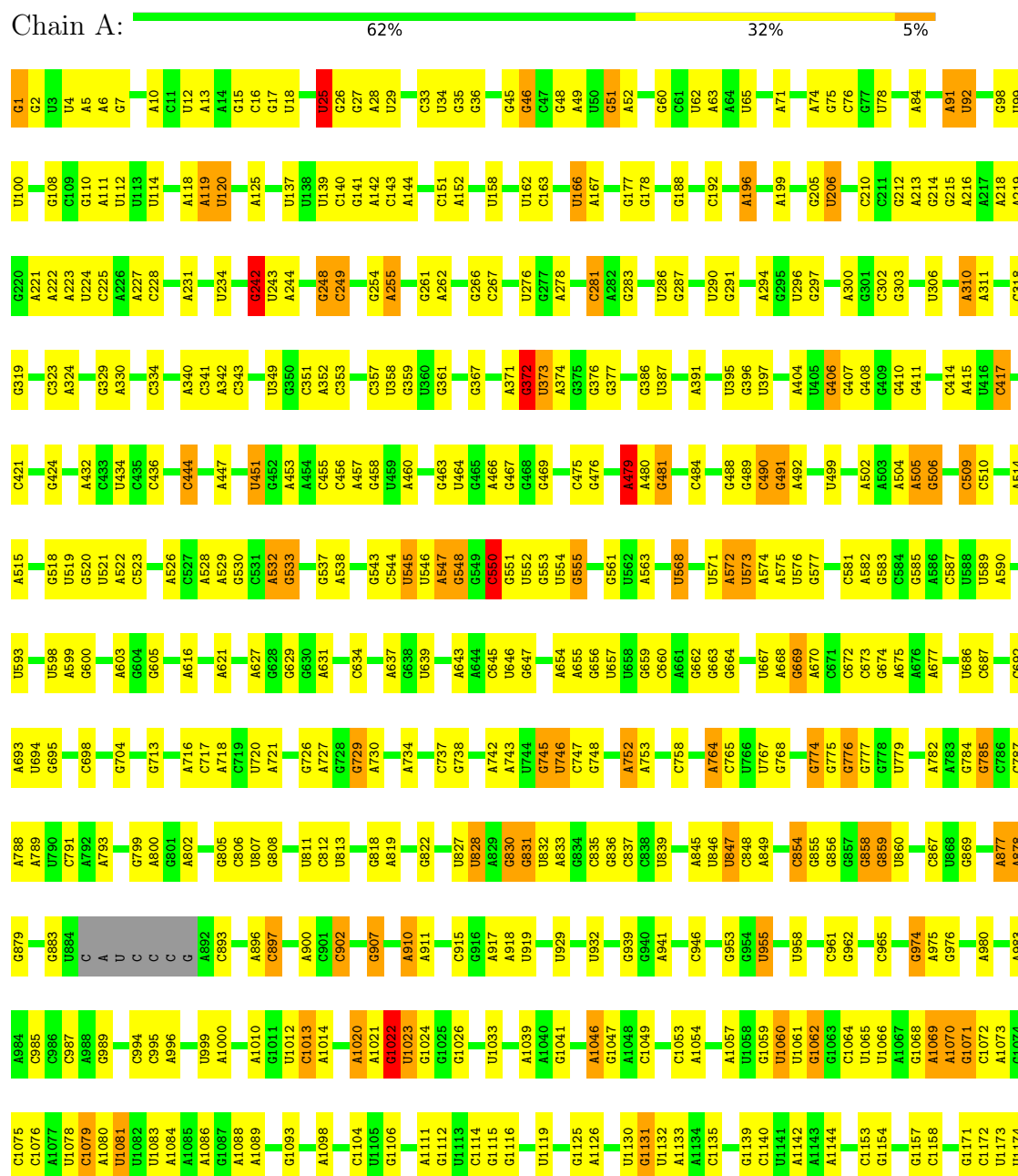


Mol	Chain	Residues	Atoms					AltConf
59	w	1	Total	C	N	O	P	0
			31	11	4	13	3	

### 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

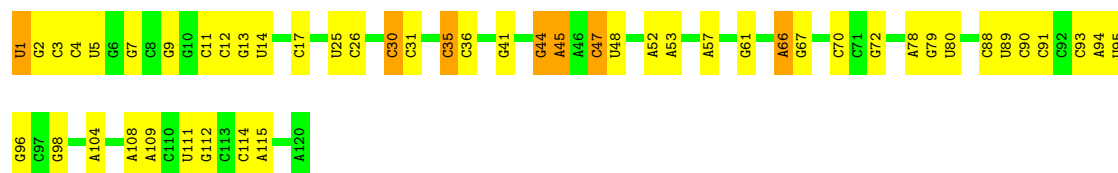


A2820	G2722	G2621	C2520	A2430	A2322	G2229	G2118	C2021	A1912	A1801	G1682	C1536	G1416	G1295	A1175
A2821	A2726	G2629	G2523	U2431	G2325	G2230	G2119	U2022	A1913	A1802	G1687	C1537	C1417	G1296	U1176
A2822	G2731	G2630	G2524	A2432	C2326	U2231	G2120	C2023	C1914	C1806	C1694	A1544	G1418	G1300	C1178
C2824	G2732	G2631	G2525	A2435	A2327	C2232	G2121	C2024	U1917	G1807	C1695	G1555	A1419	A1301	C1179
G2825	A2733	G2634	G2526	U2441	U2329	G2234	G2127	C2025	U1918	A1808	G1699	G1559	A1420	U1180	U1181
U2832		A2634	G2529	C2442	G2330	G2238	U2131	U2028	G1921	A1809	G1704	U1559	G1421	C1306	U1182
U2833	U2739	A2635	A2530	C2443	U2333	G2239	U2132	G2029	G1922	G1810	A1700	G1560	C1422	U1313	G1183
G2834	U2743	G2636	A2531	G2444	U2334	U2240	G2133	A2030	A1927	U1812	A1701	C1565	G1429	C1314	U1188
A2835	U2744	C2646	G2535	G2447	A2335	U2241	G2136	A2033	G1929	G1816	G1705	A1569	G1430	A1321	G1190
U2836	C2745	U2647	A2536	A2448	A2336	U2245	G2140	U2034	G1930	G1817	C1706	A1578	G1431	A1322	A1204
A2837	U2746	G2648	A2537	U2449	A2336	U2246	G2141	G2035	U1936	U1818	G1707	A1579	G1432	C1323	A1205
G2846	G2747					G2248	G2144	C2036	A1937	G1823	G1715	A1585	A1433	G1324	G1206
U2847	A2748	A2654	U2552	U2457	G2345	C2249	G2145	A2037	A1938	G1827	G1716	C1585	A1434	U1325	U1209
G2848	U2749	G2655	G2553	G2458	A2346	U2249	C2146	C2043	U1939	G1828	A1717	C1592	G1435	U1326	C1210
U2849	C2752	U2656	U2554	A2459	A2346	G2250	C2147	U2047	U1940	A1829	G1724	C1593	G1436	C1330	C1211
A2850		G2659	C2559	U2460	C2350	G2251	A2147	C2048	C1941	G1830	C1732	A1603	C1437	U1329	G1212
A2851	C2755		A2560	C2463	G2357	G2252	G2157	G2049	U1944	G1831	U1729	A1597	C1447	G1331	G1215
U2861	A2757	A2662	A2564	G2464	C2354	C2254	G2162	C2050	G1945	G1832	U1730	A1598	G1450	G1332	
C2862	C2762	G2665	A2565	U2473	G2357	C2258	A2163	A2052	A1953	U1834	G1731	A1603	G1451	G1333	C1221
G2863	G2763	C2666	A2566	U2474	G2372	A2267	A2171	C2055	G1954	G1835	C1732	A1604	G1452	U1222	U1223
G2864	A2764		G2567	C2475	C2374	U2268	U2172	A2060	A1960	G1841	G1737	C1607	C1454	G1224	G1225
G2867	A2765	G2673		U2476	C2374	G2279	C2174	G2061	C1961	G1842	G1738	C1607	C1461	C1348	A1237
A2868				A2477	C2380	C2283	C2175	A2062	C1962	G1847	U1744	A1610	A1469	C1349	
A2872	U2768	C2676	G2570	G2477	A2381	G2286	C2176	U2068	C1967	G1858	A1745	C1611	G1475	A1353	U1242
A2873	U2769	U2682	A2572	A2478	G2382	G2287	C2177	G2069	U1971	G1859	A1746	C1612	U1476	G1355	A1247
	G2770	C2683	C2573	C2483	U2384	A2287	C2178	A2070	C1986	G1862	G1753	A1634	G1482	G1356	G1248
C2880	C2771		U2580	G2484	C2385	G2288	C2179	A2071	A1970	G1862	A1754	U1635	A1490	U1249	
A2883	A2776	U2687	G2581	G2487	A2386	G2289	U2185	C2072	U1971	C1870	U1757	U1636	A1491	G1250	
U2884	G2777	G2688	G2582	G2488	G2387	G2290	G2186	A2076	G1972	A1871	U1758	A1637	G1492	C1251	G1252
A2893	U2778	U2689	U2585	A2491	U2388	U2291	U2178	A2077	C1987	G1872	U1759	C1638	C1493	A1253	A1254
G2894	G2780	C2691	U2586		C2385	G2292	U2189	U2076	A1987	G1873	C1760	C1646	G1500	U1255	
U2898	A2781	G2692	A2590	G2494	G2391	G2293	U2189	U2081	U1991	U1880	C1764	U1647	G1500	G1376	G1256
A2899	G2782	G2693	C2591	C2498	A2392	G2294	U2189	A2082	G1992	U1880	C1764	U1648	A1504	A1376	
A2900	C2788	G2694	G2595	G2508	C2395	G2295	U2189	U2082	U1991	G1886	C1764	U1648	A1504	G1376	G1266
C2901	G2791	U2698	A2596	G2502	G2396	C2296	U2189	A2082	G1992	G1886	C1764	U1648	A1504	G1376	G1266
C2902	C2794	C2703	A2598	A2503	U2402	U2296	A2198	U2086	C1996	G1886	C1764	U1648	A1504	G1376	G1266
U2903	C2795	C2704	A2602	U2504	U2402	A2297	A2198	U2086	C1996	G1886	C1764	U1648	A1504	G1376	G1266
	U2796	G2708	G2603	G2505	A2407	A2298	G2201	G2087	C1997	G1886	C1764	U1648	A1504	G1376	G1266
	U2797	G2709	U2604	C2507	A2407	U2299	G2201	G2087	C1997	G1886	C1764	U1648	A1504	G1376	G1266
	U2798	G2709	U2605	G2508	G2415	G2300	G2204	G2093	A1998	G1886	C1764	U1648	A1504	G1376	G1266
A2799	A2799	C2712	U2609	U2511	A2418	U2305	A2211	A2095	G2002	G1886	C1764	U1648	A1504	G1376	G1266
A2800	A2800	U2713	C2610	A2512	A2418	C2306	A2212	G2100	C2006	A1889	U1781	A1665	A1515	C1386	A1272
G2801	G2801	G2714	U2613	A2513	U2423	A2309	U2213	A2108	C2007	A1900	U1782	A1666	A1515	C1387	A1287
G2802	G2802	C2715	U2614	A2514	C2424	A2309	U2213	A2108	C2007	A1900	U1782	A1666	A1515	C1387	A1287
		C2716	U2615	A2515	A2425	A2313	U2215	U2109	C2008	A1901	U1796	A1667	A1515	C1387	A1287
G2808	G2808	C2717	U2616	A2516	A2426	C2314	U2216	G2110	C2009	A1901	U1796	A1667	A1515	C1387	A1287
A2809	A2809	G2718	U2617	C2517	C2427	A2314	U2216	G2111	A2009	G1906	U1797	A1667	A1515	C1387	A1287
		U2719	G2618	A2518	G2428	U2320	A2225	G2112	G2010	G1907	U1799	A1667	A1515	C1387	A1287
U2818	U2818	U2720	U2619	C2519	G2429	U2321	A2226	U2113	A2020	U1911	C1800	C1675	A1535	U1401	U1294




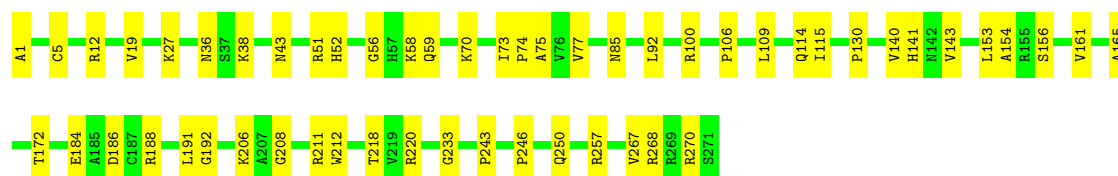
- Molecule 2: 5S ribosomal RNA

Chain B: 




- Molecule 3: 50S ribosomal protein L2

Chain C: 




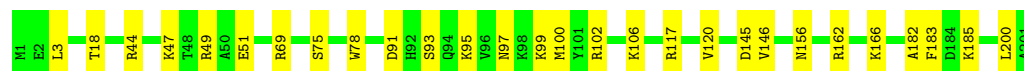
- Molecule 4: 50S ribosomal protein L3

Chain D: 




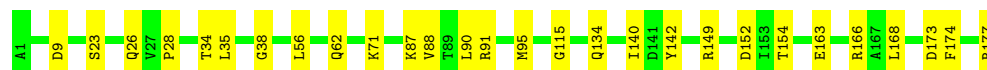
- Molecule 5: 50S ribosomal protein L4

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: 



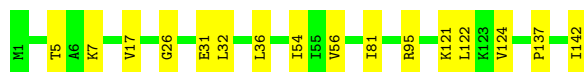
- Molecule 9: 50S ribosomal protein L11

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%



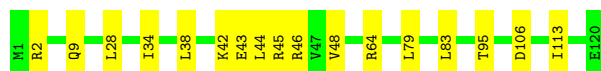
- Molecule 13: 50S ribosomal protein L16

Chain M: 86% 13%



- Molecule 14: 50S ribosomal protein L17

Chain N: 86% 14%



- Molecule 15: 50S ribosomal protein L18

Chain O: 89% 11%




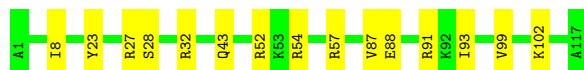
- Molecule 16: 50S ribosomal protein L19

Chain P:  87% 13%




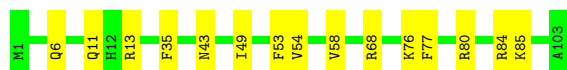
- Molecule 17: 50S ribosomal protein L20

Chain Q:  87% 13%




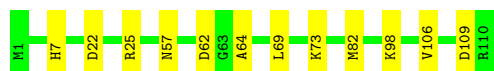
- Molecule 18: 50S ribosomal protein L21

Chain R:  85% 15%




- Molecule 19: 50S ribosomal protein L22

Chain S:  89% 11%




- Molecule 20: 50S ribosomal protein L23

Chain T:  77% 23%




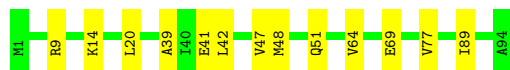
- Molecule 21: 50S ribosomal protein L24

Chain U:  86% 13%



- Molecule 22: 50S ribosomal protein L25

Chain V:  86% 14%



- 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%




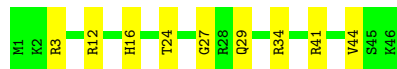
- Molecule 28: 50S ribosomal protein L33

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

Chain 4: 84% 16%



- Molecule 32: 50S ribosomal protein L10

Chain 5: 80% 20%



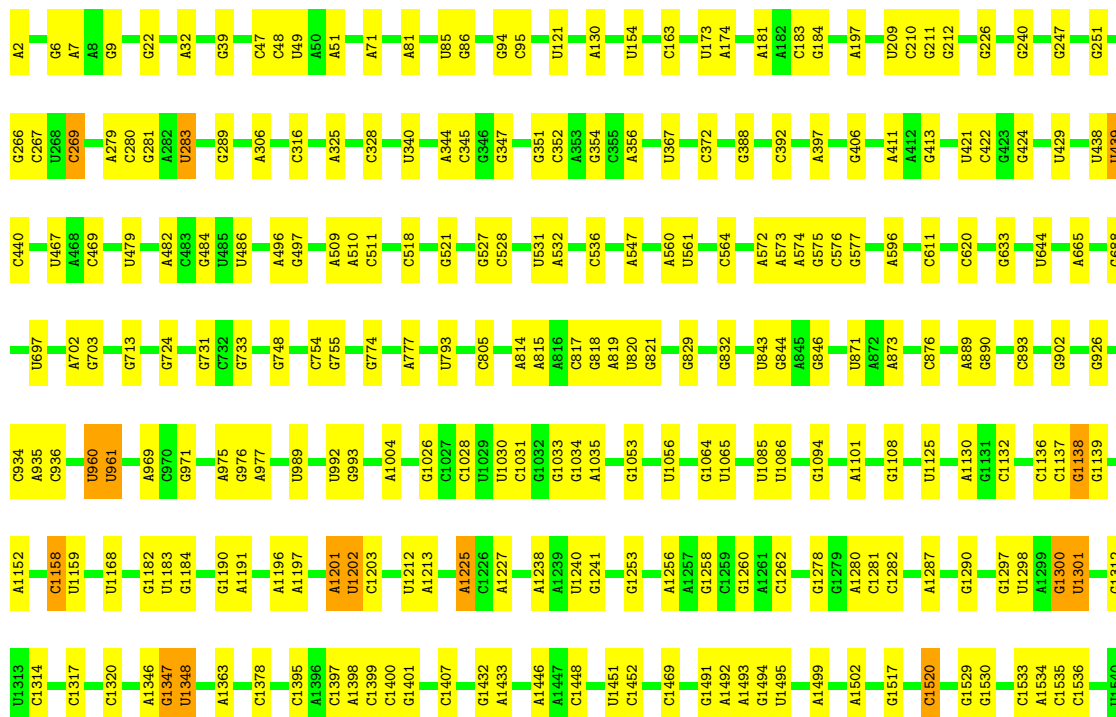
- Molecule 33: mRNA

Chain 7: 14% 43% 43%



- Molecule 34: 16S ribosomal RNA

Chain a: 84% 15%



- Molecule 35: 30S ribosomal protein S2

Chain b:  97% .



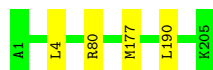
- Molecule 36: 30S ribosomal protein S3

Chain c:  99% .



- Molecule 37: 30S ribosomal protein S4

Chain d:  98% .



- Molecule 38: 30S ribosomal protein S5

Chain e:  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.

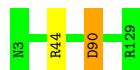
- Molecule 41: 30S ribosomal protein S8

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%



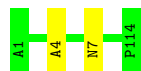
- Molecule 45: 30S ribosomal protein S12

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.

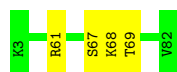
- Molecule 49: 30S ribosomal protein S16

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%



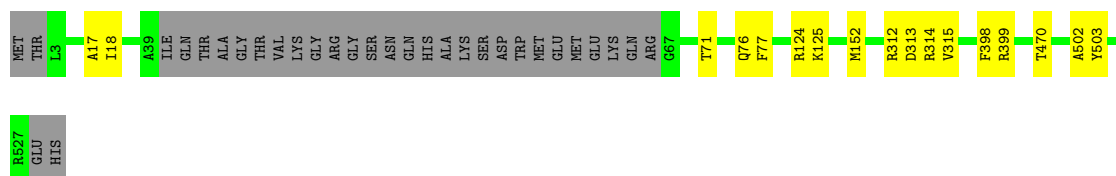
- Molecule 55: Peptide chain release factor RF1

Chain v:  96%



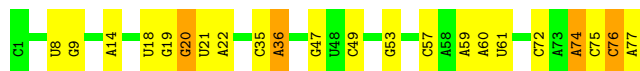
- Molecule 56: Peptide chain release factor RF3

Chain w:  91%



- Molecule 57: fMet-tRNA

Chain x:  71%



- Molecule 58: Apidaecin

Chain z:  93%





## 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

All (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
2	B	1	U	OP3-P	-10.57	1.48	1.61
34	a	2	A	OP3-P	-10.55	1.48	1.61
1	A	1913	A	C2-N3	10.02	1.42	1.33

All (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
55	v	191	GLU	CA-C-N	-14.18	86.01	117.20
1	A	1912	A	O3'-P-O5'	-12.89	79.50	104.00
57	x	36	A	P-O3'-C3'	12.52	134.72	119.70
1	A	1913	A	O3'-P-O5'	-11.99	81.22	104.00
1	A	2604	U	C2-N1-C1'	10.35	130.12	117.70
55	v	191	GLU	C-N-CA	-10.25	96.08	121.70
1	A	1913	A	C2-N3-C4	-9.89	105.65	110.60
1	A	2063	C	N1-C2-O2	9.78	124.77	118.90
57	x	74	A	C2'-C3'-O3'	9.47	130.33	109.50
1	A	2226	C	N1-C2-O2	9.18	124.41	118.90
2	B	36	C	N1-C2-O2	9.10	124.36	118.90
1	A	1313	U	N3-C2-O2	-9.04	115.87	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1348	C	N1-C2-O2	8.96	124.27	118.90
1	A	1326	U	N3-C2-O2	-8.92	115.96	122.20
55	v	329	LEU	O-C-N	-8.82	108.59	122.70
1	A	2473	U	N1-C2-O2	8.69	128.88	122.80
1	A	2473	U	N3-C2-O2	-8.53	116.23	122.20
1	A	1326	U	N1-C2-O2	8.44	128.71	122.80
34	a	611	C	N1-C2-O2	8.41	123.95	118.90
1	A	1313	U	N1-C2-O2	8.32	128.62	122.80
1	A	847	U	N3-C2-O2	-8.30	116.39	122.20
1	A	955	U	C2-N1-C1'	8.24	127.59	117.70
57	x	36	A	OP1-P-O3'	8.15	123.13	105.20
1	A	1774	C	N3-C2-O2	-8.13	116.21	121.90
1	A	2794	C	N3-C2-O2	-8.11	116.22	121.90
34	a	1407	C	N1-C2-O2	8.10	123.76	118.90
1	A	2605	U	N1-C2-O2	8.07	128.45	122.80
1	A	1313	U	C2-N1-C1'	8.07	127.39	117.70
2	B	35	C	N1-C2-O2	8.04	123.73	118.90
2	B	26	C	N1-C2-O2	7.97	123.68	118.90
1	A	847	U	N1-C2-O2	7.96	128.37	122.80
1	A	2063	C	N3-C2-O2	-7.94	116.34	121.90
1	A	2072	C	C2-N1-C1'	7.92	127.51	118.80
2	B	36	C	N3-C2-O2	-7.90	116.37	121.90
1	A	2604	U	C6-N1-C1'	-7.84	110.22	121.20
1	A	2605	U	C2-N1-C1'	7.83	127.10	117.70
34	a	754	C	C2-N1-C1'	7.78	127.35	118.80
1	A	2457	U	C2-N1-C1'	7.71	126.95	117.70
57	x	57	C	N3-C2-O2	-7.65	116.55	121.90
1	A	1180	U	N1-C2-O2	7.60	128.12	122.80
1	A	2605	U	N3-C2-O2	-7.59	116.89	122.20
34	a	1348	U	N1-C2-O2	7.58	128.10	122.80
1	A	1893	C	N3-C2-O2	-7.57	116.60	121.90
2	B	12	C	N1-C2-O2	7.55	123.43	118.90
1	A	847	U	C2-N1-C1'	7.54	126.74	117.70
1	A	2063	C	C2-N1-C1'	7.53	127.08	118.80
1	A	1893	C	N1-C2-O2	7.52	123.41	118.90
1	A	2473	U	C2-N1-C1'	7.49	126.69	117.70
1	A	2226	C	N3-C2-O2	-7.35	116.76	121.90
1	A	1326	U	C2-N1-C1'	7.33	126.49	117.70
1	A	1917	U	N1-C2-O2	7.21	127.84	122.80
34	a	1407	C	C6-N1-C2	-7.20	117.42	120.30
1	A	1914	C	N1-C2-O2	7.20	123.22	118.90
1	A	2580	U	C2-N1-C1'	7.19	126.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2063	C	C6-N1-C2	-7.19	117.42	120.30
1	A	1774	C	N1-C2-O2	7.16	123.19	118.90
1	A	1348	C	N3-C2-O2	-7.12	116.91	121.90
1	A	1049	C	N1-C2-O2	7.12	123.17	118.90
57	x	76	C	C5'-C4'-O4'	7.09	117.61	109.10
1	A	867	C	N1-C2-O2	7.06	123.13	118.90
1	A	2226	C	C2-N1-C1'	7.05	126.56	118.80
1	A	1180	U	N3-C2-O2	-7.03	117.28	122.20
2	B	36	C	C2-N1-C1'	7.01	126.52	118.80
2	B	36	C	C6-N1-C2	-6.99	117.50	120.30
1	A	1378	A	P-O3'-C3'	6.97	128.07	119.70
1	A	752	A	P-O3'-C3'	6.93	128.02	119.70
1	A	192	C	N1-C2-O2	6.93	123.06	118.90
34	a	1158	C	C2-N1-C1'	6.91	126.40	118.80
1	A	2043	C	C2-N1-C1'	6.91	126.39	118.80
1	A	1049	C	N3-C2-O2	-6.89	117.08	121.90
1	A	1378	A	OP1-P-O3'	6.87	120.31	105.20
1	A	897	C	N1-C2-O2	6.85	123.01	118.90
1	A	919	U	N1-C2-O2	6.83	127.58	122.80
1	A	2604	U	N1-C2-O2	6.83	127.58	122.80
57	x	57	C	N1-C2-O2	6.83	123.00	118.90
34	a	1407	C	N3-C2-O2	-6.81	117.13	121.90
57	x	20	G	C4-N9-C1'	-6.80	117.66	126.50
1	A	1917	U	N3-C2-O2	-6.77	117.46	122.20
1	A	854	C	N3-C2-O2	-6.76	117.16	121.90
34	a	611	C	N3-C2-O2	-6.76	117.17	121.90
1	A	2580	U	N3-C2-O2	-6.75	117.48	122.20
1	A	2580	U	O4'-C1'-N1	6.74	113.59	108.20
1	A	1022	G	P-O3'-C3'	6.72	127.76	119.70
34	a	1201	A	P-O3'-C3'	6.71	127.75	119.70
1	A	2072	C	C5-C6-N1	6.70	124.35	121.00
34	a	1297	G	P-O3'-C3'	6.66	127.69	119.70
2	B	31	C	C2-N1-C1'	6.66	126.12	118.80
1	A	25	U	C2-N1-C1'	6.65	125.67	117.70
2	B	35	C	N3-C2-O2	-6.64	117.25	121.90
1	A	2794	C	N1-C2-O2	6.63	122.88	118.90
34	a	1348	U	N3-C2-O2	-6.62	117.57	122.20
1	A	1914	C	C2-N1-C1'	6.60	126.06	118.80
1	A	1020	A	P-O3'-C3'	6.59	127.61	119.70
1	A	1956	U	N1-C2-O2	6.57	127.40	122.80
34	a	439	U	N1-C2-O2	6.53	127.37	122.80
1	A	2072	C	C6-N1-C2	-6.52	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1917	U	C2-N1-C1'	6.51	125.51	117.70
2	B	12	C	N3-C2-O2	-6.50	117.35	121.90
1	A	2704	C	N1-C2-O2	6.50	122.80	118.90
57	x	20	G	N3-C4-N9	-6.48	122.11	126.00
34	a	644	U	N3-C2-O2	-6.46	117.68	122.20
34	a	1301	U	C2-N1-C1'	6.46	125.45	117.70
57	x	20	G	C8-N9-C1'	6.44	135.37	127.00
1	A	1348	C	C6-N1-C2	-6.40	117.74	120.30
1	A	2636	C	N1-C2-O2	6.40	122.74	118.90
1	A	1956	U	N3-C2-O2	-6.39	117.73	122.20
1	A	114	U	C2-N1-C1'	6.37	125.34	117.70
2	B	17	C	C2-N1-C1'	6.36	125.79	118.80
1	A	2226	C	C6-N1-C2	-6.35	117.76	120.30
34	a	611	C	C2-N1-C1'	6.35	125.78	118.80
1	A	752	A	OP2-P-O3'	6.34	119.14	105.20
2	B	12	C	C6-N1-C2	-6.33	117.77	120.30
2	B	35	C	C6-N1-C2	-6.33	117.77	120.30
34	a	1132	C	N1-C2-O2	6.32	122.69	118.90
2	B	26	C	N3-C2-O2	-6.31	117.48	121.90
1	A	2604	U	C5-C6-N1	6.29	125.84	122.70
1	A	1348	C	C2-N1-C1'	6.28	125.70	118.80
1	A	2752	C	N1-C2-O2	6.27	122.66	118.90
1	A	2214	C	N1-C2-O2	6.26	122.66	118.90
1	A	1774	C	C6-N1-C2	-6.25	117.80	120.30
1	A	915	C	C2-N1-C1'	6.24	125.67	118.80
2	B	26	C	C2-N1-C1'	6.24	125.67	118.80
34	a	1348	U	C2-N1-C1'	6.23	125.17	117.70
1	A	2457	U	N1-C2-O2	6.22	127.16	122.80
1	A	1081	U	C2-N1-C1'	6.19	125.13	117.70
1	A	1180	U	C2-N1-C1'	6.19	125.13	117.70
1	A	2072	C	N1-C2-O2	6.19	122.61	118.90
34	a	644	U	N1-C2-O2	6.19	127.13	122.80
1	A	2604	U	O4'-C1'-N1	6.14	113.11	108.20
37	d	4	LEU	CA-CB-CG	6.14	129.41	115.30
1	A	919	U	N3-C2-O2	-6.12	117.92	122.20
1	A	1294	U	N1-C2-O2	6.11	127.08	122.80
1	A	2504	U	C2-N1-C1'	6.11	125.03	117.70
34	a	1182	G	P-O3'-C3'	6.11	127.03	119.70
1	A	1086	A	C2-N3-C4	6.10	113.65	110.60
1	A	2474	U	N1-C2-O2	6.10	127.07	122.80
2	B	11	C	N1-C2-O2	6.10	122.56	118.90
34	a	528	C	N1-C2-O2	6.07	122.54	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	936	C	N1-C2-O2	6.07	122.54	118.90
34	a	611	C	C6-N1-C2	-6.06	117.88	120.30
1	A	1081	U	N1-C2-O2	6.06	127.04	122.80
1	A	25	U	N1-C2-O2	6.04	127.03	122.80
2	B	3	C	P-O3'-C3'	6.04	126.95	119.70
34	a	85	U	P-O3'-C3'	6.03	126.94	119.70
13	M	70	ASP	CB-CG-OD1	6.03	123.72	118.30
34	a	1158	C	N1-C2-O2	6.01	122.51	118.90
55	v	187	VAL	N-CA-C	-6.01	94.78	111.00
1	A	2703	C	C6-N1-C2	-6.00	117.90	120.30
1	A	2794	C	C6-N1-C2	-5.99	117.90	120.30
1	A	1294	U	N3-C2-O2	-5.99	118.01	122.20
34	a	697	U	N1-C2-O2	5.98	126.99	122.80
34	a	989	U	N3-C2-O2	-5.98	118.02	122.20
34	a	316	C	C2-N1-C1'	5.97	125.37	118.80
34	a	1407	C	C2-N1-C1'	5.97	125.37	118.80
55	v	194	GLY	N-CA-C	5.97	128.03	113.10
1	A	2720	U	N3-C2-O2	-5.95	118.03	122.20
16	P	113	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	2580	U	N1-C2-O2	5.95	126.96	122.80
34	a	269	C	C2-N1-C1'	5.93	125.32	118.80
34	a	1399	C	P-O3'-C3'	5.93	126.81	119.70
1	A	2590	A	N9-C4-C5	5.93	108.17	105.80
1	A	1070	A	P-O3'-C3'	5.92	126.81	119.70
34	a	936	C	N3-C2-O2	-5.92	117.76	121.90
1	A	242	G	P-O3'-C3'	5.90	126.78	119.70
34	a	1202	U	N1-C2-O2	5.89	126.93	122.80
1	A	1221	C	C2-N1-C1'	5.89	125.28	118.80
1	A	1349	C	C2-N1-C1'	5.89	125.28	118.80
1	A	2590	A	N1-C6-N6	-5.89	115.07	118.60
1	A	1940	U	P-O3'-C3'	5.87	126.74	119.70
1	A	143	C	C2-N1-C1'	5.86	125.24	118.80
1	A	51	G	P-O3'-C3'	5.86	126.73	119.70
34	a	440	C	N1-C2-O2	5.85	122.41	118.90
1	A	2457	U	N3-C2-O2	-5.84	118.11	122.20
34	a	960	U	P-O3'-C3'	5.84	126.71	119.70
34	a	439	U	C5-C6-N1	5.80	125.60	122.70
1	A	2474	U	N3-C2-O2	-5.79	118.15	122.20
1	A	2286	G	P-O3'-C3'	5.78	126.64	119.70
1	A	985	C	C2-N1-C1'	5.76	125.14	118.80
1	A	1348	C	C5-C6-N1	5.75	123.88	121.00
1	A	1314	C	C2-N1-C1'	5.75	125.12	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	17	C	C6-N1-C2	-5.74	118.00	120.30
1	A	192	C	N3-C2-O2	-5.74	117.88	121.90
34	a	316	C	N1-C2-O2	5.74	122.34	118.90
1	A	2636	C	C2-N1-C1'	5.73	125.11	118.80
57	x	20	G	OP2-P-O3'	5.73	117.81	105.20
1	A	1914	C	N3-C2-O2	-5.72	117.89	121.90
1	A	2474	U	C2-N1-C1'	5.72	124.56	117.70
1	A	372	G	P-O3'-C3'	5.72	126.56	119.70
1	A	985	C	N1-C2-O2	5.72	122.33	118.90
1	A	2192	U	C2-N1-C1'	5.71	124.55	117.70
2	B	31	C	N1-C2-O2	5.71	122.32	118.90
1	A	2063	C	C5-C6-N1	5.70	123.85	121.00
1	A	859	G	P-O3'-C3'	5.69	126.53	119.70
1	A	2683	C	N1-C2-O2	5.69	122.31	118.90
34	a	754	C	N1-C2-O2	5.69	122.31	118.90
57	x	57	C	C6-N1-C2	-5.68	118.03	120.30
2	B	12	C	C2-N1-C1'	5.68	125.05	118.80
34	a	439	U	N3-C2-O2	-5.67	118.23	122.20
34	a	1190	G	P-O3'-C3'	5.67	126.50	119.70
1	A	2666	C	N1-C2-O2	5.66	122.30	118.90
34	a	1407	C	C5-C6-N1	5.66	123.83	121.00
34	a	754	C	C6-N1-C1'	-5.66	114.01	120.80
2	B	25	U	N1-C2-O2	5.65	126.75	122.80
1	A	353	C	N1-C2-O2	5.64	122.28	118.90
34	a	1225	A	C4-N9-C1'	5.64	136.45	126.30
1	A	1839	G	C4-N9-C1'	5.64	133.83	126.50
34	a	1132	C	C2-N1-C1'	5.63	125.00	118.80
1	A	2617	U	N3-C2-O2	-5.63	118.26	122.20
1	A	2566	A	P-O3'-C3'	5.63	126.45	119.70
1	A	902	C	C2-N1-C1'	5.62	124.99	118.80
34	a	697	U	N3-C2-O2	-5.62	118.26	122.20
34	a	1432	G	P-O3'-C3'	5.62	126.45	119.70
34	a	1125	U	N1-C2-O2	5.62	126.73	122.80
1	A	353	C	C2-N1-C1'	5.62	124.98	118.80
1	A	1913	A	N3-C4-C5	5.61	130.73	126.80
1	A	2457	U	O4'-C1'-N1	5.60	112.68	108.20
34	a	1347	G	P-O3'-C3'	5.60	126.42	119.70
34	a	1300	G	P-O3'-C3'	5.59	126.41	119.70
1	A	634	C	N1-C2-O2	5.59	122.25	118.90
1	A	867	C	N3-C2-O2	-5.59	117.99	121.90
1	A	2473	U	C5-C6-N1	5.59	125.49	122.70
2	B	31	C	C6-N1-C2	-5.58	118.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2655	G	P-O3'-C3'	5.58	126.40	119.70
34	a	1520	C	C2-N1-C1'	5.58	124.94	118.80
1	A	2504	U	N1-C2-O2	5.58	126.70	122.80
2	B	30	C	N1-C2-O2	5.56	122.24	118.90
1	A	897	C	C2-N1-C1'	5.55	124.90	118.80
1	A	897	C	N3-C2-O2	-5.54	118.02	121.90
34	a	989	U	N1-C2-O2	5.54	126.67	122.80
1	A	1079	C	N1-C2-O2	5.53	122.22	118.90
34	a	438	U	P-O3'-C3'	5.53	126.33	119.70
34	a	439	U	C2-N1-C1'	5.52	124.32	117.70
1	A	1818	U	C2-N1-C1'	5.52	124.32	117.70
1	A	837	C	N3-C2-O2	-5.50	118.05	121.90
1	A	206	U	N1-C2-O2	5.50	126.65	122.80
2	B	26	C	C6-N1-C2	-5.49	118.10	120.30
34	a	961	U	N1-C2-O2	5.49	126.64	122.80
57	x	20	G	C6-C5-N7	5.49	133.69	130.40
1	A	2178	C	N1-C2-O2	5.49	122.19	118.90
34	a	283	U	N1-C2-O2	5.49	126.64	122.80
1	A	479	A	P-O3'-C3'	5.49	126.28	119.70
1	A	2192	U	N1-C2-O2	5.48	126.64	122.80
1	A	2703	C	C2-N1-C1'	5.48	124.83	118.80
1	A	2739	U	N3-C2-O2	-5.48	118.36	122.20
34	a	1138	G	C4-N9-C1'	5.48	133.63	126.50
1	A	2703	C	N1-C2-O2	5.48	122.19	118.90
1	A	955	U	C6-N1-C1'	-5.48	113.53	121.20
1	A	2179	C	N1-C2-O2	5.47	122.19	118.90
1	A	2769	U	N1-C2-O2	5.47	126.63	122.80
1	A	2617	U	N1-C2-O2	5.45	126.61	122.80
34	a	1125	U	N3-C2-O2	-5.45	118.39	122.20
1	A	2739	U	N1-C2-O2	5.44	126.61	122.80
34	a	1202	U	N3-C2-O2	-5.44	118.39	122.20
1	A	2720	U	N1-C2-O2	5.44	126.61	122.80
1	A	2615	U	N3-C2-O2	-5.43	118.40	122.20
2	B	11	C	N3-C2-O2	-5.43	118.10	121.90
1	A	2192	U	N3-C2-O2	-5.42	118.41	122.20
1	A	444	C	N1-C2-O2	5.42	122.15	118.90
2	B	11	C	C6-N1-C2	-5.42	118.13	120.30
1	A	1086	A	C4-N9-C1'	5.41	136.03	126.30
1	A	919	U	C2-N1-C1'	5.39	124.17	117.70
30	3	31	ILE	CG1-CB-CG2	-5.39	99.54	111.40
1	A	417	C	C2-N1-C1'	5.39	124.72	118.80
1	A	1294	U	C2-N1-C1'	5.38	124.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	313	ASP	C-N-CA	5.38	135.16	121.70
34	a	269	C	C6-N1-C2	-5.38	118.15	120.30
1	A	2254	C	N1-C2-O2	5.37	122.12	118.90
37	d	190	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	166	U	N1-C2-O2	5.36	126.55	122.80
34	a	440	C	C6-N1-C2	-5.36	118.16	120.30
1	A	234	U	N3-C2-O2	-5.36	118.45	122.20
1	A	1086	A	N3-C4-N9	5.36	131.69	127.40
34	a	620	C	N1-C2-O2	5.36	122.11	118.90
1	A	206	U	N3-C2-O2	-5.36	118.45	122.20
1	A	2552	U	C2-N1-C1'	5.35	124.12	117.70
1	A	1818	U	N1-C2-O2	5.35	126.55	122.80
1	A	1349	C	C6-N1-C2	-5.34	118.16	120.30
34	a	1262	C	N1-C2-O2	5.34	122.10	118.90
1	A	137	U	N3-C2-O2	-5.33	118.47	122.20
1	A	2884	U	C2-N1-C1'	5.33	124.10	117.70
1	A	1760	C	N1-C2-O2	5.32	122.09	118.90
2	B	3	C	OP1-P-O3'	5.32	116.90	105.20
1	A	2504	U	N3-C2-O2	-5.31	118.48	122.20
1	A	1912	A	OP2-P-O3'	-5.31	93.53	105.20
1	A	2473	U	C6-N1-C2	-5.30	117.82	121.00
34	a	154	U	N3-C2-O2	-5.30	118.49	122.20
1	A	1188	U	N1-C2-O2	5.29	126.50	122.80
1	A	166	U	N3-C2-O2	-5.28	118.50	122.20
1	A	669	G	C4-N9-C1'	5.28	133.37	126.50
1	A	1812	U	C2-N1-C1'	5.27	124.02	117.70
1	A	2300	C	C2-N1-C1'	5.27	124.59	118.80
1	A	1839	G	N3-C4-N9	5.26	129.16	126.00
34	a	469	C	N1-C2-O2	5.25	122.05	118.90
1	A	1880	U	N3-C2-O2	-5.25	118.53	122.20
1	A	1893	C	C6-N1-C2	-5.25	118.20	120.30
1	A	353	C	C6-N1-C2	-5.24	118.20	120.30
1	A	2043	C	C6-N1-C2	-5.22	118.21	120.30
1	A	1812	U	N3-C2-O2	-5.22	118.55	122.20
1	A	2457	U	C5-C4-O4	5.22	129.03	125.90
1	A	2615	U	N1-C2-O2	5.22	126.45	122.80
34	a	1469	C	N1-C2-O2	5.22	122.03	118.90
2	B	25	U	N3-C2-O2	-5.21	118.55	122.20
1	A	114	U	N1-C2-O2	5.21	126.45	122.80
1	A	2254	C	C6-N1-C2	-5.21	118.22	120.30
57	x	20	G	P-O3'-C3'	5.20	125.94	119.70
1	A	25	U	N3-C2-O2	-5.20	118.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1203	C	C2-N1-C1'	5.20	124.52	118.80
1	A	1818	U	N3-C2-O2	-5.20	118.56	122.20
1	A	1376	C	C2-N1-C1'	5.19	124.51	118.80
1	A	837	C	N1-C2-O2	5.18	122.01	118.90
1	A	2460	U	N1-C2-O2	5.17	126.42	122.80
1	A	484	C	C6-N1-C2	-5.17	118.23	120.30
1	A	2604	U	C5-C4-O4	-5.17	122.80	125.90
1	A	2342	C	N3-C2-O2	-5.17	118.28	121.90
34	a	154	U	N1-C2-O2	5.17	126.42	122.80
1	A	550	C	N1-C2-O2	5.16	121.99	118.90
1	A	1417	C	C2-N1-C1'	5.15	124.47	118.80
34	a	1225	A	N3-C4-N9	5.15	131.52	127.40
1	A	1081	U	N3-C2-O2	-5.15	118.60	122.20
34	a	1086	U	N1-C2-O2	5.14	126.39	122.80
1	A	1306	C	C2-N1-C1'	5.13	124.44	118.80
1	A	2043	C	C5-C6-N1	5.13	123.57	121.00
1	A	1913	A	OP2-P-O3'	-5.13	93.92	105.20
34	a	283	U	N3-C2-O2	-5.13	118.61	122.20
34	a	1158	C	N3-C2-O2	-5.13	118.31	121.90
1	A	1880	U	C2-N1-C1'	5.12	123.85	117.70
1	A	1321	A	C2-N3-C4	5.11	113.16	110.60
1	A	758	C	N1-C2-O2	5.11	121.97	118.90
1	A	1892	C	N1-C2-O2	5.11	121.97	118.90
34	a	316	C	C6-N1-C2	-5.11	118.26	120.30
34	a	1138	G	N3-C4-C5	-5.11	126.05	128.60
34	a	893	C	N1-C2-O2	5.11	121.96	118.90
1	A	2769	U	N3-C2-O2	-5.10	118.63	122.20
1	A	1079	C	N3-C2-O2	-5.10	118.33	121.90
1	A	2076	U	C2-N1-C1'	5.09	123.81	117.70
34	a	1314	C	N1-C2-O2	5.09	121.96	118.90
57	x	72	C	C6-N1-C2	-5.09	118.26	120.30
34	a	961	U	N3-C2-O2	-5.09	118.64	122.20
1	A	62	U	C2-N1-C1'	5.09	123.81	117.70
1	A	2226	C	C5-C6-N1	5.09	123.54	121.00
1	A	417	C	C5-C6-N1	5.08	123.54	121.00
1	A	985	C	C6-N1-C2	-5.08	118.27	120.30
1	A	1911	U	C2-N1-C1'	5.06	123.78	117.70
1	A	955	U	O4'-C1'-N1	5.05	112.24	108.20
1	A	2072	C	C6-N1-C1'	-5.05	114.74	120.80
2	B	66	A	P-O3'-C3'	5.05	125.76	119.70
2	B	47	C	N1-C2-O2	5.04	121.93	118.90
2	B	30	C	C6-N1-C2	-5.04	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	440	C	C2-N1-C1'	5.04	124.35	118.80
1	A	1945	G	C4-N9-C1'	5.04	133.05	126.50
34	a	340	U	N1-C2-O2	5.04	126.33	122.80
1	A	634	C	C5-C6-N1	5.04	123.52	121.00
1	A	1398	C	C2-N1-C1'	5.04	124.34	118.80
1	A	1880	U	N1-C2-O2	5.03	126.32	122.80
34	a	1399	C	OP2-P-O3'	5.03	116.27	105.20
1	A	2604	U	N3-C4-O4	5.03	122.92	119.40
2	B	17	C	C5-C6-N1	5.03	123.52	121.00
1	A	634	C	C6-N1-C2	-5.03	118.29	120.30
1	A	2704	C	N3-C2-O2	-5.03	118.38	121.90
1	A	2591	C	N1-C2-O2	5.01	121.91	118.90
34	a	805	C	C2-N1-C1'	5.01	124.31	118.80
1	A	2752	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1812	U	N1-C2-O2	5.01	126.31	122.80
7	G	45	ALA	C-N-CA	5.01	134.22	121.70
1	A	1839	G	N3-C4-C5	-5.00	126.10	128.60
13	M	96	ILE	C-N-CA	5.00	134.21	121.70
1	A	137	U	N1-C2-O2	5.00	126.30	122.80
1	A	2636	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	3	30	HIS	Peptide
32	5	80	THR	Peptide
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
13	M	57	VAL	Peptide
18	R	53	PHE	Peptide
21	U	88	ASP	Peptide
35	b	15	PHE	Peptide
35	b	16	GLY	Peptide
35	b	18	GLN	Peptide
38	e	121	ASN	Peptide
39	f	52	ASN	Peptide
39	f	95	ALA	Peptide
42	i	90	ASP	Peptide

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Mol	Chain	Res	Type	Group
43	j	57	VAL	Peptide
45	l	101	LEU	Peptide
46	m	4	ALA	Peptide
50	q	67	SER	Peptide
50	q	68	LYS	Peptide
56	w	17	ALA	Peptide
56	w	314	ARG	Peptide
56	w	398	PHE	Peptide
56	w	470	THR	Peptide
56	w	502	ALA	Peptide
56	w	503	TYR	Peptide
56	w	76	GLN	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62177	0	31271	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.



All (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
1:A:1401:G:OP1	33:7:20:U:OP1	143.72	0.91
1:A:2028:U:H3	1:A:2033:A:H62	1.13	0.89
1:A:2457:U:H5	1:A:2494:G:N1	1.73	0.86
1:A:2475:C:H42	1:A:2529:G:N2	1.75	0.84
1:A:2514:U:H3	1:A:2570:G:H1	1.26	0.83
1:A:745:G:N7	1:A:746:U:C4	2.48	0.81
1:A:2505:G:O2'	1:A:2506:U:C2	2.32	0.81
1:A:2457:U:H5	1:A:2494:G:H1	0.88	0.81
1:A:306:U:H3	1:A:310:A:N6	1.79	0.79
1:A:2508:G:N1	1:A:2580:U:O4	2.17	0.77
1:A:745:G:C8	1:A:746:U:N3	2.54	0.76
1:A:2475:C:H42	1:A:2529:G:H22	1.32	0.75
33:7:20:U:H6	33:7:20:U:H5'	1.51	0.74
23:W:61:GLY:HA3	23:W:79:GLU:O	1.88	0.73
1:A:600:G:H1	1:A:657:U:H3	1.36	0.72
1:A:2475:C:N4	1:A:2529:G:H22	1.89	0.70
1:A:955:U:C5	1:A:962:G:N1	2.58	0.69
2:B:78:A:H62	2:B:98:G:H21	1.38	0.69
1:A:2506:U:H2'	1:A:2506:U:O2	1.92	0.68
33:7:18:U:O2'	33:7:19:G:OP1	2.12	0.68
1:A:745:G:N7	1:A:746:U:C2	2.62	0.67
1:A:2457:U:O4	1:A:2494:G:O6	2.13	0.67
16:P:59:THR:HG22	16:P:72:VAL:HG12	1.77	0.67
1:A:78:U:H3	1:A:108:G:H1	1.42	0.67
1:A:1687:G:H21	1:A:1701:A:H62	1.42	0.67
1:A:1476:U:H3	1:A:1515:A:N6	1.84	0.66
1:A:1666:G:H4'	11:K:6:THR:HG23	1.78	0.66
1:A:2508:G:C6	1:A:2580:U:O4	2.50	0.65
1:A:955:U:H5	1:A:962:G:H1	1.43	0.64
1:A:1418:G:N2	1:A:1579:A:N7	2.46	0.64
1:A:244:A:H62	1:A:254:G:H21	1.44	0.64
1:A:818:G:H21	1:A:1189:A:H62	1.44	0.63
1:A:955:U:H5	1:A:962:G:N1	1.96	0.63
14:N:28:LEU:HD23	14:N:48:VAL:HG21	1.81	0.63
5:E:146:VAL:HG12	5:E:185:LYS:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:109:LYS:HD2	12:L:126:ARG:HH11	1.64	0.62
1:A:2508:G:O6	1:A:2580:U:O4	2.16	0.62
1:A:2062:A:H62	1:A:2503:A:H62	1.47	0.62
2:B:78:A:H62	2:B:98:G:N2	1.97	0.62
1:A:1093:G:H21	1:A:1098:A:H62	1.48	0.62
1:A:2253:G:C6	1:A:2254:C:C4	2.88	0.62
1:A:745:G:C8	1:A:746:U:C2	2.88	0.61
1:A:2514:U:H5''	10:J:81:ILE:HD11	1.82	0.61
1:A:1422:G:H5'	11:K:48:PRO:HG3	98.56	0.61
4:D:34:VAL:HA	4:D:50:VAL:HG12	1.83	0.61
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.33	0.61
1:A:281:C:H42	1:A:359:G:H1	1.49	0.60
1:A:2028:U:H3	1:A:2033:A:N6	1.92	0.60
29:2:34:ARG:NH2	29:2:41:ARG:O	2.33	0.60
1:A:1081:U:H4'	9:I:123:ALA:HB1	1.82	0.60
1:A:629:G:N3	1:A:639:U:O2'	2.33	0.60
5:E:117:ARG:NH2	5:E:183:PHE:O	2.35	0.60
22:V:64:VAL:HG22	22:V:69:GLU:HG2	1.83	0.60
1:A:955:U:O4	1:A:962:G:O6	2.20	0.60
20:T:8:LEU:HA	20:T:50:LEU:HD21	1.84	0.60
1:A:746:U:H5''	1:A:748:G:O4'	2.01	0.60
1:A:1060:U:H5'	1:A:1062:G:H5'	1.84	0.59
1:A:585:G:H21	1:A:1254:A:H62	1.50	0.59
1:A:1433:A:H61	1:A:1560:G:H1	1.47	0.59
1:A:488:G:H22	1:A:491:G:H5''	1.66	0.59
1:A:839:U:H3	1:A:939:G:H1	1.49	0.59
33:7:18:U:H2'	33:7:19:G:H8	1.67	0.59
1:A:1862:G:H1	1:A:1880:U:H3	1.49	0.59
1:A:306:U:O4	1:A:310:A:N7	2.35	0.59
1:A:1154:G:OP2	17:Q:57:ARG:NH1	2.35	0.59
15:O:40:ILE:HG12	15:O:47:VAL:HG12	1.84	0.59
19:S:82:MET:HB2	19:S:98:LYS:HB2	1.84	0.59
33:7:18:U:H2'	33:7:19:G:C8	2.37	0.59
2:B:30:C:H1'	2:B:57:A:H61	1.68	0.59
8:H:39:ALA:HA	8:H:43:ASN:HB2	1.85	0.59
1:A:1046:A:H62	32:5:4:ASN:HD21	1.48	0.59
1:A:538:A:H4'	10:J:7:LYS:HG2	1.85	0.59
1:A:674:G:O6	1:A:716:A:N1	100.64	0.59
1:A:2295:C:OP1	15:O:10:ARG:NH1	2.35	0.59
1:A:2656:U:O2	1:A:2665:A:N7	2.35	0.59
2:B:72:G:H21	2:B:104:A:H62	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:5:58:THR:HG21	32:5:82:ILE:H	1.69	0.58
1:A:1798:U:H5''	3:C:257:ARG:HB2	1.85	0.58
1:A:1252:G:N2	17:Q:32:ARG:O	2.36	0.58
26:Z:8:GLN:HB2	26:Z:28:LEU:HD13	1.86	0.58
1:A:745:G:H2'	1:A:746:U:H5'	1.85	0.57
6:F:23:SER:HB3	6:F:26:GLN:HG3	1.85	0.57
20:T:23:ALA:HB1	20:T:29:THR:HB	1.86	0.57
6:F:134:GLN:NE2	6:F:149:ARG:O	2.38	0.57
24:X:6:VAL:HG21	24:X:58:ILE:HD11	1.86	0.57
29:2:24:THR:HG23	29:2:27:GLY:H	1.68	0.57
1:A:1986:C:H2'	1:A:1987:A:H8	1.70	0.57
1:A:2185:U:H2'	1:A:2186:G:H8	1.69	0.57
1:A:713:G:H21	1:A:718:A:H62	1.53	0.57
1:A:2515:C:H2'	1:A:2516:A:H8	1.70	0.57
22:V:42:LEU:HD13	22:V:47:VAL:HG21	1.87	0.57
27:0:30:ASP:HB3	27:0:34:GLY:H	1.70	0.56
1:A:585:G:H21	1:A:1254:A:N6	2.03	0.56
1:A:144:A:H4'	20:T:2:ILE:HD11	1.88	0.56
1:A:2748:A:H5'	7:G:3:VAL:HG21	1.87	0.56
1:A:2028:U:O4	1:A:2033:A:N7	2.38	0.56
1:A:2692:G:H1'	1:A:2847:U:H1'	1.87	0.56
1:A:605:G:H1'	1:A:657:U:H1'	1.88	0.56
3:C:92:LEU:HD11	3:C:100:ARG:HB3	1.86	0.56
1:A:2394:C:H5''	12:L:63:LYS:HE3	1.87	0.56
24:X:39:VAL:HG12	24:X:42:GLU:H	1.69	0.56
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.87	0.56
1:A:1450:G:H21	1:A:1452:G:H1	1.54	0.56
1:A:1992:G:N2	1:A:1996:C:O2'	2.38	0.56
1:A:1476:U:O4	1:A:1515:A:N7	2.39	0.56
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.86	0.56
1:A:605:G:OP1	5:E:99:LYS:NZ	2.39	0.56
11:K:40:LYS:HE3	11:K:57:VAL:HG12	1.88	0.56
13:M:40:ARG:HH11	13:M:93:VAL:HG11	1.69	0.56
23:W:33:ILE:HG22	23:W:34:VAL:HG23	1.88	0.56
1:A:962:G:O2'	1:A:2250:G:N2	2.39	0.56
1:A:2291:U:H1'	1:A:2374:C:H1'	1.88	0.56
6:F:62:GLN:HE22	6:F:90:LEU:HB3	1.71	0.56
1:A:1668:A:N3	1:A:1670:C:N4	2.54	0.55
2:B:48:U:OP2	15:O:30:ARG:NH2	2.39	0.55
1:A:587:C:O2	12:L:33:ARG:NH1	2.39	0.55
2:B:79:G:N7	22:V:14:LYS:NZ	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:35:PHE:O	18:R:58:VAL:HA	2.06	0.55
1:A:647:G:N2	1:A:2350:C:O2'	2.40	0.55
7:G:88:LEU:HG	7:G:161:VAL:HG22	1.87	0.55
9:I:11:GLN:NE2	9:I:54:ILE:O	2.38	0.55
11:K:43:ILE:HD12	11:K:56:ASP:HB2	1.89	0.55
17:Q:43:GLN:HE21	18:R:77:PHE:HB3	1.70	0.55
1:A:1432:G:O5'	16:P:105:LYS:HG2	54.31	0.55
21:U:33:VAL:HG13	21:U:66:VAL:HG22	1.88	0.55
32:5:22:ALA:HB3	32:5:87:GLU:HB2	1.89	0.55
1:A:2893:A:H5''	1:A:2894:G:H5'	1.88	0.55
24:X:58:ILE:HG12	24:X:66:VAL:HG21	1.87	0.55
1:A:318:C:H2'	1:A:319:G:H8	1.72	0.55
1:A:605:G:N3	1:A:657:U:O2'	2.38	0.55
1:A:45:G:H5''	1:A:46:G:H5'	1.88	0.55
1:A:514:A:N3	1:A:581:C:O2'	2.36	0.55
1:A:589:U:H2'	1:A:590:A:H8	1.72	0.55
7:G:94:ARG:HB2	7:G:105:SER:HB2	1.89	0.55
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.52	0.55
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.41	0.54
3:C:70:LYS:HB3	3:C:73:ILE:HD12	1.90	0.54
12:L:23:ILE:HD13	18:R:84:ARG:HH22	1.71	0.54
20:T:6:ARG:NH2	20:T:37:ASP:OD2	2.41	0.54
30:3:32:LEU:HD23	30:3:35:LYS:HD2	1.88	0.54
1:A:297:G:N2	1:A:300:A:OP2	12.73	0.54
4:D:15:PHE:H	16:P:11:GLN:HE22	1.56	0.54
1:A:1204:A:N6	1:A:1242:U:O4	2.40	0.54
3:C:51:ARG:HH22	3:C:246:PRO:HG2	1.72	0.54
26:Z:10:ARG:HB2	26:Z:53:MET:HB2	1.89	0.54
1:A:550:C:H2'	1:A:551:G:H8	1.73	0.54
24:X:39:VAL:O	24:X:43:LYS:N	2.40	0.54
1:A:358:U:H2'	1:A:359:G:H8	2.41	0.54
3:C:165:ALA:HB3	3:C:172:THR:HB	1.90	0.54
1:A:1223:G:OP1	18:R:68:ARG:NH2	2.41	0.54
1:A:2861:U:H2'	1:A:2862:G:H8	1.73	0.54
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.41	0.54
1:A:2229:U:H2'	1:A:2230:G:H8	1.72	0.53
1:A:660:C:O2'	12:L:13:LYS:NZ	2.40	0.53
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.90	0.53
1:A:1818:U:H5'	3:C:156:SER:HB2	1.89	0.53
11:K:30:ARG:NH2	11:K:37:ASP:OD2	2.40	0.53
1:A:2320:U:O2'	1:A:2322:A:N6	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:U:OP2	13:M:14:LYS:NZ	2.42	0.53
1:A:1288:G:OP2	1:A:1288:G:N2	2.40	0.53
1:A:2659:G:N2	1:A:2662:A:OP2	2.42	0.53
1:A:538:A:N6	1:A:555:G:O2'	2.42	0.53
1:A:2296:U:OP2	15:O:9:ARG:NH2	2.40	0.53
10:J:56:VAL:HB	10:J:124:VAL:HG12	1.90	0.53
3:C:1:ALA:N	3:C:19:VAL:O	2.38	0.53
4:D:148:GLN:HB2	4:D:152:PRO:HG2	1.91	0.53
32:5:3:LEU:HD12	32:5:5:LEU:H	1.72	0.53
1:A:1724:G:O6	1:A:1737:G:N2	2.42	0.53
1:A:2523:G:HO2'	1:A:2764:A:HO2'	1.54	0.53
1:A:1953:A:O2'	1:A:2559:C:O2	2.25	0.53
1:A:377:G:H1	1:A:397:U:H3	1.57	0.53
1:A:406:G:H5'	4:D:4:LEU:HD22	165.74	0.53
8:H:30:LEU:HB3	8:H:36:ALA:HB3	1.90	0.53
1:A:1069:A:N7	1:A:1073:A:N6	2.57	0.53
1:A:1800:C:N4	1:A:1818:U:O2'	2.42	0.53
1:A:1428:C:OP2	3:C:27:LYS:NZ	2.42	0.53
1:A:523:C:O2	1:A:554:U:O2'	2.27	0.52
1:A:196:A:H61	1:A:831:G:H21	1.57	0.52
1:A:177:G:H3'	1:A:178:G:H8	1.73	0.52
1:A:576:U:H2'	1:A:577:G:C8	2.45	0.52
3:C:77:VAL:HG21	3:C:109:LEU:HD11	1.91	0.52
15:O:108:ASP:OD1	15:O:111:ARG:NH1	2.41	0.52
1:A:1779:U:OP2	1:A:1784:A:N6	2.42	0.52
1:A:2693:G:H2'	1:A:2694:G:H8	1.74	0.52
1:A:537:G:H4'	10:J:5:THR:HG21	1.92	0.52
1:A:444:C:OP2	5:E:44:ARG:NH2	2.42	0.52
5:E:18:THR:HA	5:E:106:LYS:HE3	1.92	0.52
1:A:1753:G:H5''	16:P:92:ARG:HD3	1.91	0.52
21:U:36:GLU:HA	21:U:61:GLU:HG2	1.91	0.52
1:A:1270:C:H5''	1:A:1271:G:H5'	1.92	0.52
1:A:1912:A:H5'	1:A:1913:A:OP2	2.09	0.52
3:C:184:GLU:HG3	3:C:186:ASP:H	1.75	0.52
13:M:35:ALA:O	13:M:99:GLY:N	2.42	0.52
1:A:2692:G:N3	1:A:2847:U:O2'	2.40	0.52
1:A:2743:U:OP2	1:A:2755:C:N4	2.43	0.52
1:A:475:C:H4'	1:A:510:C:H5'	1.90	0.52
10:J:17:VAL:HG23	10:J:137:PRO:HB2	1.91	0.52
1:A:119:A:H4'	1:A:120:U:H5'	1.91	0.52
4:D:131:ASP:O	4:D:136:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:0:27:LEU:HD23	27:0:36:LYS:HB3	1.93	0.51
1:A:460:A:H62	1:A:469:G:H21	1.58	0.51
13:M:75:GLU:HB3	13:M:90:GLU:HG3	1.91	0.51
1:A:2253:G:C5	1:A:2254:C:C5	2.98	0.51
1:A:2848:G:O2'	1:A:2868:A:N6	2.43	0.51
20:T:38:ALA:HB1	20:T:43:ILE:HD11	1.92	0.51
1:A:1013:C:H2'	1:A:1014:A:H8	1.74	0.51
1:A:2081:U:H2'	1:A:2082:A:H8	1.75	0.51
1:A:835:C:H2'	1:A:836:G:H8	1.74	0.51
1:A:2298:A:H5''	6:F:71:LYS:HD3	1.92	0.51
8:H:47:PHE:HA	8:H:51:ARG:HB2	1.91	0.51
11:K:12:ASP:HB3	11:K:99:ILE:HG12	1.91	0.51
1:A:227:A:H61	1:A:410:G:H21	1.58	0.51
1:A:2023:C:H2'	1:A:2024:G:H8	1.75	0.51
1:A:854:C:H2'	1:A:855:G:H8	1.75	0.51
14:N:44:LEU:HD23	14:N:113:ILE:HD13	1.92	0.51
1:A:1796:U:H3	1:A:1823:G:H1	1.58	0.51
1:A:407:G:H2'	1:A:408:G:H8	1.76	0.51
1:A:2314:A:OP1	6:F:87:LYS:NZ	2.42	0.51
8:H:38:PRO:O	8:H:43:ASN:ND2	2.41	0.51
1:A:76:C:OP1	25:Y:48:ARG:NH1	2.44	0.51
1:A:1041:G:H1	1:A:1114:C:H42	1.59	0.51
1:A:2233:U:H2'	1:A:2234:G:H8	1.75	0.51
24:X:4:CYS:HB3	24:X:9:LYS:H	1.75	0.51
1:A:807:U:O2'	1:A:2060:A:N1	2.39	0.51
1:A:2110:G:N2	1:A:2179:C:N3	2.59	0.51
1:A:340:A:O2'	5:E:162:ARG:NH1	2.44	0.51
1:A:99:U:H5''	1:A:100:U:H5'	1.91	0.51
19:S:73:LYS:HB2	19:S:106:VAL:HB	1.92	0.51
22:V:9:ARG:HD3	22:V:39:ALA:HB1	1.92	0.51
3:C:5:CYS:SG	3:C:12:ARG:NH2	2.83	0.51
1:A:2020:A:N7	27:0:5:ASN:ND2	2.59	0.51
32:5:68:PRO:HA	32:5:72:LEU:HG	1.93	0.51
1:A:1326:U:H5'	1:A:2010:G:H21	1.76	0.51
1:A:2008:C:H2'	1:A:2009:A:H8	1.75	0.51
5:E:75:SER:HB3	5:E:78:TRP:HD1	1.74	0.51
16:P:25:VAL:HG22	16:P:85:VAL:HG22	1.93	0.51
1:A:1432:G:P	16:P:105:LYS:HG2	54.64	0.50
1:A:629:G:H1'	1:A:639:U:H1'	1.92	0.50
5:E:102:ARG:NH1	5:E:200:LEU:O	2.44	0.50
1:A:2746:U:H5''	7:G:137:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:G:H2'	1:A:675:A:H8	3.80	0.50
1:A:907:G:N2	13:M:70:ASP:OD2	2.44	0.50
32:5:26:VAL:HG21	32:5:114:GLU:HG2	1.92	0.50
1:A:1394:U:O2	20:T:19:LYS:NZ	2.44	0.50
1:A:463:G:N2	1:A:466:A:OP2	2.35	0.50
1:A:481:G:O2'	1:A:506:G:N2	2.45	0.50
1:A:779:U:O2	1:A:785:G:O6	2.29	0.50
1:A:848:C:H2'	1:A:849:A:H8	1.76	0.50
8:H:132:PHE:H	8:H:140:ALA:HB3	1.75	0.50
1:A:1024:G:HO2'	1:A:1144:A:HO2'	1.60	0.50
1:A:283:G:H1	1:A:357:C:H42	1.58	0.50
6:F:34:THR:HB	6:F:154:THR:HB	1.93	0.50
22:V:77:VAL:HG23	22:V:89:ILE:HG12	1.93	0.50
8:H:1:MET:N	8:H:20:ASN:OD1	2.44	0.50
1:A:2291:U:O2'	1:A:2374:C:O2	2.30	0.50
1:A:2822:G:O2'	1:A:2825:G:N1	2.40	0.50
1:A:1022:G:N2	1:A:1023:U:O4	2.45	0.50
1:A:2258:C:O2'	1:A:2427:C:OP2	2.29	0.50
1:A:451:U:O2	1:A:453:A:N6	2.45	0.50
1:A:994:C:OP1	17:Q:52:ARG:NH2	2.45	0.50
6:F:9:ASP:N	6:F:9:ASP:OD1	2.45	0.50
12:L:127:VAL:HG21	12:L:142:ILE:HD13	1.94	0.50
1:A:2788:C:O2'	1:A:2809:A:N3	2.41	0.49
1:A:776:G:H22	1:A:2072:C:H5'	1.77	0.49
25:Y:49:ASP:OD1	25:Y:52:ARG:NH2	2.45	0.49
1:A:111:A:O2'	25:Y:58:ASN:ND2	2.46	0.49
1:A:476:G:N1	1:A:479:A:OP2	2.40	0.49
1:A:532:A:N6	1:A:1206:G:O2'	61.85	0.49
3:C:140:VAL:HG12	3:C:191:LEU:HD23	1.93	0.49
4:D:55:LYS:HE2	4:D:77:ARG:HA	1.94	0.49
7:G:8:VAL:HB	7:G:49:LEU:HB2	1.94	0.49
1:A:1173:U:O2'	1:A:1177:G:N2	2.40	0.49
1:A:1080:A:H1'	9:I:127:SER:HA	1.94	0.49
1:A:242:G:N2	1:A:255:A:OP2	2.44	0.49
1:A:2768:U:O2'	10:J:95:ARG:NH2	2.46	0.49
1:A:590:A:H61	1:A:667:U:H3	1.61	0.49
1:A:1158:C:H5''	26:Z:30:ARG:HD2	1.95	0.49
1:A:737:C:N4	1:A:738:G:O6	2.45	0.49
14:N:43:GLU:OE2	14:N:46:ARG:NH2	2.45	0.49
1:A:1682:G:OP2	1:A:1699:G:N2	2.45	0.49
1:A:1807:G:N2	1:A:1810:A:OP2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:A:OP2	1:A:1431:A:O2'	2.31	0.49
1:A:2002:G:OP2	14:N:9:GLN:NE2	2.46	0.49
2:B:95:U:H2'	2:B:96:G:H8	1.78	0.49
6:F:152:ASP:N	6:F:152:ASP:OD1	2.45	0.49
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.77	0.49
1:A:177:G:N2	1:A:177:G:OP2	2.36	0.49
1:A:2458:G:O2'	1:A:2460:U:O4	2.30	0.49
2:B:5:U:OP1	2:B:61:G:O2'	2.29	0.49
1:A:659:G:O2'	5:E:95:LYS:O	2.31	0.49
12:L:17:LYS:HE3	12:L:27:LEU:HD22	1.95	0.49
20:T:13:ALA:HB3	20:T:33:LYS:HD3	1.94	0.49
1:A:48:G:N2	1:A:177:G:OP2	2.45	0.49
1:A:2505:G:O2'	1:A:2506:U:O2	2.17	0.49
1:A:2113:U:O4	1:A:2119:A:N6	2.45	0.48
1:A:537:G:H22	1:A:555:G:H2'	1.78	0.48
8:H:94:ILE:HG23	8:H:98:ASP:HB2	1.95	0.48
1:A:2076:U:OP2	1:A:2238:G:N2	2.45	0.48
1:A:28:A:O2'	1:A:296:U:OP1	49.01	0.48
1:A:1806:C:H1'	3:C:43:ASN:HD21	1.78	0.48
1:A:533:G:O5'	17:Q:27:ARG:NH1	2.47	0.48
3:C:267:VAL:HG12	3:C:268:ARG:HG2	1.96	0.48
9:I:45:THR:HG22	9:I:50:LYS:HG2	1.94	0.48
1:A:1500:G:H4'	3:C:100:ARG:HH12	1.78	0.48
1:A:776:G:N2	1:A:802:A:OP2	24.20	0.48
1:A:793:A:OP2	1:A:2071:A:O2'	2.28	0.48
3:C:243:PRO:O	3:C:250:GLN:NE2	2.46	0.48
1:A:2060:A:H62	5:E:69:ARG:HH22	1.61	0.48
1:A:818:G:N2	1:A:1189:A:H62	2.11	0.48
1:A:1899:A:H4'	1:A:1901:A:H5''	1.94	0.48
1:A:519:U:H2'	1:A:520:G:H8	1.79	0.48
26:Z:16:LEU:HB2	26:Z:19:HIS:HD2	1.78	0.48
1:A:1469:A:OP2	1:A:1522:A:N6	2.47	0.48
1:A:2618:G:H21	4:D:155:VAL:HG21	1.78	0.48
1:A:2647:U:H2'	1:A:2648:G:H8	1.78	0.48
1:A:774:G:N2	1:A:787:C:O2'	2.46	0.48
21:U:14:THR:OG1	21:U:68:ASN:ND2	2.45	0.48
1:A:2851:A:O2'	14:N:64:ARG:NH2	2.47	0.48
1:A:917:A:H5''	1:A:2268:A:H61	1.78	0.48
10:J:36:LEU:HD22	10:J:121:LYS:HB2	1.94	0.48
12:L:20:GLY:H	12:L:28:GLY:HA2	1.78	0.48
1:A:249:C:O2	30:3:11:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:A:N3	1:A:2415:G:O2'	2.41	0.48
9:I:44:LYS:HG2	9:I:70:THR:HG21	1.96	0.48
22:V:20:LEU:HD11	22:V:41:GLU:HG3	1.96	0.48
1:A:1830:C:H2'	1:A:1831:G:H8	1.79	0.48
1:A:2345:G:H4'	1:A:2346:A:H3'	1.95	0.48
1:A:2512:C:OP2	4:D:128:ARG:NH2	2.47	0.48
14:N:28:LEU:HD13	14:N:34:ILE:HG12	1.95	0.48
1:A:2306:C:N4	6:F:38:GLY:O	2.47	0.47
1:A:505:A:HO2'	1:A:509:C:HO2'	1.62	0.47
1:A:911:A:N6	13:M:11:LYS:O	2.37	0.47
17:Q:87:VAL:HG13	18:R:49:ILE:HD11	1.97	0.47
31:4:30:GLU:HG3	31:4:32:LYS:H	1.77	0.47
1:A:1046:A:H4'	32:5:61:ARG:HB3	1.97	0.47
1:A:2581:G:N2	1:A:2581:G:OP2	2.38	0.47
1:A:1613:G:H4'	29:2:3:ARG:HE	1.78	0.47
1:A:1323:C:OP1	19:S:98:LYS:NZ	2.46	0.47
1:A:213:A:H2'	1:A:214:G:C8	2.50	0.47
1:A:767:U:H2'	1:A:768:G:H8	1.79	0.47
6:F:140:ILE:HG22	6:F:142:TYR:H	1.79	0.47
1:A:585:G:N2	1:A:1254:A:H62	2.12	0.47
1:A:806:C:O2	1:A:2444:G:O2'	2.32	0.47
2:B:1:U:H2'	2:B:2:G:H8	1.79	0.47
8:H:17:ASP:HB3	8:H:19:VAL:HG23	1.96	0.47
1:A:290:U:H2'	1:A:291:G:H8	1.80	0.47
1:A:26:G:H1'	1:A:515:A:H61	1.78	0.47
1:A:2361:G:OP1	30:3:25:HIS:ND1	2.39	0.47
1:A:291:G:H1	1:A:349:U:H3	1.61	0.47
1:A:673:C:OP1	5:E:49:ARG:NH2	2.47	0.47
1:A:698:C:O2'	1:A:734:A:N6	2.35	0.47
11:K:121:GLU:HG2	11:K:122:VAL:HG23	1.97	0.47
16:P:84:SER:OG	16:P:86:LYS:NZ	2.48	0.47
1:A:410:G:N3	1:A:432:A:N6	41.51	0.47
4:D:36:GLN:OE1	4:D:49:GLN:NE2	2.48	0.47
1:A:582:A:H2'	1:A:583:G:H8	1.80	0.47
18:R:76:LYS:HB2	18:R:85:LYS:HB3	1.96	0.47
1:A:1429:G:H2'	1:A:1430:G:H8	1.79	0.47
1:A:1687:G:N2	1:A:1701:A:H62	2.12	0.47
1:A:720:U:H2'	1:A:721:A:H8	1.80	0.47
3:C:141:HIS:ND1	3:C:192:GLY:O	2.42	0.47
27:0:42:ILE:HG22	27:0:48:TYR:HB2	1.97	0.47
1:A:302:C:H2'	1:A:303:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:U:H4'	1:A:1212:G:H4'	1.97	0.46
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.97	0.46
1:A:1291:C:H2'	1:A:1292:G:H8	1.80	0.46
1:A:1333:G:H2'	1:A:1334:G:H8	1.81	0.46
21:U:20:LYS:HB3	21:U:38:ILE:HD12	1.98	0.46
1:A:1378:A:O2'	1:A:1380:G:OP2	2.31	0.46
1:A:2506:U:O2	1:A:2506:U:C2'	2.61	0.46
2:B:114:C:H2'	2:B:115:A:H8	1.79	0.46
6:F:163:GLU:OE1	6:F:166:ARG:NH1	2.49	0.46
6:F:35:LEU:HB2	6:F:88:VAL:HB	1.97	0.46
17:Q:99:VAL:O	17:Q:102:LYS:NZ	2.48	0.46
1:A:210:C:OP1	29:2:29:GLN:NE2	2.48	0.46
1:A:244:A:OP2	30:3:7:ARG:NH1	2.45	0.46
4:D:37:VAL:HG22	4:D:48:ILE:HG22	1.97	0.46
9:I:102:ARG:NH1	9:I:106:GLN:OE1	2.48	0.46
2:B:7:G:O2'	15:O:38:GLN:NE2	2.48	0.46
3:C:130:PRO:HA	3:C:188:ARG:HA	1.98	0.46
1:A:1638:C:O2	1:A:2698:U:O2'	2.33	0.46
1:A:1921:G:H2'	1:A:1922:G:H8	1.80	0.46
1:A:1801:A:N6	1:A:2201:G:O2'	2.43	0.46
1:A:2245:U:H5''	1:A:2246:G:H5'	1.95	0.46
32:5:24:SER:HB2	32:5:116:GLU:HG3	1.97	0.46
1:A:1447:C:O2'	1:A:1544:A:N3	2.39	0.46
1:A:577:G:O2'	1:A:1254:A:OP1	2.33	0.46
1:A:2052:A:O2'	4:D:149:ASN:O	2.34	0.46
5:E:182:ALA:HB2	12:L:3:LEU:HD22	1.96	0.46
8:H:70:GLU:HB2	8:H:134:VAL:HG21	1.98	0.46
1:A:1368:G:H2'	1:A:1369:G:H8	1.81	0.46
1:A:1432:G:H2'	1:A:1433:A:C8	2.51	0.46
2:B:111:U:H2'	2:B:112:G:H8	1.81	0.46
1:A:1254:A:H5''	1:A:1255:U:H5''	1.98	0.46
1:A:2313:C:H2'	1:A:2314:A:H8	1.81	0.46
1:A:746:U:O4'	1:A:748:G:N2	2.49	0.46
1:A:1386:C:H2'	1:A:1387:A:C8	2.51	0.46
1:A:1387:A:H5'	1:A:1469:A:H1'	1.97	0.46
1:A:1432:G:H2'	1:A:1433:A:H8	1.81	0.46
1:A:351:C:H2'	1:A:352:A:H8	1.81	0.46
1:A:878:A:H3'	1:A:879:G:H8	1.80	0.46
1:A:372:G:O6	24:X:56:ARG:NH2	2.50	0.45
1:A:376:G:H2'	1:A:377:G:H8	2.07	0.45
1:A:877:A:O2'	1:A:900:A:N6	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:C:H2'	2:B:94:A:H8	1.80	0.45
3:C:74:PRO:HB3	3:C:114:GLN:HE21	1.81	0.45
1:A:1071:G:N2	1:A:1089:A:O2'	2.44	0.45
1:A:212:G:H2'	1:A:213:A:C8	2.50	0.45
1:A:33:C:O2	1:A:447:A:N6	2.49	0.45
6:F:115:GLY:HA3	6:F:177:ARG:HB2	1.98	0.45
20:T:54:GLU:HB3	20:T:88:LYS:HD2	1.97	0.45
1:A:1936:A:OP2	1:A:1962:C:N4	2.43	0.45
1:A:694:U:OP1	3:C:58:LYS:NZ	2.39	0.45
15:O:8:ILE:O	15:O:12:THR:OG1	2.29	0.45
1:A:1171:G:N2	1:A:1179:G:N7	2.65	0.45
1:A:2086:U:H2'	1:A:2087:G:C8	2.52	0.45
1:A:2719:G:H4'	1:A:2846:G:H4'	1.97	0.45
1:A:2771:C:O2'	4:D:173:GLN:NE2	2.47	0.45
19:S:69:LEU:HA	19:S:109:ASP:HA	1.99	0.45
32:5:30:SER:HB3	32:5:109:LYS:HD2	1.98	0.45
1:A:1997:C:H2'	1:A:1998:A:H8	1.82	0.45
1:A:532:A:OP1	1:A:561:G:N2	2.40	0.45
2:B:52:A:N7	15:O:33:ARG:NH2	2.65	0.45
1:A:476:G:O2'	1:A:502:A:N6	2.45	0.45
5:E:75:SER:HB3	5:E:78:TRP:CD1	2.52	0.45
24:X:6:VAL:HA	24:X:73:ARG:HH22	1.80	0.45
1:A:2047:C:H2'	1:A:2048:G:H8	1.82	0.45
1:A:2086:U:H2'	1:A:2087:G:H8	1.81	0.45
1:A:373:U:H2'	1:A:374:A:H8	1.81	0.45
1:A:581:C:H2'	1:A:582:A:C8	2.52	0.45
17:Q:93:ILE:HG23	18:R:13:ARG:HB2	1.99	0.45
1:A:1597:A:H4'	1:A:1598:A:H8	1.82	0.45
1:A:91:A:O2'	1:A:92:U:O4'	2.32	0.45
6:F:56:LEU:HD13	6:F:88:VAL:HG23	1.99	0.45
3:C:154:ALA:HB2	3:C:161:VAL:HG23	1.98	0.45
13:M:47:GLU:OE2	13:M:51:ARG:NE	2.50	0.45
32:5:33:VAL:HG12	32:5:35:VAL:H	1.81	0.45
1:A:1509:A:H2'	1:A:1510:G:C8	2.52	0.45
1:A:1636:U:H2'	1:A:1637:A:H8	1.82	0.45
1:A:16:C:H2'	1:A:17:G:H8	1.80	0.45
1:A:302:C:H2'	1:A:303:G:C8	2.52	0.45
1:A:918:A:N3	2:B:80:U:O2'	2.42	0.45
2:B:45:A:O4'	6:F:91:ARG:NH2	2.50	0.45
13:M:66:ARG:NH1	13:M:104:GLU:OE2	2.50	0.45
33:7:20:U:C6	33:7:20:U:H5'	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2656:U:C2	1:A:2665:A:N7	2.85	0.44
1:A:2818:U:H2'	1:A:2819:G:C8	2.52	0.44
1:A:572:A:H61	1:A:2029:G:H21	1.65	0.44
1:A:589:U:H2'	1:A:590:A:C8	2.51	0.44
9:I:89:SER:HB3	9:I:135:MET:HA	1.99	0.44
3:C:56:GLY:HA2	3:C:212:TRP:HA	1.99	0.44
6:F:28:PRO:HB2	6:F:168:LEU:HD22	1.99	0.44
1:A:2070:A:H2'	1:A:2071:A:H8	1.82	0.44
1:A:224:U:OP2	1:A:408:G:N2	2.42	0.44
1:A:286:U:H2'	1:A:287:G:H8	1.82	0.44
1:A:692:C:H5''	3:C:38:LYS:HB3	2.00	0.44
4:D:109:VAL:HG22	4:D:203:VAL:HG22	1.99	0.44
13:M:42:THR:HG22	13:M:93:VAL:HG12	1.99	0.44
1:A:552:U:H2'	1:A:553:G:H8	1.82	0.44
1:A:605:G:O2'	1:A:657:U:O2	2.33	0.44
1:A:526:A:O2'	1:A:2043:C:O2	2.30	0.44
1:A:598:U:H2'	1:A:599:A:H8	1.81	0.44
1:A:1827:U:OP2	3:C:220:ARG:NH1	2.49	0.44
1:A:2293:G:OP1	15:O:94:ARG:NH1	2.50	0.44
1:A:787:C:H5''	1:A:788:A:H5'	2.00	0.44
1:A:2443:C:H2'	1:A:2444:G:C8	2.52	0.44
8:H:125:THR:HG23	8:H:146:VAL:HG12	1.99	0.44
1:A:1796:U:H2'	1:A:1797:G:C8	2.53	0.44
1:A:2251:G:H2'	1:A:2252:G:H8	1.82	0.44
1:A:2598:A:H5''	3:C:233:GLY:HA3	1.99	0.44
1:A:2776:A:O2'	1:A:2782:G:N7	2.46	0.44
1:A:29:U:O2	1:A:1215:G:O2'	2.34	0.44
1:A:581:C:H2'	1:A:582:A:H8	1.82	0.44
1:A:745:G:C2'	1:A:746:U:H5'	2.48	0.44
1:A:764:A:N3	3:C:211:ARG:NH1	2.65	0.44
4:D:47:ALA:HB2	4:D:83:ARG:HD2	1.99	0.44
25:Y:37:LEU:HD11	25:Y:42:LEU:HD12	1.98	0.44
31:4:19:ARG:HD2	31:4:24:ARG:HD2	2.00	0.44
1:A:13:A:O2'	1:A:15:G:N7	2.46	0.44
1:A:2144:G:H1'	1:A:2147:A:H61	1.83	0.44
1:A:2898:U:H2'	1:A:2899:A:C8	2.53	0.44
1:A:672:C:OP2	12:L:42:SER:OG	2.32	0.44
5:E:47:LYS:HB2	5:E:51:GLU:HB2	1.99	0.44
20:T:37:ASP:OD1	20:T:37:ASP:N	2.50	0.44
1:A:1754:A:N1	1:A:2716:C:O2'	2.47	0.43
1:A:18:U:O2'	1:A:554:U:OP1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2372:U:H2'	1:A:2373:G:H8	1.82	0.43
1:A:248:G:O2'	1:A:2432:A:OP1	2.30	0.43
30:3:31:ILE:HG13	30:3:31:ILE:H	1.48	0.43
1:A:693:A:O2'	1:A:1353:A:N3	2.51	0.43
1:A:2899:A:H2'	1:A:2900:A:C8	2.53	0.43
1:A:4:U:H2'	1:A:5:A:H8	1.84	0.43
4:D:9:VAL:HA	4:D:197:THR:HG23	2.00	0.43
10:J:36:LEU:HD11	10:J:122:LEU:HD13	2.00	0.43
4:D:115:GLY:HA2	4:D:166:GLY:HA3	1.99	0.43
10:J:32:LEU:HD22	10:J:54:ILE:HG21	2.01	0.43
1:A:573:U:OP2	18:R:80:ARG:NH2	2.52	0.43
1:A:1700:A:H3'	1:A:1701:A:H8	1.83	0.43
1:A:2246:G:H2'	1:A:2247:A:H8	1.83	0.43
11:K:76:VAL:H	16:P:72:VAL:HG22	1.83	0.43
32:5:119:PRO:HG2	32:5:121:SER:HB2	2.00	0.43
1:A:1266:G:N2	1:A:1269:A:OP2	13.20	0.43
1:A:1841:U:H2'	1:A:1842:G:H8	1.83	0.43
9:I:117:THR:HG22	32:5:42:ARG:HH21	1.84	0.43
11:K:87:LEU:HD13	11:K:92:GLU:HB3	1.99	0.43
21:U:28:LEU:HD12	21:U:32:LYS:HB2	2.00	0.43
24:X:39:VAL:O	24:X:43:LYS:CA	2.66	0.43
1:A:112:U:H5'	25:Y:58:ASN:HD21	1.83	0.43
1:A:2291:U:O2	1:A:2374:C:O2'	2.33	0.43
1:A:2559:C:H2'	1:A:2560:A:H8	1.83	0.43
1:A:2691:C:H2'	1:A:2692:G:H8	1.82	0.43
1:A:854:C:H2'	1:A:855:G:C8	2.53	0.43
1:A:1039:A:H2	1:A:1116:G:H22	1.66	0.43
1:A:2457:U:C5	1:A:2494:G:N1	2.61	0.43
1:A:2676:C:O2	1:A:2732:G:N2	2.48	0.43
1:A:396:G:N2	1:A:2231:U:O2'	2.50	0.43
1:A:674:G:H2'	1:A:675:A:C8	4.23	0.43
1:A:1:G:H2'	1:A:2:G:C8	2.54	0.43
1:A:2505:G:N2	1:A:2610:C:O2	2.46	0.43
1:A:883:G:N2	1:A:893:C:O2	2.42	0.43
1:A:568:U:N3	1:A:571:U:OP2	2.45	0.43
1:A:414:C:H2'	1:A:415:A:H8	1.83	0.43
6:F:91:ARG:HA	6:F:95:MET:HB3	2.01	0.43
12:L:28:GLY:H	12:L:31:GLY:HA2	1.83	0.43
1:A:1287:A:H62	14:N:106:ASP:HB3	1.84	0.42
1:A:2883:A:OP1	27:O:48:TYR:OH	2.37	0.42
1:A:490:C:H2'	1:A:491:G:H8	8.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:A:H4'	1:A:656:G:H5'	2.00	0.42
8:H:30:LEU:HA	8:H:35:LYS:HB2	2.01	0.42
14:N:79:LEU:HD23	14:N:83:LEU:HD12	2.01	0.42
20:T:8:LEU:HD11	25:Y:22:LEU:HD12	2.00	0.42
1:A:166:U:H2'	1:A:167:A:H8	2.16	0.42
1:A:720:U:H2'	1:A:721:A:C8	2.54	0.42
14:N:42:LYS:HA	14:N:45:ARG:HE	1.84	0.42
20:T:37:ASP:O	20:T:81:LYS:NZ	2.52	0.42
1:A:2595:G:N2	1:A:2598:A:OP2	2.38	0.42
1:A:2691:C:H2'	1:A:2692:G:C8	2.54	0.42
3:C:52:HIS:CE1	3:C:218:THR:HA	2.55	0.42
10:J:31:GLU:HG2	10:J:142:ILE:HG12	1.99	0.42
11:K:9:ASN:OD1	11:K:18:ARG:NH1	2.51	0.42
25:Y:24:GLU:HB3	25:Y:46:VAL:HG21	2.00	0.42
31:4:36:ARG:HG2	31:4:37:GLN:H	1.84	0.42
1:A:1295:C:H2'	1:A:1296:G:H8	1.84	0.42
1:A:2395:C:H2'	1:A:2396:G:H8	1.85	0.42
1:A:2525:G:H2'	1:A:2526:G:H8	1.84	0.42
1:A:546:U:H2'	1:A:547:A:H4'	2.00	0.42
1:A:828:U:O4	1:A:858:G:N2	39.88	0.42
1:A:849:A:H61	1:A:929:U:H3	1.68	0.42
2:B:78:A:N6	2:B:98:G:H21	2.13	0.42
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.01	0.42
20:T:6:ARG:NH1	20:T:42:GLU:OE1	2.52	0.42
1:A:2240:U:H2'	1:A:2241:A:H8	1.84	0.42
1:A:2418:A:OP1	30:3:44:ARG:NH2	2.50	0.42
1:A:244:A:H5''	12:L:67:THR:HG21	2.02	0.42
1:A:2630:G:H2'	1:A:2631:G:C8	2.55	0.42
1:A:2832:U:H1'	1:A:2834:G:C2	2.54	0.42
1:A:1131:G:HO2'	1:A:2025:C:HO2'	1.63	0.42
1:A:2836:U:H2'	1:A:2837:A:H8	1.85	0.42
3:C:38:LYS:HE3	3:C:59:GLN:HG2	2.02	0.42
24:X:39:VAL:O	24:X:43:LYS:HA	2.20	0.42
32:5:48:ALA:HB3	32:5:51:TYR:HE1	1.83	0.42
1:A:1431:A:H2'	1:A:1432:G:H8	1.83	0.42
1:A:1604:C:O2'	1:A:1610:A:N1	2.47	0.42
1:A:2175:C:H2'	1:A:2176:A:H8	1.85	0.42
1:A:2215:C:H2'	1:A:2216:G:C8	2.55	0.42
1:A:2781:A:H5''	1:A:2782:G:H5'	2.01	0.42
1:A:2313:C:H2'	1:A:2314:A:C8	2.54	0.42
5:E:97:ASN:ND2	5:E:100:MET:SD	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:SER:O	8:H:116:ARG:NH1	2.46	0.42
1:A:976:G:O2'	17:Q:54:ARG:NH2	2.53	0.42
1:A:1093:G:N2	1:A:1098:A:H62	2.15	0.42
14:N:45:ARG:HG2	14:N:95:THR:HG21	2.01	0.42
1:A:1665:A:H2'	1:A:1666:G:H8	1.84	0.42
1:A:2035:G:H5''	1:A:2036:C:H5	1.85	0.42
1:A:2327:A:H2'	1:A:2328:A:C8	2.55	0.42
1:A:25:U:H3'	1:A:26:G:C8	2.54	0.42
1:A:4:U:H2'	1:A:5:A:C8	2.55	0.42
1:A:813:U:OP1	18:R:84:ARG:NH1	2.53	0.42
17:Q:23:TYR:HB2	17:Q:28:SER:HB3	2.00	0.42
1:A:813:U:HO2'	1:A:1225:G:HO2'	1.54	0.41
1:A:1675:C:O2	4:D:133:THR:OG1	2.37	0.41
1:A:2497:A:H1'	1:A:2498:C:H5	1.85	0.41
1:A:518:G:OP2	27:O:12:ARG:NH2	2.46	0.41
9:I:56:VAL:HG22	9:I:68:PHE:HB2	2.02	0.41
14:N:38:LEU:HG	14:N:42:LYS:HE2	2.02	0.41
28:1:36:LYS:HG3	28:1:47:ILE:HG13	2.02	0.41
1:A:1716:U:H2'	1:A:1717:A:H8	1.85	0.41
1:A:1858:A:N6	1:A:1884:G:O2'	2.47	0.41
1:A:2023:C:H2'	1:A:2024:G:C8	2.55	0.41
1:A:2131:U:H5'	1:A:2132:U:H5''	2.01	0.41
1:A:2110:G:N1	1:A:2120:G:N7	2.69	0.41
1:A:2279:G:O2'	1:A:2327:A:O2'	2.30	0.41
1:A:2380:C:H2'	1:A:2381:A:C8	2.55	0.41
1:A:2463:C:H2'	1:A:2464:G:H8	1.84	0.41
1:A:5:A:H2'	1:A:6:A:C8	2.55	0.41
1:A:662:G:H2'	1:A:663:G:H8	1.85	0.41
9:I:53:PRO:HG2	9:I:77:VAL:HG11	2.03	0.41
16:P:29:VAL:HG22	16:P:80:VAL:HG12	2.02	0.41
1:A:1433:A:H2'	1:A:1434:A:C8	2.55	0.41
1:A:151:C:H2'	1:A:152:A:H8	1.86	0.41
1:A:492:A:H2	19:S:7:HIS:HE1	1.69	0.41
1:A:65:U:O2'	20:T:73:ARG:NH2	2.53	0.41
1:A:1251:C:O2'	1:A:1253:A:OP2	2.38	0.41
1:A:2036:C:H2'	1:A:2037:A:C8	2.56	0.41
1:A:2692:G:H2'	1:A:2693:G:C8	2.56	0.41
1:A:2801:G:H2'	1:A:2802:G:H8	1.85	0.41
1:A:2863:C:H2'	1:A:2864:G:H8	1.86	0.41
1:A:406:G:H2'	1:A:407:G:H8	1.84	0.41
1:A:974:G:H1'	1:A:975:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:8:ILE:HG13	17:Q:8:ILE:H	1.70	0.41
18:R:6:GLN:HE21	18:R:11:GLN:NE2	2.17	0.41
20:T:22:THR:HA	20:T:25:GLU:HG2	2.01	0.41
1:A:1435:G:H2'	1:A:1436:G:C8	2.56	0.41
1:A:414:C:H2'	1:A:415:A:C8	2.56	0.41
1:A:910:A:H62	13:M:12:MET:HA	1.84	0.41
1:A:1209:U:H2'	1:A:1210:G:H21	1.86	0.41
1:A:1433:A:H2'	1:A:1434:A:H8	1.85	0.41
1:A:225:C:N3	1:A:231:A:N6	2.69	0.41
1:A:2329:U:H2'	1:A:2330:G:C8	2.55	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.56	0.41
17:Q:88:GLU:O	18:R:11:GLN:NE2	2.53	0.41
22:V:48:MET:SD	22:V:51:GLN:NE2	2.94	0.41
1:A:1431:A:H2'	1:A:1432:G:C8	2.56	0.41
1:A:1515:A:H3'	1:A:1516:G:H8	1.86	0.41
1:A:1592:C:H2'	1:A:1593:A:H8	1.85	0.41
1:A:2140:G:H2'	1:A:2141:G:H8	1.85	0.41
1:A:2006:C:O2'	1:A:2823:A:N3	2.53	0.41
1:A:2002:G:H5''	14:N:9:GLN:HE21	1.86	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.97	0.41
1:A:1744:A:H3'	1:A:1745:A:H8	1.86	0.41
1:A:2656:U:N3	1:A:2665:A:C8	2.76	0.41
2:B:114:C:H2'	2:B:115:A:C8	2.55	0.41
3:C:75:ALA:HB3	3:C:115:ILE:HG13	2.02	0.41
23:W:61:GLY:CA	23:W:79:GLU:O	2.66	0.41
1:A:1999:C:O2	1:A:2687:U:O2'	2.34	0.41
1:A:261:G:H2'	1:A:262:A:H8	1.85	0.41
1:A:576:U:H2'	1:A:577:G:H8	1.86	0.41
2:B:44:G:H1'	2:B:47:C:H42	1.85	0.41
19:S:22:ASP:OD1	19:S:25:ARG:NH2	2.53	0.41
21:U:88:ASP:O	21:U:90:LYS:N	2.53	0.41
27:O:39:ARG:O	27:O:41:HIS:ND1	2.54	0.41
1:A:1125:G:OP2	1:A:1126:A:O2'	2.35	0.41
1:A:1313:U:H4'	1:A:1332:G:H4'	2.03	0.41
1:A:1422:G:OP1	11:K:48:PRO:HG3	96.66	0.41
1:A:572:A:N6	1:A:2029:G:H21	2.18	0.41
1:A:2487:G:H2'	1:A:2488:G:H8	1.86	0.41
1:A:2511:U:H1'	4:D:130:GLN:HE21	1.86	0.41
1:A:466:A:OP1	29:2:34:ARG:NH1	2.54	0.41
2:B:14:U:OP2	2:B:70:C:O2'	2.38	0.41
3:C:206:LYS:HE2	3:C:208:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:LEU:HD21	8:H:56:ALA:HB1	2.03	0.41
15:O:4:LYS:HE2	15:O:8:ILE:HD11	2.03	0.41
16:P:91:VAL:HG21	16:P:96:LEU:HD11	2.03	0.41
1:A:16:C:H2'	1:A:17:G:C8	2.56	0.40
1:A:2289:G:H2'	1:A:2290:G:H8	1.86	0.40
1:A:2821:A:OP2	4:D:115:GLY:N	2.52	0.40
1:A:434:U:O2'	1:A:436:C:N4	2.55	0.40
1:A:729:G:OP2	3:C:206:LYS:NZ	2.41	0.40
1:A:788:A:OP1	1:A:791:C:N4	2.44	0.40
19:S:62:ASP:OD1	19:S:62:ASP:N	2.54	0.40
1:A:987:C:O2'	1:A:1000:A:N3	2.47	0.40
1:A:1355:G:H2'	1:A:1356:G:C8	2.80	0.40
1:A:318:C:H2'	1:A:319:G:C8	2.54	0.40
1:A:395:U:H2'	1:A:396:G:C8	2.56	0.40
20:T:58:VAL:HG22	20:T:85:VAL:HG13	2.03	0.40
1:A:499:U:H5''	21:U:42:LYS:HE2	2.02	0.40
32:5:56:ARG:HE	32:5:83:ALA:HB2	1.86	0.40
1:A:1114:C:H2'	1:A:1115:G:H8	1.86	0.40
1:A:1190:G:H5''	12:L:32:GLY:HA2	2.03	0.40
1:A:1745:A:H2'	1:A:1746:A:H8	1.86	0.40
1:A:574:A:N6	1:A:2034:U:OP1	2.42	0.40
1:A:6:A:H2'	1:A:7:G:C8	2.56	0.40
5:E:91:ASP:OD2	5:E:93:SER:OG	2.33	0.40
1:A:2863:C:H2'	1:A:2864:G:C8	2.57	0.40
1:A:341:C:H2'	1:A:342:A:C8	2.57	0.40
1:A:464:U:O2	29:2:16:HIS:NE2	2.54	0.40
1:A:832:U:H2'	1:A:833:A:C8	2.56	0.40
1:A:1140:C:H5'	10:J:26:GLY:HA3	2.03	0.40
1:A:1704:C:H2'	1:A:1705:A:C8	2.57	0.40
1:A:1913:A:H4'	1:A:1914:C:OP2	2.22	0.40
1:A:2483:C:N3	13:M:123:LYS:NZ	2.67	0.40
1:A:2708:G:H2'	1:A:2709:G:H8	1.87	0.40
1:A:521:U:H2'	1:A:522:A:H8	1.85	0.40
1:A:545:U:N3	1:A:548:G:N1	2.45	0.40
1:A:807:U:OP1	1:A:830:G:N2	2.55	0.40
1:A:807:U:H2'	1:A:808:G:H8	1.86	0.40
11:K:21:CYS:HA	11:K:41:ILE:HG22	2.03	0.40
12:L:55:MET:HA	12:L:56:PRO:HD3	1.90	0.40
12:L:96:LYS:HE3	12:L:103:ILE:HA	2.04	0.40

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

All (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
55	v	329	LEU
56	w	315	VAL
7	G	47	ASN
30	3	32	LEU
38	e	122	VAL
39	f	53	LYS
45	l	102	ASP
21	U	89	GLY
39	f	55	HIS
55	v	189	ALA
56	w	18	ILE
36	c	97	PRO
38	e	121	ASN
54	u	37	TYR
55	v	322	ILE
56	w	399	ARG
12	L	128	THR
42	i	90	ASP
56	w	77	PHE
19	S	64	ALA
58	z	16	PRO
18	R	54	VAL

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
4	D	33	ARG
5	E	156	ASN
14	N	2	ARG
18	R	43	ASN
19	S	57	ASN
23	W	51	ARG
24	X	26	ARG
35	b	23	ASN
35	b	35	ASN
35	b	202	ASN
37	d	80	ARG

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Mol	Chain	Res	Type
37	d	177	MET
38	e	69	ASN
42	i	44	ARG
44	k	12	ARG
46	m	7	ASN
50	q	61	ARG
55	v	133	ARG
55	v	303	ARG
55	v	339	MET
56	w	71	THR
56	w	124	ARG
56	w	125	LYS
56	w	152	MET
56	w	312	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
3	C	114	GLN
3	C	238	ASN
3	C	250	GLN
4	D	150	GLN
5	E	156	ASN
7	G	63	GLN
14	N	9	GLN
15	O	38	GLN
16	P	11	GLN
16	P	55	HIS
17	Q	43	GLN
18	R	6	GLN
18	R	18	GLN
18	R	43	ASN
18	R	91	GLN
19	S	7	HIS
19	S	57	ASN
23	W	42	HIS
25	Y	58	ASN
28	1	18	HIS
31	4	37	GLN
32	5	4	ASN

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Mol	Chain	Res	Type
35	b	23	ASN
35	b	35	ASN
37	d	115	GLN
38	e	69	ASN
39	f	11	HIS
39	f	58	HIS
41	h	3	GLN
41	h	75	GLN
42	i	4	GLN
42	i	36	GLN
42	i	74	GLN
43	j	58	ASN
44	k	100	ASN
48	o	45	HIS
49	p	18	GLN
50	q	30	HIS
51	r	51	GLN
53	t	2	ASN
55	v	156	HIS
55	v	182	HIS
55	v	236	HIS
55	v	296	ASN
55	v	307	ASN
55	v	311	ASN
56	w	311	HIS
56	w	381	GLN
56	w	445	GLN
56	w	489	ASN

### 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%)

All (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
1	A	34	U
1	A	35	G
1	A	36	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	60	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	91	A
1	A	92	U
1	A	98	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	158	U
1	A	162	U
1	A	163	C
1	A	188	G
1	A	196	A
1	A	199	A
1	A	205	G
1	A	206	U
1	A	215	G
1	A	216	A
1	A	218	A
1	A	219	A
1	A	221	A
1	A	222	A

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Mol	Chain	Res	Type
1	A	223	A
1	A	228	C
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	276	U
1	A	278	A
1	A	281	C
1	A	294	A
1	A	310	A
1	A	311	A
1	A	323	C
1	A	324	A
1	A	329	G
1	A	330	A
1	A	334	C
1	A	343	C
1	A	361	G
1	A	367	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	391	A
1	A	404	A
1	A	406	G
1	A	411	G
1	A	417	C
1	A	421	C
1	A	424	G
1	A	451	U
1	A	455	C
1	A	456	C
1	A	457	A
1	A	458	G
1	A	467	G
1	A	480	A

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Mol	Chain	Res	Type
1	A	481	G
1	A	489	G
1	A	490	C
1	A	491	G
1	A	504	A
1	A	505	A
1	A	506	G
1	A	509	C
1	A	528	A
1	A	529	A
1	A	530	G
1	A	532	A
1	A	533	G
1	A	543	G
1	A	544	C
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	555	G
1	A	563	A
1	A	568	U
1	A	572	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	616	A
1	A	621	A
1	A	627	A
1	A	637	A
1	A	643	A
1	A	645	C
1	A	646	U
1	A	654	A
1	A	668	A
1	A	669	G
1	A	670	A
1	A	677	A
1	A	686	U
1	A	687	C
1	A	695	G
1	A	704	G

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Mol	Chain	Res	Type
1	A	717	C
1	A	726	G
1	A	729	G
1	A	730	A
1	A	745	G
1	A	746	U
1	A	747	C
1	A	752	A
1	A	753	A
1	A	764	A
1	A	765	C
1	A	774	G
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	799	G
1	A	800	A
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	828	U
1	A	830	G
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	858	G
1	A	859	G
1	A	860	U
1	A	869	G
1	A	877	A
1	A	878	A
1	A	896	A
1	A	897	C

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Mol	Chain	Res	Type
1	A	902	C
1	A	907	G
1	A	910	A
1	A	932	U
1	A	941	A
1	A	946	C
1	A	953	G
1	A	961	C
1	A	965	C
1	A	974	G
1	A	980	A
1	A	983	A
1	A	989	G
1	A	995	C
1	A	996	A
1	A	999	U
1	A	1010	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C
1	A	1076	C

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Mol	Chain	Res	Type
1	A	1078	U
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1088	A
1	A	1104	C
1	A	1106	G
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1157	G
1	A	1172	C
1	A	1174	U
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1204	A
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1225	G
1	A	1237	A
1	A	1247	A
1	A	1248	G
1	A	1250	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1289	C
1	A	1300	G
1	A	1301	A
1	A	1321	A

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Mol	Chain	Res	Type
1	A	1325	U
1	A	1329	U
1	A	1330	C
1	A	1341	G
1	A	1345	C
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1395	A
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1428	C
1	A	1437	C
1	A	1454	C
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1504	A
1	A	1515	A
1	A	1524	G
1	A	1532	A
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1555	G
1	A	1559	U
1	A	1560	G
1	A	1565	C
1	A	1569	A
1	A	1578	U
1	A	1585	C
1	A	1598	A
1	A	1603	A
1	A	1607	C

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Mol	Chain	Res	Type
1	A	1610	A
1	A	1611	C
1	A	1634	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1651	G
1	A	1660	G
1	A	1664	A
1	A	1665	A
1	A	1669	A
1	A	1670	C
1	A	1674	G
1	A	1694	C
1	A	1695	G
1	A	1707	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1733	G
1	A	1738	G
1	A	1757	A
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1780	A
1	A	1781	U
1	A	1782	U
1	A	1784	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1835	G
1	A	1847	G
1	A	1870	C
1	A	1871	A
1	A	1873	G

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Mol	Chain	Res	Type
1	A	1896	G
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1917	U
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1940	U
1	A	1941	C
1	A	1944	U
1	A	1955	U
1	A	1960	A
1	A	1962	C
1	A	1963	U
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1992	G
1	A	1997	C
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2030	A
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2050	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	U

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Mol	Chain	Res	Type
1	A	2069	G
1	A	2072	C
1	A	2093	G
1	A	2095	A
1	A	2100	G
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2136	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2178	C
1	A	2189	U
1	A	2192	U
1	A	2198	A
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2249	U
1	A	2250	G
1	A	2251	G
1	A	2266	A
1	A	2279	G
1	A	2283	C

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Mol	Chain	Res	Type
1	A	2286	G
1	A	2287	A
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2325	G
1	A	2327	A
1	A	2334	U
1	A	2335	A
1	A	2336	A
1	A	2350	C
1	A	2354	C
1	A	2357	G
1	A	2361	G
1	A	2383	G
1	A	2385	C
1	A	2391	G
1	A	2392	A
1	A	2402	U
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2426	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2447	G
1	A	2448	A
1	A	2449	U
1	A	2473	U
1	A	2476	A
1	A	2478	A
1	A	2484	G
1	A	2491	U
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U

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Mol	Chain	Res	Type
1	A	2506	U
1	A	2513	A
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2531	A
1	A	2535	G
1	A	2547	A
1	A	2554	U
1	A	2564	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2580	U
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2604	U
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2621	G
1	A	2629	U
1	A	2634	A
1	A	2636	C
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2656	U
1	A	2673	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2712	C
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2722	G
1	A	2726	A

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Mol	Chain	Res	Type
1	A	2731	G
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2791	G
1	A	2794	C
1	A	2796	U
1	A	2797	U
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2834	G
1	A	2835	A
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2884	U
1	A	2902	C
2	B	4	C
2	B	9	G
2	B	13	G
2	B	35	C
2	B	41	G
2	B	44	G
2	B	45	A
2	B	53	A
2	B	67	G
2	B	89	U

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Mol	Chain	Res	Type
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
33	7	18	U
33	7	19	G
33	7	20	U
33	7	21	A
33	7	22	A
33	7	23	A
34	a	6	G
34	a	7	A
34	a	9	G
34	a	22	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	51	A
34	a	71	A
34	a	81	A
34	a	86	G
34	a	94	G
34	a	95	C
34	a	121	U
34	a	130	A
34	a	163	C
34	a	173	U
34	a	174	A
34	a	181	A
34	a	183	C
34	a	184	G
34	a	197	A
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	226	G
34	a	240	G
34	a	247	G
34	a	251	G

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Mol	Chain	Res	Type
34	a	266	G
34	a	267	C
34	a	269	C
34	a	279	A
34	a	280	C
34	a	281	G
34	a	283	U
34	a	289	G
34	a	306	A
34	a	325	A
34	a	328	C
34	a	344	A
34	a	345	C
34	a	347	G
34	a	351	G
34	a	352	C
34	a	354	G
34	a	356	A
34	a	367	U
34	a	372	C
34	a	388	G
34	a	392	C
34	a	397	A
34	a	406	G
34	a	411	A
34	a	413	G
34	a	421	U
34	a	422	C
34	a	424	G
34	a	429	U
34	a	439	U
34	a	467	U
34	a	479	U
34	a	482	A
34	a	484	G
34	a	486	U
34	a	496	A
34	a	497	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	518	C

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Mol	Chain	Res	Type
34	a	521	G
34	a	527	G
34	a	531	U
34	a	532	A
34	a	536	C
34	a	547	A
34	a	560	A
34	a	561	U
34	a	564	C
34	a	572	A
34	a	573	A
34	a	574	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	596	A
34	a	633	G
34	a	665	A
34	a	688	G
34	a	702	A
34	a	703	G
34	a	713	G
34	a	724	G
34	a	731	G
34	a	733	G
34	a	748	G
34	a	755	G
34	a	774	G
34	a	777	A
34	a	793	U
34	a	814	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	820	U
34	a	821	G
34	a	829	G
34	a	832	G
34	a	843	U
34	a	844	G
34	a	846	G

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Mol	Chain	Res	Type
34	a	871	U
34	a	873	A
34	a	876	C
34	a	889	A
34	a	890	G
34	a	902	G
34	a	926	G
34	a	934	C
34	a	935	A
34	a	960	U
34	a	961	U
34	a	969	A
34	a	971	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	992	U
34	a	993	G
34	a	1004	A
34	a	1026	G
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1053	G
34	a	1056	U
34	a	1064	G
34	a	1065	U
34	a	1085	U
34	a	1094	G
34	a	1101	A
34	a	1108	G
34	a	1130	A
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1152	A
34	a	1158	C
34	a	1159	U

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Mol	Chain	Res	Type
34	a	1168	U
34	a	1183	U
34	a	1184	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1212	U
34	a	1213	A
34	a	1225	A
34	a	1227	A
34	a	1238	A
34	a	1240	U
34	a	1241	G
34	a	1253	G
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1287	A
34	a	1290	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1363	A
34	a	1378	C
34	a	1395	C
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1401	G
34	a	1433	A

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Mol	Chain	Res	Type
34	a	1446	A
34	a	1448	C
34	a	1451	U
34	a	1452	C
34	a	1491	G
34	a	1492	A
34	a	1493	A
34	a	1494	G
34	a	1495	U
34	a	1499	A
34	a	1502	A
34	a	1517	G
34	a	1520	C
34	a	1529	G
34	a	1530	G
34	a	1533	C
34	a	1534	A
34	a	1535	C
34	a	1536	C
57	x	8	U
57	x	9	G
57	x	14	A
57	x	18	U
57	x	19	G
57	x	20	G
57	x	21	U
57	x	22	A
57	x	35	C
57	x	36	A
57	x	47	G
57	x	49	C
57	x	53	G
57	x	59	A
57	x	60	A
57	x	61	U
57	x	74	A
57	x	75	C
57	x	76	C
57	x	77	A

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	242	G
1	A	372	G
1	A	479	A
1	A	490	C
1	A	752	A
1	A	858	G
1	A	859	G
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1130	U
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1913	A
1	A	1940	U
1	A	2286	G
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2506	U
1	A	2566	A
1	A	2655	G
1	A	2756	U
1	A	2808	G
2	B	66	A
2	B	88	C
33	7	18	U
33	7	20	U

## 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

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

All (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
59	w	601	GCP	PG-O1G	2.50	1.55	1.50
59	w	601	GCP	C5-C4	-2.28	1.38	1.52
59	w	601	GCP	C8-N9	-2.16	1.37	1.45
59	w	601	GCP	PB-O2B	-2.16	1.51	1.56

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.

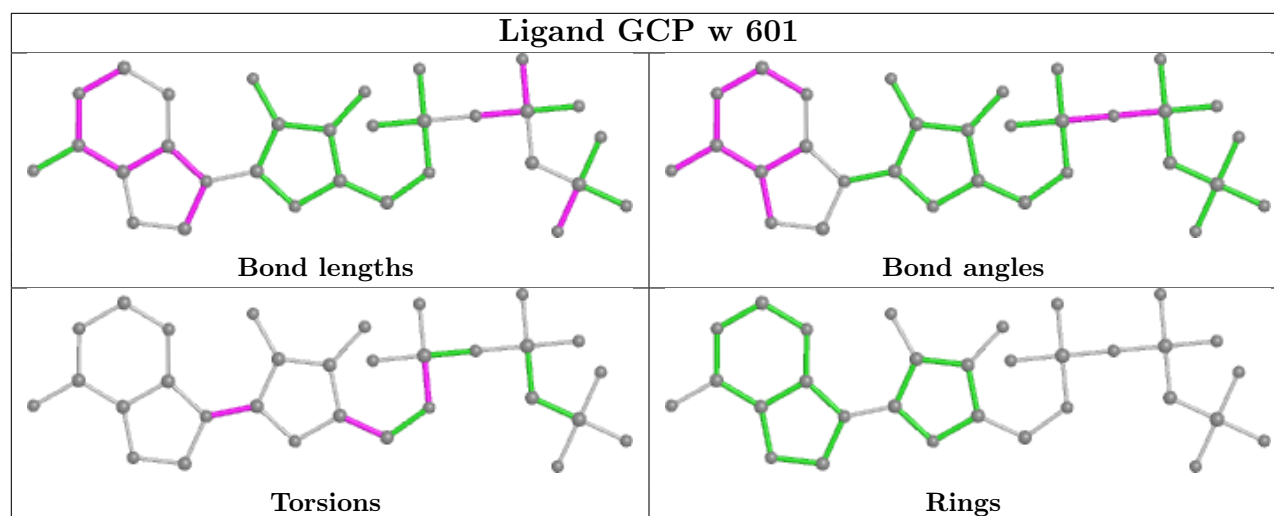
All (8) torsion outliers are listed below:

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'
59	w	601	GCP	C3'-C4'-C5'-O5'
59	w	601	GCP	C5'-O5'-PA-O1A
59	w	601	GCP	C5'-O5'-PA-O2A

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