



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Oct 17, 2018 – 04:37 PM EDT

PDB ID : 6GXO
EMDB ID: : EMD-0082
Title : Cryo-EM structure of a rotated E. coli 70S ribosome in complex with RF3-GDPCP, RF1(GAQ) and P/E-tRNA (State IV)
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.
Deposited on : 2018-06-27
Resolution : 3.90 Å(reported)

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

We welcome your comments at 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.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

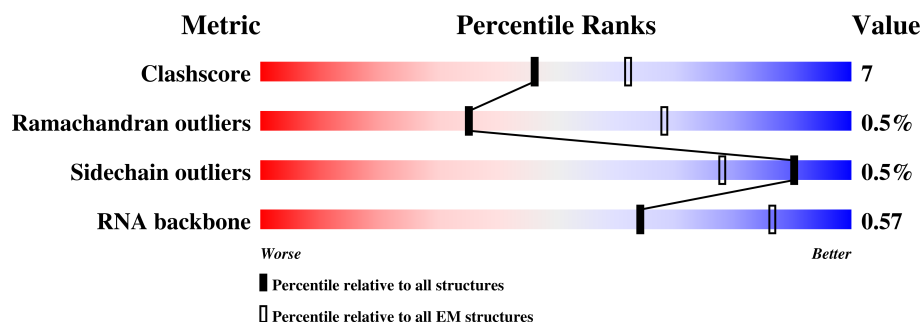
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















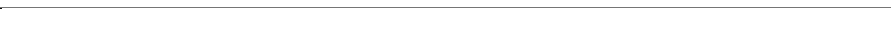

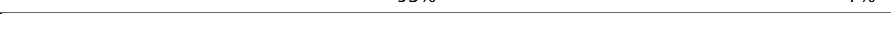
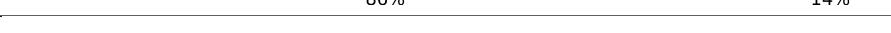
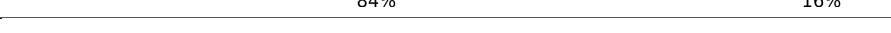







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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% 37% 5%
3	C	271	83% 17%
4	D	209	85% 15%
5	E	201	86% 14%
6	F	177	84% 16%
7	G	176	93% 6% .
8	H	149	83% 17%

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

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Mol	Chain	Length	Quality of chain
34	a	1539	84% 15% .
35	b	218	97% .
36	c	206	100%
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	100%
44	k	116	99% .
45	l	123	98% .
46	m	114	98% .
47	n	101	100%
48	o	88	100%
49	p	82	99% .
50	q	80	95% . .
51	r	65	100%
52	s	79	100%
53	t	85	100%
54	u	65	97% .
55	v	248	95% 5%
56	w	529	92% . 6%
57	x	77	45% 47% 8%
58	z	14	93% 7%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 151479 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	2900	Total	C	N	O	P	0	0
			62262	27774	11460	20128	2900		

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	-	expression tag	GB 1373146531

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	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
			1639	732	297	534	76		

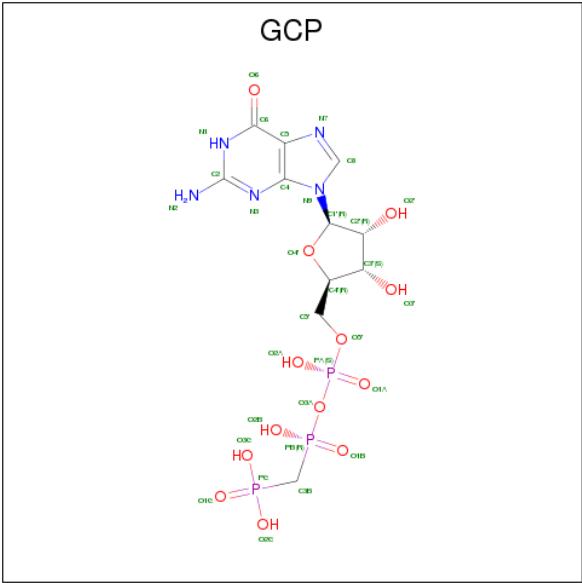
- Molecule 58 is a protein called Apidaecin.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



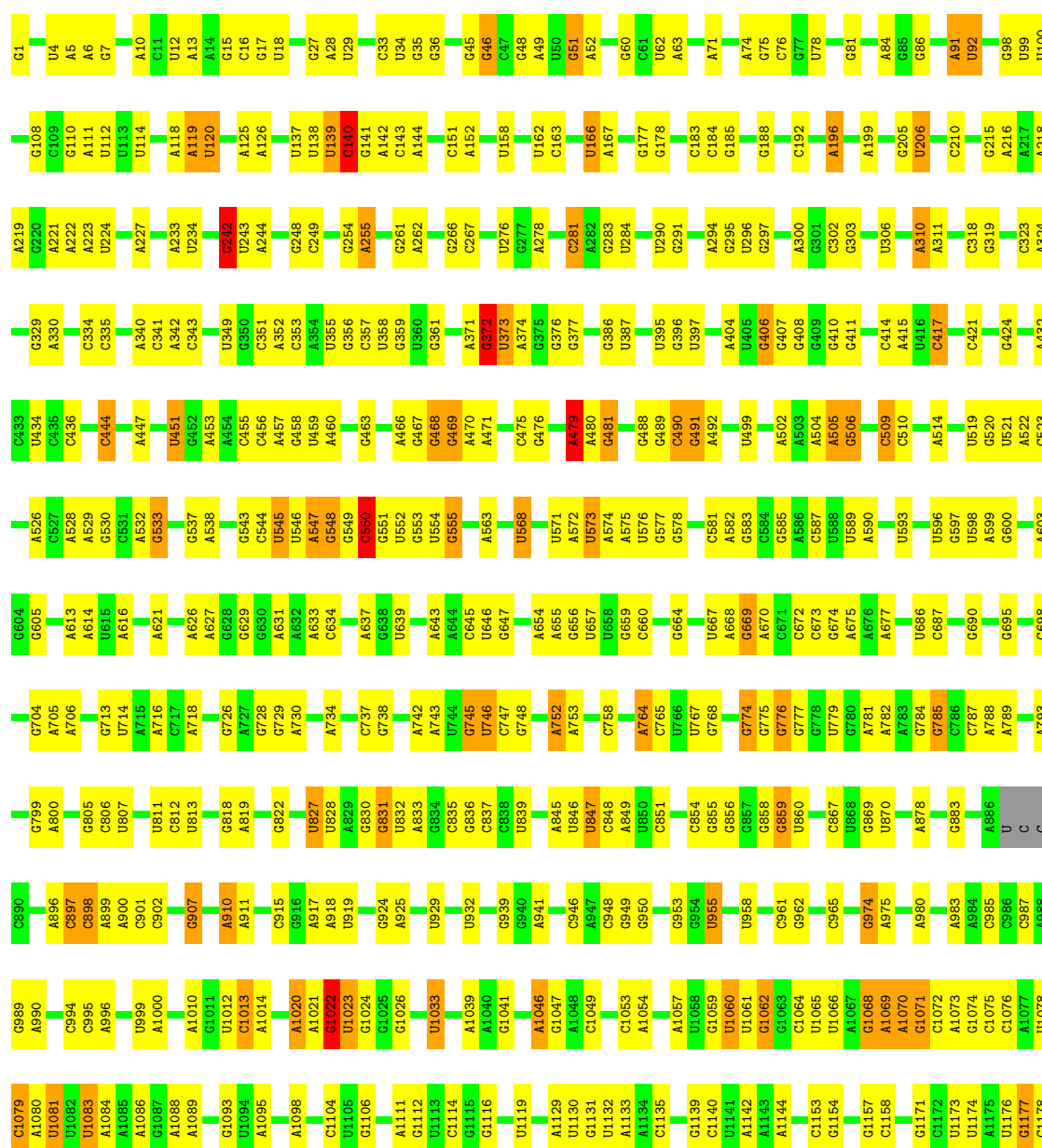
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	w	1	32	11	5	13	3	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA

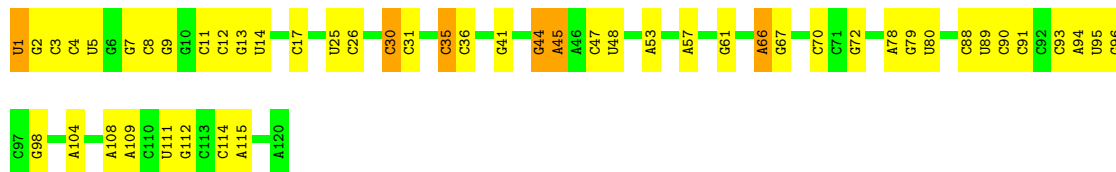
Chain A: 




A2821	G2719	U2511	A2088	A1988	A1900	G1797	C1536	C1417	A1301	G1179
G2822	U2720	C2512	G2093	C1999	A1901	U1798	G1537	G1418	C1306	U1180
A2823	A2721	A2513	A2094	G2002	C1905	G1799	A1544	A1419	G1309	U1181
G2824	G2722	C2514	A2095	A2003	A1906	A1801	G1555	A1420	G1310	G1182
G2825	A2726	C2515	A2096	G2004	U1911	A1802	G1555	G1421	G1310	U1188
U2832	G2731	C2516	A2111	A2005	A1912	G1687	U1559	G1422	U1313	A1189
U2833	G2732	A2518	A2212	C2006	A1913	C1806	U1560	C1428	G1314	G1190
G2834	U2733	C2519	G2110	U2007	A1914	G1807	G1560	G1429	C1315	G1191
A2835	A2734	C2520	G2111	C2008	U1917	A1809	C1565	G1430	A1204	A1204
U2836	G2735	C2521	U2111	A2009	A1918	A1810	U1569	A1431	A1321	A1205
A2837	U2739	G2522	G2112	G2010	A1919	G1811	A1433	G1432	A1322	G1206
G2846	U2743	C2523	U2113	A2020	A1920	U1812	A1434	A1433	G1323	U1209
U2847	G2744	G2524	U2220	C2021	G1921	G1816	G1435	G1436	U1210	U1210
G2848	U2745	C2525	G2223	U2022	G1922	G1817	A1437	G1437	C1211	G1211
U2849	G2746	G2526	G2224	G2023	G1925	U1818	C1585	C1447	A1327	G1212
A2850	U2747	C2527	G2225	G2024	U1926	G1823	C1585	C1447	U1328	G1215
G2851	G2748	U2528	G2226	U2028	A1927	G1826	U1592	G1450	U1329	G1215
U2852	A2749	C2529	C2226	G2029	U1928	U1827	A1593	C1451	C1330	C1221
U2861	A2750	G2530	U2229	U2030	G1929	G1828	A1597	G1452	G1333	U1222
G2862	U2751	C2531	G2230	A2031	G1930	U1829	A1598	C1453	G1334	G1223
U2863	C2752	A2547	U2231	G2032	U1931	C1830	U1602	C1454	G1341	U1224
A2864	G2753	U2552	G2232	U2033	A1932	G1831	A1603	C1461	C1345	G1225
G2865	U2754	C2553	U2233	U2034	U1936	U1832	A1604	C1462	C1345	A1226
U2866	G2755	G2554	G2234	G2035	A1937	C1833	U1607	C1469	C1348	A1237
A2867	C2756	U2555	U2235	U2036	U1938	U1834	C1607	C1469	C1349	U1242
G2872	U2757	C2556	G2236	G2037	U1940	G1835	A1610	G1475	G1355	A1247
A2873	A2758	G2557	U2237	C2043	C1941	C1837	C1611	U1476	G1356	G1248
U2880	U2759	U2558	G2238	C2047	U1944	U1841	G1613	G1482	A1365	U1249
A2883	G2760	C2559	U2239	G2048	A1953	G1842	A1634	A1490	G1250	G1250
U2884	U2761	U2560	G2240	U2049	G1954	G1847	A1635	G1491	C1251	C1251
A2889	A2762	A2561	U2241	A2051	U1955	A1848	U1636	G1492	G1369	A1252
U2890	G2763	C2562	G2242	C2052	U1956	U1849	A1637	C1493	A1253	A1254
G2901	U2764	G2243	U2243	C2055	A1960	U1858	C1638	G1500	U1372	U1255
U2902	A2765	U2244	G2244	G2056	U1961	G1862	C1646	A1504	C1376	G1256
U2903	U2766	C2563	U2245	A2060	C1962	U1862	U1647	A1504	G1377	G1266
G2904	U2767	G2246	U2246	G2061	U1963	C1870	U1648	A1509	A1378	G1266
A2905	A2768	A2247	A2247	A2062	C1967	A1871	G1649	G1510	U1379	A1269
U2906	G2769	C2248	G2248	C2063	G1968	A1872	A1651	G1516	G1380	C1270
A2907	U2770	G2249	G2249	U2068	A1969	G1873	G1652	A1515	A1383	G1271
G2908	U2771	C2250	U2250	G2069	U1970	U1880	G1653	G1517	C1386	A1272
U2909	A2772	G2251	G2251	A2071	U1971	G1884	G1660	A1522	A1387	A1287
A2910	G2773	C2252	U2252	C2072	C1972	G1891	A1664	U1523	U1394	G1288
U2911	U2774	G2253	G2253	U2076	C1986	G1892	A1665	G1524	A1395	U1294
G2912	A2775	C2254	U2254	A2081	U1987	C1893	A1666	G1524	A1395	U1294
A2913	U2776	G2255	U2255	A2082	U1991	G1896	G1667	A1532	C1398	C1297
U2914	G2777	C2256	U2256	U2086	G1992	A1896	A1668	U1533	C1399	G1298
G2915	U2778	G2257	U2257	G2087	C1996	A1899	A1669	U1534	C1416	G1300
A2916	A2779	C2258	U2258	G2087	C1997	A1899	C1670	A1535		

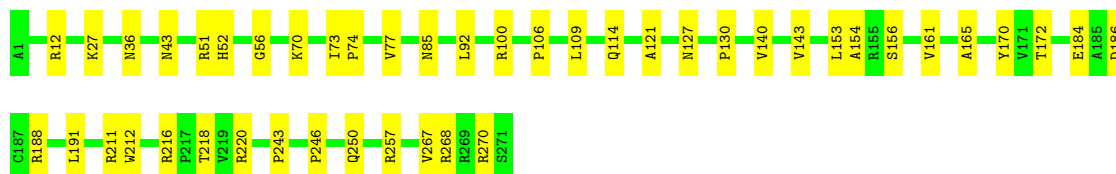
- Molecule 2: 5S ribosomal RNA

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: 



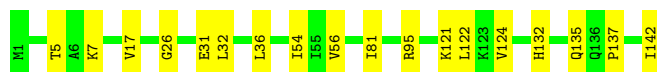
- Molecule 9: 50S ribosomal protein L11

Chain I: 87% 13%



- Molecule 10: 50S ribosomal protein L13

Chain J: 87% 13%



- Molecule 11: 50S ribosomal protein L14

Chain K: 80% 20%



- 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: 83% 16%

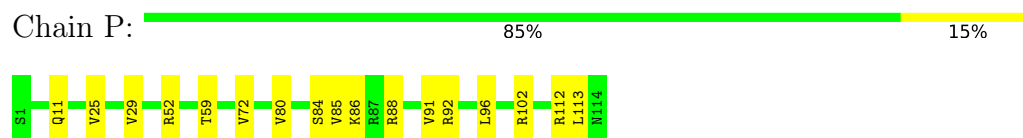


- Molecule 15: 50S ribosomal protein L18

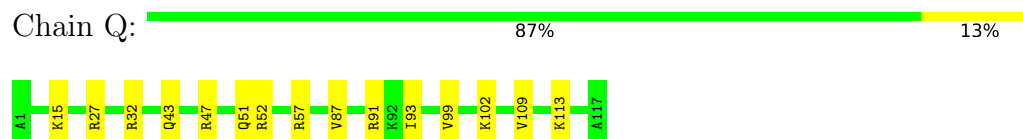
Chain O: 89% 11%



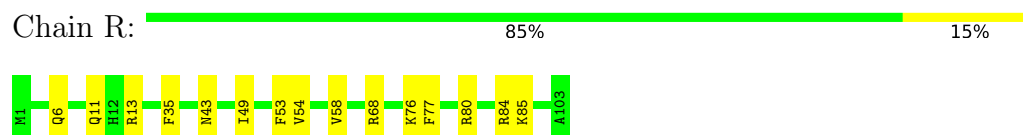
- Molecule 16: 50S ribosomal protein L19



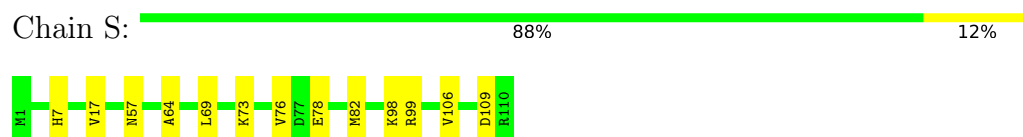
- Molecule 17: 50S ribosomal protein L20



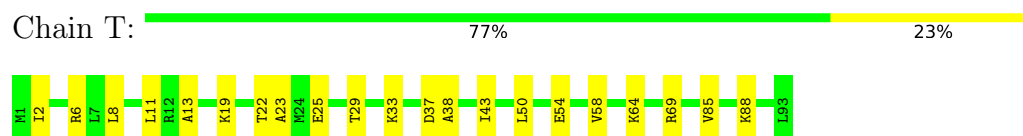
- Molecule 18: 50S ribosomal protein L21



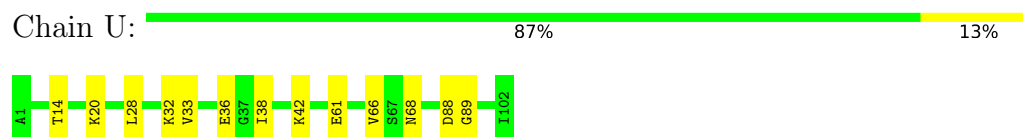
- Molecule 19: 50S ribosomal protein L22



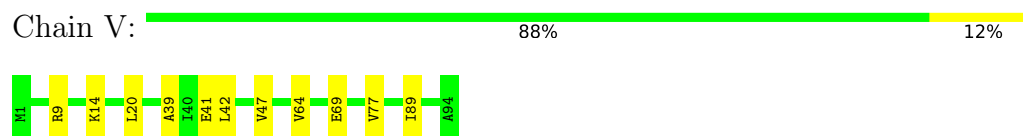
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25




- Molecule 23: 50S ribosomal protein L27

Chain W:  93% 7%




- Molecule 24: 50S ribosomal protein L28

Chain X:  86% 14%




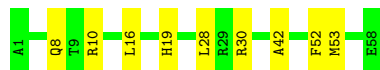
- Molecule 25: 50S ribosomal protein L29

Chain Y:  84% 16%




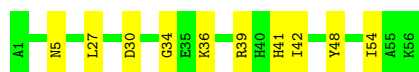
- Molecule 26: 50S ribosomal protein L30

Chain Z:  84% 16%




- Molecule 27: 50S ribosomal protein L32

Chain 0:  82% 18%




- Molecule 28: 50S ribosomal protein L33

Chain 1:  90% 10%




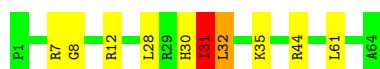
- Molecule 29: 50S ribosomal protein L34

Chain 2:  80% 20%

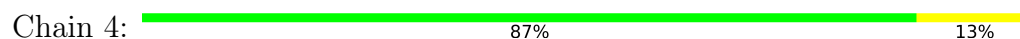


- Molecule 30: 50S ribosomal protein L35

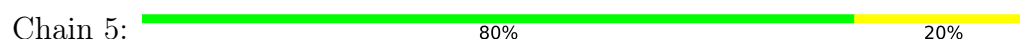
Chain 3:  84% 13% ..



- Molecule 31: 50S ribosomal protein L36



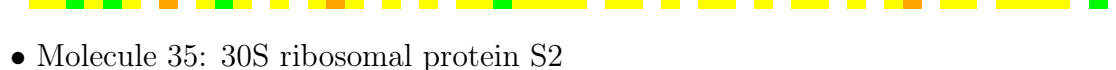
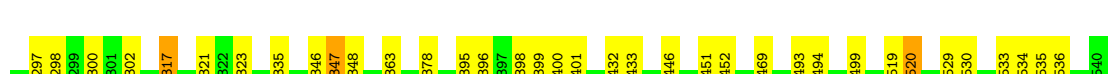
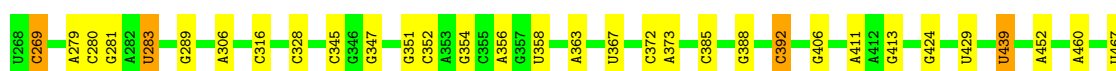
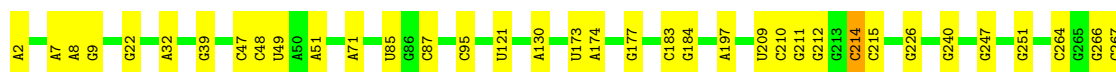
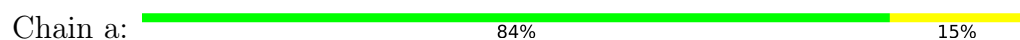
- Molecule 32: 50S ribosomal protein L10



- Molecule 33: mRNA



- Molecule 34: 16S ribosomal RNA



- Molecule 35: 30S ribosomal protein S2

Chain b:  97% .



- Molecule 36: 30S ribosomal protein S3

Chain c:  100%

There are no outlier residues recorded for this chain.

- 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.

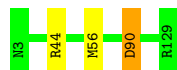
- Molecule 41: 30S ribosomal protein S8

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:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 30S ribosomal protein S11

Chain k:  99%



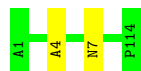
- Molecule 45: 30S ribosomal protein S12

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.

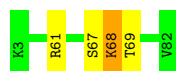
- Molecule 49: 30S ribosomal protein S16

Chain p:  99%



- Molecule 50: 30S ribosomal protein S17

Chain q:  95%



- 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.

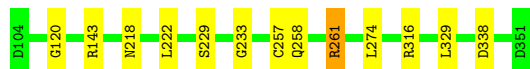
- Molecule 54: 30S ribosomal protein S21

Chain u:  97%



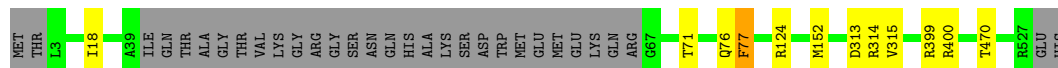
- Molecule 55: Peptide chain release factor RF1

Chain v:  95%



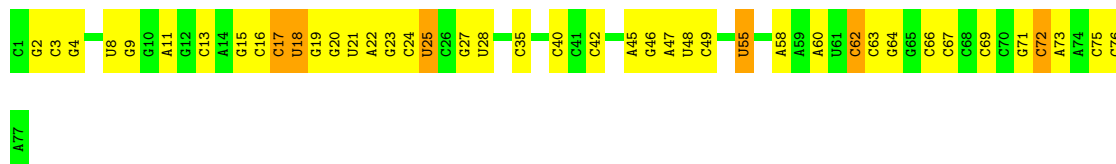
- Molecule 56: Peptide chain release factor RF3

Chain w:  92%



- Molecule 57: fMet-tRNA

Chain x:  45%



- 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	46814	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.9	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.29	1/69729 (0.0%)	1.00	228/108768 (0.2%)
10	J	0.25	0/1152	0.46	0/1551
11	K	0.27	0/947	0.52	0/1268
12	L	0.27	0/1054	0.54	0/1403
13	M	0.27	0/1093	0.57	1/1460 (0.1%)
14	N	0.27	0/973	0.52	0/1301
15	O	0.25	0/902	0.47	0/1209
16	P	0.25	0/929	0.51	1/1242 (0.1%)
17	Q	0.26	0/960	0.45	0/1278
18	R	0.26	0/829	0.50	0/1107
19	S	0.24	0/864	0.50	0/1156
2	B	0.39	1/2876 (0.0%)	1.16	32/4483 (0.7%)
20	T	0.25	0/744	0.51	0/994
21	U	0.29	0/787	0.55	0/1051
22	V	0.25	0/766	0.49	0/1025
23	W	0.26	0/582	0.41	0/769
24	X	0.24	0/635	0.46	0/848
25	Y	0.23	0/510	0.47	0/677
26	Z	0.24	0/453	0.47	0/605
27	0	0.24	0/450	0.46	0/599
28	1	0.26	0/416	0.50	0/554
29	2	0.24	0/380	0.45	0/498
3	C	0.26	0/2121	0.51	0/2852
30	3	0.26	0/513	0.64	2/676 (0.3%)
31	4	0.28	0/303	0.52	0/397
32	5	0.30	0/1001	0.64	0/1350
33	7	0.33	0/169	0.84	0/261
34	a	0.29	1/36967 (0.0%)	0.98	80/57666 (0.1%)
35	b	0.28	0/1735	0.55	0/2338
36	c	0.25	0/1651	0.47	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	0.30	0/835	0.62	0/1128
4	D	0.26	0/1586	0.51	0/2134
40	g	0.27	0/1195	0.52	0/1602
41	h	0.26	0/989	0.55	0/1326
42	i	0.27	0/1034	0.56	0/1375
43	j	0.27	0/796	0.60	0/1077
44	k	0.26	0/885	0.51	0/1195
45	l	0.28	0/969	0.59	0/1300
46	m	0.26	0/892	0.56	0/1193
47	n	0.24	0/811	0.51	0/1081
48	o	0.24	0/722	0.52	0/964
49	p	0.26	0/659	0.51	0/884
5	E	0.25	0/1571	0.47	0/2113
50	q	0.28	0/657	0.60	1/881 (0.1%)
51	r	0.23	0/511	0.48	0/689
52	s	0.26	0/652	0.50	0/877
53	t	0.29	0/671	0.49	0/888
54	u	0.32	0/500	0.66	0/668
55	v	0.46	1/1962 (0.1%)	0.89	6/2643 (0.2%)
56	w	0.27	0/4011	0.61	5/5421 (0.1%)
57	x	0.38	0/1831	1.42	44/2853 (1.5%)
58	z	1.04	1/127 (0.8%)	1.45	3/175 (1.7%)
6	F	0.28	0/1434	0.54	0/1926
7	G	0.26	0/1343	0.52	1/1816 (0.1%)
8	H	0.26	0/1122	0.47	0/1515
9	I	0.29	0/1046	0.55	0/1410
All	All	0.29	5/164121 (0.0%)	0.90	406/244526 (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	2
38	e	0	1
39	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	i	0	2
45	l	0	1
46	m	0	1
49	p	0	1
5	E	0	1
50	q	0	2
54	u	0	1
56	w	0	1
6	F	0	2
7	G	0	3
All	All	0	25

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	257	CYS	C-N	15.26	1.69	1.34
58	z	5	PRO	C-N	11.35	1.60	1.34
1	A	1	G	OP3-P	-10.60	1.48	1.61
2	B	1	U	OP3-P	-10.56	1.48	1.61
34	a	2	A	OP3-P	-10.53	1.48	1.61

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	257	CYS	O-C-N	-28.49	77.11	122.70
58	z	5	PRO	O-C-N	11.62	141.28	122.70
57	x	62	C	N1-C2-O2	10.90	125.44	118.90
1	A	2604	U	C2-N1-C1'	10.62	130.45	117.70
58	z	5	PRO	CA-C-N	-10.55	93.99	117.20
1	A	1893	C	N1-C2-O2	9.81	124.79	118.90
2	B	36	C	N1-C2-O2	9.49	124.59	118.90
56	w	399	ARG	N-CA-C	9.45	136.52	111.00
1	A	2063	C	N1-C2-O2	9.45	124.57	118.90
57	x	62	C	C2-N1-C1'	9.28	129.01	118.80
57	x	17	C	N1-C2-O2	9.22	124.43	118.90
1	A	1326	U	N3-C2-O2	-9.20	115.76	122.20
1	A	1313	U	N3-C2-O2	-9.02	115.88	122.20
58	z	5	PRO	C-N-CA	-8.99	99.22	121.70
1	A	1348	C	N1-C2-O2	8.95	124.27	118.90
57	x	67	C	C2-N1-C1'	8.88	128.57	118.80
1	A	2506	U	C2-N1-C1'	8.87	128.35	117.70
1	A	898	C	C2-N1-C1'	8.80	128.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2226	C	N1-C2-O2	8.79	124.17	118.90
1	A	2473	U	N1-C2-O2	8.75	128.93	122.80
1	A	1326	U	N1-C2-O2	8.71	128.90	122.80
1	A	1893	C	N3-C2-O2	-8.70	115.81	121.90
1	A	2506	U	N1-C2-O2	8.67	128.87	122.80
57	x	17	C	C2-N1-C1'	8.61	128.27	118.80
1	A	897	C	N1-C2-O2	8.56	124.04	118.90
1	A	1313	U	N1-C2-O2	8.45	128.71	122.80
57	x	67	C	N1-C2-O2	8.41	123.95	118.90
1	A	2473	U	N3-C2-O2	-8.38	116.33	122.20
57	x	62	C	N3-C2-O2	-8.38	116.03	121.90
1	A	2605	U	N1-C2-O2	8.38	128.66	122.80
1	A	1774	C	N3-C2-O2	-8.27	116.11	121.90
1	A	847	U	N3-C2-O2	-8.25	116.42	122.20
1	A	955	U	C2-N1-C1'	8.25	127.60	117.70
2	B	36	C	N3-C2-O2	-8.20	116.16	121.90
1	A	1313	U	C2-N1-C1'	8.17	127.51	117.70
1	A	2604	U	C6-N1-C1'	-8.12	109.84	121.20
1	A	2506	U	N3-C2-O2	-8.08	116.54	122.20
34	a	754	C	C2-N1-C1'	8.01	127.61	118.80
2	B	26	C	N1-C2-O2	7.97	123.68	118.90
1	A	2063	C	N3-C2-O2	-7.95	116.34	121.90
1	A	847	U	N1-C2-O2	7.88	128.31	122.80
1	A	2072	C	C2-N1-C1'	7.87	127.46	118.80
2	B	35	C	N1-C2-O2	7.85	123.61	118.90
1	A	2605	U	N3-C2-O2	-7.81	116.73	122.20
1	A	2605	U	C2-N1-C1'	7.70	126.94	117.70
56	w	470	THR	N-CA-C	7.69	131.76	111.00
1	A	2457	U	C2-N1-C1'	7.68	126.92	117.70
1	A	1180	U	N1-C2-O2	7.66	128.16	122.80
1	A	898	C	C5-C6-N1	7.60	124.80	121.00
34	a	214	C	N1-C2-O2	7.57	123.44	118.90
1	A	847	U	C2-N1-C1'	7.56	126.77	117.70
2	B	12	C	N1-C2-O2	7.54	123.42	118.90
34	a	528	C	N1-C2-O2	7.52	123.41	118.90
1	A	2063	C	C2-N1-C1'	7.52	127.07	118.80
57	x	62	C	C6-N1-C2	-7.45	117.32	120.30
1	A	1049	C	N1-C2-O2	7.45	123.37	118.90
57	x	17	C	N3-C2-O2	-7.43	116.70	121.90
1	A	2473	U	C2-N1-C1'	7.36	126.53	117.70
1	A	2580	U	C2-N1-C1'	7.36	126.53	117.70
1	A	867	C	N1-C2-O2	7.34	123.30	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	72	C	C5-C6-N1	7.28	124.64	121.00
34	a	611	C	N1-C2-O2	7.25	123.25	118.90
1	A	2063	C	C6-N1-C2	-7.23	117.41	120.30
56	w	399	ARG	CB-CA-C	-7.21	95.97	110.40
1	A	1326	U	C2-N1-C1'	7.21	126.35	117.70
1	A	192	C	N1-C2-O2	7.18	123.21	118.90
1	A	1774	C	N1-C2-O2	7.17	123.20	118.90
1	A	897	C	C2-N1-C1'	7.17	126.69	118.80
1	A	1180	U	N3-C2-O2	-7.17	117.18	122.20
57	x	67	C	C6-N1-C2	-7.16	117.44	120.30
2	B	36	C	C2-N1-C1'	7.15	126.66	118.80
1	A	1049	C	N3-C2-O2	-7.14	116.90	121.90
34	a	439	U	N1-C2-O2	7.14	127.80	122.80
57	x	69	C	C2-N1-C1'	7.13	126.65	118.80
57	x	66	C	N1-C2-O2	7.10	123.16	118.90
1	A	1348	C	N3-C2-O2	-7.07	116.95	121.90
2	B	36	C	C6-N1-C2	-7.07	117.47	120.30
57	x	40	C	N1-C2-O2	7.07	123.14	118.90
1	A	898	C	C6-N1-C2	-7.05	117.48	120.30
1	A	2226	C	N3-C2-O2	-7.02	116.98	121.90
34	a	516	U	N3-C2-O2	-7.01	117.29	122.20
1	A	1378	A	P-O3'-C3'	6.98	128.07	119.70
1	A	140	C	N1-C2-O2	6.97	123.08	118.90
34	a	1158	C	C2-N1-C1'	6.97	126.46	118.80
34	a	806	C	C6-N1-C2	-6.96	117.52	120.30
34	a	936	C	N1-C2-O2	6.96	123.08	118.90
1	A	2604	U	N1-C2-O2	6.94	127.66	122.80
1	A	752	A	P-O3'-C3'	6.86	127.94	119.70
1	A	2072	C	C5-C6-N1	6.86	124.43	121.00
34	a	516	U	N1-C2-O2	6.83	127.58	122.80
1	A	897	C	N3-C2-O2	-6.82	117.13	121.90
1	A	140	C	C2-N1-C1'	6.81	126.29	118.80
1	A	1378	A	OP1-P-O3'	6.80	120.16	105.20
57	x	67	C	N3-C2-O2	-6.80	117.14	121.90
57	x	55	U	N1-C2-O2	6.79	127.55	122.80
34	a	1201	A	P-O3'-C3'	6.77	127.83	119.70
1	A	2580	U	O4'-C1'-N1	6.77	113.62	108.20
1	A	183	C	N1-C2-O2	6.77	122.96	118.90
1	A	2072	C	C6-N1-C2	-6.76	117.60	120.30
1	A	1022	G	P-O3'-C3'	6.75	127.81	119.70
1	A	2043	C	C2-N1-C1'	6.74	126.21	118.80
1	A	2794	C	N1-C2-O2	6.73	122.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1297	G	P-O3'-C3'	6.73	127.77	119.70
1	A	2226	C	C2-N1-C1'	6.71	126.18	118.80
1	A	919	U	N1-C2-O2	6.66	127.46	122.80
1	A	1020	A	P-O3'-C3'	6.59	127.61	119.70
2	B	35	C	N3-C2-O2	-6.58	117.29	121.90
2	B	12	C	N3-C2-O2	-6.58	117.30	121.90
57	x	18	U	P-O3'-C3'	6.56	127.57	119.70
1	A	2704	C	N1-C2-O2	6.56	122.83	118.90
1	A	183	C	N3-C2-O2	-6.55	117.31	121.90
1	A	1956	U	N1-C2-O2	6.54	127.38	122.80
55	v	257	CYS	C-N-CA	-6.53	105.38	121.70
2	B	31	C	C2-N1-C1'	6.52	125.97	118.80
2	B	12	C	C6-N1-C2	-6.50	117.70	120.30
55	v	233	GLY	N-CA-C	6.49	129.32	113.10
34	a	214	C	N3-C2-O2	-6.47	117.37	121.90
57	x	40	C	C2-N1-C1'	6.46	125.91	118.80
1	A	1893	C	C2-N1-C1'	6.44	125.89	118.80
57	x	62	C	C5-C6-N1	6.44	124.22	121.00
1	A	2580	U	N3-C2-O2	-6.43	117.70	122.20
1	A	2752	C	N1-C2-O2	6.42	122.75	118.90
57	x	25	U	N1-C2-O2	6.42	127.29	122.80
34	a	1158	C	N1-C2-O2	6.41	122.75	118.90
1	A	1956	U	N3-C2-O2	-6.41	117.71	122.20
2	B	35	C	C6-N1-C2	-6.41	117.74	120.30
1	A	114	U	C2-N1-C1'	6.40	125.38	117.70
1	A	2636	C	N1-C2-O2	6.38	122.73	118.90
1	A	2457	U	N1-C2-O2	6.38	127.26	122.80
34	a	805	C	C6-N1-C2	-6.37	117.75	120.30
2	B	26	C	N3-C2-O2	-6.35	117.45	121.90
34	a	1125	U	N1-C2-O2	6.35	127.25	122.80
1	A	1774	C	C6-N1-C2	-6.32	117.77	120.30
2	B	17	C	C2-N1-C1'	6.31	125.74	118.80
1	A	1348	C	C6-N1-C2	-6.31	117.78	120.30
1	A	752	A	OP2-P-O3'	6.30	119.07	105.20
1	A	1917	U	N1-C2-O2	6.30	127.21	122.80
34	a	1202	U	N1-C2-O2	6.30	127.21	122.80
1	A	2590	A	N9-C4-C5	6.29	108.32	105.80
1	A	897	C	C6-N1-C2	-6.29	117.78	120.30
1	A	1348	C	C2-N1-C1'	6.28	125.71	118.80
1	A	1917	U	N3-C2-O2	-6.28	117.81	122.20
1	A	1081	U	C2-N1-C1'	6.27	125.22	117.70
1	A	1917	U	C2-N1-C1'	6.26	125.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	C	C2-N1-C1'	6.26	125.69	118.80
1	A	2604	U	C5-C6-N1	6.26	125.83	122.70
1	A	1081	U	N1-C2-O2	6.24	127.17	122.80
1	A	2226	C	C6-N1-C2	-6.22	117.81	120.30
1	A	2504	U	C2-N1-C1'	6.22	125.16	117.70
57	x	72	C	C6-N1-C2	-6.21	117.82	120.30
2	B	11	C	N1-C2-O2	6.20	122.62	118.90
57	x	18	U	OP1-P-O3'	6.19	118.81	105.20
34	a	439	U	N3-C2-O2	-6.18	117.87	122.20
1	A	915	C	C2-N1-C1'	6.17	125.59	118.80
57	x	55	U	N3-C2-O2	-6.17	117.88	122.20
1	A	1180	U	C2-N1-C1'	6.16	125.09	117.70
55	v	257	CYS	CA-C-N	-6.16	103.65	117.20
57	x	55	U	C2-N1-C1'	6.16	125.09	117.70
2	B	26	C	C2-N1-C1'	6.15	125.56	118.80
13	M	70	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	2590	A	N1-C6-N6	-6.14	114.92	118.60
57	x	69	C	N1-C2-O2	6.12	122.58	118.90
34	a	1182	G	P-O3'-C3'	6.11	127.03	119.70
2	B	3	C	P-O3'-C3'	6.10	127.02	119.70
37	d	4	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	1086	A	C2-N3-C4	6.09	113.65	110.60
34	a	439	U	C2-N1-C1'	6.08	125.00	117.70
1	A	143	C	C2-N1-C1'	6.08	125.48	118.80
16	P	113	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	2474	U	N1-C2-O2	6.07	127.05	122.80
1	A	902	C	C2-N1-C1'	6.06	125.47	118.80
34	a	644	U	N3-C2-O2	-6.06	117.96	122.20
1	A	2072	C	N1-C2-O2	6.04	122.53	118.90
34	a	979	C	N1-C2-O2	6.04	122.53	118.90
1	A	2286	G	P-O3'-C3'	6.03	126.94	119.70
57	x	35	C	N1-C2-O2	6.03	122.52	118.90
57	x	17	C	C6-N1-C2	-6.03	117.89	120.30
1	A	2457	U	N3-C2-O2	-6.01	117.99	122.20
34	a	1125	U	N3-C2-O2	-6.01	117.99	122.20
57	x	62	C	C6-N1-C1'	-6.00	113.60	120.80
57	x	66	C	C6-N1-C2	-6.00	117.90	120.30
1	A	2703	C	C6-N1-C2	-5.99	117.90	120.30
1	A	919	U	N3-C2-O2	-5.98	118.01	122.20
34	a	1347	G	P-O3'-C3'	5.97	126.87	119.70
1	A	1349	C	C2-N1-C1'	5.97	125.37	118.80
1	A	2666	C	N1-C2-O2	5.97	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	697	U	N1-C2-O2	5.97	126.98	122.80
2	B	30	C	N1-C2-O2	5.96	122.48	118.90
1	A	140	C	N3-C2-O2	-5.96	117.73	121.90
57	x	25	U	N3-C2-O2	-5.95	118.04	122.20
1	A	1893	C	C6-N1-C2	-5.94	117.92	120.30
34	a	805	C	C2-N1-C1'	5.94	125.34	118.80
34	a	754	C	C6-N1-C1'	-5.92	113.69	120.80
1	A	242	G	P-O3'-C3'	5.92	126.80	119.70
1	A	2636	C	C2-N1-C1'	5.91	125.30	118.80
34	a	806	C	N3-C2-O2	-5.90	117.77	121.90
1	A	192	C	N3-C2-O2	-5.90	117.77	121.90
1	A	2604	U	O4'-C1'-N1	5.89	112.91	108.20
57	x	66	C	C2-N1-C1'	5.89	125.28	118.80
1	A	372	G	P-O3'-C3'	5.89	126.76	119.70
34	a	611	C	N3-C2-O2	-5.88	117.78	121.90
34	a	960	U	P-O3'-C3'	5.88	126.76	119.70
34	a	528	C	N3-C2-O2	-5.88	117.78	121.90
34	a	1399	C	P-O3'-C3'	5.88	126.75	119.70
1	A	1070	A	P-O3'-C3'	5.87	126.75	119.70
34	a	806	C	C2-N1-C1'	5.87	125.26	118.80
34	a	269	C	C2-N1-C1'	5.87	125.25	118.80
1	A	51	G	P-O3'-C3'	5.86	126.74	119.70
57	x	40	C	N3-C2-O2	-5.86	117.80	121.90
57	x	67	C	C5-C6-N1	5.86	123.93	121.00
1	A	1940	U	P-O3'-C3'	5.84	126.71	119.70
34	a	806	C	N1-C2-O2	5.83	122.40	118.90
34	a	936	C	N3-C2-O2	-5.83	117.82	121.90
34	a	961	U	N1-C2-O2	5.83	126.88	122.80
1	A	1221	C	C2-N1-C1'	5.82	125.21	118.80
1	A	2720	U	N3-C2-O2	-5.81	118.13	122.20
1	A	867	C	N3-C2-O2	-5.80	117.84	121.90
34	a	1432	G	P-O3'-C3'	5.80	126.67	119.70
1	A	2655	G	P-O3'-C3'	5.80	126.66	119.70
57	x	17	C	C6-N1-C1'	-5.80	113.84	120.80
1	A	1314	C	C2-N1-C1'	5.80	125.18	118.80
1	A	2474	U	N3-C2-O2	-5.80	118.14	122.20
34	a	1202	U	N3-C2-O2	-5.79	118.14	122.20
57	x	66	C	N3-C2-O2	-5.79	117.84	121.90
1	A	2214	C	N1-C2-O2	5.79	122.37	118.90
2	B	17	C	C6-N1-C2	-5.77	117.99	120.30
1	A	2580	U	N1-C2-O2	5.76	126.83	122.80
34	a	989	U	N3-C2-O2	-5.76	118.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	985	C	C2-N1-C1'	5.75	125.12	118.80
1	A	985	C	N1-C2-O2	5.74	122.35	118.90
1	A	468	G	P-O3'-C3'	5.72	126.57	119.70
1	A	898	C	C6-N1-C1'	-5.72	113.93	120.80
1	A	1930	G	P-O3'-C3'	5.72	126.56	119.70
34	a	754	C	N1-C2-O2	5.71	122.33	118.90
57	x	67	C	C6-N1-C1'	-5.71	113.94	120.80
2	B	25	U	N1-C2-O2	5.69	126.78	122.80
1	A	2703	C	N1-C2-O2	5.69	122.31	118.90
1	A	2504	U	N1-C2-O2	5.68	126.78	122.80
56	w	77	PHE	N-CA-C	5.68	126.35	111.00
34	a	1190	G	P-O3'-C3'	5.68	126.52	119.70
34	a	1469	C	N1-C2-O2	5.68	122.31	118.90
34	a	1225	A	C4-N9-C1'	5.65	136.48	126.30
1	A	2473	U	C5-C6-N1	5.65	125.53	122.70
1	A	2192	U	C2-N1-C1'	5.65	124.48	117.70
34	a	1317	C	N1-C2-O2	5.64	122.29	118.90
1	A	859	G	P-O3'-C3'	5.62	126.45	119.70
1	A	898	C	N1-C2-O2	5.62	122.27	118.90
1	A	2474	U	C2-N1-C1'	5.62	124.44	117.70
1	A	2566	A	P-O3'-C3'	5.62	126.44	119.70
1	A	2194	U	P-O3'-C3'	5.61	126.44	119.70
57	x	25	U	C2-N1-C1'	5.61	124.44	117.70
1	A	2457	U	O4'-C1'-N1	5.61	112.69	108.20
34	a	385	C	N1-C2-O2	5.61	122.27	118.90
1	A	2506	U	C6-N1-C1'	-5.60	113.36	121.20
34	a	283	U	N1-C2-O2	5.60	126.72	122.80
34	a	611	C	C2-N1-C1'	5.59	124.95	118.80
2	B	12	C	C2-N1-C1'	5.59	124.95	118.80
34	a	697	U	N3-C2-O2	-5.59	118.29	122.20
57	x	72	C	C2-N3-C4	5.59	122.69	119.90
1	A	1348	C	C5-C6-N1	5.59	123.79	121.00
34	a	516	U	C2-N1-C1'	5.58	124.40	117.70
34	a	611	C	C6-N1-C2	-5.57	118.07	120.30
1	A	2617	U	N3-C2-O2	-5.56	118.31	122.20
34	a	961	U	N3-C2-O2	-5.55	118.31	122.20
34	a	620	C	N1-C2-O2	5.53	122.22	118.90
34	a	316	C	N1-C2-O2	5.53	122.22	118.90
2	B	31	C	C6-N1-C2	-5.52	118.09	120.30
34	a	644	U	N1-C2-O2	5.50	126.65	122.80
1	A	955	U	C6-N1-C1'	-5.50	113.51	121.20
1	A	1349	C	C6-N1-C2	-5.49	118.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	72	C	C2-N1-C1'	5.49	124.84	118.80
1	A	837	C	N3-C2-O2	-5.49	118.06	121.90
1	A	2794	C	N3-C2-O2	-5.49	118.06	121.90
1	A	206	U	N1-C2-O2	5.47	126.63	122.80
2	B	11	C	N3-C2-O2	-5.47	118.07	121.90
1	A	2615	U	N3-C2-O2	-5.46	118.38	122.20
34	a	989	U	N1-C2-O2	5.46	126.62	122.80
2	B	26	C	C6-N1-C2	-5.46	118.12	120.30
34	a	469	C	N1-C2-O2	5.45	122.17	118.90
57	x	48	U	C2-N1-C1'	5.44	124.23	117.70
1	A	2769	U	N1-C2-O2	5.44	126.61	122.80
34	a	1225	A	N3-C4-N9	5.43	131.75	127.40
1	A	479	A	P-O3'-C3'	5.43	126.22	119.70
1	A	669	G	C4-N9-C1'	5.43	133.56	126.50
1	A	1079	C	N1-C2-O2	5.43	122.16	118.90
1	A	1926	U	P-O3'-C3'	5.43	126.21	119.70
57	x	13	C	N1-C2-O2	5.42	122.15	118.90
1	A	2504	U	N3-C2-O2	-5.42	118.41	122.20
37	d	190	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	2683	C	N1-C2-O2	5.41	122.14	118.90
1	A	2457	U	C5-C4-O4	5.40	129.14	125.90
1	A	1905	C	N1-C2-O2	5.40	122.14	118.90
1	A	2703	C	C2-N1-C1'	5.40	124.74	118.80
1	A	1086	A	N3-C4-N9	5.40	131.72	127.40
1	A	166	U	N1-C2-O2	5.39	126.58	122.80
1	A	417	C	C2-N1-C1'	5.39	124.73	118.80
34	a	1132	C	N1-C2-O2	5.39	122.13	118.90
34	a	269	C	C6-N1-C2	-5.39	118.15	120.30
1	A	2300	C	C2-N1-C1'	5.38	124.72	118.80
1	A	1188	U	N1-C2-O2	5.38	126.56	122.80
1	A	2552	U	C2-N1-C1'	5.37	124.14	117.70
1	A	2720	U	N1-C2-O2	5.37	126.56	122.80
1	A	634	C	N1-C2-O2	5.37	122.12	118.90
1	A	2604	U	C5-C4-O4	-5.36	122.68	125.90
1	A	1086	A	C4-N9-C1'	5.36	135.94	126.30
30	3	31	ILE	CG1-CB-CG2	-5.35	99.63	111.40
1	A	166	U	N3-C2-O2	-5.35	118.46	122.20
1	A	1760	C	N1-C2-O2	5.34	122.11	118.90
1	A	2739	U	N3-C2-O2	-5.34	118.46	122.20
1	A	444	C	N1-C2-O2	5.34	122.10	118.90
2	B	31	C	N1-C2-O2	5.34	122.10	118.90
2	B	11	C	C6-N1-C2	-5.33	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2617	U	N1-C2-O2	5.33	126.53	122.80
1	A	1081	U	N3-C2-O2	-5.33	118.47	122.20
1	A	919	U	C2-N1-C1'	5.32	124.09	117.70
1	A	2884	U	C2-N1-C1'	5.32	124.09	117.70
1	A	1818	U	C2-N1-C1'	5.32	124.08	117.70
57	x	72	C	N1-C2-O2	5.32	122.09	118.90
1	A	234	U	N3-C2-O2	-5.32	118.48	122.20
1	A	1911	U	C2-N1-C1'	5.31	124.07	117.70
1	A	1812	U	C2-N1-C1'	5.29	124.05	117.70
1	A	2739	U	N1-C2-O2	5.29	126.50	122.80
2	B	3	C	OP1-P-O3'	5.28	116.83	105.20
2	B	25	U	N3-C2-O2	-5.28	118.50	122.20
1	A	758	C	N1-C2-O2	5.27	122.06	118.90
1	A	1812	U	N3-C2-O2	-5.26	118.52	122.20
34	a	392	C	C2-N1-C1'	5.26	124.59	118.80
2	B	30	C	C6-N1-C2	-5.26	118.20	120.30
34	a	439	U	C5-C6-N1	5.26	125.33	122.70
55	v	120	GLY	N-CA-C	5.26	126.24	113.10
1	A	2604	U	N3-C4-O4	5.25	123.08	119.40
1	A	2636	C	C6-N1-C2	-5.25	118.20	120.30
57	x	40	C	C6-N1-C2	-5.25	118.20	120.30
1	A	2494	G	C4-N9-C1'	5.25	133.32	126.50
30	3	61	LEU	CA-CB-CG	5.25	127.36	115.30
34	a	470	C	N1-C2-O2	5.25	122.05	118.90
1	A	985	C	C6-N1-C2	-5.24	118.20	120.30
1	A	143	C	C6-N1-C2	-5.24	118.20	120.30
1	A	1880	U	N3-C2-O2	-5.24	118.53	122.20
1	A	2096	C	C6-N1-C2	-5.23	118.21	120.30
1	A	2254	C	N1-C2-O2	5.23	122.04	118.90
1	A	2615	U	N1-C2-O2	5.23	126.46	122.80
1	A	206	U	N3-C2-O2	-5.23	118.54	122.20
1	A	2506	U	C5-C6-N1	5.23	125.31	122.70
1	A	1376	C	C2-N1-C1'	5.23	124.55	118.80
1	A	2460	U	N1-C2-O2	5.21	126.45	122.80
1	A	114	U	N1-C2-O2	5.21	126.45	122.80
1	A	837	C	N1-C2-O2	5.21	122.02	118.90
34	a	1132	C	C2-N1-C1'	5.20	124.52	118.80
34	a	1158	C	N3-C2-O2	-5.20	118.26	121.90
55	v	274	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	2043	C	C6-N1-C2	-5.19	118.22	120.30
1	A	62	U	C2-N1-C1'	5.19	123.93	117.70
1	A	2704	C	N3-C2-O2	-5.19	118.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2063	C	C5-C6-N1	5.18	123.59	121.00
1	A	2043	C	C5-C6-N1	5.18	123.59	121.00
1	A	1398	C	C2-N1-C1'	5.18	124.50	118.80
1	A	2076	U	C2-N1-C1'	5.18	123.92	117.70
2	B	30	C	N3-C2-O2	-5.18	118.28	121.90
34	a	936	C	C6-N1-C2	-5.18	118.23	120.30
1	A	353	C	N1-C2-O2	5.17	122.00	118.90
1	A	353	C	C2-N1-C1'	5.17	124.48	118.80
1	A	2656	U	N1-C2-O2	5.16	126.41	122.80
2	B	17	C	C5-C6-N1	5.16	123.58	121.00
1	A	898	C	P-O3'-C3'	5.14	125.87	119.70
1	A	2473	U	C6-N1-C2	-5.14	117.92	121.00
1	A	2752	C	C6-N1-C2	-5.14	118.25	120.30
7	G	45	ALA	C-N-CA	5.14	134.54	121.70
34	a	283	U	N3-C2-O2	-5.13	118.61	122.20
1	A	2556	C	N1-C2-O2	5.13	121.98	118.90
50	q	68	LYS	C-N-CA	5.13	134.51	121.70
1	A	550	C	N1-C2-O2	5.12	121.97	118.90
1	A	1818	U	N1-C2-O2	5.11	126.38	122.80
1	A	634	C	C6-N1-C2	-5.10	118.26	120.30
1	A	1880	U	C2-N1-C1'	5.10	123.82	117.70
34	a	358	U	N3-C2-O2	-5.10	118.63	122.20
34	a	1262	C	N1-C2-O2	5.10	121.96	118.90
1	A	2752	C	N3-C2-O2	-5.09	118.34	121.90
34	a	479	U	N1-C2-O2	5.09	126.36	122.80
1	A	1417	C	C2-N1-C1'	5.08	124.39	118.80
1	A	1306	C	C2-N1-C1'	5.08	124.39	118.80
1	A	955	U	O4'-C1'-N1	5.07	112.26	108.20
1	A	2794	C	C6-N1-C2	-5.07	118.27	120.30
1	A	479	A	OP1-P-O3'	5.07	116.36	105.20
34	a	1225	A	C2-N3-C4	5.07	113.14	110.60
34	a	961	U	C2-N1-C1'	5.07	123.78	117.70
34	a	1138	G	C4-N9-C1'	5.07	133.09	126.50
1	A	1880	U	N1-C2-O2	5.06	126.34	122.80
56	w	313	ASP	C-N-CA	5.06	134.35	121.70
57	x	69	C	C6-N1-C1'	-5.06	114.72	120.80
1	A	2769	U	N3-C2-O2	-5.06	118.66	122.20
1	A	1321	A	C2-N3-C4	5.06	113.13	110.60
1	A	2329	U	C5-C6-N1	5.05	125.23	122.70
34	a	891	U	N1-C2-O2	5.05	126.34	122.80
34	a	392	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1818	U	N3-C2-O2	-5.05	118.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	C	C5-C6-N1	5.04	123.52	121.00
34	a	264	C	N1-C2-O2	5.04	121.92	118.90
34	a	1520	C	C2-N1-C1'	5.04	124.34	118.80
1	A	897	C	C5-C6-N1	5.04	123.52	121.00
1	A	2226	C	C5-C6-N1	5.04	123.52	121.00
34	a	1203	C	C6-N1-C2	-5.03	118.29	120.30
2	B	66	A	P-O3'-C3'	5.03	125.73	119.70
1	A	140	C	P-O3'-C3'	5.03	125.73	119.70
34	a	979	C	N3-C2-O2	-5.03	118.38	121.90
34	a	1109	C	N1-C2-O2	5.02	121.91	118.90

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	3	30	HIS	Peptide
32	5	80	THR	Peptide
5	E	82	GLY	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
38	e	121	ASN	Peptide
39	f	52	ASN	Peptide
39	f	95	ALA	Peptide
42	i	56	MET	Peptide
42	i	90	ASP	Peptide
45	l	101	LEU	Peptide
46	m	4	ALA	Peptide
49	p	44	SER	Peptide
50	q	67	SER	Peptide
50	q	68	LYS	Peptide
54	u	23	GLU	Peptide
56	w	314	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62262	0	31318	464	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	29	0
4	D	1565	0	1616	19	0
5	E	1552	0	1619	18	0
6	F	1410	0	1447	18	0
7	G	1323	0	1374	5	0
8	H	1111	0	1148	15	0
9	I	1032	0	1088	11	0
10	J	1129	0	1162	13	0
11	K	938	0	1012	15	0
12	L	1045	0	1117	14	0
13	M	1074	0	1157	11	0
14	N	960	0	1000	15	0
15	O	892	0	923	10	0
16	P	917	0	965	11	0
17	Q	947	0	1022	12	0
18	R	816	0	839	10	0
19	S	857	0	922	7	0
20	T	738	0	807	15	0
21	U	779	0	834	6	0
22	V	753	0	780	6	0
23	W	575	0	592	3	0
24	X	625	0	655	9	0
25	Y	509	0	543	8	0
26	Z	449	0	491	6	0
27	0	444	0	461	7	0
28	1	409	0	440	3	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	5	0
34	a	33016	0	16615	0	0
35	b	1704	0	1732	0	0
36	c	1624	0	1699	0	0
37	d	1643	0	1710	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	1141	0	1170	0	0
39	f	817	0	808	0	0
40	g	1181	0	1240	0	0
41	h	979	0	1034	0	0
42	i	1022	0	1070	0	0
43	j	786	0	828	0	0
44	k	869	0	878	0	0
45	l	955	0	1019	0	0
46	m	883	0	944	0	0
47	n	799	0	841	0	0
48	o	714	0	737	0	0
49	p	649	0	666	0	0
50	q	648	0	691	0	0
51	r	504	0	502	0	0
52	s	637	0	665	0	0
53	t	665	0	714	0	0
54	u	495	0	486	0	0
55	v	1932	0	1881	0	0
56	w	3938	0	3929	0	0
57	x	1639	0	837	0	0
58	z	120	0	128	0	0
59	w	32	0	13	0	0
All	All	151479	0	104064	695	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 7.

All (695) 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:1517:G:N1	1:A:1920:C:H5'	103.03	1.10
1:A:306:U:H3	1:A:310:A:H62	1.06	0.99
1:A:593:U:H3	1:A:664:G:H1	1.14	0.94
1:A:1476:U:H3	1:A:1515:A:H62	0.99	0.92
1:A:1517:G:H1	1:A:1920:C:H5'	103.44	0.91
1:A:545:U:H3	1:A:548:G:H1	0.99	0.90
1:A:745:G:N7	1:A:746:U:C4	2.40	0.90
1:A:2028:U:H3	1:A:2033:A:H62	1.15	0.88
1:A:1517:G:N2	1:A:1920:C:O5'	103.41	0.88
1:A:2457:U:H5	1:A:2494:G:H1	0.90	0.88
1:A:1074:G:H1	1:A:1083:U:H3	29.79	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1517:G:C2	1:A:1920:C:O5'	102.68	0.85
1:A:1517:G:N1	1:A:1920:C:C5'	103.28	0.83
1:A:2457:U:H5	1:A:2494:G:N1	1.75	0.81
1:A:2475:C:H42	1:A:2529:G:N2	1.80	0.80
1:A:745:G:N7	1:A:746:U:N3	2.30	0.79
1:A:1932:A:H62	1:A:1968:G:H21	1.33	0.77
1:A:2508:G:N1	1:A:2580:U:O4	2.18	0.76
23:W:61:GLY:HA3	23:W:79:GLU:O	1.87	0.74
1:A:2475:C:H42	1:A:2529:G:H22	1.34	0.74
1:A:1517:G:H1	1:A:1920:C:C5'	103.71	0.73
1:A:306:U:H3	1:A:310:A:N6	1.86	0.72
1:A:600:G:H1	1:A:657:U:H3	1.37	0.71
1:A:1517:G:H21	1:A:1919:A:H2'	104.22	0.70
1:A:1517:G:C2	1:A:1920:C:C5'	103.34	0.69
1:A:955:U:C5	1:A:962:G:N1	2.58	0.68
1:A:1476:U:H3	1:A:1515:A:N6	1.83	0.68
1:A:2457:U:O4	1:A:2494:G:O6	2.12	0.68
1:A:2475:C:N4	1:A:2529:G:H22	1.92	0.67
16:P:59:THR:HG22	16:P:72:VAL:HG12	1.77	0.67
1:A:1912:A:N7	1:A:1917:U:O4	2.27	0.67
1:A:1433:A:H61	1:A:1560:G:H1	1.41	0.67
2:B:78:A:H62	2:B:98:G:H21	1.41	0.66
6:F:62:GLN:HE22	6:F:90:LEU:HB3	1.61	0.66
12:L:109:LYS:HD2	12:L:126:ARG:HH11	1.62	0.65
1:A:2508:G:C6	1:A:2580:U:O4	2.51	0.64
33:7:18:U:H6	33:7:18:U:H5''	1.63	0.64
1:A:2508:G:O6	1:A:2580:U:O4	2.16	0.64
1:A:459:U:H3	1:A:470:A:H62	1.47	0.64
1:A:955:U:H5	1:A:962:G:H1	1.44	0.64
5:E:146:VAL:HG12	5:E:185:LYS:HB2	1.80	0.64
1:A:78:U:H3	1:A:108:G:H1	1.45	0.63
5:E:18:THR:HA	5:E:106:LYS:HE3	1.81	0.63
14:N:28:LEU:HD23	14:N:48:VAL:HG21	1.81	0.63
1:A:2514:U:H5''	10:J:81:ILE:HD11	1.80	0.63
1:A:1039:A:H2	1:A:1116:G:H1	1.42	0.62
1:A:955:U:H5	1:A:962:G:N1	1.97	0.62
1:A:1905:C:H4'	1:A:1929:G:H21	1.64	0.62
1:A:1687:G:H21	1:A:1701:A:H62	1.47	0.62
1:A:244:A:H62	1:A:254:G:H21	1.47	0.62
1:A:1418:G:N2	1:A:1579:A:N7	2.48	0.61
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1798:U:H5"	3:C:257:ARG:HB2	1.82	0.61
1:A:1046:A:H62	32:5:4:ASN:HD21	1.47	0.61
1:A:1060:U:H5'	1:A:1062:G:H5'	1.83	0.61
1:A:1517:G:H22	1:A:1920:C:C4'	105.96	0.61
1:A:1154:G:OP2	17:Q:57:ARG:NH1	2.34	0.61
1:A:1666:G:H4'	11:K:6:THR:HG23	1.83	0.61
33:7:18:U:C6	33:7:18:U:C5'	2.83	0.61
1:A:2514:U:H3	1:A:2570:G:H1	1.48	0.61
1:A:2656:U:O2	1:A:2665:A:N7	2.34	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
1:A:488:G:H22	1:A:491:G:H5"	1.66	0.60
1:A:281:C:H42	1:A:359:G:H1	1.49	0.60
1:A:1081:U:H4'	9:I:123:ALA:HB1	1.83	0.60
3:C:51:ARG:HH22	3:C:246:PRO:HG2	1.67	0.60
30:3:32:LEU:HD23	30:3:35:LYS:HD2	1.84	0.60
19:S:82:MET:HB2	19:S:98:LYS:HB2	1.84	0.60
1:A:2062:A:H62	1:A:2503:A:H62	1.49	0.60
1:A:629:G:N3	1:A:639:U:O2'	2.33	0.60
4:D:34:VAL:HA	4:D:50:VAL:HG12	1.84	0.60
32:5:58:THR:HG21	32:5:82:ILE:H	1.67	0.60
1:A:818:G:H21	1:A:1189:A:H62	1.47	0.60
11:K:40:LYS:HE3	11:K:57:VAL:HG12	1.84	0.60
1:A:1252:G:N2	17:Q:32:ARG:O	2.35	0.60
6:F:134:GLN:NE2	6:F:149:ARG:O	2.35	0.60
8:H:39:ALA:HA	8:H:43:ASN:HB2	1.85	0.59
1:A:839:U:H3	1:A:939:G:H1	1.50	0.59
1:A:1862:G:H1	1:A:1880:U:H3	1.49	0.59
2:B:78:A:H62	2:B:98:G:N2	2.00	0.59
5:E:117:ARG:NH2	5:E:183:PHE:O	2.36	0.59
1:A:538:A:H4'	10:J:7:LYS:HG2	1.85	0.59
1:A:2296:U:OP2	15:O:9:ARG:NH2	2.36	0.59
1:A:1093:G:H21	1:A:1098:A:H62	1.51	0.59
1:A:1500:G:H4'	3:C:100:ARG:HH12	1.68	0.59
1:A:6:A:HO2'	10:J:132:HIS:HD1	1.51	0.58
12:L:23:ILE:HD13	18:R:84:ARG:HH22	1.68	0.58
1:A:196:A:H61	1:A:831:G:H21	1.52	0.58
22:V:42:LEU:HD13	22:V:47:VAL:HG21	1.85	0.58
1:A:2185:U:H2'	1:A:2186:G:H8	1.69	0.58
1:A:674:G:O6	1:A:716:A:N1	105.62	0.58
26:Z:8:GLN:HB2	26:Z:28:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:11:GLN:NE2	9:I:54:ILE:O	2.37	0.57
1:A:1517:G:H22	1:A:1920:C:H4'	106.18	0.57
1:A:2094:A:O3'	8:H:11:ASN:ND2	2.38	0.57
1:A:745:G:O6	1:A:746:U:C5	2.58	0.57
32:5:3:LEU:HD12	32:5:5:LEU:H	1.68	0.57
1:A:1476:U:O4	1:A:1515:A:N7	2.38	0.57
1:A:306:U:O4	1:A:310:A:N7	2.37	0.57
3:C:92:LEU:HD11	3:C:100:ARG:HB3	1.86	0.57
29:2:24:THR:HG23	29:2:27:GLY:H	1.69	0.57
1:A:318:C:H2'	1:A:319:G:H8	1.70	0.57
4:D:15:PHE:H	16:P:11:GLN:HE22	1.52	0.57
1:A:2515:C:H2'	1:A:2516:A:H8	1.70	0.57
2:B:48:U:OP2	15:O:30:ARG:NH2	2.38	0.57
23:W:33:ILE:HG22	23:W:34:VAL:HG23	1.87	0.57
27:O:30:ASP:HB3	27:O:34:GLY:H	1.70	0.57
1:A:962:G:O2'	1:A:2250:G:N2	2.38	0.57
1:A:1986:C:H2'	1:A:1987:A:H8	1.71	0.56
18:R:35:PHE:O	18:R:58:VAL:HA	2.05	0.56
24:X:6:VAL:HG21	24:X:58:ILE:HD11	1.87	0.56
1:A:605:G:H1'	1:A:657:U:H1'	1.88	0.56
2:B:72:G:H21	2:B:104:A:H62	1.53	0.56
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.39	0.56
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.87	0.56
20:T:23:ALA:HB1	20:T:29:THR:HB	1.87	0.56
1:A:1754:A:O2'	16:P:102:ARG:NH2	2.38	0.56
24:X:39:VAL:HG12	24:X:42:GLU:H	1.70	0.56
1:A:1173:U:O2'	1:A:1177:G:N2	2.39	0.56
1:A:1223:G:OP1	18:R:68:ARG:NH2	2.39	0.56
1:A:1517:G:N2	1:A:1920:C:C5'	104.07	0.56
1:A:1992:G:N2	1:A:1996:C:O2'	2.36	0.55
1:A:2692:G:H1'	1:A:2847:U:H1'	1.88	0.55
1:A:605:G:N3	1:A:657:U:O2'	2.38	0.55
2:B:79:G:N7	22:V:14:LYS:NZ	2.53	0.55
5:E:102:ARG:NH1	5:E:200:LEU:O	2.39	0.55
1:A:605:G:OP1	5:E:99:LYS:NZ	2.40	0.55
6:F:23:SER:HB3	6:F:26:GLN:HG3	1.87	0.55
15:O:40:ILE:HG12	15:O:47:VAL:HG12	1.88	0.55
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.40	0.55
7:G:88:LEU:HG	7:G:161:VAL:HG22	1.87	0.55
1:A:1932:A:H62	1:A:1968:G:N2	2.02	0.55
1:A:2893:A:H5''	1:A:2894:G:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:G:N2	1:A:2350:C:O2'	2.40	0.55
1:A:907:G:N2	13:M:70:ASP:OD2	2.40	0.55
1:A:144:A:H4'	20:T:2:ILE:HD11	1.89	0.55
1:A:2028:U:O4	1:A:2033:A:N7	2.39	0.55
1:A:2229:U:H2'	1:A:2230:G:H8	1.71	0.55
24:X:4:CYS:HB3	24:X:9:LYS:H	1.72	0.55
1:A:1204:A:N6	1:A:1242:U:O4	2.40	0.55
1:A:2291:U:H1'	1:A:2374:C:H1'	1.89	0.55
1:A:2861:U:H2'	1:A:2862:G:H8	1.72	0.55
14:N:43:GLU:OE2	14:N:46:ARG:NH2	2.40	0.55
24:X:58:ILE:HG12	24:X:66:VAL:HG21	1.89	0.55
1:A:1428:C:OP2	3:C:27:LYS:NZ	2.40	0.55
1:A:585:G:H21	1:A:1254:A:H62	1.55	0.55
11:K:30:ARG:NH2	11:K:37:ASP:OD2	2.39	0.54
1:A:2523:G:HO2'	1:A:2764:A:HO2'	1.56	0.54
1:A:460:A:H62	1:A:469:G:H21	1.54	0.54
1:A:475:C:H4'	1:A:510:C:H5'	1.88	0.54
1:A:2748:A:H5'	7:G:3:VAL:HG21	1.89	0.54
24:X:39:VAL:O	24:X:43:LYS:N	2.40	0.54
1:A:2320:U:O2'	1:A:2322:A:N6	2.40	0.54
1:A:514:A:N3	1:A:581:C:O2'	2.37	0.54
11:K:43:ILE:HD12	11:K:56:ASP:HB2	1.90	0.54
1:A:2028:U:H3	1:A:2033:A:N6	1.94	0.54
1:A:2394:C:H5''	12:L:63:LYS:HE3	1.90	0.54
1:A:550:C:H2'	1:A:551:G:H8	1.73	0.54
1:A:589:U:H2'	1:A:590:A:H8	1.73	0.54
1:A:444:C:OP2	5:E:44:ARG:NH2	2.41	0.54
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.40	0.54
2:B:30:C:H1'	2:B:57:A:H61	1.71	0.54
3:C:70:LYS:HB3	3:C:73:ILE:HD12	1.90	0.54
7:G:94:ARG:HB2	7:G:105:SER:HB2	1.90	0.54
20:T:8:LEU:HA	20:T:50:LEU:HD21	1.89	0.54
32:5:22:ALA:HB3	32:5:87:GLU:HB2	1.88	0.54
1:A:587:C:O2	12:L:33:ARG:NH1	2.41	0.54
15:O:108:ASP:OD1	15:O:111:ARG:NH1	2.40	0.54
1:A:538:A:N6	1:A:555:G:O2'	2.41	0.53
27:0:27:LEU:HD23	27:0:36:LYS:HB3	1.91	0.53
1:A:1779:U:OP2	1:A:1784:A:N6	2.42	0.53
1:A:2110:G:N1	1:A:2120:G:N7	2.57	0.53
1:A:2659:G:N2	1:A:2662:A:OP2	2.41	0.53
3:C:165:ALA:HB3	3:C:172:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:G:H5'	4:D:4:LEU:HD22	165.61	0.53
1:A:533:G:O5'	17:Q:27:ARG:NH1	2.42	0.53
4:D:148:GLN:HB2	4:D:152:PRO:HG2	1.91	0.53
1:A:1753:G:H5''	16:P:92:ARG:HD3	1.90	0.53
1:A:994:C:OP1	17:Q:52:ARG:NH2	2.41	0.53
1:A:210:C:OP1	29:2:29:GLN:NE2	2.42	0.53
1:A:1668:A:N3	1:A:1670:C:N4	2.57	0.53
1:A:2020:A:N7	27:0:5:ASN:ND2	2.57	0.53
13:M:75:GLU:HB3	13:M:90:GLU:HG3	1.91	0.53
26:Z:10:ARG:HB2	26:Z:53:MET:HB2	1.90	0.53
1:A:698:C:HO2'	1:A:734:A:H61	1.54	0.53
21:U:36:GLU:HA	21:U:61:GLU:HG2	1.90	0.53
1:A:523:C:O2	1:A:554:U:O2'	2.27	0.53
1:A:1422:G:H5'	11:K:48:PRO:HG3	98.98	0.53
1:A:2306:C:N4	6:F:38:GLY:O	2.41	0.53
1:A:2746:U:H5''	7:G:137:LYS:HE2	1.90	0.53
1:A:177:G:H3'	1:A:178:G:H8	1.73	0.52
32:5:26:VAL:HG21	32:5:114:GLU:HG2	1.91	0.52
1:A:576:U:H2'	1:A:577:G:C8	2.45	0.52
8:H:1:MET:N	8:H:20:ASN:OD1	2.42	0.52
1:A:1818:U:H5'	3:C:156:SER:HB2	1.91	0.52
1:A:1899:A:H4'	1:A:1901:A:H5''	1.91	0.52
1:A:463:G:N2	1:A:466:A:OP2	2.34	0.52
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.92	0.52
8:H:47:PHE:HA	8:H:51:ARG:HB2	1.90	0.52
22:V:9:ARG:HD3	22:V:39:ALA:HB1	1.91	0.52
1:A:1450:G:H21	1:A:1452:G:H1	1.56	0.52
17:Q:43:GLN:HE21	18:R:77:PHE:HB3	1.74	0.52
1:A:1613:G:H4'	29:2:3:ARG:HE	1.74	0.52
1:A:2110:G:N2	1:A:2179:C:O2	2.43	0.52
1:A:585:G:H21	1:A:1254:A:N6	2.08	0.52
20:T:38:ALA:HB1	20:T:43:ILE:HD11	1.90	0.52
1:A:1024:G:HO2'	1:A:1144:A:HO2'	1.58	0.52
1:A:335:C:O2'	1:A:1433:A:N3	112.64	0.52
1:A:76:C:OP1	25:Y:48:ARG:NH1	2.43	0.52
1:A:111:A:O2'	25:Y:58:ASN:ND2	2.42	0.52
1:A:451:U:O2	1:A:453:A:N6	2.42	0.52
1:A:45:G:H5''	1:A:46:G:H5'	1.92	0.52
4:D:131:ASP:O	4:D:136:ASN:ND2	2.40	0.52
1:A:1270:C:H5''	1:A:1271:G:H5'	1.92	0.52
1:A:827:U:H2'	1:A:870:U:H3	55.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:17:LYS:HE3	12:L:27:LEU:HD22	1.92	0.52
1:A:958:U:OP2	13:M:14:LYS:NZ	2.42	0.52
1:A:2023:C:H2'	1:A:2024:G:H8	1.74	0.51
1:A:835:C:H2'	1:A:836:G:H8	1.74	0.51
3:C:184:GLU:HG3	3:C:186:ASP:H	1.75	0.51
10:J:56:VAL:HB	10:J:124:VAL:HG12	1.91	0.51
1:A:1800:C:N4	1:A:1818:U:O2'	2.43	0.51
1:A:924:G:H2'	1:A:925:A:H8	1.74	0.51
2:B:5:U:OP1	2:B:61:G:O2'	2.28	0.51
6:F:163:GLU:OE1	6:F:166:ARG:NH1	2.43	0.51
8:H:30:LEU:HB3	8:H:36:ALA:HB3	1.91	0.51
1:A:2768:U:O2'	10:J:95:ARG:NH2	2.43	0.51
14:N:44:LEU:HD23	14:N:113:ILE:HD13	1.92	0.51
20:T:13:ALA:HB3	20:T:33:LYS:HD3	1.92	0.51
1:A:1013:C:H2'	1:A:1014:A:H8	1.74	0.51
1:A:119:A:H4'	1:A:120:U:H5'	1.92	0.51
1:A:2113:U:O4	1:A:2119:A:N6	2.44	0.51
1:A:1953:A:O2'	1:A:2559:C:O2	2.28	0.51
1:A:407:G:H2'	1:A:408:G:H8	1.76	0.51
1:A:2081:U:H2'	1:A:2082:A:H8	1.75	0.51
1:A:2848:G:O2'	1:A:2868:A:N6	2.43	0.51
1:A:410:G:N3	1:A:432:A:N6	41.54	0.51
8:H:38:PRO:O	8:H:43:ASN:ND2	2.41	0.51
1:A:99:U:H5''	1:A:100:U:H5'	1.91	0.51
1:A:2656:U:N3	1:A:2665:A:C8	2.72	0.51
1:A:2743:U:OP2	1:A:2755:C:N4	2.43	0.51
1:A:698:C:O2'	1:A:734:A:N6	2.35	0.51
1:A:112:U:H5'	25:Y:58:ASN:HD21	1.76	0.51
1:A:1724:G:O6	1:A:1737:G:N2	2.43	0.51
1:A:574:A:N6	1:A:2034:U:OP1	2.41	0.51
10:J:17:VAL:HG23	10:J:137:PRO:HB2	1.93	0.51
1:A:1068:G:N2	1:A:1095:A:O2'	2.36	0.51
1:A:2008:C:H2'	1:A:2009:A:H8	1.75	0.51
32:5:68:PRO:HA	32:5:72:LEU:HG	1.93	0.50
21:U:33:VAL:HG13	21:U:66:VAL:HG22	1.93	0.50
1:A:227:A:H61	1:A:410:G:H21	1.59	0.50
1:A:629:G:H1'	1:A:639:U:H1'	1.92	0.50
1:A:291:G:H1	1:A:349:U:H3	1.59	0.50
3:C:77:VAL:HG21	3:C:109:LEU:HD11	1.92	0.50
1:A:660:C:O2'	12:L:13:LYS:NZ	2.44	0.50
13:M:66:ARG:NH1	13:M:104:GLU:OE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2693:G:H2'	1:A:2694:G:H8	1.75	0.50
1:A:242:G:N2	1:A:255:A:OP2	2.44	0.50
11:K:12:ASP:HB3	11:K:99:ILE:HG12	1.93	0.50
19:S:73:LYS:HB2	19:S:106:VAL:HB	1.92	0.50
1:A:1069:A:N7	1:A:1073:A:N6	2.60	0.50
1:A:673:C:OP1	5:E:49:ARG:NH2	2.43	0.50
13:M:35:ALA:O	13:M:99:GLY:N	2.44	0.50
31:4:30:GLU:HG3	31:4:32:LYS:H	1.76	0.50
1:A:2291:U:O2'	1:A:2374:C:O2	2.30	0.50
1:A:2656:U:C2	1:A:2665:A:N7	2.80	0.50
2:B:7:G:O2'	15:O:38:GLN:NE2	2.45	0.50
1:A:537:G:H4'	10:J:5:THR:HG21	1.92	0.50
1:A:1807:G:N2	1:A:1810:A:OP2	2.44	0.50
1:A:1517:G:N2	1:A:1919:A:H2'	104.17	0.50
1:A:2692:G:N3	1:A:2847:U:O2'	2.42	0.50
1:A:481:G:O2'	1:A:506:G:N2	2.45	0.50
1:A:1323:C:OP1	19:S:98:LYS:NZ	2.43	0.50
1:A:1022:G:N2	1:A:1023:U:O4	2.44	0.50
1:A:1602:U:OP2	20:T:64:LYS:NZ	2.45	0.50
1:A:2788:C:O2'	1:A:2809:A:N3	2.41	0.50
1:A:358:U:H2'	1:A:359:G:H8	2.44	0.49
8:H:94:ILE:HG23	8:H:98:ASP:HB2	1.94	0.49
12:L:20:GLY:H	12:L:28:GLY:HA2	1.76	0.49
1:A:139:U:O2'	1:A:140:C:O2	2.30	0.49
1:A:776:G:H22	1:A:2072:C:H5'	1.75	0.49
3:C:140:VAL:HG12	3:C:191:LEU:HD23	1.93	0.49
1:A:2002:G:OP2	14:N:9:GLN:NE2	2.45	0.49
1:A:573:U:OP2	18:R:80:ARG:NH2	2.45	0.49
5:E:75:SER:HB3	5:E:78:TRP:HD1	1.77	0.49
1:A:2647:U:H2'	1:A:2648:G:H8	1.77	0.49
1:A:377:G:H1	1:A:397:U:H3	1.60	0.49
1:A:746:U:H5''	1:A:748:G:O4'	2.11	0.49
20:T:6:ARG:NH2	20:T:37:ASP:OD2	2.45	0.49
1:A:537:G:H22	1:A:555:G:H2'	1.77	0.49
1:A:764:A:N3	3:C:211:ARG:NH1	2.61	0.49
17:Q:87:VAL:HG13	18:R:49:ILE:HD11	1.95	0.49
25:Y:49:ASP:OD1	25:Y:52:ARG:NH2	2.45	0.49
1:A:1682:G:OP2	1:A:1699:G:N2	2.45	0.49
1:A:2076:U:OP2	1:A:2238:G:N2	2.45	0.49
1:A:745:G:C8	1:A:746:U:N3	2.79	0.49
16:P:84:SER:OG	16:P:86:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:25:VAL:HG22	16:P:85:VAL:HG22	1.93	0.49
1:A:2286:G:H3'	28:1:29:LYS:HE2	1.94	0.49
1:A:848:C:H2'	1:A:849:A:H8	1.78	0.49
1:A:1080:A:H1'	9:I:127:SER:HA	1.94	0.49
1:A:774:G:N2	1:A:787:C:O2'	2.45	0.49
2:B:95:U:H2'	2:B:96:G:H8	1.78	0.49
31:4:19:ARG:HD2	31:4:24:ARG:HD2	1.95	0.48
1:A:2258:C:O2'	1:A:2427:C:OP2	2.30	0.48
1:A:659:G:O2'	5:E:95:LYS:O	2.31	0.48
1:A:2305:U:N3	6:F:150:GLY:O	2.45	0.48
22:V:20:LEU:HD11	22:V:41:GLU:HG3	1.95	0.48
32:5:33:VAL:HG12	32:5:35:VAL:H	1.78	0.48
1:A:471:A:OP1	5:E:79:ARG:NH1	2.42	0.48
1:A:781:A:OP1	3:C:216:ARG:NH2	2.42	0.48
2:B:114:C:H2'	2:B:115:A:H8	1.77	0.48
1:A:2293:G:OP1	15:O:94:ARG:NH1	2.46	0.48
33:7:18:U:H6	33:7:18:U:C5'	2.22	0.48
1:A:1936:A:OP2	1:A:1962:C:N4	2.40	0.48
1:A:28:A:O2'	1:A:296:U:OP1	48.99	0.48
1:A:590:A:H61	1:A:667:U:H3	1.61	0.48
1:A:1288:G:N2	1:A:1288:G:OP2	2.42	0.48
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.78	0.48
1:A:290:U:H2'	1:A:291:G:H8	1.79	0.48
1:A:297:G:N2	1:A:300:A:OP2	12.76	0.48
1:A:355:U:H2'	1:A:356:G:H8	1.79	0.48
4:D:36:GLN:OE1	4:D:49:GLN:NE2	2.46	0.48
1:A:911:A:N6	13:M:11:LYS:O	2.37	0.48
18:R:76:LYS:HB2	18:R:85:LYS:HB3	1.95	0.48
33:7:17:A:C3'	33:7:18:U:H5''	2.44	0.48
1:A:48:G:N2	1:A:177:G:OP2	2.45	0.48
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.95	0.48
10:J:36:LEU:HD22	10:J:121:LYS:HB2	1.94	0.48
1:A:177:G:N2	1:A:177:G:OP2	2.36	0.48
1:A:1129:A:O2'	1:A:2515:C:O2	2.30	0.48
9:I:45:THR:HG22	9:I:50:LYS:HG2	1.94	0.48
26:Z:16:LEU:HB2	26:Z:19:HIS:HD2	1.78	0.48
1:A:1266:G:N2	1:A:1269:A:OP2	13.27	0.48
9:I:102:ARG:NH1	9:I:106:GLN:OE1	2.47	0.48
20:T:8:LEU:HD11	25:Y:22:LEU:HD12	1.96	0.48
8:H:132:PHE:H	8:H:140:ALA:HB3	1.78	0.48
17:Q:93:ILE:HG23	18:R:13:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:A:OP2	30:3:7:ARG:NH1	2.44	0.47
1:A:2539:C:O2'	31:4:36:ARG:NH1	2.42	0.47
1:A:302:C:H2'	1:A:303:G:H8	1.79	0.47
1:A:519:U:H2'	1:A:520:G:H8	1.79	0.47
1:A:582:A:H2'	1:A:583:G:H8	1.79	0.47
1:A:745:G:H2'	1:A:746:U:H5'	1.95	0.47
3:C:243:PRO:O	3:C:250:GLN:NE2	2.46	0.47
1:A:1469:A:OP2	1:A:1522:A:N6	2.47	0.47
1:A:283:G:H1	1:A:357:C:H42	1.61	0.47
9:I:44:LYS:HG2	9:I:70:THR:HG21	1.96	0.47
1:A:1830:C:H2'	1:A:1831:G:H8	1.79	0.47
1:A:2233:U:H2'	1:A:2234:G:H8	1.77	0.47
1:A:793:A:OP2	1:A:2071:A:O2'	2.29	0.47
32:5:30:SER:HB3	32:5:109:LYS:HD2	1.97	0.47
1:A:1432:G:H2'	1:A:1433:A:H8	1.80	0.47
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.52	0.47
1:A:2618:G:H21	4:D:155:VAL:HG21	1.79	0.47
1:A:2822:G:O2'	1:A:2825:G:N1	2.40	0.47
1:A:2345:G:H4'	1:A:2346:A:H3'	1.96	0.47
1:A:713:G:H21	1:A:718:A:H62	1.61	0.47
1:A:806:C:O2	1:A:2444:G:O2'	2.33	0.47
2:B:1:U:H2'	2:B:2:G:H8	1.79	0.47
6:F:28:PRO:HB2	6:F:168:LEU:HD22	1.96	0.47
11:K:9:ASN:OD1	11:K:18:ARG:NH1	2.47	0.47
1:A:807:U:O2'	1:A:2060:A:N1	2.43	0.47
1:A:728:G:H4'	3:C:12:ARG:HD3	1.97	0.47
7:G:8:VAL:HB	7:G:49:LEU:HB2	1.97	0.47
29:2:34:ARG:NH2	29:2:41:ARG:O	2.48	0.47
1:A:1827:U:OP2	3:C:220:ARG:NH1	2.47	0.47
1:A:672:C:OP2	12:L:42:SER:OG	2.30	0.47
3:C:154:ALA:HB2	3:C:161:VAL:HG23	1.96	0.47
1:A:340:A:O2'	5:E:162:ARG:NH1	2.45	0.47
17:Q:99:VAL:O	17:Q:102:LYS:NZ	2.47	0.47
21:U:14:THR:OG1	21:U:68:ASN:ND2	2.46	0.47
1:A:631:A:N3	1:A:2415:G:O2'	2.41	0.47
22:V:77:VAL:HG23	22:V:89:ILE:HG12	1.96	0.47
1:A:1378:A:O2'	1:A:1380:G:OP2	2.30	0.47
2:B:8:C:O2'	15:O:25:ARG:NH1	2.47	0.47
8:H:17:ASP:HB3	8:H:19:VAL:HG23	1.97	0.47
3:C:267:VAL:HG12	3:C:268:ARG:HG2	1.97	0.46
11:K:121:GLU:HG2	11:K:122:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:G:H2'	1:A:1334:G:H8	1.81	0.46
1:A:1806:C:H1'	3:C:43:ASN:HD21	1.80	0.46
1:A:2245:U:H5''	1:A:2246:G:H5'	1.95	0.46
1:A:29:U:O2	1:A:1215:G:O2'	2.34	0.46
1:A:849:A:H61	1:A:929:U:H3	1.63	0.46
3:C:130:PRO:HA	3:C:188:ARG:HA	1.98	0.46
1:A:2052:A:O2'	4:D:149:ASN:O	2.34	0.46
1:A:767:U:H2'	1:A:768:G:H8	1.80	0.46
1:A:779:U:O2	1:A:785:G:O6	2.34	0.46
8:H:70:GLU:HB2	8:H:134:VAL:HG21	1.98	0.46
14:N:28:LEU:HD13	14:N:34:ILE:HG12	1.96	0.46
27:O:42:ILE:HG22	27:O:48:TYR:HB2	1.98	0.46
1:A:1071:G:N2	1:A:1089:A:O2'	2.44	0.46
1:A:1429:G:H2'	1:A:1430:G:H8	1.79	0.46
1:A:1432:G:H2'	1:A:1433:A:C8	2.51	0.46
1:A:1447:C:O2'	1:A:1544:A:N3	2.39	0.46
1:A:2851:A:O2'	14:N:64:ARG:NH2	2.49	0.46
1:A:918:A:N3	2:B:80:U:O2'	2.42	0.46
1:A:2060:A:H62	5:E:69:ARG:HH22	1.63	0.46
1:A:505:A:HO2'	1:A:509:C:HO2'	1.64	0.46
10:J:36:LEU:HD11	10:J:122:LEU:HD13	1.98	0.46
1:A:16:C:H2'	1:A:17:G:H8	1.78	0.46
4:D:55:LYS:HE2	4:D:77:ARG:HA	1.98	0.46
1:A:1254:A:H5''	1:A:1255:U:H5''	1.98	0.46
1:A:1462:C:HO2'	1:A:2702:G:HO2'	1.64	0.46
1:A:351:C:H2'	1:A:352:A:H8	1.81	0.46
2:B:111:U:H2'	2:B:112:G:H8	1.81	0.46
1:A:1386:C:H2'	1:A:1387:A:C8	2.51	0.46
1:A:1636:U:H2'	1:A:1637:A:H8	1.81	0.46
1:A:2086:U:H2'	1:A:2087:G:C8	2.51	0.46
1:A:376:G:H2'	1:A:377:G:H8	2.04	0.46
2:B:44:G:H1'	2:B:47:C:H42	1.82	0.46
1:A:1046:A:H4'	32:5:61:ARG:HB3	1.98	0.45
1:A:577:G:O2'	1:A:1254:A:OP1	2.33	0.45
1:A:1997:C:H2'	1:A:1998:A:H8	1.82	0.45
19:S:69:LEU:HA	19:S:109:ASP:HA	1.98	0.45
1:A:2086:U:H2'	1:A:2087:G:H8	1.81	0.45
1:A:581:C:H2'	1:A:582:A:C8	2.51	0.45
1:A:1368:G:H2'	1:A:1369:G:H8	1.81	0.45
1:A:1387:A:H5'	1:A:1469:A:H1'	1.97	0.45
1:A:2525:G:H2'	1:A:2526:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:C:H2'	1:A:582:A:H8	1.81	0.45
4:D:109:VAL:HG22	4:D:203:VAL:HG22	1.98	0.45
4:D:37:VAL:HG22	4:D:48:ILE:HG22	1.99	0.45
19:S:78:GLU:OE1	19:S:99:ARG:NH2	2.49	0.45
1:A:1334:G:H5''	20:T:69:ARG:HH22	1.81	0.45
1:A:2313:C:H2'	1:A:2314:A:C8	2.52	0.45
5:E:75:SER:HB3	5:E:78:TRP:CD1	2.51	0.45
1:A:244:A:H5''	12:L:67:THR:HG21	1.99	0.45
12:L:96:LYS:HE3	12:L:103:ILE:HA	1.99	0.45
1:A:2223:G:OP1	3:C:170:TYR:OH	2.32	0.45
1:A:2771:C:O2'	4:D:173:GLN:NE2	2.45	0.45
1:A:466:A:OP1	29:2:34:ARG:NH1	2.48	0.45
6:F:91:ARG:HA	6:F:95:MET:HB3	1.99	0.45
19:S:17:VAL:HG12	19:S:76:VAL:HG21	1.99	0.45
1:A:1509:A:H2'	1:A:1510:G:C8	2.52	0.45
1:A:917:A:H5''	1:A:2268:A:H61	1.82	0.45
1:A:2458:G:O2'	1:A:2460:U:O4	2.34	0.45
1:A:33:C:O2	1:A:447:A:N6	2.50	0.45
25:Y:37:LEU:HD11	25:Y:42:LEU:HD12	1.98	0.45
33:7:17:A:C5	33:7:18:U:C5	3.05	0.45
1:A:813:U:OP1	18:R:84:ARG:NH1	2.50	0.45
20:T:11:LEU:O	25:Y:29:ARG:NH1	2.50	0.45
26:Z:10:ARG:NH2	26:Z:52:PHE:O	2.50	0.45
5:E:182:ALA:HB2	12:L:3:LEU:HD22	1.97	0.45
1:A:490:C:H2'	1:A:491:G:H8	8.65	0.44
4:D:9:VAL:HA	4:D:197:THR:HG23	1.99	0.44
1:A:2144:G:H1'	1:A:2147:A:H61	1.82	0.44
1:A:459:U:O4	1:A:470:A:N7	2.50	0.44
14:N:45:ARG:HG2	14:N:95:THR:HG21	1.98	0.44
1:A:2818:U:H2'	1:A:2819:G:C8	2.52	0.44
1:A:302:C:H2'	1:A:303:G:C8	2.53	0.44
1:A:737:C:N4	1:A:738:G:O6	2.51	0.44
6:F:9:ASP:OD1	6:F:9:ASP:N	2.48	0.44
8:H:30:LEU:HA	8:H:35:LYS:HB2	1.99	0.44
11:K:87:LEU:HD13	11:K:92:GLU:HB3	1.99	0.44
1:A:1041:G:H1	1:A:1114:C:H42	1.66	0.44
9:I:89:SER:HB3	9:I:135:MET:HA	1.99	0.44
14:N:38:LEU:HG	14:N:42:LYS:HE2	1.99	0.44
32:5:119:PRO:HG2	32:5:121:SER:HB2	2.00	0.44
1:A:1287:A:OP2	14:N:103:ARG:NH1	2.46	0.44
1:A:18:U:O2'	1:A:554:U:OP1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:G:O2'	1:A:657:U:O2	2.33	0.44
6:F:147:ARG:HG3	6:F:149:ARG:H	1.82	0.44
14:N:42:LYS:HA	14:N:45:ARG:HE	1.83	0.44
1:A:1431:A:H2'	1:A:1432:G:H8	1.81	0.44
1:A:2298:A:H5''	6:F:71:LYS:HD3	1.99	0.44
1:A:2443:C:H2'	1:A:2444:G:C8	2.52	0.44
1:A:476:G:O2'	1:A:502:A:N6	2.46	0.44
11:K:76:VAL:H	16:P:72:VAL:HG22	1.82	0.44
32:5:24:SER:HB2	32:5:116:GLU:HG3	1.99	0.44
1:A:1796:U:H2'	1:A:1797:G:C8	2.53	0.44
1:A:2070:A:H2'	1:A:2071:A:H8	1.82	0.44
1:A:2683:C:O2	11:K:70:ARG:NH2	2.50	0.44
1:A:2883:A:OP1	27:0:48:TYR:OH	2.36	0.44
1:A:674:G:H2'	1:A:675:A:H8	3.82	0.44
1:A:910:A:H62	13:M:12:MET:HA	1.82	0.44
30:3:8:GLY:O	30:3:12:ARG:NH2	2.48	0.44
1:A:2719:G:H4'	1:A:2846:G:H4'	1.99	0.44
1:A:2898:U:H2'	1:A:2899:A:C8	2.53	0.44
1:A:589:U:H2'	1:A:590:A:C8	2.52	0.44
1:A:2047:C:H2'	1:A:2048:G:H8	1.83	0.44
1:A:2899:A:H2'	1:A:2900:A:C8	2.53	0.44
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.00	0.44
6:F:115:GLY:HA3	6:F:177:ARG:HB2	1.98	0.44
32:5:48:ALA:HB3	32:5:51:TYR:HE1	1.82	0.43
1:A:2246:G:H2'	1:A:2247:A:H8	1.83	0.43
3:C:56:GLY:HA2	3:C:212:TRP:HA	2.00	0.43
8:H:125:THR:HG23	8:H:146:VAL:HG12	1.99	0.43
24:X:39:VAL:O	24:X:43:LYS:CA	2.66	0.43
24:X:6:VAL:HA	24:X:73:ARG:HH22	1.81	0.43
25:Y:24:GLU:HB3	25:Y:46:VAL:HG21	1.99	0.43
1:A:224:U:OP2	1:A:408:G:N2	2.43	0.43
1:A:2372:U:H2'	1:A:2373:G:H8	1.82	0.43
1:A:2491:U:H4'	1:A:2570:G:H5'	2.00	0.43
1:A:552:U:H2'	1:A:553:G:H8	1.83	0.43
1:A:787:C:H5''	1:A:788:A:H5'	2.00	0.43
2:B:93:C:H2'	2:B:94:A:H8	1.83	0.43
9:I:91:LYS:HG3	9:I:94:LYS:HE2	2.00	0.43
13:M:17:ASN:O	13:M:38:ARG:NH1	2.47	0.43
20:T:58:VAL:HG22	20:T:85:VAL:HG13	2.01	0.43
1:A:1796:U:H3	1:A:1823:G:H1	1.66	0.43
1:A:2220:U:H4'	8:H:97:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1638:C:O2	1:A:2698:U:O2'	2.36	0.43
1:A:598:U:H2'	1:A:599:A:H8	1.82	0.43
8:H:113:SER:O	8:H:116:ARG:NH1	2.45	0.43
13:M:47:GLU:OE2	13:M:51:ARG:NE	2.51	0.43
1:A:1209:U:H4'	1:A:1212:G:H4'	2.00	0.43
1:A:2691:C:H2'	1:A:2692:G:H8	1.82	0.43
1:A:284:U:H3	1:A:356:G:H1	1.65	0.43
1:A:476:G:N1	1:A:479:A:OP2	2.39	0.43
1:A:13:A:O2'	1:A:15:G:N7	2.46	0.43
1:A:1858:A:N6	1:A:1884:G:O2'	2.47	0.43
1:A:91:A:O2'	1:A:92:U:O4'	2.33	0.43
1:A:1033:U:O2'	1:A:2750:A:N6	2.52	0.43
1:A:2035:G:H5''	1:A:2036:C:H5	1.84	0.43
1:A:2295:C:OP1	15:O:10:ARG:NH1	2.39	0.43
11:K:114:LYS:HE3	11:K:118:LEU:HD11	2.00	0.43
1:A:1158:C:H5''	26:Z:30:ARG:HD2	2.01	0.43
1:A:2313:C:H2'	1:A:2314:A:H8	1.84	0.43
1:A:2505:G:O2'	1:A:2506:U:O4'	2.37	0.43
2:B:45:A:O4'	6:F:91:ARG:NH2	2.52	0.43
1:A:499:U:H5''	21:U:42:LYS:HE2	2.00	0.43
1:A:1171:G:N2	1:A:1179:G:N7	2.67	0.43
1:A:1431:A:H2'	1:A:1432:G:C8	2.53	0.43
1:A:2251:G:H2'	1:A:2252:G:H8	1.83	0.43
10:J:32:LEU:HD22	10:J:54:ILE:HG21	2.01	0.43
16:P:88:ARG:HB3	16:P:112:ARG:HD3	2.01	0.43
16:P:91:VAL:HG21	16:P:96:LEU:HD11	2.00	0.43
30:3:28:LEU:HA	30:3:32:LEU:HD11	2.00	0.43
9:I:117:THR:HG22	32:5:42:ARG:HH21	1.83	0.43
1:A:1394:U:O2	20:T:19:LYS:NZ	2.46	0.43
1:A:1665:A:H2'	1:A:1666:G:H8	1.83	0.43
1:A:1709:U:H2'	1:A:1710:G:H8	1.84	0.43
1:A:1891:G:O2'	1:A:2235:G:O2'	2.37	0.43
1:A:373:U:H2'	1:A:374:A:H8	1.83	0.43
1:A:2131:U:H5'	1:A:2132:U:H5''	2.01	0.42
1:A:655:A:H4'	1:A:656:G:H5'	2.00	0.42
17:Q:47:ARG:NH2	17:Q:51:GLN:OE1	2.51	0.42
1:A:2512:C:OP2	4:D:128:ARG:NH2	2.52	0.42
24:X:39:VAL:O	24:X:43:LYS:HA	2.19	0.42
1:A:1372:U:O2'	1:A:2212:A:N3	2.41	0.42
1:A:434:U:O2'	1:A:436:C:N4	2.53	0.42
12:L:127:VAL:HG21	12:L:142:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:G:O6	24:X:56:ARG:NH2	2.52	0.42
32:5:56:ARG:HE	32:5:83:ALA:HB2	1.85	0.42
1:A:2289:G:H2'	1:A:2290:G:H8	1.84	0.42
1:A:2630:G:H2'	1:A:2631:G:C8	2.55	0.42
3:C:121:ALA:HB1	3:C:127:ASN:HB3	2.01	0.42
1:A:585:G:N2	1:A:1254:A:H62	2.16	0.42
1:A:1515:A:H3'	1:A:1516:G:H8	1.85	0.42
1:A:1700:A:H3'	1:A:1701:A:H8	1.85	0.42
1:A:2832:U:H1'	1:A:2834:G:C2	2.54	0.42
1:A:2705:A:O2'	1:A:2852:G:OP1	2.34	0.42
6:F:152:ASP:N	6:F:152:ASP:OD1	2.52	0.42
1:A:818:G:N2	1:A:1189:A:H62	2.14	0.42
1:A:568:U:N3	1:A:571:U:OP2	2.46	0.42
4:D:47:ALA:HB2	4:D:83:ARG:HD2	2.01	0.42
1:A:1709:U:H2'	1:A:1710:G:C8	2.55	0.42
4:D:115:GLY:HA2	4:D:166:GLY:HA3	2.01	0.42
20:T:54:GLU:HB3	20:T:88:LYS:HD2	2.00	0.42
1:A:1140:C:H5'	10:J:26:GLY:HA3	2.02	0.42
1:A:1597:A:H4'	1:A:1598:A:H8	1.85	0.42
1:A:184:C:H2'	1:A:185:G:H8	1.83	0.42
1:A:2327:A:H2'	1:A:2328:A:C8	2.55	0.42
1:A:2418:A:OP1	30:3:44:ARG:NH2	2.47	0.42
1:A:2006:C:O2'	1:A:2823:A:N3	2.50	0.42
6:F:56:LEU:HD13	6:F:88:VAL:HG23	2.01	0.42
1:A:1251:C:O2'	1:A:1253:A:OP2	2.38	0.42
1:A:1604:C:O2'	1:A:1610:A:N1	2.47	0.42
1:A:16:C:H2'	1:A:17:G:C8	2.55	0.42
1:A:2781:A:H5''	1:A:2782:G:H5'	2.01	0.42
2:B:114:C:H2'	2:B:115:A:C8	2.54	0.42
9:I:53:PRO:HG2	9:I:77:VAL:HG11	2.02	0.42
1:A:1435:G:H2'	1:A:1436:G:C8	2.55	0.42
1:A:2691:C:H2'	1:A:2692:G:C8	2.54	0.42
1:A:546:U:H2'	1:A:547:A:H4'	2.00	0.42
6:F:35:LEU:HB2	6:F:88:VAL:HB	2.02	0.42
1:A:6:A:N3	10:J:135:GLN:NE2	2.68	0.42
10:J:31:GLU:HG2	10:J:142:ILE:HG12	2.00	0.42
15:O:4:LYS:HE2	15:O:8:ILE:HD11	2.02	0.42
1:A:1675:C:O2	4:D:133:THR:OG1	2.37	0.41
1:A:2240:U:H2'	1:A:2241:A:H8	1.84	0.41
1:A:633:A:O2'	1:A:2404:U:OP1	2.36	0.41
1:A:2497:A:H1'	1:A:2498:C:H5	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:G:C6	1:A:746:U:C5	3.07	0.41
2:B:14:U:OP2	2:B:70:C:O2'	2.37	0.41
5:E:149:ILE:HD11	5:E:172:ALA:HA	2.02	0.41
1:A:1227:G:OP2	17:Q:15:LYS:NZ	2.47	0.41
1:A:1841:U:H2'	1:A:1842:G:H8	1.85	0.41
1:A:526:A:O2'	1:A:2043:C:O2	2.28	0.41
1:A:2457:U:C5	1:A:2494:G:N1	2.63	0.41
1:A:5:A:H2'	1:A:6:A:C8	2.55	0.41
5:E:47:LYS:HB2	5:E:51:GLU:HB2	2.01	0.41
1:A:2002:G:H5''	14:N:9:GLN:HE21	1.85	0.41
1:A:151:C:H2'	1:A:152:A:H8	1.86	0.41
1:A:1687:G:N2	1:A:1701:A:H62	2.17	0.41
1:A:2175:C:H2'	1:A:2176:A:H8	1.83	0.41
1:A:2329:U:H2'	1:A:2330:G:C8	2.55	0.41
1:A:4:U:H2'	1:A:5:A:H8	1.86	0.41
1:A:674:G:H2'	1:A:675:A:C8	4.25	0.41
14:N:79:LEU:HD23	14:N:83:LEU:HD12	2.02	0.41
23:W:61:GLY:CA	23:W:79:GLU:O	2.65	0.41
1:A:1716:U:H2'	1:A:1717:A:H8	1.85	0.41
6:F:140:ILE:HG22	6:F:142:TYR:H	1.85	0.41
11:K:21:CYS:HA	11:K:41:ILE:HG22	2.02	0.41
12:L:95:LEU:HD22	12:L:100:ILE:HD11	2.03	0.41
13:M:50:ARG:HD3	13:M:65:ILE:HD11	2.02	0.41
21:U:28:LEU:HD12	21:U:32:LYS:HB2	2.01	0.41
1:A:1309:G:H2'	1:A:1310:G:C8	4.07	0.41
1:A:2036:C:H2'	1:A:2037:A:C8	2.56	0.41
1:A:2581:G:N2	1:A:2581:G:OP2	2.38	0.41
1:A:2836:U:H2'	1:A:2837:A:H8	1.86	0.41
1:A:4:U:H2'	1:A:5:A:C8	2.55	0.41
3:C:74:PRO:HB3	3:C:114:GLN:HE21	1.85	0.41
1:A:851:C:O2'	26:Z:42:ALA:O	2.38	0.41
1:A:1327:A:H3'	1:A:1328:A:H8	1.85	0.41
1:A:1433:A:H2'	1:A:1434:A:H8	1.86	0.41
1:A:2279:G:O2'	1:A:2327:A:O2'	2.30	0.41
1:A:2511:U:H1'	4:D:130:GLN:HE21	1.86	0.41
1:A:406:G:H2'	1:A:407:G:H8	1.84	0.41
1:A:578:G:OP1	1:A:1255:U:O2'	2.38	0.41
1:A:626:A:N3	12:L:78:ARG:NH2	2.66	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.56	0.41
1:A:854:C:H2'	1:A:855:G:H8	1.85	0.41
9:I:56:VAL:HG22	9:I:68:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:31:ILE:HG13	30:3:31:ILE:H	1.49	0.41
1:A:1297:C:H2'	1:A:1298:C:C6	2.55	0.41
1:A:1433:A:H2'	1:A:1434:A:C8	2.55	0.41
1:A:1592:C:H2'	1:A:1593:A:H8	1.85	0.41
1:A:1744:A:H3'	1:A:1745:A:H8	1.86	0.41
1:A:2291:U:O2	1:A:2374:C:O2'	2.36	0.41
1:A:987:C:O2'	1:A:1000:A:N3	2.47	0.41
1:A:1837:C:O2'	1:A:1927:A:N3	2.42	0.41
11:K:103:VAL:HG21	11:K:116:ILE:HG22	2.01	0.41
27:0:39:ARG:O	27:0:41:HIS:ND1	2.54	0.41
1:A:1826:G:O2'	1:A:1971:U:OP2	2.35	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.98	0.41
1:A:1969:A:O2'	1:A:1972:G:N3	2.40	0.41
1:A:2380:C:H2'	1:A:2381:A:C8	2.56	0.41
1:A:974:G:H1'	1:A:975:A:C8	2.56	0.41
16:P:29:VAL:HG22	16:P:80:VAL:HG12	2.02	0.41
20:T:37:ASP:N	20:T:37:ASP:OD1	2.53	0.41
1:A:1355:G:H2'	1:A:1356:G:C8	2.80	0.41
1:A:1745:A:H2'	1:A:1746:A:H8	1.86	0.41
1:A:1921:G:H2'	1:A:1922:G:H8	1.85	0.41
1:A:2120:G:H2'	1:A:2121:G:C8	2.56	0.41
1:A:492:A:H2	19:S:7:HIS:HE1	1.68	0.41
6:F:48:LEU:HD11	6:F:149:ARG:HH12	1.86	0.41
13:M:58:LYS:HB3	13:M:59:ARG:H	1.72	0.41
1:A:1653:G:H5''	14:N:2:ARG:HG2	2.03	0.41
1:A:1190:G:H2'	1:A:1191:G:H8	1.86	0.40
1:A:1649:G:H2'	1:A:1650:A:H8	1.86	0.40
1:A:410:G:H21	1:A:432:A:H62	42.27	0.40
1:A:705:A:H2'	1:A:706:A:H8	1.85	0.40
1:A:81:G:O2'	1:A:295:G:O2'	2.39	0.40
1:A:832:U:H2'	1:A:833:A:C8	2.55	0.40
18:R:6:GLN:HE21	18:R:11:GLN:NE2	2.18	0.40
14:N:118:ARG:NH2	27:0:54:ILE:O	2.54	0.40
1:A:813:U:HO2'	1:A:1225:G:HO2'	1.50	0.40
1:A:1834:U:H5''	1:A:1835:G:H5'	2.03	0.40
1:A:1326:U:H5'	1:A:2010:G:H21	1.86	0.40
1:A:2087:G:H2'	1:A:2088:A:C8	2.55	0.40
1:A:2140:G:H2'	1:A:2141:G:H8	1.85	0.40
1:A:2334:U:O2	15:O:13:ARG:NH1	2.45	0.40
1:A:2559:C:H2'	1:A:2560:A:H8	1.86	0.40
1:A:1940:U:OP1	1:A:2603:G:N2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:G:H2'	1:A:262:A:H8	1.85	0.40
1:A:2632:A:H2'	1:A:2633:G:C8	2.57	0.40
1:A:521:U:H2'	1:A:522:A:H8	1.85	0.40
1:A:948:C:H2'	1:A:949:G:C8	2.57	0.40
1:A:2630:G:H2'	1:A:2631:G:H8	1.85	0.40
1:A:395:U:H2'	1:A:396:G:C8	2.56	0.40
1:A:414:C:H2'	1:A:415:A:C8	2.56	0.40
1:A:690:G:H4'	3:C:216:ARG:HH22	1.85	0.40
1:A:6:A:H2'	1:A:7:G:C8	2.56	0.40
3:C:52:HIS:CE1	3:C:218:THR:HA	2.56	0.40
8:H:12:LEU:HD13	8:H:19:VAL:HB	2.03	0.40
17:Q:109:VAL:HG12	17:Q:113:LYS:HE2	2.02	0.40
20:T:22:THR:HA	20:T:25:GLU:HG2	2.02	0.40
28:1:10:LEU:HB3	28:1:48:TYR:HB3	2.02	0.40
28:1:36:LYS:HG3	28:1:47:ILE:HG13	2.03	0.40
1:A:126:A:H61	29:2:42:LEU:HD23	1.87	0.40
1:A:1636:U:H2'	1:A:1637:A:C8	2.56	0.40
1:A:166:U:H2'	1:A:167:A:H8	2.16	0.40
1:A:1997:C:H2'	1:A:1998:A:C8	2.57	0.40
1:A:1999:C:O2	1:A:2687:U:O2'	2.33	0.40
1:A:949:G:H2'	1:A:950:G:H8	1.86	0.40
21:U:20:LYS:HB3	21:U:38:ILE:HD12	2.03	0.40
1:A:2215:C:H2'	1:A:2216:G:C8	2.57	0.40
1:A:2675:A:H5''	11:K:31:ARG:HH11	1.86	0.40
1:A:2692:G:H2'	1:A:2693:G:C8	2.57	0.40
1:A:341:C:H2'	1:A:342:A:C8	2.57	0.40
1:A:596:U:H2'	1:A:597:G:H8	1.86	0.40
14:N:56:LYS:NZ	14:N:87:PHE:O	2.53	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%)	260 (97%)	9 (3%)	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%)	160 (91%)	15 (9%)	0	100	100
7	G	174/176 (99%)	161 (92%)	11 (6%)	2 (1%)	16	56
8	H	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
9	I	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
12	L	141/143 (99%)	124 (88%)	15 (11%)	2 (1%)	12	51
13	M	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	24	64
14	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
15	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	P	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	17	57
19	S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	19	59
20	T	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
21	U	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	17	57
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%)	73 (97%)	2 (3%)	0	100	100
25	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
26	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
28	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
29	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	55 (89%)	5 (8%)	2 (3%)	4	36
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
32	5	129/131 (98%)	104 (81%)	25 (19%)	0	100	100
35	b	216/218 (99%)	195 (90%)	20 (9%)	1 (0%)	31	71
36	c	204/206 (99%)	199 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	d	203/205 (99%)	181 (89%)	22 (11%)	0	100	100
38	e	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	13	53
39	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	8	45
40	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
41	h	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
42	i	125/127 (98%)	108 (86%)	16 (13%)	1 (1%)	21	62
43	j	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
44	k	114/116 (98%)	99 (87%)	15 (13%)	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%)	76 (88%)	10 (12%)	0	100	100
49	p	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
50	q	78/80 (98%)	67 (86%)	10 (13%)	1 (1%)	13	53
51	r	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
52	s	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
53	t	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
54	u	63/65 (97%)	49 (78%)	13 (21%)	1 (2%)	11	49
55	v	244/248 (98%)	221 (91%)	16 (7%)	7 (3%)	5	38
56	w	494/529 (93%)	435 (88%)	55 (11%)	4 (1%)	21	62
58	z	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
All	All	6533/6674 (98%)	5966 (91%)	537 (8%)	30 (0%)	35	71

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	46	ASP
13	M	58	LYS
30	3	31	ILE
50	q	69	THR
55	v	143	ARG
55	v	229	SER
55	v	258	GLN
55	v	261	ARG
55	v	329	LEU

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Mol	Chain	Res	Type
55	v	338	ASP
56	w	315	VAL
7	G	47	ASN
21	U	89	GLY
30	3	32	LEU
38	e	122	VAL
39	f	53	LYS
45	l	102	ASP
56	w	18	ILE
35	b	17	HIS
39	f	55	HIS
54	u	37	TYR
56	w	77	PHE
38	e	121	ASN
56	w	400	ARG
12	L	128	THR
19	S	64	ALA
42	i	90	ASP
55	v	218	ASN
12	L	31	GLY
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	90
4	D	164/164 (100%)	163 (99%)	1 (1%)	87	94
5	E	165/165 (100%)	164 (99%)	1 (1%)	87	94
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	137 (100%)	0	100	100
8	H	114/114 (100%)	114 (100%)	0	100	100
9	I	109/109 (100%)	109 (100%)	0	100	100
10	J	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	103/103 (100%)	103 (100%)	0	100	100
12	L	102/102 (100%)	102 (100%)	0	100	100
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	100/100 (100%)	99 (99%)	1 (1%)	78	89
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	99 (100%)	0	100	100
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	83 (99%)	1 (1%)	74	87
19	S	93/93 (100%)	92 (99%)	1 (1%)	76	88
20	T	80/80 (100%)	80 (100%)	0	100	100
21	U	83/83 (100%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/57 (100%)	56 (98%)	1 (2%)	62	83
24	X	67/67 (100%)	66 (98%)	1 (2%)	67	85
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/48 (100%)	48 (100%)	0	100	100
27	0	47/47 (100%)	47 (100%)	0	100	100
28	1	45/45 (100%)	45 (100%)	0	100	100
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	83
36	c	170/170 (100%)	170 (100%)	0	100	100
37	d	172/172 (100%)	170 (99%)	2 (1%)	74	87
38	e	114/119 (96%)	113 (99%)	1 (1%)	81	90
39	f	87/87 (100%)	87 (100%)	0	100	100
40	g	124/124 (100%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	423 (99%)	4 (1%)	81	90
58	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5406/5460 (99%)	5380 (100%)	26 (0%)	90	95

All (26) 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
37	d	177	MET
38	e	69	ASN
42	i	44	ARG
44	k	12	ARG
46	m	7	ASN

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Mol	Chain	Res	Type
50	q	61	ARG
55	v	222	LEU
55	v	261	ARG
55	v	316	ARG
56	w	71	THR
56	w	76	GLN
56	w	124	ARG
56	w	152	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
3	C	114	GLN
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
25	Y	58	ASN
28	1	18	HIS
32	5	4	ASN
35	b	23	ASN
35	b	35	ASN
37	d	115	GLN
38	e	69	ASN
38	e	88	HIS
38	e	134	ASN
39	f	58	HIS
41	h	3	GLN
41	h	75	GLN

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Mol	Chain	Res	Type
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	235	GLN
55	v	238	ASN
55	v	263	GLN
56	w	409	GLN
56	w	445	GLN
56	w	510	ASN
58	z	15	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	540 (18%)	34 (1%)
2	B	119/120 (99%)	14 (11%)	2 (1%)
33	7	6/7 (85%)	5 (83%)	1 (16%)
34	a	1538/1539 (99%)	223 (14%)	0
57	x	76/77 (98%)	35 (46%)	0
All	All	4632/4646 (99%)	817 (17%)	37 (0%)

All (817) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	46	G
1	A	49	A
1	A	51	G

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Mol	Chain	Res	Type
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	137	U
1	A	138	U
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
1	A	223	A
1	A	233	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A

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Mol	Chain	Res	Type
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	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
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	469	G
1	A	480	A
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

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Mol	Chain	Res	Type
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	613	A
1	A	614	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
1	A	714	U
1	A	726	G
1	A	729	G
1	A	730	A
1	A	745	G
1	A	746	U

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Mol	Chain	Res	Type
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	878	A
1	A	883	G
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	907	G
1	A	910	A
1	A	932	U

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Mol	Chain	Res	Type
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	990	A
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
1	A	1078	U
1	A	1079	C
1	A	1083	U

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Mol	Chain	Res	Type
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	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	1294	U
1	A	1300	G
1	A	1301	A
1	A	1315	C
1	A	1321	A
1	A	1325	U
1	A	1329	U
1	A	1330	C

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Mol	Chain	Res	Type
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
1	A	1610	A
1	A	1611	C
1	A	1634	A

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Mol	Chain	Res	Type
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	1848	A
1	A	1870	C
1	A	1871	A
1	A	1873	G
1	A	1893	C
1	A	1896	G

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Mol	Chain	Res	Type
1	A	1901	A
1	A	1913	A
1	A	1914	C
1	A	1917	U
1	A	1918	A
1	A	1925	C
1	A	1926	U
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
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	2004	G
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

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Mol	Chain	Res	Type
1	A	2068	U
1	A	2069	G
1	A	2072	C
1	A	2093	G
1	A	2096	C
1	A	2100	G
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	2195	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	2226	C
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

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Mol	Chain	Res	Type
1	A	2283	C
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	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2506	U

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Mol	Chain	Res	Type
1	A	2518	A
1	A	2520	C
1	A	2529	G
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	2574	G
1	A	2580	U
1	A	2582	G
1	A	2585	U
1	A	2586	U
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	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
1	A	2731	G
1	A	2733	A
1	A	2744	G
1	A	2748	A

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Mol	Chain	Res	Type
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
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
33	7	18	U

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Mol	Chain	Res	Type
33	7	20	U
33	7	21	A
33	7	22	A
33	7	23	A
34	a	7	A
34	a	8	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	85	U
34	a	87	C
34	a	95	C
34	a	121	U
34	a	130	A
34	a	173	U
34	a	174	A
34	a	177	G
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	214	C
34	a	215	C
34	a	226	G
34	a	240	G
34	a	247	G
34	a	251	G
34	a	266	G
34	a	267	C
34	a	269	C
34	a	279	A
34	a	280	C
34	a	281	G

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Mol	Chain	Res	Type
34	a	283	U
34	a	289	G
34	a	306	A
34	a	328	C
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	363	A
34	a	367	U
34	a	372	C
34	a	373	A
34	a	388	G
34	a	392	C
34	a	406	G
34	a	411	A
34	a	413	G
34	a	424	G
34	a	429	U
34	a	439	U
34	a	452	A
34	a	460	A
34	a	467	U
34	a	468	A
34	a	479	U
34	a	482	A
34	a	484	G
34	a	485	U
34	a	486	U
34	a	496	A
34	a	497	G
34	a	510	A
34	a	511	C
34	a	516	U
34	a	519	C
34	a	521	G
34	a	527	G
34	a	531	U
34	a	532	A
34	a	547	A

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Mol	Chain	Res	Type
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	687	A
34	a	688	G
34	a	701	U
34	a	703	G
34	a	713	G
34	a	718	A
34	a	719	C
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	755	G
34	a	777	A
34	a	812	G
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	828	U
34	a	829	G
34	a	832	G
34	a	843	U
34	a	844	G
34	a	846	G
34	a	871	U
34	a	872	A
34	a	876	C

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Mol	Chain	Res	Type
34	a	889	A
34	a	890	G
34	a	902	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	1014	A
34	a	1022	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	1065	U
34	a	1085	U
34	a	1094	G
34	a	1101	A
34	a	1108	G
34	a	1127	G
34	a	1130	A
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1140	C
34	a	1152	A
34	a	1158	C
34	a	1159	U
34	a	1168	U

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Mol	Chain	Res	Type
34	a	1181	G
34	a	1183	U
34	a	1184	G
34	a	1191	A
34	a	1196	A
34	a	1201	A
34	a	1202	U
34	a	1208	C
34	a	1212	U
34	a	1213	A
34	a	1225	A
34	a	1227	A
34	a	1236	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	1261	A
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1286	U
34	a	1287	A
34	a	1298	U
34	a	1300	G
34	a	1302	C
34	a	1317	C
34	a	1321	U
34	a	1323	G
34	a	1335	U
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	1396	A
34	a	1398	A

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Mol	Chain	Res	Type
34	a	1400	C
34	a	1401	G
34	a	1433	A
34	a	1446	A
34	a	1451	U
34	a	1452	C
34	a	1493	A
34	a	1494	G
34	a	1499	A
34	a	1519	A
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	2	G
57	x	3	C
57	x	4	G
57	x	8	U
57	x	9	G
57	x	11	A
57	x	15	G
57	x	16	C
57	x	17	C
57	x	18	U
57	x	19	G
57	x	20	G
57	x	21	U
57	x	22	A
57	x	23	G
57	x	24	C
57	x	25	U
57	x	27	G
57	x	28	U
57	x	42	C
57	x	45	A
57	x	46	G
57	x	47	A
57	x	49	C
57	x	55	U

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Mol	Chain	Res	Type
57	x	58	A
57	x	60	A
57	x	62	C
57	x	63	C
57	x	64	G
57	x	71	G
57	x	72	C
57	x	73	A
57	x	75	C
57	x	76	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	86	G
1	A	140	C
1	A	242	G
1	A	372	G
1	A	468	G
1	A	479	A
1	A	490	C
1	A	549	G
1	A	746	U
1	A	752	A
1	A	858	G
1	A	859	G
1	A	898	C
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	1378	A
1	A	1399	C
1	A	1432	G
1	A	1926	U
1	A	1930	G
1	A	1940	U
1	A	2194	U
1	A	2286	G

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Mol	Chain	Res	Type
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2566	A
1	A	2655	G
1	A	2808	G
2	B	66	A
2	B	88	C
33	7	18	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 [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
59	GCP	w	601	56	25,34,34	2.48	8 (32%)	31,54,54	1.75	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GCP	w	601	56	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	601	GCP	C4-N9	-7.34	1.38	1.47
59	w	601	GCP	C5-C6	-4.58	1.44	1.52
59	w	601	GCP	C8-N9	-3.19	1.37	1.46
59	w	601	GCP	C5-C4	-2.29	1.38	1.52
59	w	601	GCP	PB-O2B	-2.15	1.51	1.56
59	w	601	GCP	PG-O1G	2.51	1.55	1.50
59	w	601	GCP	C6-N1	3.08	1.38	1.33
59	w	601	GCP	PB-O3A	5.76	1.64	1.58

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	w	601	GCP	C5-C6-N1	-5.28	111.97	118.27
59	w	601	GCP	PA-O3A-PB	-2.38	124.69	132.42
59	w	601	GCP	O6-C6-C5	3.69	127.44	119.82
59	w	601	GCP	C4-C5-N7	6.08	110.52	102.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
55	v	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	891:G	O3'	892:A	P	9.09

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	884:U	O3'	885:C	P	7.63
1	A	1905:C	O3'	1906:G	P	3.75
1	A	2107:G	O3'	2108:A	P	3.38
1	A	2094:A	O3'	2095:A	P	3.36
1	v	288:GLN	C	289:ALA	N	2.14
1	v	257:CYS	C	258:GLN	N	1.69