



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 18, 2017 – 04:34 AM EDT

PDB ID : 5U4I
EMDB ID: : EMD-8505
Title : Structural Basis of Co-translational Quality Control by ArfA and RF2 Bound to Ribosome
Authors : Zeng, F.; Chen, Y.; Remis, J.; Shekhar, M.; Phillips, J.C.; Tajkhorshid, E.; Jin, H.
Deposited on : unknown
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

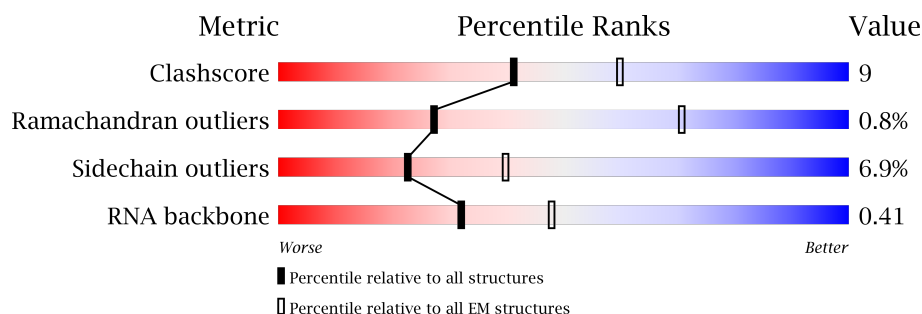
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.





















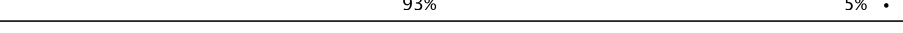






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	2904	40% 47% 13%
2	B	118	43% 47% 10%
3	C	273	78% 19% ..
4	D	209	83% 16% .
5	E	201	84% 15% .
6	F	179	82% 16% ..
7	G	177	86% 13% .
8	H	149	88% 11% .






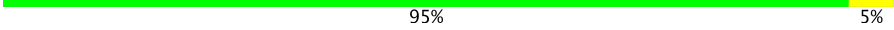


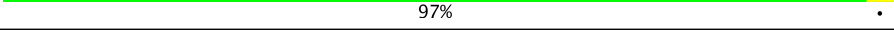
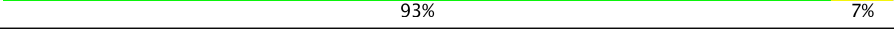

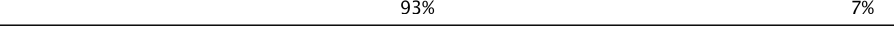

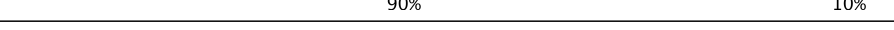



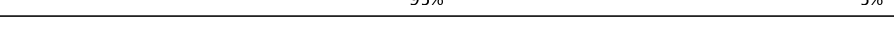



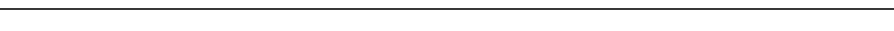


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Mol	Chain	Length	Quality of chain
9	J	142	 84% 14% ..
10	K	142	 92% 8% .
11	L	123	 80% 17% .
12	M	144	 83% 15% .
13	N	136	 85% 14% .
14	O	127	 73% 20% . 6%
15	P	117	 88% 11% .
16	Q	115	 89% 10% .
17	R	118	 80% 17% ..
18	S	103	 83% 15% ..
19	T	110	 79% 20% .
20	U	100	 83% 10% 7%
21	V	104	 79% 19% .
22	W	94	 82% 16% .
23	X	85	 75% 13% . 9%
24	Y	78	 76% 21% ..
25	Z	63	 87% 10% ..
26	0	59	 93% 5% .
27	1	57	 86% 11% ..
28	2	55	 73% 18% 9%
29	3	46	 89% 11%
30	4	65	 77% 22% .
31	5	38	 89% 11%
32	a	1533	 68% 32%
33	b	241	 87% 6% 7%

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Mol	Chain	Length	Quality of chain
34	c	233	
35	d	206	
36	e	167	
37	f	135	
38	g	179	
39	h	129	
40	i	130	
41	j	103	
42	k	117	
43	l	123	
44	m	118	
45	n	100	
46	o	88	
47	p	82	
48	q	84	
49	r	75	
50	s	82	
51	t	86	
52	u	71	
53	v	383	
54	w	57	
55	x	77	
55	y	77	
56	z	18	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	2504	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 149495 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2904	Total	C	N	O	P	0	0
			62351	27820	11472	20155	2904		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 42756

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- 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	J	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	K	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	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	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	T	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	U	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	V	102	Total	C	N	O	S	0	0
			779	492	146	141			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	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	X	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	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	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	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	1	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	2	50	Total	C	N	O		0	0
			409	263	75	71			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	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	4	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	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1533	Total	C	N	O	P	0	0
			32906	14683	6036	10654	1533		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	527	A	G	conflict	GB 817573384

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	204	Total	C	N	O	S	0	0
			1633	1020	313	296	4		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	65	Total	C	N	O	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	15	GLU	ALA	conflict	UNP P0A7T7

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 53 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	357	Total	C	N	O	S	0	0
			2836	1744	498	584	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 54 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	47	Total	C	N	O	S	0	0
			388	239	82	66	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

- Molecule 55 is a RNA chain called P-site or E-site fMet-tRNA(fMet).

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

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

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	B	4	Total	Mg	0
			4	4	
57	A	100	Total	Mg	0
			100	100	
57	a	20	Total	Mg	0
			20	20	

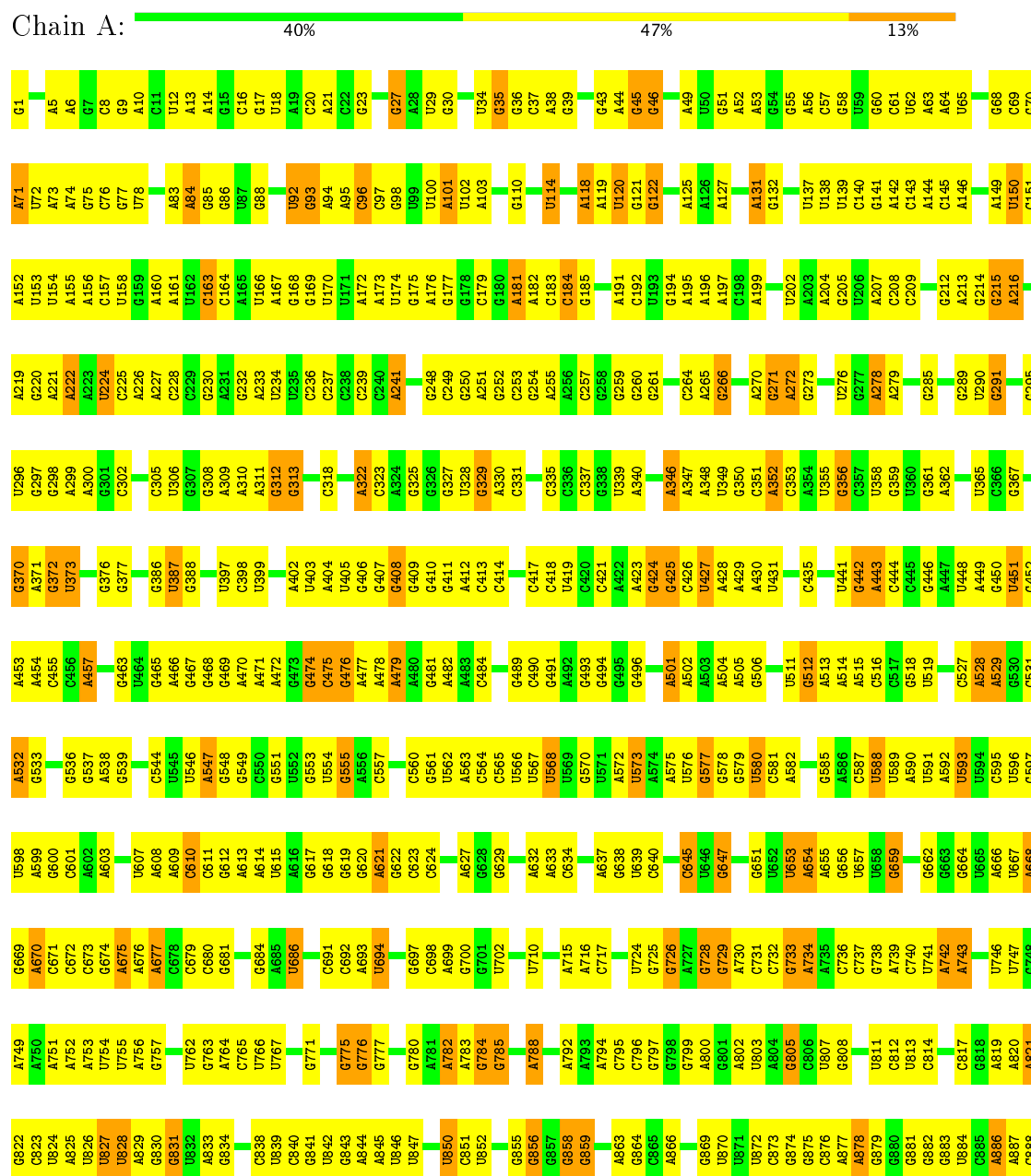
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	5	1	Total	Zn	0
			1	1	

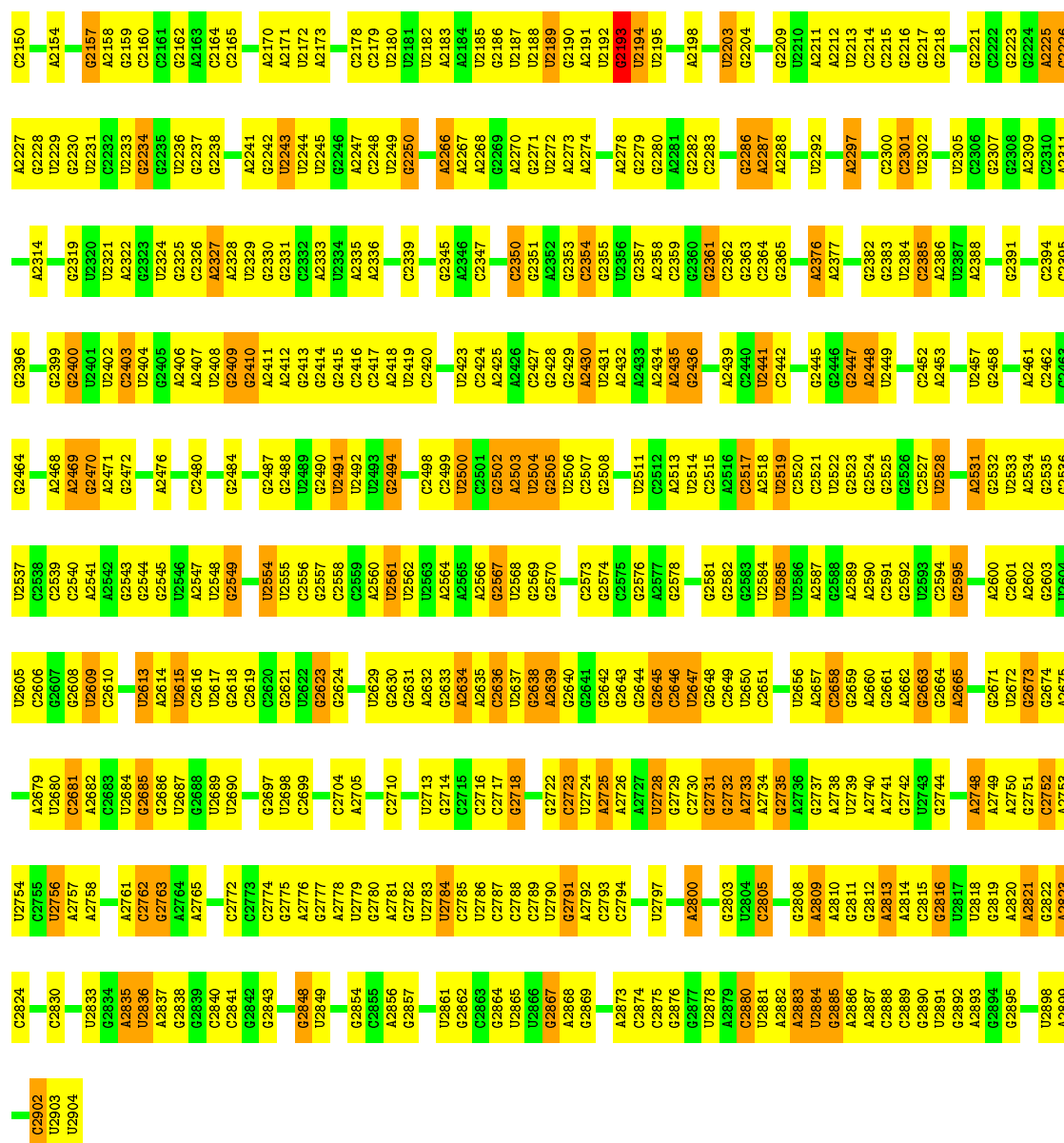
3 Residue-property plots

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.

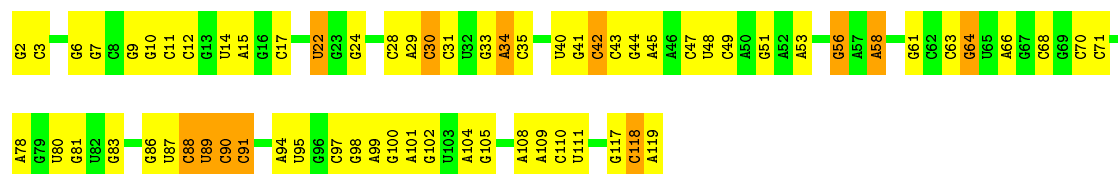
• Molecule 1: 23S rRNA



U2074	U2007	G1830	C1748	G1675	G1500	A1431	A1354	A1269	U1181	G1115	C1043	A972	C889
U2075	C2008	G1831	A1749	A1676	G1492	G1432	G1355	C1270	G1182	G1116	C1044	A973	C890
U2076	A2009	C1832	G1750	A1677	A1501	A1433	G1356	G1271	U1183	C1117	A1046	6974	6891
		C1833	U1751	A1678	A1502	A1434	G1357	A1272			G1047		6892
C2078	G2012	G1834	C1752	A1679	A1503	G1435	G1358	U1273	G1186	U1119		6978	C893
U2079	A2013	G1835	G1753			G1436	G1359	A1274	G1187	G1120	A1050		6894
A2080		C1836		G1682	C1507	C1437	G1360	A1275	U1188	G1121	A1051	A983	6895
U2081	U2016		U1758	U1683	A1508	U1438	G1361	A1276	U1189	C1122	G1052	A984	A896
A2082	U2017	C1843	A1759		A1509		C1362	G1277	G1190	G1123	C1053		6897
G2083	C2018	C1844		U1687	G1510	U1442		G1278	G1195	G1124	A1054	6987	6904
C2084	A2019		C1764	U1688	G1511	U1443		G1279	G1125	A988	G1055	A983	A905
	A2020	A1847	A1773	A1689	U1512	G1444	G1368	G1280	U1199	A1126	G1056	6989	U906
U2086	U1939	A1848	C1774	A1690	U1513	G1445	G1369		G1200	A1127	A1057	A990	6907
C2087	U2022	G1849			G1514	C1446	G1370	A1284	U1201	G1128	U1058		
	C2023	U1850		G1695	A1515	C1447	G1371	A1285	G1288	A1129	G1059	C991	A910
U2092	G2024	U1851	U1778	A1696	A1516	G1448			A1205	U1130	U1060	C992	A911
C2093	C2025	G1857	U1779	G1697	G1517	G1449	U1379	C1289	G1206	G1131	U1061	6994	6912
A2094	U2026	A1610		A1610	U1519	G1451	G1380	C1290		U1132	G1062	C995	6913
A2095	C2027	G1613	U1700		U1520	G1452			G1210	A1133		A996	G914
	U2028	U1858	A1701		A1521	A1453	A1383	C1293	G1211	A1134	U1065	6997	C915
U2099	G2029	G1860	A1783		U1522	G1454	A1384	U1294	G1212	G1135	U1066	C998	6916
G2100	A2030	G1861	A1785	C1708	U1523	G1455	A1385			G1136	A1067	U999	6917
A2101	A2031	G1862	U1786	U1709		G1456	G1386		G1216	G1137	G1068	A1000	A918
G2102	G2032	G1863	A1787	G1710		G1457	A1387	C1298	U1217	G1138	A1069	A1001	U919
	A2033	G1864	G1788	A1711	C1531	U1458	G1388	G1299	G1218	G1139	A1070	G1002	
	C2034	U1865	A1789	U1712	A1532	U1459			U1219	U1140	C1071	G1003	6926
	G2035	A1866	C1790	A1713	C1533	U1460	U1390	A1301	G1220	U1141	C1072	A927	A928
	C2036	G1964		U1714	U1534	C1461	U1391	A1302		A1142	G1073	C1006	
U2110	A2037	G1965		G1715	A1535	G1462	U1394	C1306	G1223	A1143	G1074	C1007	U931
G2112	G2038	G1967	U1716	G1716	C1536	G1463	U1395		U1224	A1144	C1075	A1008	U932
U2113	U2039	A1871	G1717		G1537	G1464	A1395	G1311	G1225		A1076	A1009	6933
A2114	G2040	G1872	U1718	G1642	U1539	G1465	U1396	U1312	A1226	G1149	A1077	G1010	6934
G2115	U2041	U1873	G1719	G1643		U1466	U1397	U1313	G1227	C1150	U1078	G1011	U934
G2116	A2042	G1874	U1720	C1644	A1548	U1467	C1398	G1314		A1151	G1079	U1012	C935
A2117	G2043	G1875	G1721	G1645		U1468	C1399	C1315	G1236	C1152	A1080	C1013	
C2044	G1973	A1876	A1722	C1646	A1549	U1468			A1237	G1153			A941
U2118	C2045	G1877	G1723	U1647	C1550		A1403	U1316	G1238	G1154	U1083	G1017	C942
	G2046	A1801	G1724	U1648	G1555	G1471	C1404	U1317	G1239	A1155	A1084	U1018	A943
		A1802		G1649		G1472	U1405	U1318	U1240	A1156	A1085	U1019	
		G1803	U1725		C1558	U1473	U1406	C1319		U1159	G1087	A1021	A947
	G2049	C1804	C1726			U1474	G1408	A1321	C1243	G1160	A1088	G1022	C948
	A2051	A1805		U1652	G1558	U1475	U1409		C1245	C1161	A1089	U1023	
	A2052	C1806	G1730	G1653	A1566	U1476		U1326	G1246	G1162	A1090	G1024	6953
		G1807	G1731	A1654	G1567	A1477	G1416	A1327	A1247	G1163	A1096	G1026	C957
		A1808	C1732	A1655	C1568	G1478	C1417	A1328	G1248	G1164	U1097	A1027	U958
			G1733	C1656	A1569		G1418	U1329	U1249	A1165	A1098	A1028	A959
		G1811	U1729	U1657	A1570	G1482						A1029	A960
		U1812	G1735	G1658	A1571		A1419					C1030	C961
		G1813	A1736	G1660	C1575	U1486	A1420	G1338	G1252	G1170	U1101		
		A1814	G1737	G1661		U1487	G1421		A1253	G1171	C1102	6962	
		C1815			U1578	C1488	G1422	G1341	A1254	C1172		U1033	6963
		U1816	G1738	U1662	A1579	C1489	G1423	A1342	U1255	U1173	U1105	G1034	C964
		G1817	A1739	G1663	A1580	G1491	G1424	U1343	G1256	U1174	G1106	U1035	C965
		U1818	G1740	A1664	G1581	G1492	G1425	U1344		A1175		G1036	
		A1819	C1741	A1665	G1582	C1493	G1426	C1345	U1263	U1176	C1109	G1037	6968
		U1820	U1742	G1666	G1583	A1494	A1427		A1264	G1177	A1038	G1037	6969
		A1821	G1743	G1667	A1584	A1495	C1428	U1352	G1178	C1179	A1111	A1039	
		C1822	A1744	A1668	U1586		G1430		G1266	U1180	G1112		6971
			A1745	A1669									
		G1828	A1746	G1674									
		A1829	U1747										



Chain B:



• Molecule 3: 50S ribosomal protein L2

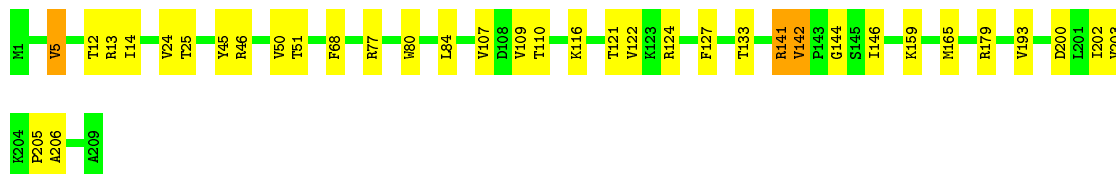
Chain C:





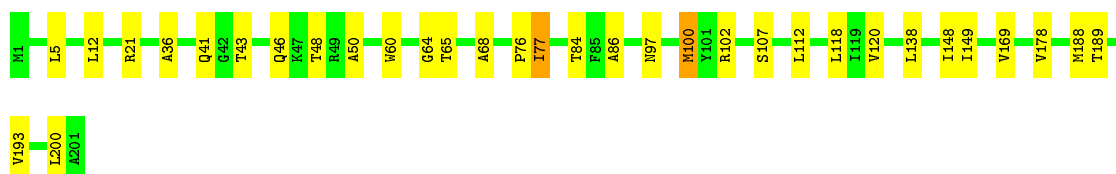
• Molecule 4: 50S ribosomal protein L3

Chain D: 83% 16% .



• Molecule 5: 50S ribosomal protein L4

Chain E: 84% 15% .



• Molecule 6: 50S ribosomal protein L5

Chain F: 82% 16% ..



• Molecule 7: 50S ribosomal protein L6

Chain G: 86% 13% .



• Molecule 8: 50S ribosomal protein L9

Chain H: 88% 11% .



• Molecule 9: 50S ribosomal protein L11

Chain J: 84% 14% ..



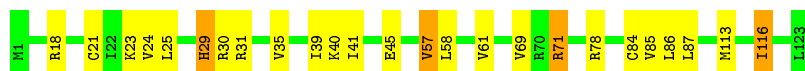
- Molecule 10: 50S ribosomal protein L13

Chain K:  92% 8% .




- Molecule 11: 50S ribosomal protein L14

Chain L:  80% 17% .




- Molecule 12: 50S ribosomal protein L15

Chain M:  83% 15% .



- Molecule 13: 50S ribosomal protein L16

Chain N:  85% 14% .




- Molecule 14: 50S ribosomal protein L17

Chain O:  73% 20% 6% .




- Molecule 15: 50S ribosomal protein L18

Chain P:  88% 11% .




- Molecule 16: 50S ribosomal protein L19

Chain Q:  89% 10% .




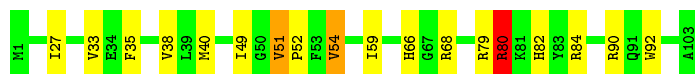
- Molecule 17: 50S ribosomal protein L20

Chain R:  80% 17% ..




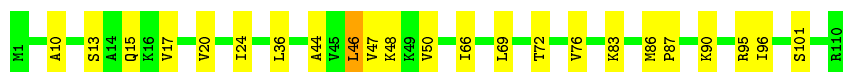
- Molecule 18: 50S ribosomal protein L21

Chain S:  83% 15% ..




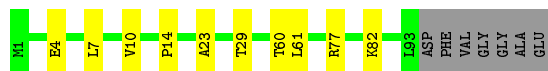
- Molecule 19: 50S ribosomal protein L22

Chain T:  79% 20% .




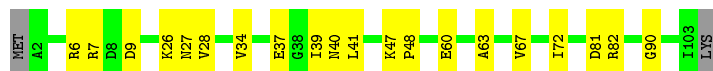
- Molecule 20: 50S ribosomal protein L23

Chain U:  83% 10% 7%




- Molecule 21: 50S ribosomal protein L24

Chain V:  79% 19% .



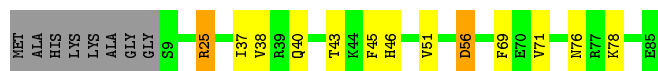
- Molecule 22: 50S ribosomal protein L25

Chain W:  82% 16% .



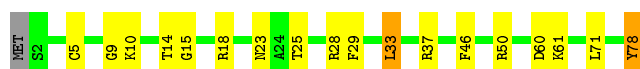
- Molecule 23: 50S ribosomal protein L27

Chain X:  75% 13% . 9%



- Molecule 24: 50S ribosomal protein L28

Chain Y:  76% 21% ..



- Molecule 25: 50S ribosomal protein L29

Chain Z: 87% 10% . .



- Molecule 26: 50S ribosomal protein L30

Chain 0: 93% 5% .



- Molecule 27: 50S ribosomal protein L32

Chain 1: 86% 11% . .



- Molecule 28: 50S ribosomal protein L33

Chain 2: 73% 18% 9%



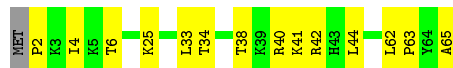
- Molecule 29: 50S ribosomal protein L34

Chain 3: 89% 11%



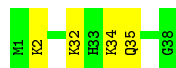
- Molecule 30: 50S ribosomal protein L35

Chain 4: 77% 22% .



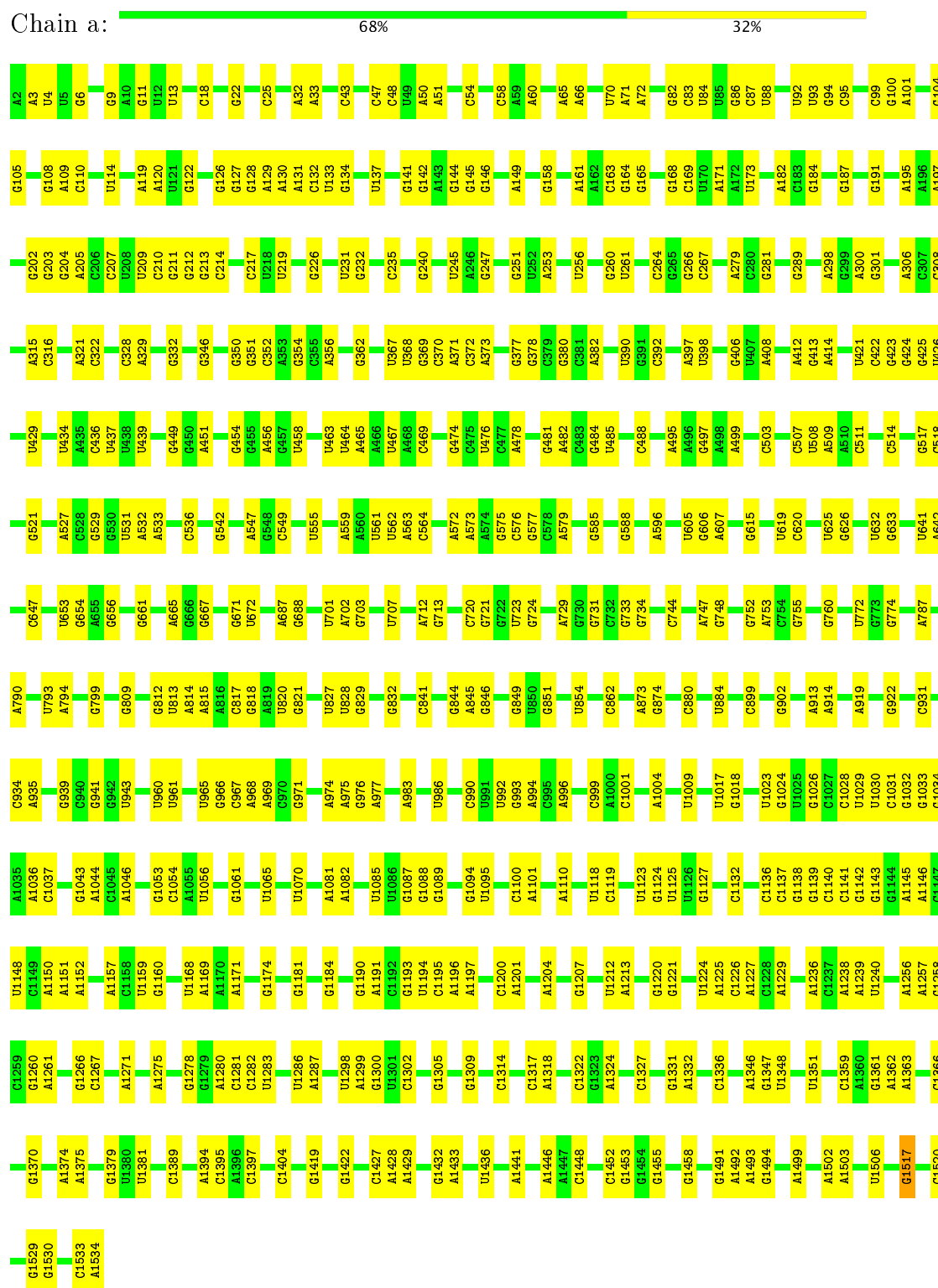
- Molecule 31: 50S ribosomal protein L36

Chain 5: 89% 11%



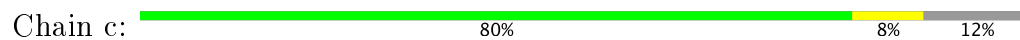
• Molecule 32: 16S rRNA

Chain a:





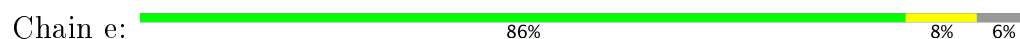
- Molecule 34: 30S ribosomal protein S3



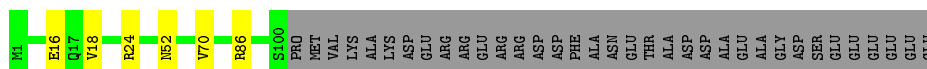
- Molecule 35: 30S ribosomal protein S4



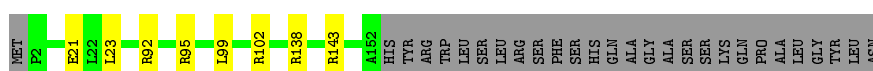
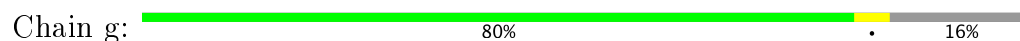
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9





- Molecule 41: 30S ribosomal protein S10

Chain j: 83% 13% 5%



- Molecule 42: 30S ribosomal protein S11

Chain k: 97% .



- Molecule 43: 30S ribosomal protein S12

Chain l: 93% 7%



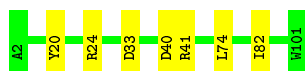
- Molecule 44: 30S ribosomal protein S13

Chain m: 91% 5% . .



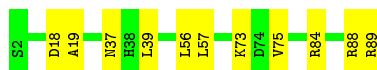
- Molecule 45: 30S ribosomal protein S14

Chain n: 93% 7%



- Molecule 46: 30S ribosomal protein S15

Chain o: 88% 13%




- Molecule 47: 30S ribosomal protein S16

Chain p: 90% 10%




- Molecule 48: 30S ribosomal protein S17

Chain q:  87% 8% 5%




- Molecule 49: 30S ribosomal protein S18

Chain r:  81% 5% 13%



- Molecule 50: 30S ribosomal protein S19

Chain s:  90% 9% .



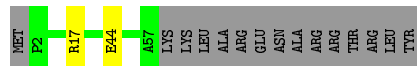
- Molecule 51: 30S ribosomal protein S20

Chain t:  95% 5%




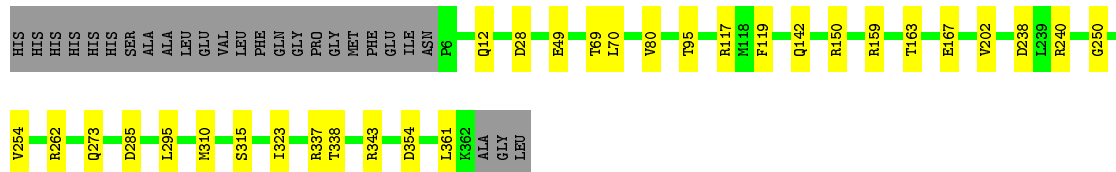
- Molecule 52: 30S ribosomal protein S21

Chain u:  76% . 21%



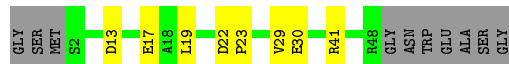
- Molecule 53: Peptide chain release factor 2

Chain v:  85% 8% 7%

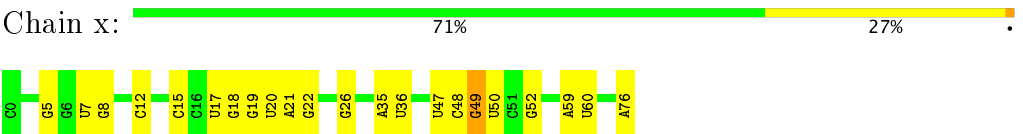


- Molecule 54: Alternative ribosome-rescue factor A

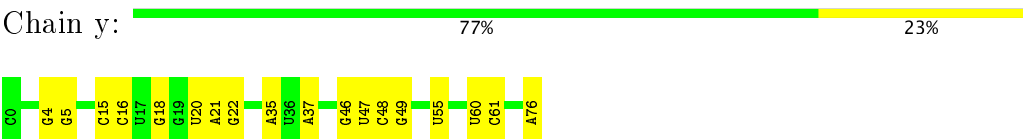
Chain w:  68% 14% 18%



• Molecule 55: P-site or E-site fMet-tRNA(fMet)



• Molecule 55: P-site or E-site fMet-tRNA(fMet)



• Molecule 56: mRNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (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: 5MU, OMC, ZN, OMG, OMU, MA6, MG, MEQ, 2MG, 5MC, UR3, 4OC, 1MG, PSU

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	0.23	0/69434	0.65	2/108325 (0.0%)
10	K	0.37	0/1152	0.65	0/1551
11	L	0.35	0/955	0.62	0/1279
12	M	0.37	0/1062	0.64	0/1413
13	N	0.39	0/1093	0.66	0/1460
14	O	0.42	0/973	0.74	0/1301
15	P	0.36	0/902	0.67	0/1209
16	Q	0.37	0/929	0.64	0/1242
17	R	0.41	0/960	0.70	0/1278
18	S	0.39	0/829	0.62	0/1107
19	T	0.34	0/864	0.69	0/1156
2	B	0.23	0/2828	0.65	0/4410
20	U	0.36	0/744	0.67	0/994
21	V	0.40	0/787	0.61	0/1051
22	W	0.38	0/766	0.61	0/1025
23	X	0.38	0/595	0.62	0/787
24	Y	0.38	0/635	0.67	0/848
25	Z	0.33	0/502	0.69	1/667 (0.1%)
26	0	0.36	0/453	0.68	1/605 (0.2%)
27	1	0.36	0/450	0.64	0/599
28	2	0.40	0/416	0.57	0/554
29	3	0.41	0/380	0.73	0/498
3	C	0.36	0/2121	0.65	0/2852
30	4	0.36	0/513	0.67	0/676
31	5	0.33	0/303	0.62	0/397
32	a	0.23	0/36593	0.66	1/57081 (0.0%)
33	b	0.40	0/1784	0.62	0/2403
34	c	0.38	0/1651	0.66	0/2225
35	d	0.38	0/1655	0.68	0/2216
36	e	0.37	0/1169	0.65	0/1573
37	f	0.40	0/835	0.62	0/1128
38	g	0.38	0/1195	0.69	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	h	0.36	0/989	0.65	0/1326
4	D	0.38	0/1586	0.61	0/2134
40	i	0.39	0/1034	0.70	0/1375
41	j	0.37	0/796	0.70	0/1077
42	k	0.38	0/893	0.60	0/1205
43	l	0.35	0/969	0.66	0/1300
44	m	0.62	2/892 (0.2%)	0.84	1/1193 (0.1%)
45	n	0.38	0/817	0.69	0/1088
46	o	0.37	0/722	0.68	0/964
47	p	0.39	0/659	0.64	0/884
48	q	0.38	0/657	0.66	0/881
49	r	0.40	0/548	0.63	0/736
5	E	0.36	0/1571	0.66	0/2113
50	s	0.46	1/675 (0.1%)	0.69	1/908 (0.1%)
51	t	0.37	0/676	0.67	0/895
52	u	0.43	0/472	0.73	0/627
53	v	0.38	0/2865	0.65	0/3858
54	w	0.35	0/394	0.63	0/519
55	x	0.24	0/1832	0.68	1/2855 (0.0%)
55	y	0.23	0/1832	0.65	0/2855
56	z	0.21	0/147	0.62	0/227
6	F	0.41	0/1434	0.65	0/1926
7	G	0.41	0/1343	0.64	0/1816
8	H	0.38	0/1122	0.63	0/1515
9	J	0.40	0/1046	0.61	0/1410
All	All	0.29	3/161499 (0.0%)	0.66	8/241199 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	m	90	ARG	CZ-NH1	13.28	1.50	1.33
44	m	90	ARG	CD-NE	5.57	1.55	1.46
50	s	55	ARG	CZ-NH1	5.15	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	m	90	ARG	NE-CZ-NH2	-14.43	113.09	120.30
50	s	55	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	2193	G	C2'-C3'-O3'	6.96	124.83	113.70
55	x	49	G	C2'-C3'-O3'	6.73	124.47	113.70
32	a	1517	G	C2'-C3'-O3'	6.38	123.91	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1730	C	C2'-C3'-O3'	5.50	122.49	113.70
26	0	25	LEU	CA-CB-CG	5.35	127.61	115.30
25	Z	18	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

There are no planarity outliers.

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	62351	0	31373	1018	0
2	B	2529	0	1281	33	0
3	C	2082	0	2154	28	0
4	D	1565	0	1616	17	0
5	E	1552	0	1619	17	0
6	F	1410	0	1444	12	0
7	G	1323	0	1371	10	0
8	H	1111	0	1148	8	0
9	J	1032	0	1088	6	0
10	K	1129	0	1162	6	0
11	L	946	0	1023	13	0
12	M	1053	0	1129	12	0
13	N	1074	0	1157	10	0
14	O	960	0	1000	16	0
15	P	892	0	923	2	0
16	Q	917	0	962	4	0
17	R	947	0	1019	15	0
18	S	816	0	839	12	0
19	T	857	0	922	16	0
20	U	738	0	807	3	0
21	V	779	0	831	8	0
22	W	753	0	780	9	0
23	X	588	0	604	6	0
24	Y	625	0	652	9	0
25	Z	501	0	531	3	0
26	0	449	0	488	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	1	444	0	458	6	0
28	2	409	0	440	5	0
29	3	377	0	418	3	0
30	4	504	0	572	10	0
31	5	302	0	341	3	0
32	a	32906	0	16575	0	0
33	b	1753	0	1780	0	0
34	c	1624	0	1696	0	0
35	d	1633	0	1694	0	0
36	e	1156	0	1199	0	0
37	f	817	0	808	0	0
38	g	1181	0	1238	0	0
39	h	979	0	1031	0	0
40	i	1022	0	1070	0	0
41	j	786	0	828	0	0
42	k	877	0	887	0	0
43	l	955	0	1016	0	0
44	m	883	0	941	0	0
45	n	805	0	844	0	0
46	o	714	0	734	0	0
47	p	649	0	666	0	0
48	q	648	0	691	0	0
49	r	539	0	553	0	0
50	s	658	0	683	0	0
51	t	670	0	719	0	0
52	u	465	0	491	0	0
53	v	2836	0	2735	0	0
54	w	388	0	400	0	0
55	x	1640	0	837	0	0
55	y	1640	0	837	0	0
56	z	131	0	66	0	0
57	A	100	0	0	0	0
57	B	4	0	0	0	0
57	a	20	0	0	0	0
58	5	1	0	0	0	0
All	All	149495	0	101171	1250	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 9.

All (1250) 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:2244:U:N3	1:A:2435:A:N6	1.68	1.35
1:A:2013:A:N6	1:A:2613:U:H3	1.26	1.31
1:A:2067:G:O2'	1:A:2069:G:H8	1.16	1.28
1:A:2067:G:O2'	1:A:2069:G:C8	1.88	1.22
1:A:2500:U:O2	1:A:2504:PSU:N1	1.71	1.20
1:A:2013:A:N1	1:A:2613:U:O4	1.81	1.14
1:A:1248:G:H3'	1:A:1249:U:H5''	1.32	1.10
1:A:2244:U:N3	1:A:2435:A:C6	2.23	1.05
1:A:1596:A:H2'	1:A:1597:A:C8	1.93	1.04
1:A:2500:U:C2	1:A:2504:PSU:C2	2.49	1.01
1:A:465:G:H2'	1:A:466:A:C8	1.96	1.00
1:A:2500:U:O2	1:A:2504:PSU:C2	2.14	1.00
1:A:2244:U:C2	1:A:2435:A:N6	2.30	0.99
1:A:2244:U:C4	1:A:2435:A:N6	2.34	0.95
1:A:234:U:O4	1:A:430:A:N1	2.00	0.95
1:A:2068:U:O4	1:A:2430:A:C8	2.19	0.95
1:A:1802:A:H2'	1:A:1803:A:C8	2.01	0.95
1:A:2068:U:N3	1:A:2430:A:N7	2.15	0.94
1:A:814:C:H1'	1:A:1225:G:H21	1.30	0.93
1:A:827:U:H2'	1:A:2068:U:C2	2.03	0.93
1:A:2500:U:C2	1:A:2504:PSU:N1	2.36	0.93
1:A:2074:U:H3	1:A:2435:A:H2	1.16	0.92
1:A:1255:U:OP2	1:A:2502:G:N2	2.02	0.92
1:A:172:A:H2'	1:A:173:A:C8	2.05	0.92
1:A:2500:U:O2	1:A:2504:PSU:C6	2.24	0.91
1:A:2748:A:H5'	1:A:2753:A:H61	1.33	0.91
1:A:653:U:H3'	1:A:654:A:H5''	1.52	0.91
1:A:2060:A:O4'	1:A:2502:G:H1'	1.71	0.90
1:A:234:U:H3	1:A:430:A:H61	1.13	0.90
1:A:2244:U:O2	1:A:2435:A:N7	2.06	0.88
1:A:2452:C:H42	1:A:2504:PSU:HN3	1.22	0.85
1:A:910:A:H2'	1:A:911:A:C8	2.12	0.84
1:A:1353:A:H2'	1:A:1354:A:C8	2.12	0.84
1:A:1300:G:H4'	1:A:1301:A:H5''	1.58	0.84
1:A:2756:U:C4	1:A:2758:A:N6	2.45	0.84
1:A:1394:U:H4'	1:A:1603:A:H4'	1.58	0.83
1:A:1405:U:H2'	1:A:1406:U:C6	2.14	0.83
1:A:2788:C:H2'	1:A:2789:C:C6	2.14	0.83
1:A:2646:C:H2'	1:A:2647:U:O4'	1.79	0.82
1:A:2036:C:H2'	1:A:2037:A:C8	2.14	0.82
1:A:94:A:H2'	1:A:95:A:C8	2.14	0.82
1:A:2756:U:N3	1:A:2758:A:C6	2.48	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:U:O2'	1:A:2502:G:O6	1.96	0.82
1:A:2452:C:H2'	1:A:2453:A:C8	2.15	0.82
1:A:1433:A:H2'	1:A:1434:A:C8	2.14	0.81
1:A:2036:C:H2'	1:A:2037:A:H8	1.46	0.81
1:A:1326:U:H2'	1:A:1327:A:C8	2.16	0.81
1:A:2500:U:N3	1:A:2504:PSU:O2	2.14	0.80
1:A:675:A:H2'	1:A:676:A:C8	2.17	0.80
8:H:47:PHE:HA	8:H:51:ARG:HB2	1.64	0.80
6:F:105:THR:O	6:F:109:PRO:HD2	1.81	0.80
1:A:2060:A:O4'	1:A:2502:G:C1'	2.30	0.80
1:A:2020:A:H5'	27:1:9:THR:HG23	1.64	0.79
1:A:927:A:H2'	1:A:928:A:C8	2.17	0.79
1:A:632:A:H2'	1:A:633:A:C8	2.18	0.78
1:A:1779:U:H5	1:A:1784:A:N7	1.82	0.78
1:A:532:A:H4'	1:A:533:G:C8	2.19	0.78
1:A:2752:C:H3'	1:A:2753:A:H8	1.49	0.78
1:A:2722:G:H2'	1:A:2723:C:C6	2.19	0.77
1:A:2557:G:H2'	1:A:2558:C:C6	2.19	0.77
1:A:827:U:H2'	1:A:2068:U:N3	2.00	0.77
1:A:2068:U:O4	1:A:2430:A:H8	1.67	0.77
1:A:1357:C:H2'	1:A:1358:G:O4'	1.85	0.76
1:A:2567:G:H2'	1:A:2568:U:C6	2.21	0.76
1:A:2117:A:H61	1:A:2170:A:H61	1.32	0.76
1:A:1862:G:O6	1:A:1880:U:O2	2.03	0.76
18:S:51:VAL:HB	18:S:52:PRO:HD2	1.66	0.75
1:A:581:C:H2'	1:A:582:A:C8	2.21	0.75
1:A:1270:C:H5''	1:A:1271:G:H5'	1.68	0.75
1:A:191:A:H2'	1:A:192:C:C6	2.22	0.75
1:A:2093:G:N7	1:A:2225:A:H2'	2.02	0.74
1:A:1432:G:H2'	1:A:1433:A:C8	2.22	0.74
1:A:886:A:H1'	1:A:889:C:H5	1.53	0.74
1:A:1028:A:H2'	1:A:1029:A:C8	2.22	0.74
1:A:2868:A:H2'	1:A:2869:G:C8	2.22	0.74
1:A:1248:G:H3'	1:A:1249:U:C5'	2.13	0.73
1:A:2532:G:O2'	1:A:2665:A:H1'	1.88	0.73
1:A:1548:A:H2'	1:A:1549:A:C8	2.23	0.73
1:A:2882:A:H3'	1:A:2883:A:H5''	1.71	0.73
1:A:2756:U:N3	1:A:2758:A:N6	2.36	0.73
1:A:2836:U:H2'	1:A:2837:A:C8	2.23	0.73
17:R:24:TYR:HB3	17:R:28:ARG:HB3	1.71	0.73
1:A:172:A:H2'	1:A:173:A:H8	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:C:H2'	1:A:797:G:C8	2.25	0.72
1:A:2086:U:H2'	1:A:2087:G:C8	2.24	0.72
1:A:2273:A:H2'	1:A:2274:A:C8	2.25	0.72
1:A:2006:C:H2'	1:A:2007:U:H6	1.54	0.72
1:A:814:C:H1'	1:A:1225:G:N2	2.04	0.71
22:W:20:LEU:O	22:W:20:LEU:HD22	3.69	0.71
1:A:2658:C:H2'	1:A:2659:G:O4'	1.90	0.71
9:J:105:LEU:HD13	9:J:129:GLU:HG2	1.73	0.71
1:A:1434:A:H2'	1:A:1435:G:C8	2.26	0.70
3:C:144:VAL:HB	3:C:154:LEU:HB2	1.72	0.70
1:A:1326:U:H2'	1:A:1327:A:H8	1.54	0.70
1:A:1648:U:H2'	1:A:1649:G:O4'	1.92	0.70
1:A:250:G:H2'	1:A:251:A:C8	2.27	0.70
1:A:2704:C:H2'	1:A:2705:A:O4'	1.92	0.70
1:A:827:U:C2'	1:A:2068:U:C2	2.75	0.69
1:A:2752:C:H3'	1:A:2753:A:C8	2.28	0.69
1:A:2300:C:H2'	1:A:2301:C:C6	2.27	0.69
1:A:2748:A:H5'	1:A:2753:A:N6	2.06	0.69
1:A:161:A:H2	1:A:2217:G:HO2'	1.39	0.69
1:A:2452:C:N4	1:A:2504:PSU:HN3	1.90	0.69
18:S:51:VAL:HB	18:S:52:PRO:CD	2.22	0.69
1:A:2241:A:H2'	1:A:2242:G:C8	2.28	0.68
1:A:851:C:H2'	1:A:852:U:C6	2.29	0.68
1:A:181:A:H2'	1:A:182:A:C8	2.28	0.68
1:A:158:U:H3	1:A:168:G:H1	1.41	0.68
1:A:2500:U:N3	1:A:2504:PSU:C2	2.62	0.68
3:C:84:ASP:HB2	3:C:91:ILE:HG12	1.76	0.68
1:A:2547:A:H2'	1:A:2548:U:C6	2.29	0.67
1:A:1863:G:H2'	1:A:1864:U:C6	2.28	0.67
1:A:327:G:H1	1:A:335:C:H42	1.41	0.67
1:A:2532:G:H2'	1:A:2533:U:C6	2.30	0.67
1:A:2698:U:H2'	1:A:2699:C:C6	2.30	0.67
1:A:2733:A:H3'	1:A:2734:A:H8	1.59	0.67
1:A:308:G:H2'	1:A:309:A:C8	2.30	0.67
1:A:576:U:O2'	1:A:2502:G:C6	2.47	0.67
1:A:2067:G:C2'	1:A:2069:G:C8	2.77	0.66
1:A:56:A:H2'	1:A:57:C:C6	2.29	0.66
1:A:191:A:H2'	1:A:192:C:H6	1.60	0.66
1:A:12:U:H2'	1:A:12:U:O2	1.95	0.66
1:A:1899:A:H4'	1:A:1901:A:H5''	1.77	0.66
1:A:1717:A:H2'	1:A:1718:G:O4'	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:C:H2'	1:A:999:U:O4'	1.95	0.66
1:A:1805:A:H2'	1:A:1806:C:C6	2.31	0.66
1:A:2006:C:H2'	1:A:2007:U:C6	2.31	0.66
1:A:234:U:H3	1:A:430:A:N6	1.92	0.66
1:A:715:A:H2'	1:A:716:A:C8	2.81	0.66
1:A:234:U:C4	1:A:430:A:N1	2.64	0.66
2:B:80:U:H2'	2:B:81:G:C8	2.31	0.66
1:A:1548:A:H2'	1:A:1549:A:H8	1.60	0.66
1:A:1802:A:H2'	1:A:1803:A:H8	1.57	0.66
1:A:2788:C:H2'	1:A:2789:C:H6	1.61	0.66
1:A:1043:C:H42	1:A:1112:G:H1	1.42	0.65
1:A:1736:U:H2'	1:A:1737:G:H8	1.61	0.65
1:A:2409:G:H2'	1:A:2410:G:O4'	1.97	0.65
2:B:80:U:H2'	2:B:81:G:H8	1.61	0.64
1:A:1709:U:H2'	1:A:1710:G:C8	2.32	0.64
1:A:2514:U:H2'	1:A:2515:C:C6	2.32	0.64
1:A:1570:A:H2'	1:A:1571:A:C8	2.32	0.64
1:A:538:A:H2'	1:A:539:G:O4'	1.97	0.64
7:G:9:VAL:HG23	7:G:69:ARG:HD2	1.78	0.64
1:A:1117:C:HO2'	1:A:1118:C:H6	1.44	0.64
1:A:570:G:H2'	1:A:2030:A:N7	2.13	0.64
1:A:2500:U:H2'	1:A:2504:PSU:HN1	1.61	0.64
1:A:2399:G:H1	1:A:2417:C:H42	1.46	0.64
3:C:240:PHE:O	3:C:242:LYS:N	2.31	0.64
1:A:537:G:H22	1:A:555:G:H2'	1.62	0.64
1:A:588:U:H2'	1:A:589:U:C6	2.32	0.64
1:A:84:A:H62	1:A:101:A:H8	1.44	0.64
5:E:97:ASN:HB2	5:E:100:MET:HB2	1.79	0.64
6:F:105:THR:O	6:F:109:PRO:CD	2.45	0.64
1:A:1201:U:H3	1:A:1244:A:H61	1.45	0.64
1:A:2880:C:H2'	1:A:2881:U:C6	2.31	0.63
8:H:132:PHE:H	8:H:140:ALA:HB3	1.63	0.63
18:S:79:ARG:HG2	18:S:80:ARG:HG3	1.78	0.63
1:A:2811:G:H1	1:A:2889:C:H42	1.47	0.63
1:A:161:A:H2	1:A:2217:G:O2'	1.81	0.63
1:A:2674:G:H4'	11:L:30:ARG:HG3	1.80	0.63
1:A:1434:A:H2'	1:A:1435:G:H8	1.62	0.62
1:A:2500:U:C2	1:A:2504:PSU:O2	2.49	0.62
1:A:2060:A:H5''	1:A:2502:G:O2'	1.99	0.62
1:A:840:C:H2'	1:A:841:G:H8	1.62	0.62
1:A:645:C:H2'	1:A:647:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:G:H2'	1:A:1188:U:H5	1.65	0.62
1:A:992:C:H42	1:A:1162:G:H1	1.47	0.62
1:A:1665:A:H2'	1:A:1666:G:O4'	2.00	0.62
1:A:2013:A:N1	1:A:2613:U:C4	2.66	0.62
1:A:290:U:H3	1:A:350:G:H1	1.47	0.62
1:A:224:U:H2'	1:A:225:C:C6	3.27	0.62
1:A:2079:U:H2'	1:A:2080:A:O4'	1.99	0.62
1:A:2074:U:O4	1:A:2435:A:N1	2.33	0.62
1:A:796:C:H2'	1:A:797:G:H8	1.64	0.61
1:A:253:C:H2'	1:A:254:G:O4'	1.99	0.61
1:A:1599:U:H2'	1:A:1600:C:C6	2.35	0.61
1:A:1476:U:H3	1:A:1515:A:H62	1.46	0.61
1:A:2327:A:H2'	1:A:2328:A:C8	2.36	0.61
1:A:57:C:H42	1:A:70:G:H1	1.49	0.61
1:A:850:U:H2'	1:A:851:C:C6	2.36	0.61
1:A:1284:A:H2'	1:A:1285:A:C8	2.35	0.61
2:B:90:C:H2'	2:B:91:C:O4'	2.00	0.61
3:C:137:VAL:HG21	3:C:167:ARG:HB2	1.83	0.61
1:A:589:U:H2'	1:A:590:A:H8	1.66	0.60
2:B:63:C:H2'	2:B:64:G:C8	2.35	0.60
1:A:1656:C:H2'	1:A:1657:U:C6	2.36	0.60
1:A:291:G:O6	1:A:349:U:O2	2.19	0.60
1:A:1783:A:N1	1:A:2587:A:H2'	2.16	0.60
1:A:2187:U:H2'	1:A:2188:U:C6	2.35	0.60
1:A:339:U:H2'	1:A:340:A:H8	1.67	0.60
1:A:743:A:O2'	1:A:1659:G:OP1	2.20	0.60
1:A:1865:U:H2'	1:A:1875:G:N2	2.16	0.60
1:A:1689:A:H2'	1:A:1690:A:C8	2.36	0.60
1:A:1076:C:H2'	1:A:1077:A:C8	2.36	0.60
1:A:1486:U:H3	1:A:1503:A:H61	1.48	0.60
1:A:1736:U:H2'	1:A:1737:G:C8	2.36	0.60
1:A:581:C:H2'	1:A:582:A:H8	1.67	0.60
1:A:978:G:H1	1:A:985:C:H42	1.48	0.60
4:D:116:LYS:HB2	4:D:165:MET:HB3	1.82	0.60
1:A:1361:G:H2'	1:A:1362:C:C6	2.37	0.60
6:F:126:GLY:HA2	6:F:163:ASP:HA	1.83	0.60
1:A:1744:A:H3'	1:A:1745:A:H8	1.67	0.59
1:A:2532:G:H2'	1:A:2533:U:H6	1.67	0.59
1:A:2836:U:H2'	1:A:2837:A:H8	1.65	0.59
1:A:305:C:H2'	1:A:306:U:C6	2.36	0.59
1:A:1592:C:H2'	1:A:1593:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1597:A:H4'	1:A:1598:A:H8	1.65	0.59
1:A:2547:A:H2'	1:A:2548:U:H6	1.67	0.59
1:A:1682:G:H2'	1:A:1683:U:C6	2.37	0.59
1:A:424:G:HO2'	1:A:425:G:H8	6.25	0.59
1:A:1795:C:H2'	1:A:1796:U:O4'	2.02	0.59
1:A:2013:A:N6	1:A:2613:U:N3	2.05	0.59
1:A:2100:G:H2'	1:A:2101:A:H5'	1.84	0.59
1:A:2244:U:C2	1:A:2435:A:C6	2.88	0.59
1:A:1746:A:H2'	1:A:1747:U:C6	2.38	0.59
1:A:2403:C:H42	1:A:2414:G:H1	1.49	0.59
1:A:2686:G:H2'	1:A:2687:U:O4'	2.01	0.59
1:A:2016:U:H2'	1:A:2017:U:C6	2.37	0.59
1:A:501:A:H2'	1:A:502:A:C8	2.37	0.59
1:A:589:U:H2'	1:A:590:A:C8	2.38	0.59
13:N:33:LEU:HD13	13:N:117:PHE:HB3	1.85	0.59
18:S:27:ILE:HD13	18:S:33:VAL:HG11	1.84	0.59
22:W:20:LEU:O	22:W:20:LEU:HD13	4.86	0.59
1:A:1038:G:H2'	1:A:1039:A:C8	2.38	0.58
1:A:1752:C:H2'	1:A:1753:G:C8	2.37	0.58
1:A:659:G:H1'	5:E:97:ASN:HD21	1.68	0.58
1:A:184:C:H2'	1:A:185:G:H8	1.68	0.58
1:A:241:A:N1	1:A:255:A:H5''	2.18	0.58
1:A:2403:C:H2'	1:A:2404:U:O4'	2.04	0.58
1:A:451:U:H2'	1:A:453:A:N7	2.18	0.58
1:A:753:A:H2'	1:A:754:U:C6	2.38	0.58
1:A:1423:G:H1	1:A:1575:C:H42	1.52	0.58
1:A:2394:C:H5''	12:M:63:LYS:HE2	1.85	0.58
22:W:72:VAL:HG12	22:W:93:ARG:HA	1.84	0.58
1:A:68:G:N2	1:A:152:A:H1'	41.59	0.58
1:A:1742:U:H2'	1:A:1743:G:C8	2.39	0.58
1:A:358:U:H2'	1:A:359:G:C8	2.71	0.58
1:A:418:C:H2'	1:A:419:U:O4'	2.04	0.58
1:A:754:U:H2'	1:A:755:U:C6	2.38	0.58
17:R:49:ASP:O	17:R:53:ARG:HB3	2.03	0.58
1:A:1821:A:H2'	1:A:1822:C:C6	2.38	0.58
1:A:1873:G:H2'	1:A:1874:C:C6	2.38	0.58
1:A:2837:A:H2'	1:A:2838:G:C8	2.39	0.58
1:A:1298:C:H42	1:A:1642:G:H1	1.52	0.58
1:A:2068:U:C4	1:A:2430:A:C8	2.91	0.58
1:A:917:A:H5''	1:A:2268:A:H61	1.68	0.58
1:A:325:G:H1	1:A:337:C:H42	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:G:H2'	1:A:36:G:O4'	2.04	0.58
2:B:45:A:H8	6:F:92:ARG:HD2	1.69	0.58
1:A:1115:G:O2'	1:A:1116:G:H5''	2.04	0.57
1:A:1172:C:H2'	1:A:1173:U:C6	5.08	0.57
1:A:44:A:H2'	1:A:45:G:O4'	2.04	0.57
1:A:532:A:H2'	1:A:532:A:N3	2.55	0.57
1:A:1019:U:H2'	1:A:1020:A:H8	1.68	0.57
1:A:1726:C:H42	1:A:1734:G:H1	1.50	0.57
1:A:2505:G:O6	1:A:2610:C:O2	2.23	0.57
1:A:1932:A:H2'	1:A:1933:G:O4'	2.04	0.57
1:A:2328:A:H2'	1:A:2329:U:C6	2.38	0.57
1:A:2697:G:H2'	1:A:2698:U:O4'	2.04	0.57
1:A:441:U:H2'	1:A:442:G:O4'	2.04	0.57
1:A:623:C:H2'	1:A:624:C:C6	2.48	0.57
1:A:184:C:H2'	1:A:185:G:C8	2.40	0.57
1:A:121:G:H4'	1:A:149:A:H5'	1.85	0.57
1:A:2192:U:H2'	1:A:2193:G:O4'	2.04	0.57
1:A:580:U:H2'	1:A:581:C:C6	2.39	0.57
1:A:629:G:H1	1:A:634:C:H42	1.52	0.57
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.86	0.57
19:T:46:LEU:O	19:T:50:VAL:HG23	2.05	0.57
1:A:443:A:H2'	1:A:443:A:N3	2.18	0.57
1:A:2061:G:H4'	1:A:2503:A:C2	2.40	0.57
1:A:289:G:H2'	1:A:290:U:C6	2.40	0.57
1:A:1473:G:H2'	1:A:1474:U:O4'	2.51	0.57
1:A:1269:A:H2'	1:A:1270:C:C6	2.40	0.57
1:A:1406:U:O4	1:A:1596:A:N1	2.37	0.57
1:A:739:A:H1'	1:A:740:C:H5	1.70	0.56
4:D:46:ARG:HB3	4:D:84:LEU:HB2	1.87	0.56
5:E:148:ILE:HB	5:E:169:VAL:HG22	1.85	0.56
1:A:1266:G:N2	1:A:1269:A:N7	8.89	0.56
1:A:2078:C:H2'	1:A:2079:U:C6	2.40	0.56
1:A:2068:U:C4	1:A:2430:A:N7	2.72	0.56
12:M:62:PRO:HG2	30:4:25:LYS:HB3	1.85	0.56
2:B:45:A:C8	6:F:92:ARG:HD2	2.41	0.56
1:A:1351:C:H2'	1:A:1352:U:C6	2.40	0.56
1:A:2647:U:H2'	1:A:2648:G:C8	2.41	0.56
1:A:17:G:H2'	1:A:18:U:C6	2.39	0.56
1:A:2783:U:H2'	1:A:2784:U:C6	2.40	0.56
1:A:1430:G:H2'	1:A:1431:A:O4'	2.06	0.56
1:A:2037:A:H2'	1:A:2038:G:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:A:H2'	1:A:821:A:C8	2.41	0.56
1:A:893:C:H2'	1:A:894:U:H4'	1.88	0.56
1:A:971:G:H2'	1:A:972:A:O4'	2.05	0.56
29:3:24:THR:HG23	29:3:27:GLY:H	1.69	0.56
1:A:2732:G:H5''	1:A:2733:A:O4'	2.05	0.56
1:A:45:G:H2'	1:A:46:G:C8	5.55	0.56
1:A:2791:G:H1	1:A:2805:C:H42	1.53	0.56
1:A:457:A:N1	1:A:470:A:H5''	2.21	0.56
1:A:621:A:C5	1:A:622:G:H1'	2.41	0.56
1:A:653:U:H3'	1:A:654:A:C5'	2.31	0.56
1:A:957:C:H5'	13:N:75:GLU:HG2	1.87	0.56
1:A:1009:A:H2'	1:A:1010:A:C8	2.41	0.56
1:A:2400:G:H4'	28:2:18:GLY:HA3	1.87	0.56
1:A:329:G:O4'	1:A:477:A:H1'	2.06	0.56
1:A:843:G:H2'	1:A:844:A:C8	2.41	0.56
1:A:1454:C:H5'	14:O:63:ARG:CZ	2.36	0.56
1:A:450:G:N2	1:A:482:A:N6	32.48	0.55
1:A:5:A:H2'	1:A:6:A:C8	2.40	0.55
1:A:150:U:H2'	1:A:151:C:C6	2.41	0.55
8:H:69:ALA:HA	8:H:72:ILE:HD12	1.87	0.55
1:A:1406:U:N3	1:A:1596:A:C2	2.74	0.55
22:W:31:TYR:HE1	22:W:90:ASP:HB3	1.71	0.55
1:A:1860:G:H2'	1:A:1861:G:C8	2.42	0.55
1:A:2674:G:H2'	1:A:2675:A:C8	2.42	0.55
1:A:1173:U:H2'	1:A:1174:U:H4'	1.89	0.55
1:A:2077:A:C6	1:A:2435:A:N6	2.74	0.55
1:A:1864:U:H4'	1:A:2410:G:O2'	2.07	0.55
1:A:1297:C:OP1	1:A:2710:C:H4'	2.07	0.55
1:A:443:A:N6	5:E:36:ALA:HB1	2.22	0.55
1:A:2675:A:H4'	11:L:29:HIS:HB3	1.89	0.55
29:3:12:ARG:HH21	29:3:44:VAL:HB	1.72	0.55
1:A:1002:G:H1	1:A:1153:C:H42	1.55	0.55
12:M:57:LEU:HD12	12:M:60:ARG:HH22	1.72	0.55
1:A:1160:G:O6	1:A:1182:G:N1	21.19	0.55
1:A:1186:G:H3'	1:A:1187:G:H8	1.72	0.55
1:A:1482:G:H1	1:A:1507:C:H42	1.55	0.55
1:A:1689:A:H2'	1:A:1690:A:H8	1.71	0.55
1:A:585:G:N7	17:R:6:ARG:NH1	2.55	0.55
1:A:840:C:H2'	1:A:841:G:C8	2.41	0.55
1:A:906:U:H4'	13:N:66:ARG:HH21	1.72	0.55
1:A:2044:C:H42	1:A:2624:G:H1	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2645:G:H3'	1:A:2646:C:C5'	2.37	0.55
1:A:2657:A:H61	1:A:2665:A:H3'	1.71	0.55
1:A:1026:G:H2'	1:A:1027:A:H8	1.72	0.54
1:A:1697:G:H4'	1:A:1978:A:H5''	1.89	0.54
1:A:964:C:O2'	1:A:2273:A:N3	2.39	0.54
1:A:2556:C:H2'	1:A:2557:G:O4'	2.06	0.54
1:A:2491:U:H5'	1:A:2570:G:H5''	1.88	0.54
1:A:2507:C:H2'	1:A:2508:G:O4'	2.07	0.54
1:A:2519:U:H2'	1:A:2541:A:H61	1.72	0.54
1:A:547:A:N3	1:A:547:A:H2'	2.22	0.54
1:A:576:U:H4'	1:A:2502:G:N7	2.22	0.54
1:A:577:G:H2'	1:A:578:G:C8	2.42	0.54
24:Y:5:CYS:HA	24:Y:33:LEU:HD21	1.89	0.54
1:A:564:C:OP2	18:S:79:ARG:HD3	2.06	0.54
10:K:37:ARG:HA	10:K:118:MET:HE2	1.90	0.54
11:L:113:MET:O	11:L:116:ILE:HG13	2.07	0.54
1:A:1123:C:H2'	1:A:1124:G:O4'	2.07	0.54
1:A:1246:A:H2'	1:A:1247:A:O4'	2.07	0.54
1:A:1280:G:H1	1:A:1290:C:H42	1.55	0.54
1:A:969:G:H2'	1:A:970:U:C6	2.42	0.54
1:A:71:A:H5''	1:A:72:U:H3'	1.89	0.54
1:A:825:A:H2'	1:A:826:U:C6	2.43	0.54
19:T:17:VAL:HB	19:T:76:VAL:HG11	1.89	0.54
1:A:2536:G:H2'	1:A:2537:U:O4'	2.06	0.54
1:A:2875:C:H2'	1:A:2876:G:C8	2.43	0.54
1:A:753:A:H2'	1:A:754:U:H6	1.71	0.54
1:A:1779:U:C5	1:A:1784:A:N7	2.72	0.54
1:A:2067:G:HO2'	1:A:2069:G:H8	0.56	0.54
8:H:84:ALA:HA	8:H:91:PHE:H	1.72	0.54
1:A:1285:A:N6	1:A:1355:G:H4'	63.66	0.54
1:A:160:A:H2'	1:A:161:A:O4'	2.83	0.54
1:A:1791:A:N6	1:A:1828:G:O2'	2.39	0.54
1:A:347:A:H2'	1:A:348:A:C8	2.43	0.54
1:A:8:C:H2'	1:A:9:G:O4'	2.08	0.54
1:A:1930:G:N2	1:A:1968:G:H2'	2.23	0.54
1:A:2728:U:O2'	1:A:2729:G:H8	1.91	0.54
1:A:1592:C:H2'	1:A:1593:A:H8	1.72	0.53
1:A:2050:C:H2'	1:A:2051:A:O4'	2.07	0.53
1:A:2447:G:C6	1:A:2504:PSU:O2	2.61	0.53
1:A:1279:G:N3	1:A:1279:G:H3'	4.67	0.53
1:A:2244:U:O2	1:A:2435:A:C5	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2671:G:H2'	1:A:2672:U:O4'	2.08	0.53
14:O:51:LEU:HD21	14:O:69:ARG:HG3	1.90	0.53
1:A:1276:A:H61	1:A:1294:U:H3	1.55	0.53
1:A:1811:G:H2'	1:A:1812:U:C6	2.44	0.53
1:A:514:A:H2'	1:A:515:A:C8	2.44	0.53
1:A:56:A:H2'	1:A:57:C:H6	1.72	0.53
1:A:639:U:H2'	1:A:640:C:C6	2.43	0.53
1:A:2522:U:O2'	1:A:2647:U:H5'	2.09	0.53
1:A:1877:A:H2'	1:A:1878:G:O4'	2.07	0.53
1:A:2740:A:C8	1:A:2763:G:N2	2.76	0.53
1:A:2882:A:C3'	1:A:2883:A:H5''	2.36	0.53
2:B:56:G:H1'	2:B:58:A:N6	2.23	0.53
1:A:1386:C:H2'	1:A:1387:A:H8	1.74	0.53
1:A:1593:A:H2'	1:A:1594:U:O4'	2.08	0.53
1:A:993:G:H5''	17:R:50:ARG:HD2	1.89	0.53
1:A:2092:U:H5''	8:H:24:GLY:HA3	1.89	0.53
13:N:69:PRO:HB2	13:N:92:TRP:HB3	1.89	0.53
1:A:489:G:H21	1:A:1320:C:H5''	1.73	0.53
1:A:1511:G:H2'	1:A:1512:C:C6	2.44	0.53
1:A:2273:A:H2'	1:A:2274:A:H8	1.72	0.53
1:A:669:G:H1	1:A:737:C:H42	64.92	0.53
1:A:1500:G:H2'	1:A:1501:G:C8	2.43	0.53
1:A:2417:C:H2'	1:A:2418:A:O4'	2.09	0.53
1:A:1434:A:H2'	1:A:1435:G:O4'	2.74	0.53
1:A:1071:G:H1'	1:A:1089:A:H2'	1.90	0.53
1:A:1130:U:C2	1:A:2025:C:H5''	2.43	0.53
1:A:1656:C:H2'	1:A:1657:U:H6	1.73	0.53
1:A:1712:U:H2'	1:A:1713:A:C8	2.44	0.53
1:A:2038:G:H2'	1:A:2039:U:O4'	2.09	0.53
1:A:2567:G:H2'	1:A:2568:U:H6	1.71	0.53
1:A:2733:A:H3'	1:A:2734:A:C8	2.43	0.53
1:A:863:A:H4'	2:B:100:G:N2	2.23	0.53
1:A:2062:A:C6	1:A:2503:A:N6	2.77	0.53
1:A:2781:A:H5''	1:A:2782:G:H5'	1.90	0.53
1:A:591:U:HO2'	30:4:2:PRO:N	2.07	0.53
1:A:947:A:H2'	1:A:948:C:C6	2.44	0.53
2:B:33:G:H2'	2:B:34:A:O4'	2.08	0.53
11:L:24:VAL:HA	11:L:39:ILE:HG22	1.90	0.53
11:L:58:LEU:HD11	11:L:86:LEU:HD23	1.91	0.53
1:A:2544:G:H2'	1:A:2545:G:C8	2.44	0.53
1:A:904:G:H2'	1:A:905:A:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:G:N2	1:A:478:A:H3'	2.25	0.52
1:A:597:G:H2'	1:A:598:U:O4'	2.46	0.52
14:O:49:GLU:HG2	14:O:94:TYR:HD2	1.74	0.52
1:A:2816:G:HO2'	1:A:2883:A:HO2'	1.57	0.52
1:A:942:G:H2'	1:A:943:A:O4'	2.10	0.52
2:B:89:U:O2	2:B:89:U:O4'	2.28	0.52
3:C:71:LYS:HB3	3:C:74:ILE:HD12	1.91	0.52
9:J:18:ASN:HB2	9:J:38:CYS:HB3	1.89	0.52
1:A:1675:C:H3'	1:A:1676:A:H8	1.74	0.52
1:A:424:G:O2'	1:A:425:G:H8	5.85	0.52
14:O:66:ALA:C	14:O:68:ALA:H	2.13	0.52
1:A:1301:A:O2'	1:A:1302:A:H3'	2.10	0.52
1:A:1406:U:H2'	1:A:1407:G:O4'	2.10	0.52
1:A:1834:U:H5''	1:A:1835:2MG:H5'	1.91	0.52
1:A:2074:U:H2'	1:A:2075:U:C6	2.44	0.52
1:A:2728:U:HO2'	1:A:2729:G:H8	1.56	0.52
1:A:377:G:H1	1:A:397:U:H3	1.56	0.52
1:A:560:C:H2'	1:A:561:G:O4'	2.09	0.52
19:T:24:ILE:HD13	19:T:36:LEU:HD11	1.91	0.52
1:A:1778:U:H3'	1:A:1784:A:N6	2.25	0.52
1:A:2531:A:H61	1:A:2662:A:H61	1.57	0.52
1:A:2717:C:H2'	1:A:2718:G:O4'	2.09	0.52
1:A:270:A:H2	1:A:370:G:H5'	1.74	0.52
10:K:17:VAL:HG23	10:K:137:PRO:HB2	1.91	0.52
1:A:2329:U:H2'	1:A:2330:G:C8	2.45	0.52
1:A:807:U:H2'	1:A:808:G:C8	2.45	0.52
1:A:1653:G:H3'	14:O:2:ARG:HG2	1.92	0.52
19:T:36:LEU:HD13	19:T:48:LYS:HA	1.92	0.52
1:A:181:A:H2'	1:A:182:A:H8	1.70	0.52
1:A:2026:U:H2'	1:A:2027:G:O4'	2.09	0.52
1:A:2233:U:H2'	1:A:2234:G:C8	2.44	0.52
2:B:22:U:H3	2:B:61:G:H1	1.57	0.52
2:B:97:C:H2'	2:B:98:G:O4'	2.10	0.52
12:M:109:LYS:HG2	12:M:126:ARG:HB2	1.92	0.52
1:A:1313:U:H2'	1:A:1314:C:C6	5.11	0.52
1:A:2548:U:H2'	1:A:2549:G:O4'	2.10	0.52
1:A:595:C:H42	1:A:662:G:H1	1.57	0.52
1:A:607:U:H2'	1:A:608:A:H8	1.75	0.52
1:A:833:A:H2'	1:A:834:G:C8	2.45	0.52
1:A:1126:A:H4'	1:A:1127:A:O5'	2.09	0.51
1:A:1:G:H1	1:A:2902:C:H42	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:G:H1	1:A:398:C:H42	1.56	0.51
1:A:875:G:C6	1:A:876:C:N4	2.78	0.51
1:A:155:A:H2	1:A:166:U:H3	19.88	0.51
1:A:2209:G:H1	1:A:2215:C:H42	1.59	0.51
1:A:272:A:H2'	1:A:273:G:C8	2.45	0.51
1:A:2730:C:H2'	1:A:2731:G:C8	2.45	0.51
1:A:450:G:N2	1:A:482:A:H62	31.94	0.51
1:A:985:C:H42	1:A:1220:G:H1	46.95	0.51
1:A:2082:A:H2'	1:A:2083:G:O4'	2.10	0.51
3:C:154:LEU:HD22	3:C:176:LEU:HD21	1.92	0.51
23:X:40:GLN:HE22	23:X:45:PHE:HB2	1.76	0.51
24:Y:5:CYS:HB3	24:Y:10:LYS:H	1.75	0.51
1:A:2002:G:O6	1:A:2003:A:N6	2.44	0.51
1:A:2134:A:N6	1:A:2157:G:H1'	2.25	0.51
7:G:145:ALA:HB1	7:G:164:TYR:HE1	1.75	0.51
1:A:1027:A:C2	1:A:2488:G:H5'	2.46	0.51
1:A:2071:A:H2'	1:A:2072:C:C6	2.46	0.51
1:A:46:G:O2'	1:A:365:U:H1'	53.68	0.51
1:A:579:G:H2'	1:A:580:U:C6	2.45	0.51
1:A:2314:A:H1'	6:F:155:THR:HG21	1.93	0.51
17:R:40:ILE:HD11	18:S:84:ARG:HE	1.76	0.51
1:A:29:U:H2'	1:A:30:G:O4'	2.09	0.51
8:H:94:ILE:HB	8:H:122:LEU:HD12	1.93	0.51
1:A:1370:C:H2'	1:A:1371:G:O4'	2.11	0.51
1:A:150:U:H2'	1:A:151:C:H6	1.75	0.51
1:A:2267:A:H5''	1:A:2268:A:H5'	1.93	0.51
1:A:2554:U:H2'	1:A:2555:U:C6	2.45	0.51
1:A:2821:A:H2'	1:A:2822:G:O4'	2.10	0.51
1:A:312:G:H2'	1:A:313:G:C8	2.46	0.51
1:A:827:U:O2'	1:A:2068:U:C2	2.64	0.51
1:A:1177:G:H2'	1:A:1178:C:O4'	2.11	0.51
1:A:1532:A:H61	1:A:1539:U:H3	1.58	0.51
1:A:1418:G:H21	1:A:1580:A:H62	1.58	0.51
1:A:77:G:H2'	1:A:78:U:C6	2.46	0.51
22:W:20:LEU:C	22:W:20:LEU:HD13	4.50	0.51
1:A:1798:U:H2'	1:A:1819:A:N6	2.26	0.51
1:A:2523:G:H1	1:A:2540:C:H42	1.59	0.51
1:A:417:C:H2'	1:A:418:C:C6	2.46	0.51
1:A:567:U:H2'	1:A:568:U:O4'	2.11	0.51
1:A:873:C:H2'	1:A:874:G:C8	2.45	0.51
1:A:1659:G:H2'	1:A:1660:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:C:O2'	1:A:839:U:H5''	2.11	0.50
1:A:1599:U:H2'	1:A:1600:C:H6	1.75	0.50
1:A:1687:G:H2'	1:A:1688:U:C6	2.47	0.50
1:A:226:A:H5'	1:A:257:C:H4'	1.93	0.50
1:A:339:U:H2'	1:A:340:A:C8	2.47	0.50
1:A:407:G:H2'	1:A:408:G:H8	1.75	0.50
1:A:1087:G:H2'	1:A:1087:G:N3	4.49	0.50
1:A:1677:A:H2'	1:A:1678:A:C8	2.47	0.50
1:A:259:G:H2'	1:A:260:G:O4'	2.77	0.50
1:A:266:G:H1	1:A:426:C:H42	1.60	0.50
1:A:855:G:H2'	1:A:856:G:O4'	2.12	0.50
1:A:878:A:H3'	1:A:879:G:H8	1.76	0.50
3:C:162:VAL:HG12	3:C:174:LEU:HD12	1.92	0.50
4:D:124:ARG:HD2	4:D:165:MET:HB2	1.94	0.50
1:A:1343:G:H1'	1:A:1597:A:C2	2.47	0.50
1:A:2077:A:C5	1:A:2435:A:C6	2.99	0.50
1:A:2241:A:H2'	1:A:2242:G:H8	1.74	0.50
1:A:57:C:H2'	1:A:58:G:O4'	2.11	0.50
1:A:784:G:H5'	1:A:785:G:OP1	2.12	0.50
21:V:28:VAL:HG12	21:V:34:VAL:HG12	1.92	0.50
1:A:2382:G:H21	30:4:42:ARG:NH1	2.10	0.50
1:A:194:G:H2'	1:A:195:A:O4'	2.11	0.50
1:A:2029:G:O6	1:A:2032:G:H5''	2.12	0.50
1:A:2623:G:H2'	1:A:2624:G:C8	2.46	0.50
1:A:1721:G:H21	1:A:1722:A:H62	1.59	0.50
1:A:2528:U:H5'	31:5:32:LYS:HE3	1.93	0.50
1:A:532:A:H4'	1:A:533:G:H8	1.74	0.50
1:A:579:G:H2'	1:A:580:U:H6	1.77	0.50
24:Y:33:LEU:HD23	24:Y:50:ARG:HG2	1.93	0.50
1:A:1090:A:H61	1:A:1101:U:H3	1.60	0.50
1:A:2266:A:H1'	1:A:2272:U:H3	1.77	0.50
1:A:236:C:H2'	1:A:237:C:C6	2.47	0.50
1:A:2560:A:H2'	1:A:2561:U:O4'	2.12	0.50
1:A:2590:A:H2'	1:A:2591:C:C6	2.45	0.50
1:A:84:A:H4'	1:A:85:G:O5'	2.11	0.50
1:A:2662:A:C5	1:A:2663:G:H1'	2.47	0.50
1:A:851:C:H2'	1:A:852:U:H6	1.77	0.50
16:Q:64:ILE:HA	16:Q:69:GLY:HA2	1.93	0.50
1:A:1054:A:H61	1:A:1105:U:H3	1.60	0.50
1:A:1277:G:H1	1:A:1293:C:H42	1.59	0.50
1:A:2385:C:H2'	1:A:2386:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:149:ILE:HB	5:E:188:MET:HG2	1.92	0.50
12:M:78:ARG:HG2	12:M:113:ALA:HB3	1.93	0.50
20:U:23:ALA:HB1	20:U:29:THR:HB	1.93	0.50
1:A:1000:A:H2'	1:A:1001:A:C8	2.47	0.49
1:A:1997:C:H2'	1:A:1998:A:H8	1.76	0.49
1:A:219:A:H2'	1:A:220:G:C8	2.47	0.49
1:A:2722:G:H2'	1:A:2723:C:H6	1.71	0.49
1:A:623:C:H2'	1:A:624:C:H6	1.87	0.49
12:M:110:VAL:HB	12:M:127:VAL:HG22	1.94	0.49
19:T:20:VAL:HG11	19:T:44:ALA:HA	1.93	0.49
1:A:927:A:H2'	1:A:928:A:H8	1.73	0.49
1:A:2217:G:H2'	1:A:2218:G:C8	2.46	0.49
1:A:2364:C:H2'	1:A:2365:G:O4'	2.11	0.49
1:A:270:A:H5'	1:A:271:G:H5''	1.94	0.49
1:A:327:G:H1	1:A:335:C:N4	2.10	0.49
1:A:673:C:H2'	1:A:674:G:O4'	2.11	0.49
2:B:70:C:H2'	2:B:71:C:C6	2.47	0.49
7:G:15:VAL:HG22	7:G:79:VAL:HG23	1.94	0.49
17:R:88:VAL:HG11	18:S:49:ILE:HD11	1.93	0.49
23:X:37:ILE:HG22	23:X:38:VAL:HG23	1.95	0.49
30:4:38:THR:HA	30:4:41:LYS:HE3	1.93	0.49
1:A:1922:G:H2'	1:A:1923:U:O4'	2.12	0.49
1:A:2301:C:H2'	1:A:2302:U:C6	2.47	0.49
1:A:697:G:H2'	1:A:698:C:O4'	2.12	0.49
1:A:95:A:H2'	1:A:96:C:O4'	2.12	0.49
6:F:108:VAL:HG12	6:F:109:PRO:HD3	1.95	0.49
8:H:69:ALA:O	8:H:72:ILE:HB	2.12	0.49
28:2:15:ALA:HB2	28:2:47:VAL:HG11	1.94	0.49
1:A:1176:U:H2'	1:A:1177:G:C8	2.47	0.49
1:A:1746:A:H2'	1:A:1747:U:H6	1.78	0.49
1:A:2660:A:H3'	1:A:2661:G:H8	1.77	0.49
2:B:110:C:H2'	2:B:111:U:O4'	2.12	0.49
2:B:51:G:H22	2:B:53:A:H62	1.59	0.49
1:A:1425:G:H2'	1:A:1426:G:C8	2.48	0.49
1:A:475:C:O2	1:A:479:A:N6	2.44	0.49
1:A:2025:C:H2'	1:A:2026:U:C6	2.48	0.49
1:A:962:G:H21	1:A:2250:G:H22	1.60	0.49
1:A:1255:U:C6	5:E:68:ALA:HA	2.47	0.49
1:A:2086:U:H2'	1:A:2087:G:H8	1.73	0.49
1:A:2684:U:H2'	1:A:2685:G:O4'	2.13	0.49
1:A:2814:A:H2'	1:A:2815:C:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:G:H3'	1:A:475:C:C5'	2.42	0.49
1:A:85:G:H1	1:A:97:C:H42	1.58	0.49
5:E:112:LEU:HB3	5:E:118:LEU:HB2	1.95	0.49
18:S:38:VAL:HG13	18:S:54:VAL:HG12	1.94	0.49
1:A:1243:C:H2'	1:A:1244:A:O4'	2.13	0.49
1:A:1964:G:H4'	1:A:1965:C:OP2	2.11	0.49
1:A:2642:G:H1	1:A:2772:C:H42	1.61	0.49
1:A:387:U:H4'	1:A:388:G:O4'	2.12	0.49
1:A:656:G:H2'	1:A:657:U:C6	2.48	0.49
1:A:77:G:H5'	25:Z:52:ARG:HG2	1.95	0.49
1:A:959:A:H2'	1:A:960:A:C8	2.47	0.49
7:G:88:GLN:HG3	7:G:163:ARG:HG3	1.95	0.49
1:A:1028:A:H2'	1:A:1029:A:H8	1.75	0.49
1:A:1030:C:H42	1:A:1124:G:H1	1.59	0.49
1:A:1398:C:H2'	1:A:1399:C:C6	2.47	0.49
1:A:155:A:H2'	1:A:156:A:C8	2.48	0.49
1:A:2052:A:H61	1:A:2617:U:H3	1.60	0.49
1:A:2748:A:H2'	1:A:2749:A:C8	2.48	0.49
2:B:10:G:H2'	2:B:11:C:O4'	2.13	0.49
1:A:1076:C:H2'	1:A:1077:A:H8	1.77	0.48
1:A:1361:G:H2'	1:A:1362:C:H6	1.75	0.48
1:A:1645:G:H5''	1:A:1646:C:H5'	1.95	0.48
1:A:2412:A:H2'	1:A:2413:G:O4'	2.13	0.48
1:A:2819:G:H2'	1:A:2821:A:N7	2.27	0.48
1:A:580:U:O3'	17:R:31:VAL:HG13	2.13	0.48
1:A:873:C:H2'	1:A:874:G:H8	1.78	0.48
2:B:63:C:H2'	2:B:64:G:H8	1.75	0.48
3:C:221:ARG:HE	3:C:221:ARG:HB2	1.41	0.48
11:L:35:VAL:HG22	11:L:69:VAL:HG11	1.94	0.48
1:A:1273:U:H4'	1:A:1275:A:OP2	2.13	0.48
1:A:2070:A:H2'	1:A:2071:A:O4'	2.14	0.48
1:A:736:C:H2'	1:A:737:C:H6	2.07	0.48
1:A:1138:G:H2'	1:A:1139:G:O4'	2.13	0.48
1:A:1201:U:H3	1:A:1244:A:N6	2.09	0.48
1:A:2395:C:H2'	1:A:2396:G:O4'	2.14	0.48
1:A:2672:U:H2'	1:A:2673:G:C8	2.48	0.48
2:B:6:G:H4'	2:B:28:C:H4'	1.95	0.48
12:M:47:ARG:HG2	12:M:50:PHE:HB2	1.93	0.48
1:A:1141:U:H4'	1:A:1142:A:O4'	2.12	0.48
1:A:1248:G:C3'	1:A:1249:U:H5''	2.24	0.48
1:A:1386:C:H2'	1:A:1387:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:U:H3'	2:B:88:C:H5'	1.95	0.48
3:C:167:ARG:HA	3:C:172:VAL:HG12	1.95	0.48
3:C:161:TYR:HB3	3:C:194:GLU:HG3	1.95	0.48
7:G:156:PRO:HB2	7:G:172:LYS:HG2	1.94	0.48
7:G:163:ARG:HH11	7:G:169:VAL:HB	1.78	0.48
17:R:24:TYR:HB3	17:R:28:ARG:CB	2.42	0.48
1:A:1821:A:H2'	1:A:1822:C:H6	1.77	0.48
1:A:2242:G:H2'	1:A:2243:U:O4'	2.14	0.48
1:A:2350:C:H2'	1:A:2351:G:O4'	2.14	0.48
1:A:2524:G:H1	1:A:2539:C:H42	1.60	0.48
9:J:79:LEU:HD12	9:J:108:ILE:HD13	1.94	0.48
1:A:222:A:N6	1:A:232:G:H1'	2.28	0.48
1:A:2354:C:H42	1:A:2363:G:H1	1.61	0.48
1:A:699:A:H2'	1:A:700:G:O4'	2.14	0.48
2:B:94:A:H2'	2:B:95:U:O4'	2.13	0.48
1:A:1448:G:H2'	1:A:1449:G:O4'	2.13	0.48
1:A:1716:U:H2'	1:A:1717:A:C8	2.49	0.48
1:A:1860:G:H2'	1:A:1861:G:H8	1.77	0.48
1:A:2521:C:H42	1:A:2544:G:H1	1.62	0.48
1:A:2615:U:C2	27:1:4:GLN:HA	2.48	0.48
1:A:2661:G:H2'	1:A:2662:A:C8	2.48	0.48
1:A:358:U:H2'	1:A:359:G:H8	2.00	0.48
1:A:725:G:C2	1:A:726:G:N2	2.81	0.48
1:A:771:G:OP1	29:3:14:ARG:HD2	2.14	0.48
1:A:1390:U:H2'	1:A:1391:U:C6	3.29	0.48
1:A:2055:C:C5'	1:A:2056:G:H5''	2.43	0.48
1:A:2557:G:H2'	1:A:2558:C:H6	1.71	0.48
1:A:2756:U:C4	1:A:2758:A:C6	3.00	0.48
18:S:68:ARG:HB3	18:S:90:ARG:HB3	1.96	0.48
23:X:71:VAL:HG22	23:X:78:LYS:HG2	1.96	0.48
1:A:1043:C:N4	1:A:1112:G:H1	2.10	0.48
1:A:1137:G:H2'	1:A:1138:G:C8	2.48	0.48
1:A:1805:A:H2'	1:A:1806:C:H6	1.77	0.48
1:A:1935:G:H3'	1:A:1962:5MC:HN41	1.78	0.48
1:A:2024:G:H2'	1:A:2025:C:C6	2.48	0.48
1:A:2225:A:H4'	1:A:2226:C:O5'	2.14	0.48
1:A:2615:U:H2'	1:A:2616:C:C6	2.49	0.48
1:A:2616:C:H2'	1:A:2617:U:C6	2.48	0.48
1:A:278:A:N3	1:A:278:A:H2'	2.28	0.48
1:A:872:U:H2'	1:A:873:C:C6	2.49	0.48
1:A:1006:C:H42	1:A:1137:G:H1	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:G:H2'	1:A:1445:G:C8	2.49	0.48
1:A:1521:G:H2'	1:A:1522:A:C8	2.49	0.48
1:A:1725:U:H2'	1:A:1726:C:C6	2.48	0.48
1:A:1967:C:H2'	1:A:1968:G:O4'	2.14	0.48
1:A:2185:U:H2'	1:A:2186:G:C8	2.49	0.48
1:A:2809:A:H2'	1:A:2810:A:C8	2.49	0.48
1:A:2885:G:H1	27:1:40:ARG:HH22	1.60	0.47
1:A:167:A:H2'	1:A:168:G:O4'	2.14	0.47
1:A:1980:G:HO2'	1:A:1982:U:H6	1.60	0.47
1:A:572:A:H2'	1:A:573:U:O4'	2.14	0.47
1:A:807:U:H2'	1:A:808:G:H8	1.79	0.47
1:A:1278:C:H2'	1:A:1279:G:H8	1.79	0.47
1:A:1510:G:H2'	1:A:1511:G:C8	2.49	0.47
1:A:1713:A:H61	1:A:1745:A:H61	1.62	0.47
1:A:2179:C:H2'	1:A:2180:U:C6	2.49	0.47
1:A:2297:A:N1	1:A:2321:U:H5	2.12	0.47
3:C:232:HIS:NE2	3:C:244:PRO:HA	2.29	0.47
21:V:7:ARG:HB2	21:V:27:ASN:HA	1.96	0.47
1:A:821:A:H3'	1:A:946:C:H6	1.79	0.47
1:A:842:U:H2'	1:A:843:G:C8	2.49	0.47
4:D:110:THR:HB	4:D:202:ILE:HB	1.95	0.47
4:D:141:ARG:HB3	4:D:141:ARG:HH11	1.79	0.47
14:O:96:ARG:HD3	14:O:98:LEU:HD11	1.96	0.47
1:A:2228:G:H2'	1:A:2229:U:C6	2.49	0.47
1:A:2452:C:N3	1:A:2504:PSU:O4	2.47	0.47
1:A:536:G:H2'	1:A:537:G:O4'	2.13	0.47
2:B:48:U:H2'	2:B:49:C:C6	2.49	0.47
1:A:1465:G:H2'	1:A:1466:U:O4'	2.15	0.47
1:A:1495:A:H3'	1:A:1496:A:C8	2.49	0.47
1:A:1722:A:H2'	1:A:1723:G:H8	1.79	0.47
1:A:1831:G:H2'	1:A:1832:C:C6	2.49	0.47
1:A:2605:PSU:H2'	1:A:2606:C:C6	2.50	0.47
1:A:2672:U:H2'	1:A:2673:G:H8	1.79	0.47
1:A:2734:A:C4	1:A:2735:G:H1'	2.49	0.47
1:A:732:C:H2'	1:A:733:G:O4'	2.13	0.47
1:A:2590:A:H2'	1:A:2591:C:H6	1.78	0.47
1:A:2673:G:H2'	1:A:2674:G:C8	2.49	0.47
1:A:805:G:H22	1:A:828:U:H5"	1.79	0.47
6:F:65:PRO:HB2	6:F:87:CYS:HB2	1.95	0.47
30:4:40:ARG:O	30:4:44:LEU:HG	2.14	0.47
1:A:2013:A:H4'	19:T:96:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:U:H1'	1:A:1226:A:N3	2.30	0.47
1:A:1419:A:H2'	1:A:1421:G:N7	2.30	0.47
1:A:2637:U:H3'	1:A:2638:G:C8	2.50	0.47
1:A:611:C:H2'	1:A:612:G:O4'	2.15	0.47
1:A:829:A:H5'	1:A:831:G:N7	2.30	0.47
20:U:4:GLU:HA	20:U:7:LEU:HD12	1.97	0.47
1:A:2812:G:H2'	1:A:2813:A:O4'	2.15	0.47
3:C:251:GLN:HB3	3:C:255:LYS:HD2	1.97	0.47
17:R:52:GLN:O	17:R:55:ARG:HG2	2.15	0.47
23:X:25:ARG:HB2	23:X:37:ILE:HA	1.97	0.47
1:A:1003:G:H1	1:A:1152:C:H42	1.63	0.47
1:A:1607:C:H4'	1:A:1608:A:O5'	2.15	0.47
1:A:1747:U:H2'	1:A:1748:C:C6	2.49	0.47
1:A:2081:U:H4'	24:Y:25:THR:HG21	1.97	0.47
1:A:2697:G:H1	1:A:2710:C:H42	1.60	0.47
1:A:736:C:H2'	1:A:737:C:C6	2.78	0.47
20:U:61:LEU:HG	20:U:82:LYS:HB3	1.96	0.47
1:A:593:U:H1'	30:4:4:ILE:HD11	1.96	0.47
1:A:1722:A:H2'	1:A:1723:G:C8	2.50	0.47
1:A:1749:A:H2'	1:A:1750:G:C8	2.49	0.47
1:A:2657:A:N1	1:A:2665:A:H2'	2.30	0.47
1:A:666:A:H2'	1:A:667:U:C6	2.49	0.47
1:A:724:U:H2'	1:A:725:G:O4'	2.15	0.47
1:A:2616:C:H2'	1:A:2617:U:H6	1.80	0.46
1:A:2635:A:H2'	1:A:2636:C:O4'	2.15	0.46
1:A:37:C:H2'	1:A:38:A:O4'	2.15	0.46
1:A:891:G:H2'	1:A:892:A:C8	2.50	0.46
1:A:1478:G:H1	1:A:1513:U:H3	1.63	0.46
1:A:174:U:H2'	1:A:175:G:C8	2.50	0.46
1:A:679:C:H2'	1:A:680:C:C6	2.51	0.46
1:A:755:U:H2'	1:A:756:A:C8	2.50	0.46
1:A:794:A:H2'	1:A:795:C:C6	2.50	0.46
1:A:2469:A:H2'	1:A:2470:G:O4'	2.16	0.46
3:C:223:THR:HA	3:C:232:HIS:O	2.15	0.46
1:A:1993:U:H4'	4:D:133:THR:HG22	1.97	0.46
28:2:11:LEU:HB3	28:2:49:TYR:HB3	1.98	0.46
1:A:1046:A:H3'	1:A:1047:G:H8	4.29	0.46
1:A:2618:G:H2'	1:A:2619:C:O4'	2.14	0.46
1:A:934:U:H2'	1:A:935:C:C6	2.51	0.46
1:A:971:G:P	1:A:989:G:H1	2.39	0.46
2:B:78:A:H62	2:B:98:G:H21	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:61:VAL:HB	11:L:87:LEU:HD11	1.97	0.46
23:X:43:THR:HB	23:X:46:HIS:CD2	2.50	0.46
1:A:968:C:O3'	26:0:18:PRO:HD3	2.15	0.46
1:A:121:G:H2'	1:A:122:G:H8	1.80	0.46
1:A:1397:U:OP2	1:A:1398:C:N4	2.48	0.46
1:A:143:C:H2'	1:A:144:A:H8	1.81	0.46
1:A:1653:G:C6	14:O:9:GLN:HB3	2.50	0.46
1:A:413:C:H42	1:A:2410:G:H1	1.62	0.46
1:A:2643:G:H2'	1:A:2644:G:O4'	2.14	0.46
1:A:477:A:H2'	1:A:478:A:O4'	2.16	0.46
1:A:1748:C:H2'	1:A:1749:A:C8	2.50	0.46
1:A:1748:C:H2'	1:A:1749:A:H8	1.81	0.46
1:A:2757:A:C5	1:A:2758:A:N7	2.83	0.46
1:A:466:A:C2	1:A:796:C:O4'	2.69	0.46
1:A:1266:G:H5''	19:T:15:GLN:HE22	1.79	0.46
28:2:37:LYS:HG2	28:2:46:HIS:HB3	1.98	0.46
1:A:68:G:H22	1:A:101:A:H2	30.40	0.46
1:A:1289:C:H2'	1:A:1290:C:H6	1.80	0.46
1:A:1843:C:H2'	1:A:1844:C:H6	1.81	0.46
1:A:1930:G:HO2'	1:A:1968:G:H1	1.61	0.46
1:A:2543:G:H2'	1:A:2544:G:C8	2.50	0.46
1:A:348:A:H2'	1:A:349:U:O4'	2.15	0.46
5:E:5:LEU:HG	5:E:120:VAL:HB	1.98	0.46
5:E:60:TRP:HB2	5:E:65:THR:HG21	1.98	0.46
18:S:66:HIS:HB3	18:S:92:TRP:HZ3	1.80	0.46
1:A:1117:C:O2'	1:A:1118:C:H6	1.96	0.46
1:A:1151:A:H2'	1:A:1152:C:C6	2.50	0.46
1:A:2039:U:H2'	1:A:2040:G:C8	2.51	0.46
1:A:227:A:H2	1:A:418:C:H1'	1.81	0.46
1:A:2544:G:H2'	1:A:2545:G:H8	1.81	0.46
1:A:2645:G:H4'	1:A:2732:G:O3'	2.16	0.46
1:A:2800:A:C2	1:A:2895:G:H1'	2.50	0.46
1:A:407:G:H2'	1:A:408:G:C8	2.50	0.46
1:A:489:G:N2	1:A:1320:C:H5''	2.31	0.46
1:A:672:C:H2'	1:A:673:C:H6	1.81	0.46
1:A:121:G:H2'	1:A:122:G:C8	2.51	0.46
1:A:428:A:H2'	1:A:429:A:C8	2.51	0.46
1:A:672:C:H2'	1:A:673:C:C6	2.50	0.46
1:A:751:A:O4'	19:T:90:LYS:HA	2.16	0.46
1:A:825:A:H2'	1:A:826:U:O4'	2.16	0.46
11:L:21:CYS:HA	11:L:41:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:5:CYS:HB3	24:Y:9:GLY:H	1.81	0.46
1:A:1002:G:H2'	1:A:1003:G:O4'	2.15	0.46
1:A:1850:G:H2'	1:A:1851:U:O4'	2.16	0.46
1:A:1067:A:N6	1:A:1109:C:H5'	54.41	0.45
1:A:1433:A:H2'	1:A:1434:A:O4'	2.58	0.45
1:A:2114:A:N6	1:A:2119:A:H62	2.14	0.45
1:A:2146:C:H4'	1:A:2147:A:O5'	2.16	0.45
1:A:2190:G:H2'	1:A:2191:A:O4'	2.15	0.45
1:A:489:G:H22	1:A:1320:C:H3'	1.81	0.45
1:A:749:A:H2	1:A:753:A:HO2'	1.57	0.45
1:A:958:U:H2'	2:B:89:U:H1'	1.97	0.45
3:C:158:ALA:HB1	3:C:197:ASN:HB3	1.98	0.45
1:A:729:G:C8	3:C:207:LYS:HD2	2.50	0.45
1:A:1021:A:H2'	1:A:1023:U:H5''	1.99	0.45
1:A:2623:G:H2'	1:A:2624:G:H8	1.81	0.45
1:A:821:A:H3'	1:A:946:C:C6	2.50	0.45
2:B:48:U:H2'	2:B:49:C:H6	1.81	0.45
6:F:92:ARG:HA	6:F:96:MET:HB2	1.96	0.45
17:R:98:ILE:HG22	17:R:106:PHE:HB2	1.99	0.45
1:A:1018:U:H3	1:A:1144:A:H61	1.65	0.45
1:A:1678:A:H2'	1:A:1679:A:O4'	2.15	0.45
1:A:1847:A:O2'	1:A:1848:A:H5''	2.16	0.45
1:A:2887:A:H2'	1:A:2888:C:H6	1.81	0.45
1:A:351:C:H2'	1:A:352:A:O4'	2.16	0.45
1:A:209:C:H4'	1:A:681:G:H4'	1.97	0.45
1:A:2385:C:H2'	1:A:2386:A:H8	1.81	0.45
1:A:2471:A:H2'	1:A:2472:G:O4'	2.16	0.45
1:A:2837:A:H2'	1:A:2838:G:H8	1.80	0.45
1:A:599:A:H2'	1:A:600:G:O4'	2.16	0.45
11:L:18:ARG:H	11:L:45:GLU:HB3	1.80	0.45
1:A:1313:U:H2'	1:A:1314:C:H6	4.28	0.45
1:A:1385:A:H1'	1:A:1386:C:C6	2.52	0.45
1:A:529:A:OP2	10:K:113:PRO:HD3	2.17	0.45
1:A:587:C:C6	1:A:671:C:H1'	2.51	0.45
1:A:752:A:H62	1:A:2609:U:H3	1.64	0.45
10:K:34:ARG:HG3	10:K:39:LYS:HB2	1.97	0.45
21:V:39:ILE:HG22	21:V:40:ASN:HD22	1.80	0.45
1:A:1056:G:H5''	1:A:1057:A:O4'	2.17	0.45
1:A:991:C:H42	1:A:1163:G:H1	1.64	0.45
1:A:1436:G:H2'	1:A:1437:C:O4'	2.16	0.45
1:A:1700:A:H3'	1:A:1701:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:C:H42	1:A:2038:G:H1	1.65	0.45
1:A:886:A:H1'	1:A:889:C:C5	2.43	0.45
1:A:992:C:H2'	1:A:993:G:O4'	2.17	0.45
10:K:32:LEU:HD22	10:K:54:ILE:HG21	1.98	0.45
1:A:1859:U:H2'	1:A:1860:G:C8	2.51	0.45
1:A:2396:G:H1	1:A:2420:C:H42	1.64	0.45
1:A:2647:U:H2'	1:A:2648:G:H8	1.79	0.45
1:A:2880:C:H2'	1:A:2881:U:H6	1.75	0.45
1:A:1722:A:N6	1:A:1737:G:H1	2.14	0.45
1:A:2062:A:N6	1:A:2503:A:N6	2.65	0.45
1:A:2244:U:H2'	1:A:2245:U:C6	2.52	0.45
1:A:2875:C:H2'	1:A:2876:G:H8	1.82	0.45
19:T:86:MET:HA	19:T:87:PRO:HD2	1.85	0.45
1:A:1806:C:H2'	1:A:1807:G:O4'	2.16	0.45
1:A:221:A:H61	1:A:428:A:H62	1.65	0.45
1:A:2680:U:H2'	1:A:2681:C:C6	2.51	0.45
1:A:417:C:H2'	1:A:418:C:H6	1.82	0.45
19:T:83:LYS:HD3	19:T:95:ARG:HD2	1.99	0.45
1:A:1939:5MU:H3'	1:A:1940:U:C5'	2.46	0.45
1:A:1998:A:H2'	1:A:1999:C:C6	2.52	0.45
1:A:2194:U:H2'	1:A:2195:U:C6	2.52	0.45
1:A:674:G:N1	1:A:716:A:N1	96.51	0.45
1:A:766:U:H2'	1:A:767:U:C6	2.52	0.45
4:D:142:VAL:HG23	4:D:144:GLY:H	1.82	0.45
11:L:71:ARG:HH22	16:Q:32:VAL:HG12	1.82	0.45
21:V:41:LEU:HB3	21:V:60:GLU:HG2	1.99	0.45
1:A:1815:A:O4'	1:A:1817:G:H1'	2.16	0.44
1:A:1935:G:H1'	1:A:1964:G:N2	2.31	0.44
1:A:2227:A:H2'	1:A:2228:G:O4'	2.17	0.44
1:A:2630:G:H2'	1:A:2631:G:C8	2.52	0.44
1:A:536:G:H1	1:A:557:C:H42	1.65	0.44
1:A:839:U:H2'	1:A:840:C:C6	2.51	0.44
4:D:109:VAL:HG22	4:D:203:VAL:HG13	1.97	0.44
8:H:15:LEU:HD21	8:H:56:ALA:HB1	1.97	0.44
19:T:36:LEU:HD22	19:T:47:VAL:HG13	2.00	0.44
1:A:694:U:H5''	1:A:1569:A:C6	2.52	0.44
1:A:2038:G:H2'	1:A:2039:U:C6	2.52	0.44
1:A:2617:U:H2'	1:A:2618:G:O4'	2.17	0.44
1:A:373:U:H4'	1:A:423:A:O2'	2.17	0.44
3:C:13:ARG:HG3	3:C:13:ARG:HH11	1.81	0.44
1:A:1077:A:H61	1:A:1088:A:H3'	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:G:H2'	1:A:1150:C:C6	2.52	0.44
1:A:1997:C:H2'	1:A:1998:A:C8	2.53	0.44
1:A:207:A:H2'	1:A:208:C:O4'	2.18	0.44
1:A:2189:U:H2'	1:A:2190:G:H8	1.80	0.44
1:A:2742:G:H1	1:A:2762:C:H42	1.66	0.44
1:A:2843:G:H1	1:A:2874:C:H42	1.65	0.44
1:A:52:A:H2'	1:A:53:A:C8	2.52	0.44
3:C:159:GLY:H	3:C:195:VAL:HB	1.83	0.44
4:D:51:THR:HG21	4:D:68:PHE:HE1	1.81	0.44
7:G:95:ARG:HH12	7:G:129:THR:HG23	1.83	0.44
13:N:41:LEU:HD11	13:N:102:LEU:HD22	1.98	0.44
18:S:38:VAL:HB	18:S:59:ILE:HD11	1.98	0.44
21:V:40:ASN:HB3	21:V:63:ALA:HB3	2.00	0.44
1:A:2884:U:H3'	1:A:2885:G:H21	1.82	0.44
1:A:45:G:H2'	1:A:46:G:H8	4.93	0.44
1:A:617:G:H1	1:A:623:C:H42	19.21	0.44
1:A:694:U:H5''	1:A:1569:A:C5	2.52	0.44
1:A:780:G:H2'	1:A:782:A:N7	2.33	0.44
1:A:934:U:H2'	1:A:935:C:H6	1.82	0.44
3:C:138:GLY:H	3:C:164:ILE:HB	1.82	0.44
21:V:34:VAL:HG13	21:V:67:VAL:HG22	1.99	0.44
1:A:131:A:H2'	1:A:132:G:C8	2.52	0.44
1:A:1811:G:H2'	1:A:1812:U:H6	1.81	0.44
1:A:2078:C:H2'	1:A:2079:U:H6	1.82	0.44
1:A:2461:A:H2'	1:A:2462:C:C6	2.52	0.44
1:A:596:U:H2'	1:A:597:G:C8	2.52	0.44
6:F:100:PHE:O	6:F:104:ILE:HG12	2.17	0.44
9:J:53:PRO:HD2	9:J:77:VAL:HG11	1.99	0.44
1:A:1137:G:H2'	1:A:1138:G:H8	1.82	0.44
1:A:1518:C:H2'	1:A:1519:G:H8	1.83	0.44
1:A:2645:G:H3'	1:A:2646:C:H5'	1.98	0.44
1:A:27:G:C2	1:A:512:G:N3	2.85	0.44
1:A:1055:G:H2'	1:A:1056:G:O4'	2.17	0.44
1:A:1277:G:H2'	1:A:1278:C:C6	2.52	0.44
1:A:1723:G:O6	1:A:1737:G:N2	2.51	0.44
1:A:2024:G:OP2	1:A:2034:U:H4'	2.18	0.44
1:A:585:G:O2'	5:E:77:ILE:HG22	2.18	0.44
1:A:895:U:H3	1:A:897:C:N4	2.16	0.44
22:W:25:LYS:HG2	22:W:43:ASP:HA	2.00	0.44
27:1:9:THR:HB	27:1:11:SER:H	1.83	0.44
28:2:24:THR:HG23	30:4:34:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:U:O2	1:A:1161:C:N4	7.13	0.44
1:A:1278:C:H2'	1:A:1279:G:C8	2.53	0.44
1:A:154:U:H2'	1:A:155:A:C8	2.53	0.44
1:A:1849:G:H2'	1:A:1850:G:H8	1.83	0.44
1:A:1959:G:H2'	1:A:1960:A:O4'	2.18	0.44
1:A:2448:A:H3'	1:A:2449:U:H2'	1.99	0.44
1:A:2638:G:H22	1:A:2775:G:H2'	1.83	0.44
1:A:297:G:H2'	1:A:298:G:O4'	2.18	0.44
1:A:346:A:H2'	1:A:347:A:O4'	2.17	0.44
1:A:692:C:H2'	1:A:693:A:C8	2.53	0.44
1:A:1447:C:H2'	1:A:1448:G:C8	2.53	0.44
1:A:1477:A:C5	1:A:1478:G:H1'	2.53	0.44
1:A:2140:G:H2'	1:A:2141:G:O4'	2.17	0.44
1:A:2270:A:H2'	1:A:2271:G:O4'	2.18	0.44
1:A:588:U:H2'	1:A:589:U:H6	1.78	0.44
1:A:824:U:H3	1:A:833:A:H61	1.64	0.44
2:B:30:C:H3'	2:B:31:C:H6	1.83	0.44
5:E:41:GLN:HB3	5:E:43:THR:HG23	1.99	0.44
14:O:103:ARG:HB3	14:O:108:ALA:HB3	2.00	0.44
1:A:1216:G:H2'	1:A:1217:U:O4'	2.18	0.43
1:A:1773:A:H2'	1:A:1774:C:O4'	2.17	0.43
1:A:2685:G:H4'	11:L:78:ARG:HH22	1.83	0.43
1:A:698:C:H5''	1:A:699:A:H5'	2.00	0.43
1:A:780:G:H21	1:A:783:A:H62	1.66	0.43
1:A:863:A:H4'	2:B:100:G:H21	1.82	0.43
1:A:1353:A:H2'	1:A:1354:A:H8	1.79	0.43
1:A:1724:G:H2'	1:A:1725:U:C6	2.52	0.43
1:A:1744:A:H3'	1:A:1745:A:C8	2.51	0.43
1:A:2060:A:O4'	1:A:2502:G:O4'	2.36	0.43
1:A:2543:G:H21	1:A:2646:C:H5''	1.83	0.43
4:D:122:VAL:HA	4:D:127:PHE:HB2	2.00	0.43
16:Q:7:GLN:O	16:Q:10:GLN:HG2	2.17	0.43
1:A:1515:A:H3'	1:A:1516:G:H8	1.84	0.43
1:A:1860:G:H1	1:A:1882:U:H3	1.64	0.43
1:A:609:A:H62	1:A:619:G:H21	1.67	0.43
1:A:754:U:H2'	1:A:755:U:H6	1.81	0.43
1:A:1264:A:OP1	27:1:16:ARG:NH1	2.49	0.43
1:A:2453:A:N6	1:A:2499:C:H42	2.16	0.43
1:A:838:C:H2'	1:A:839:U:C6	2.53	0.43
2:B:2:G:H1	2:B:118:C:H42	1.67	0.43
2:B:2:G:H2'	2:B:3:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:107:PHE:HB3	12:M:126:ARG:HH11	1.83	0.43
24:Y:14:THR:HG22	24:Y:28:ARG:HG2	2.00	0.43
1:A:749:A:H4'	1:A:1271:G:N3	2.34	0.43
1:A:1408:G:H3'	1:A:1409:U:H5''	2.00	0.43
1:A:734:A:O2'	1:A:1635:A:H4'	2.19	0.43
1:A:1652:A:H3'	1:A:1653:G:H8	1.83	0.43
1:A:173:A:H2'	1:A:174:U:C6	2.53	0.43
1:A:2016:U:H2'	1:A:2017:U:H6	1.81	0.43
1:A:213:A:H2'	1:A:214:G:C8	2.53	0.43
1:A:2244:U:O4	1:A:2436:G:O6	2.36	0.43
1:A:2584:U:H2'	1:A:2585:U:H2'	2.00	0.43
1:A:2681:C:C4	1:A:2724:U:C4	3.06	0.43
1:A:468:G:H2'	1:A:469:G:O4'	2.18	0.43
1:A:553:G:H2'	1:A:554:U:O4'	2.18	0.43
1:A:92:U:H3'	1:A:93:G:H8	1.83	0.43
2:B:101:A:H2'	2:B:102:G:O4'	2.18	0.43
5:E:102:ARG:HE	5:E:200:LEU:HA	1.83	0.43
1:A:1442:U:H2'	1:A:1443:U:O4'	2.18	0.43
1:A:2233:U:H2'	1:A:2234:G:H8	1.83	0.43
1:A:236:C:H2'	1:A:237:C:H6	1.81	0.43
1:A:728:G:H4'	3:C:13:ARG:HE	1.82	0.43
1:A:1050:A:H2'	1:A:1051:G:O4'	2.18	0.43
1:A:1585:C:O2	1:A:1585:C:H2'	2.18	0.43
1:A:1708:C:H2'	1:A:1709:U:C6	2.53	0.43
1:A:1790:C:H3'	1:A:1828:G:N2	2.34	0.43
1:A:2099:U:H2'	1:A:2100:G:H8	1.83	0.43
1:A:1654:A:C8	1:A:2823:A:O4'	2.72	0.43
1:A:2835:A:N6	1:A:2878:U:H2'	2.33	0.43
11:L:23:LYS:HB3	11:L:40:LYS:HB3	2.01	0.43
1:A:1199:U:H2'	1:A:1200:C:C6	2.54	0.43
1:A:16:C:H2'	1:A:17:G:H8	1.83	0.43
1:A:1946:U:H2'	1:A:1947:C:C6	2.53	0.43
1:A:271:G:H4'	1:A:272:A:OP1	2.18	0.43
1:A:2811:G:H1	1:A:2889:C:N4	2.15	0.43
1:A:511:U:H5'	1:A:1236:G:OP1	2.18	0.43
1:A:859:G:N2	1:A:916:G:H2'	2.34	0.43
1:A:2110:G:H5'	1:A:2118:U:O2'	2.19	0.43
1:A:2070:A:C6	1:A:2442:C:N3	2.86	0.43
1:A:2633:G:H2'	1:A:2634:A:O4'	2.18	0.43
1:A:1993:U:H4'	4:D:133:THR:CG2	2.49	0.43
9:J:24:GLY:HA3	9:J:25:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1379:U:H4'	1:A:1380:G:OP1	2.19	0.43
1:A:676:A:H2	1:A:2069:G:O2'	2.02	0.43
1:A:2361:G:H2'	1:A:2362:C:O4'	2.19	0.43
1:A:2386:A:H4'	23:X:56:ASP:HA	2.00	0.43
1:A:2591:C:H2'	1:A:2592:G:C8	2.54	0.43
1:A:2639:A:H2'	1:A:2640:G:O4'	2.19	0.43
1:A:2784:U:H2'	1:A:2785:C:H6	1.84	0.43
4:D:107:VAL:HG12	4:D:205:PRO:HA	2.00	0.43
17:R:62:ILE:HG12	17:R:76:TYR:OH	2.19	0.43
1:A:1182:G:H2'	1:A:1183:U:O4'	2.19	0.42
1:A:118:A:H2'	1:A:120:U:O4	2.18	0.42
1:A:676:A:C2	1:A:2070:A:O4'	2.72	0.42
1:A:984:A:N3	1:A:984:A:H2'	2.33	0.42
7:G:73:ASN:O	7:G:77:ILE:HG12	2.19	0.42
14:O:21:PHE:CZ	14:O:43:GLU:HB3	2.54	0.42
30:4:33:LEU:HD22	30:4:41:LYS:HD3	2.01	0.42
1:A:1531:C:H2'	1:A:1532:A:C8	2.54	0.42
1:A:1789:A:H2'	1:A:1790:C:O4'	2.18	0.42
1:A:2051:A:H4'	4:D:146:ILE:HG12	2.01	0.42
1:A:2247:A:H2'	1:A:2248:C:C6	2.54	0.42
1:A:2286:G:H4'	1:A:2287:A:O5'	2.19	0.42
1:A:2435:A:H2'	1:A:2436:G:O4'	2.19	0.42
1:A:2650:U:H2'	1:A:2651:C:C6	2.53	0.42
1:A:220:G:H1	1:A:427:U:H3'	1.84	0.42
1:A:493:G:H2'	1:A:494:G:O4'	2.19	0.42
9:J:73:PRO:HA	9:J:74:PRO:HD3	1.92	0.42
25:Z:18:LEU:HB2	25:Z:53:VAL:HG11	2.01	0.42
1:A:1662:U:H2'	1:A:1663:G:O4'	2.19	0.42
1:A:1719:G:H2'	1:A:1720:U:O4'	2.19	0.42
1:A:2439:A:H5'	1:A:2441:U:O5'	2.19	0.42
1:A:2646:C:H42	1:A:2674:G:H1	1.66	0.42
1:A:2786:U:H2'	1:A:2787:C:C6	2.54	0.42
1:A:414:C:H1'	1:A:1864:U:O2	2.19	0.42
1:A:1199:U:H2'	1:A:1200:C:O4'	2.19	0.42
1:A:1265:A:O3'	1:A:1266:G:H4'	2.19	0.42
1:A:1669:A:H2'	1:A:1669:A:N3	2.34	0.42
1:A:1726:C:N4	1:A:1734:G:H1	2.17	0.42
1:A:1849:G:H2'	1:A:1850:G:C8	2.55	0.42
1:A:2679:A:H2'	1:A:2680:U:O4'	2.20	0.42
1:A:452:G:H2'	1:A:453:A:C8	2.54	0.42
1:A:775:G:H2'	1:A:776:G:O4'	6.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:C:H2'	2:B:43:C:C6	2.55	0.42
1:A:826:U:O2'	12:M:53:GLY:HA3	2.19	0.42
1:A:2856:A:H2'	1:A:2857:G:O4'	2.20	0.42
1:A:610:C:H2'	1:A:611:C:C6	2.55	0.42
1:A:918:A:H2'	1:A:919:U:O4'	2.20	0.42
1:A:1463:C:H2'	1:A:1464:G:C8	2.55	0.42
1:A:2724:U:H2'	1:A:2725:A:C8	2.55	0.42
1:A:2741:A:H2'	1:A:2742:G:O4'	2.19	0.42
6:F:29:PRO:HB2	6:F:169:LEU:HD22	2.00	0.42
1:A:1388:G:H1	1:A:1399:C:H42	1.66	0.42
1:A:1995:U:H3'	1:A:1996:C:H2'	2.02	0.42
1:A:610:C:H42	1:A:618:G:H1	1.68	0.42
1:A:215:G:O3'	1:A:216:A:H4'	2.19	0.42
1:A:2407:A:H2'	1:A:2407:A:N3	2.34	0.42
1:A:2861:U:H2'	1:A:2862:G:C8	2.55	0.42
1:A:289:G:H2'	1:A:290:U:H6	1.84	0.42
1:A:409:G:H2'	1:A:410:G:C8	2.55	0.42
1:A:700:G:H1	1:A:732:C:H42	1.66	0.42
1:A:76:C:H2'	1:A:77:G:C8	2.54	0.42
3:C:44:ASN:HD21	3:C:46:ASN:HB2	1.85	0.42
1:A:1816:C:H3'	3:C:62:TYR:HE1	1.84	0.42
19:T:10:ALA:HB3	19:T:101:SER:HB2	2.01	0.42
1:A:1418:G:C2	1:A:1579:A:N7	2.88	0.42
1:A:1406:U:C4	1:A:1596:A:N1	2.88	0.42
1:A:1741:C:H2'	1:A:1742:U:O4'	2.20	0.42
1:A:2013:A:C2	1:A:2613:U:O4	2.64	0.42
1:A:2637:U:H3'	1:A:2638:G:H8	1.85	0.42
1:A:2638:G:N2	1:A:2775:G:H2'	2.35	0.42
1:A:514:A:N3	1:A:581:C:O2'	2.50	0.42
1:A:64:A:H2'	1:A:65:U:C6	2.55	0.42
1:A:686:U:H6	1:A:788:A:N1	2.18	0.42
1:A:802:A:H2'	1:A:803:U:O4'	2.19	0.42
3:C:147:LYS:HD2	3:C:150:LYS:HD2	2.02	0.42
4:D:14:ILE:HG12	4:D:24:VAL:HG21	2.01	0.42
14:O:28:LEU:HD23	14:O:48:VAL:HG21	2.01	0.42
17:R:62:ILE:HG23	17:R:76:TYR:CZ	2.55	0.42
21:V:26:LYS:HD3	21:V:37:GLU:HB3	2.01	0.42
30:4:62:LEU:HB3	30:4:65:ALA:HB3	2.02	0.42
31:5:2:LYS:HB2	31:5:35:GLN:HG2	2.01	0.42
1:A:2061:G:C4'	1:A:2503:A:C2	3.03	0.42
1:A:2600:A:H2'	1:A:2601:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:A:H2'	1:A:716:A:H8	2.34	0.42
1:A:2002:G:OP1	14:O:13:ASN:HA	2.19	0.42
2:B:104:A:H1'	22:W:31:TYR:HE2	1.85	0.42
1:A:1515:A:H2'	1:A:1516:G:O4'	2.20	0.41
1:A:1518:C:H2'	1:A:1519:G:C8	2.55	0.41
1:A:1835:2MG:H2'	1:A:1836:C:C6	2.55	0.41
1:A:677:A:H4'	1:A:2070:A:O2'	2.20	0.41
1:A:2813:A:H2'	1:A:2814:A:C8	2.55	0.41
1:A:327:G:H2'	1:A:328:U:C6	2.55	0.41
21:V:47:LYS:HA	21:V:48:PRO:HD3	1.94	0.41
24:Y:15:GLY:HA3	24:Y:29:PHE:HE1	1.85	0.41
1:A:1446:C:H42	1:A:1465:G:H1	1.67	0.41
1:A:1511:G:H2'	1:A:1512:C:H6	1.85	0.41
1:A:1973:G:H2'	1:A:1974:C:O4'	2.20	0.41
1:A:2527:C:H5'	31:5:34:LYS:HE2	2.02	0.41
1:A:2564:A:OP1	1:A:2648:G:O2'	2.38	0.41
1:A:2615:U:H2'	1:A:2616:C:H6	1.85	0.41
1:A:272:A:H2'	1:A:273:G:H8	1.84	0.41
1:A:2821:A:H2'	1:A:2822:G:C8	2.55	0.41
13:N:35:ALA:HA	13:N:128:THR:HG22	2.01	0.41
1:A:1266:G:O6	19:T:13:SER:HB3	2.21	0.41
1:A:56:A:N1	1:A:114:U:O4	2.53	0.41
1:A:16:C:H2'	1:A:17:G:C8	2.55	0.41
1:A:1818:U:H2'	3:C:156:ARG:HD2	2.03	0.41
1:A:20:C:H2'	1:A:21:A:C8	2.55	0.41
1:A:2453:A:H61	1:A:2499:C:H42	1.67	0.41
1:A:2774:C:H2'	1:A:2775:G:O4'	2.21	0.41
1:A:471:A:H2'	1:A:472:A:O4'	2.19	0.41
6:F:8:TYR:HA	6:F:12:VAL:HB	2.02	0.41
15:P:68:LYS:HA	15:P:102:ARG:HG2	2.02	0.41
1:A:1598:A:H3'	1:A:1599:U:H6	1.85	0.41
1:A:153:U:C2	1:A:173:A:N1	2.88	0.41
1:A:2660:A:H2'	1:A:2661:G:O4'	2.20	0.41
1:A:828:U:H4'	1:A:831:G:C6	2.55	0.41
2:B:10:G:H1	2:B:110:C:H42	1.68	0.41
5:E:48:THR:C	5:E:50:ALA:H	2.24	0.41
11:L:40:LYS:HE3	11:L:57:VAL:HB	2.02	0.41
1:A:145:C:H2'	1:A:146:A:C8	2.55	0.41
1:A:1490:A:H2'	1:A:1490:A:N3	2.35	0.41
1:A:2045:C:H2'	1:A:2046:G:O4'	2.20	0.41
1:A:2730:C:H2'	1:A:2731:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:G:H5''	1:A:46:G:OP1	2.20	0.41
1:A:538:A:N6	1:A:555:G:O2'	2.54	0.41
3:C:44:ASN:ND2	3:C:46:ASN:H	2.18	0.41
1:A:1248:G:C5	17:R:3:ARG:HB2	2.56	0.41
1:A:1317:G:H2'	1:A:1318:U:O4'	2.21	0.41
1:A:1426:G:C8	1:A:1427:A:H2'	2.54	0.41
1:A:163:C:H2'	1:A:164:C:C6	2.56	0.41
1:A:2024:G:H2'	1:A:2025:C:H6	1.84	0.41
1:A:2358:A:H2'	1:A:2359:C:O4'	2.20	0.41
1:A:1787:A:O4'	1:A:2589:A:H4'	2.21	0.41
1:A:668:A:H2'	1:A:670:A:H62	1.84	0.41
1:A:827:U:H2'	1:A:870:U:O4	57.17	0.41
3:C:53:HIS:HA	3:C:217:ARG:HB2	2.03	0.41
5:E:46:GLN:HB2	5:E:86:ALA:HB1	2.02	0.41
14:O:2:ARG:HA	14:O:5:LYS:HD2	2.03	0.41
14:O:98:LEU:HD22	27:1:54:VAL:HG21	2.03	0.41
1:A:1036:G:H2'	1:A:1037:G:C8	2.56	0.41
1:A:1023:U:H4'	1:A:1123:C:OP1	2.20	0.41
1:A:1170:C:H2'	1:A:1171:G:C8	2.56	0.41
1:A:1172:C:H2'	1:A:1173:U:H6	4.64	0.41
1:A:1266:G:N2	1:A:2012:G:H2'	2.36	0.41
1:A:1314:C:H42	1:A:1338:G:H1	1.68	0.41
1:A:1327:A:H2'	1:A:1328:A:O4'	2.21	0.41
1:A:1435:G:H2'	1:A:1436:G:O4'	2.21	0.41
1:A:160:A:H2'	1:A:161:A:C8	2.94	0.41
1:A:182:A:H2'	1:A:183:C:C6	2.56	0.41
1:A:2411:A:H2'	1:A:2412:A:C8	2.56	0.41
1:A:2415:G:H2'	1:A:2416:C:O4'	2.21	0.41
1:A:2505:G:C8	1:A:2576:G:N1	2.89	0.41
1:A:2848:G:O2'	1:A:2867:G:N2	2.51	0.41
1:A:932:U:OP2	1:A:932:U:H6	2.04	0.41
1:A:910:A:H62	13:N:12:MET:HA	1.86	0.41
15:P:5:SER:O	15:P:9:ARG:HG3	2.21	0.41
1:A:1266:G:H5''	19:T:15:GLN:NE2	2.36	0.41
1:A:1432:G:H2'	1:A:1433:A:H8	1.79	0.41
1:A:1739:A:H2'	1:A:1740:G:O4'	2.21	0.41
1:A:1790:C:H2'	1:A:1791:A:C5	2.56	0.41
1:A:2084:C:H2'	1:A:2085:U:O4'	2.21	0.41
1:A:2737:G:H2'	1:A:2738:A:C8	2.56	0.41
1:A:741:U:H2'	1:A:742:A:C8	2.56	0.41
3:C:243:HIS:HA	3:C:244:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:C:H4'	10:K:110:PRO:HD3	2.03	0.41
22:W:30:ILE:HG23	22:W:72:VAL:HG11	2.02	0.41
24:Y:71:LEU:HD21	24:Y:78:TYR:HB3	2.02	0.41
1:A:1170:C:H42	1:A:1178:C:N4	2.19	0.41
1:A:175:G:H2'	1:A:176:A:C8	2.56	0.41
1:A:2236:U:H2'	1:A:2237:G:O4'	2.21	0.41
1:A:2447:G:O6	1:A:2504:PSU:O2	2.38	0.41
1:A:2494:G:O2'	13:N:79:ALA:HA	2.21	0.41
1:A:418:C:H2'	1:A:419:U:C6	2.56	0.41
1:A:68:G:O2'	1:A:170:U:H1'	49.42	0.41
1:A:822:G:H2'	1:A:823:C:C6	2.56	0.41
1:A:872:U:H2'	1:A:873:C:H6	1.83	0.41
12:M:79:LEU:HD11	12:M:112:LEU:HD12	2.03	0.41
1:A:1249:U:H3'	12:M:18:ARG:HH22	1.86	0.41
1:A:1478:G:N2	1:A:1514:G:H1'	2.36	0.41
1:A:1843:C:H2'	1:A:1844:C:C6	2.56	0.41
1:A:2025:C:H2'	1:A:2026:U:H6	1.86	0.41
1:A:2037:A:H2'	1:A:2038:G:H8	1.86	0.41
1:A:676:A:C2	1:A:2069:G:O2'	2.74	0.41
1:A:1801:A:C8	1:A:2203:U:H2'	2.55	0.41
1:A:2533:U:H2'	1:A:2534:A:O4'	2.21	0.41
1:A:2633:G:H1	1:A:2785:C:H42	1.68	0.41
1:A:355:U:H2'	1:A:356:G:C8	2.56	0.41
1:A:406:G:H2'	1:A:407:G:C8	2.55	0.41
1:A:600:G:H1	1:A:657:U:H3	1.67	0.41
1:A:674:G:H2'	1:A:675:A:C8	5.33	0.41
1:A:783:A:H3'	1:A:783:A:C8	2.56	0.41
1:A:985:C:H2'	1:A:986:C:C6	2.56	0.41
7:G:170:ARG:HB3	7:G:170:ARG:NH2	2.35	0.41
1:A:693:A:H1'	1:A:1354:A:H1'	2.02	0.41
1:A:1664:A:H61	1:A:1996:C:H42	1.69	0.41
1:A:2061:G:OP1	1:A:2061:G:H4'	2.20	0.41
1:A:2185:U:H2'	1:A:2186:G:H8	1.86	0.41
1:A:2230:G:H2'	1:A:2231:U:C6	2.56	0.41
1:A:2594:C:H2'	1:A:2595:G:O4'	2.21	0.41
5:E:5:LEU:HD11	5:E:12:LEU:HD12	2.01	0.41
13:N:30:SER:HA	13:N:133:LYS:HB2	2.02	0.41
4:D:13:ARG:HH11	16:Q:56:HIS:HA	1.86	0.41
1:A:151:C:H2'	1:A:152:A:O4'	2.21	0.40
1:A:1880:U:H2'	1:A:1881:C:C6	2.56	0.40
1:A:1991:U:H2'	1:A:1992:G:H5'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:U:N3	1:A:2025:C:H5''	2.36	0.40
1:A:202:U:H2'	1:A:202:U:O2	2.20	0.40
1:A:2649:C:H2'	1:A:2650:U:C6	2.56	0.40
1:A:2664:G:O2'	1:A:2665:A:O4'	2.39	0.40
1:A:2786:U:H2'	1:A:2787:C:H6	1.86	0.40
1:A:2864:G:H2'	1:A:2865:U:O4'	2.21	0.40
1:A:532:A:C2'	1:A:532:A:N3	3.16	0.40
13:N:126:ILE:H	13:N:126:ILE:HG13	1.81	0.40
25:Z:39:GLN:HE21	25:Z:41:HIS:HE1	1.69	0.40
1:A:1502:A:H3'	1:A:1503:A:H5''	2.03	0.40
1:A:1804:C:N4	1:A:1814:G:N2	2.68	0.40
1:A:858:G:N3	1:A:2268:A:H2'	2.36	0.40
1:A:1128:G:H21	1:A:2517:C:H1'	1.85	0.40
1:A:2519:U:H2'	1:A:2541:A:N6	2.36	0.40
1:A:2889:C:H2'	1:A:2890:G:O4'	2.22	0.40
1:A:296:U:H2'	1:A:297:G:C8	2.56	0.40
1:A:299:A:N6	1:A:322:A:O2'	2.54	0.40
7:G:11:VAL:HA	7:G:12:PRO:HD3	1.92	0.40
1:A:715:A:C8	14:O:60:VAL:HG11	94.36	0.40
14:O:69:ARG:HG2	14:O:69:ARG:H	1.71	0.40
14:O:79:LEU:HA	14:O:83:LEU:HB2	2.03	0.40
1:A:1023:U:H1'	1:A:1122:G:H5''	2.03	0.40
1:A:992:C:N4	1:A:1162:G:H1	2.15	0.40
1:A:1186:G:H2'	1:A:1187:G:O4'	2.22	0.40
1:A:1462:C:H2'	1:A:1463:C:C6	2.56	0.40
1:A:2376:A:H2'	1:A:2377:A:O4'	2.21	0.40
1:A:2813:A:H3'	1:A:2814:A:H8	1.86	0.40
1:A:863:A:H2'	1:A:864:G:C8	2.56	0.40
1:A:978:G:H1	1:A:985:C:N4	2.16	0.40
4:D:5:VAL:HG21	4:D:80:TRP:CG	2.57	0.40
1:A:2525:G:H1'	1:A:2741:A:H2	1.86	0.40
30:4:6:THR:HG23	30:4:63:PRO:HD2	2.04	0.40
1:A:1060:U:C2	1:A:1062:G:H5'	2.56	0.40
1:A:1788:C:H2'	1:A:1789:A:O4'	2.21	0.40
1:A:528:A:C2	1:A:2042:A:H2'	2.55	0.40
1:A:2128:G:H2'	1:A:2129:C:O4'	2.22	0.40
1:A:2403:C:N4	1:A:2414:G:H1	2.17	0.40
1:A:372:G:C8	24:Y:61:LYS:HD2	2.57	0.40
5:E:76:PRO:HG2	5:E:84:THR:HB	2.03	0.40
22:W:5:ASN:HA	22:W:64:VAL:HG12	2.03	0.40
1:A:2008:C:H2'	1:A:2009:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:A:H2'	1:A:564:C:H42	74.56	0.40
2:B:56:G:H1'	2:B:58:A:H62	1.87	0.40
3:C:122:ALA:HB1	3:C:128:ASN:HD22	1.86	0.40
17:R:66:ASN:HD21	17:R:70:ARG:HE	1.70	0.40
19:T:66:ILE:HA	19:T:69:LEU:HD12	2.04	0.40
1:A:169:G:H2'	1:A:170:U:C6	2.57	0.40
1:A:1932:A:H3'	1:A:1933:G:H8	1.87	0.40
1:A:2840:C:H2'	1:A:2841:C:C6	2.57	0.40
1:A:448:U:H5''	1:A:449:A:C8	2.57	0.40
1:A:84:A:N1	1:A:98:G:O2'	2.46	0.40
1:A:866:A:H61	1:A:913:U:H1'	1.86	0.40
3:C:210:ALA:HA	3:C:213:TRP:CE3	2.57	0.40
1:A:1248:G:C4	17:R:3:ARG:HB2	2.55	0.40
18:S:35:PHE:HB2	18:S:59:ILE:HB	2.04	0.40
1:A:2505:G:C6	1:A:2610:C:O2	2.75	0.40
1:A:484:C:H42	1:A:496:G:H1	1.69	0.40
19:T:66:ILE:H	19:T:66:ILE:HG13	1.76	0.40
5:E:178:VAL:HG23	12:M:3:LEU:HD21	2.03	0.40
1:A:2043:C:H1'	1:A:2779:U:O4	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	269/273 (98%)	246 (91%)	20 (7%)	3 (1%)	17 59
4	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	32 73
5	E	199/201 (99%)	183 (92%)	14 (7%)	2 (1%)	18 61
6	F	175/179 (98%)	155 (89%)	16 (9%)	4 (2%)	7 43
7	G	174/177 (98%)	166 (95%)	8 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	13	53
9	J	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	3	28
10	K	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	25	68
11	L	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
12	M	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	25	68
13	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
14	O	118/127 (93%)	105 (89%)	12 (10%)	1 (1%)	22	65
15	P	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	20	63
16	Q	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
17	R	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
18	S	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	5	37
19	T	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	20	63
20	U	91/100 (91%)	83 (91%)	6 (7%)	2 (2%)	8	44
21	V	100/104 (96%)	82 (82%)	17 (17%)	1 (1%)	18	61
22	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
23	X	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	14	55
24	Y	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
25	Z	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	11	49
26	0	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	10	48
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	8	45
29	3	44/46 (96%)	44 (100%)	0	0	100	100
30	4	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
33	b	222/241 (92%)	207 (93%)	14 (6%)	1 (0%)	32	73
34	c	204/233 (88%)	192 (94%)	10 (5%)	2 (1%)	18	61
35	d	202/206 (98%)	192 (95%)	10 (5%)	0	100	100
36	e	155/167 (93%)	145 (94%)	8 (5%)	2 (1%)	14	55
37	f	98/135 (73%)	93 (95%)	4 (4%)	1 (1%)	18	61
38	g	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
39	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	i	125/130 (96%)	112 (90%)	10 (8%)	3 (2%)	7	42
41	j	96/103 (93%)	87 (91%)	6 (6%)	3 (3%)	5	37
42	k	115/117 (98%)	103 (90%)	11 (10%)	1 (1%)	20	63
43	l	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	22	65
44	m	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
45	n	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
46	o	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	15	57
47	p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
48	q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
49	r	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
50	s	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	14	55
51	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
52	u	54/71 (76%)	54 (100%)	0	0	100	100
53	v	354/383 (92%)	334 (94%)	19 (5%)	1 (0%)	44	80
54	w	45/57 (79%)	39 (87%)	5 (11%)	1 (2%)	8	44
All	All	6056/6398 (95%)	5615 (93%)	390 (6%)	51 (1%)	27	65

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
5	E	64	GLY
18	S	82	HIS
6	F	174	ASP
9	J	20	SER
10	K	81	ILE
14	O	67	PHE
18	S	51	VAL
34	c	4	LYS
37	f	52	ASN
41	j	36	VAL
41	j	57	VAL
3	C	255	LYS
9	J	92	PRO
19	T	72	THR
21	V	90	GLY
26	0	4	THR

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Mol	Chain	Res	Type
33	b	126	PHE
36	e	78	ASN
40	i	13	LYS
40	i	111	VAL
41	j	94	ALA
4	D	206	ALA
6	F	21	ASN
8	H	15	LEU
8	H	72	ILE
12	M	86	GLU
40	i	109	ARG
53	v	250	GLY
3	C	69	ARG
6	F	176	PRO
6	F	177	PHE
18	S	80	ARG
23	X	76	ASN
25	Z	37	LEU
42	k	39	GLY
46	o	19	ALA
9	J	18	ASN
15	P	34	HIS
20	U	10	VAL
28	2	5	ILE
43	l	42	PRO
36	e	44	GLY
54	w	23	PRO
9	J	22	PRO
9	J	31	GLY
34	c	108	LYS
5	E	77	ILE
9	J	12	VAL
50	s	29	LYS
20	U	14	PRO

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	216/218 (99%)	198 (92%)	18 (8%)	13	46
4	D	164/164 (100%)	153 (93%)	11 (7%)	19	57
5	E	165/165 (100%)	159 (96%)	6 (4%)	40	74
6	F	148/150 (99%)	136 (92%)	12 (8%)	14	48
7	G	137/138 (99%)	132 (96%)	5 (4%)	40	74
8	H	114/114 (100%)	109 (96%)	5 (4%)	33	69
9	J	109/110 (99%)	103 (94%)	6 (6%)	25	62
10	K	116/116 (100%)	114 (98%)	2 (2%)	66	87
11	L	104/104 (100%)	96 (92%)	8 (8%)	15	50
12	M	103/103 (100%)	96 (93%)	7 (7%)	18	56
13	N	109/109 (100%)	103 (94%)	6 (6%)	25	62
14	O	100/103 (97%)	95 (95%)	5 (5%)	28	65
15	P	86/87 (99%)	78 (91%)	8 (9%)	10	41
16	Q	99/100 (99%)	93 (94%)	6 (6%)	22	60
17	R	89/90 (99%)	81 (91%)	8 (9%)	11	42
18	S	84/84 (100%)	81 (96%)	3 (4%)	40	74
19	T	93/93 (100%)	92 (99%)	1 (1%)	78	91
20	U	80/84 (95%)	78 (98%)	2 (2%)	53	81
21	V	83/85 (98%)	78 (94%)	5 (6%)	22	60
22	W	78/78 (100%)	69 (88%)	9 (12%)	6	30
23	X	59/63 (94%)	55 (93%)	4 (7%)	18	56
24	Y	67/68 (98%)	60 (90%)	7 (10%)	8	36
25	Z	54/55 (98%)	53 (98%)	1 (2%)	62	85
26	0	48/49 (98%)	48 (100%)	0	100	100
27	1	47/48 (98%)	45 (96%)	2 (4%)	33	70
28	2	45/49 (92%)	44 (98%)	1 (2%)	57	83
29	3	38/38 (100%)	38 (100%)	0	100	100
30	4	51/52 (98%)	51 (100%)	0	100	100
31	5	34/34 (100%)	34 (100%)	0	100	100
33	b	186/199 (94%)	172 (92%)	14 (8%)	16	51
34	c	170/190 (90%)	153 (90%)	17 (10%)	9	37
35	d	171/173 (99%)	157 (92%)	14 (8%)	13	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	119/126 (94%)	107 (90%)	12 (10%)	9	37
37	f	87/116 (75%)	82 (94%)	5 (6%)	24	61
38	g	124/147 (84%)	116 (94%)	8 (6%)	20	58
39	h	104/104 (100%)	98 (94%)	6 (6%)	23	61
40	i	105/107 (98%)	95 (90%)	10 (10%)	10	40
41	j	86/90 (96%)	76 (88%)	10 (12%)	6	30
42	k	90/90 (100%)	88 (98%)	2 (2%)	57	83
43	l	103/103 (100%)	96 (93%)	7 (7%)	18	56
44	m	92/96 (96%)	85 (92%)	7 (8%)	15	51
45	n	83/83 (100%)	76 (92%)	7 (8%)	13	46
46	o	76/76 (100%)	66 (87%)	10 (13%)	5	24
47	p	65/65 (100%)	57 (88%)	8 (12%)	5	27
48	q	74/78 (95%)	67 (90%)	7 (10%)	10	40
49	r	57/66 (86%)	53 (93%)	4 (7%)	18	55
50	s	72/72 (100%)	65 (90%)	7 (10%)	9	38
51	t	65/65 (100%)	61 (94%)	4 (6%)	21	59
52	u	48/61 (79%)	46 (96%)	2 (4%)	34	70
53	v	304/324 (94%)	274 (90%)	30 (10%)	9	38
54	w	40/46 (87%)	33 (82%)	7 (18%)	2	13
All	All	5041/5228 (96%)	4695 (93%)	346 (7%)	23	55

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	13	ARG
3	C	33	LEU
3	C	51	THR
3	C	52	ARG
3	C	63	ARG
3	C	72	ASP
3	C	80	ARG
3	C	133	ARG
3	C	135	ILE
3	C	142	HIS
3	C	156	ARG

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Mol	Chain	Res	Type
3	C	164	ILE
3	C	175	ARG
3	C	176	LEU
3	C	182	ARG
3	C	221	ARG
3	C	264	ASP
3	C	269	ARG
4	D	5	VAL
4	D	12	THR
4	D	45	TYR
4	D	50	VAL
4	D	77	ARG
4	D	121	THR
4	D	141	ARG
4	D	142	VAL
4	D	159	LYS
4	D	179	ARG
4	D	200	ASP
5	E	21	ARG
5	E	100	MET
5	E	107	SER
5	E	138	LEU
5	E	189	THR
5	E	193	VAL
6	F	6	ASP
6	F	16	LEU
6	F	22	TYR
6	F	52	ASN
6	F	71	ARG
6	F	74	VAL
6	F	95	ARG
6	F	108	VAL
6	F	135	GLN
6	F	152	LEU
6	F	155	THR
6	F	170	LEU
7	G	45	HIS
7	G	50	LEU
7	G	89	LEU
7	G	98	VAL
7	G	148	LEU
8	H	1	MET

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Mol	Chain	Res	Type
8	H	9	VAL
8	H	27	ARG
8	H	96	THR
8	H	124	THR
9	J	8	VAL
9	J	37	PHE
9	J	60	VAL
9	J	79	LEU
9	J	133	ARG
9	J	137	LEU
10	K	28	LEU
10	K	81	ILE
11	L	25	LEU
11	L	29	HIS
11	L	31	ARG
11	L	57	VAL
11	L	71	ARG
11	L	84	CYS
11	L	85	VAL
11	L	116	ILE
12	M	23	ILE
12	M	27	LEU
12	M	46	VAL
12	M	48	ARG
12	M	110	VAL
12	M	126	ARG
12	M	132	ARG
13	N	44	ARG
13	N	60	GLN
13	N	66	ARG
13	N	74	THR
13	N	86	LYS
13	N	119	LEU
14	O	15	SER
14	O	37	THR
14	O	70	THR
14	O	79	LEU
14	O	90	ARG
15	P	7	ARG
15	P	21	LEU
15	P	30	ARG
15	P	36	TYR

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Mol	Chain	Res	Type
15	P	53	THR
15	P	83	LEU
15	P	84	GLU
15	P	106	LEU
16	Q	21	ARG
16	Q	33	VAL
16	Q	88	ARG
16	Q	93	ARG
16	Q	97	LEU
16	Q	109	ARG
17	R	11	ARG
17	R	28	ARG
17	R	30	ARG
17	R	40	ILE
17	R	51	ARG
17	R	53	ARG
17	R	74	ILE
17	R	83	LEU
18	S	40	MET
18	S	54	VAL
18	S	80	ARG
19	T	46	LEU
20	U	60	THR
20	U	77	ARG
21	V	6	ARG
21	V	9	ASP
21	V	72	ILE
21	V	81	ASP
21	V	82	ARG
22	W	9	ARG
22	W	12	GLN
22	W	18	ARG
22	W	29	ILE
22	W	43	ASP
22	W	51	GLN
22	W	61	LEU
22	W	64	VAL
22	W	82	TYR
23	X	25	ARG
23	X	51	VAL
23	X	56	ASP
23	X	69	PHE

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Mol	Chain	Res	Type
24	Y	18	ARG
24	Y	23	ASN
24	Y	33	LEU
24	Y	37	ARG
24	Y	46	PHE
24	Y	60	ASP
24	Y	78	TYR
25	Z	56	LEU
27	1	9	THR
27	1	39	LEU
28	2	32	GLU
33	b	19	GLN
33	b	35	ARG
33	b	39	HIS
33	b	51	ASN
33	b	87	CYS
33	b	97	LEU
33	b	102	THR
33	b	106	THR
33	b	114	LEU
33	b	125	THR
33	b	137	ARG
33	b	139	ARG
33	b	179	LEU
33	b	204	ASP
34	c	25	ASN
34	c	43	LEU
34	c	59	ARG
34	c	65	ARG
34	c	72	ARG
34	c	75	ILE
34	c	87	LEU
34	c	90	VAL
34	c	93	ASP
34	c	106	VAL
34	c	110	GLU
34	c	140	ASN
34	c	169	ARG
34	c	176	HIS
34	c	178	LEU
34	c	179	ARG
34	c	206	GLU

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Mol	Chain	Res	Type
35	d	3	ARG
35	d	28	ILE
35	d	35	GLU
35	d	44	ARG
35	d	55	LEU
35	d	58	LYS
35	d	73	ARG
35	d	91	LEU
35	d	93	LEU
35	d	97	ARG
35	d	116	GLN
35	d	141	ASP
35	d	159	LEU
35	d	191	LEU
36	e	31	PHE
36	e	34	THR
36	e	45	ARG
36	e	69	ARG
36	e	76	LEU
36	e	90	THR
36	e	93	ARG
36	e	120	VAL
36	e	123	VAL
36	e	131	THR
36	e	136	VAL
36	e	165	LEU
37	f	16	GLU
37	f	18	VAL
37	f	24	ARG
37	f	70	VAL
37	f	86	ARG
38	g	21	GLU
38	g	23	LEU
38	g	92	ARG
38	g	95	ARG
38	g	99	LEU
38	g	102	ARG
38	g	138	ARG
38	g	143	ARG
39	h	32	LEU
39	h	40	LEU
39	h	76	GLN

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Mol	Chain	Res	Type
39	h	83	LEU
39	h	106	THR
39	h	113	ASP
40	i	18	ARG
40	i	39	PHE
40	i	85	ARG
40	i	106	ARG
40	i	113	ARG
40	i	115	LYS
40	i	119	ARG
40	i	124	ARG
40	i	129	LYS
40	i	130	ARG
41	j	7	ARG
41	j	9	ARG
41	j	10	LEU
41	j	16	ARG
41	j	31	ARG
41	j	37	ARG
41	j	53	ILE
41	j	68	ARG
41	j	73	LEU
41	j	102	LEU
42	k	53	ARG
42	k	96	THR
43	l	31	ARG
43	l	44	LYS
43	l	56	ARG
43	l	74	LEU
43	l	94	ARG
43	l	110	ARG
43	l	115	SER
44	m	16	VAL
44	m	29	ARG
44	m	39	ILE
44	m	52	GLN
44	m	90	ARG
44	m	102	THR
44	m	113	ARG
45	n	20	TYR
45	n	24	ARG
45	n	33	ASP

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Mol	Chain	Res	Type
45	n	40	ASP
45	n	41	ARG
45	n	74	LEU
45	n	82	ILE
46	o	18	ASP
46	o	37	ASN
46	o	39	LEU
46	o	56	LEU
46	o	57	LEU
46	o	73	LYS
46	o	75	VAL
46	o	84	ARG
46	o	88	ARG
46	o	89	ARG
47	p	9	HIS
47	p	14	ARG
47	p	24	SER
47	p	25	ARG
47	p	31	ARG
47	p	51	ARG
47	p	59	HIS
47	p	66	THR
48	q	6	ARG
48	q	16	LYS
48	q	21	ILE
48	q	23	VAL
48	q	42	THR
48	q	57	ASP
48	q	79	VAL
49	r	47	THR
49	r	67	LEU
49	r	72	ASP
49	r	73	ARG
50	s	11	ILE
50	s	24	GLU
50	s	36	ARG
50	s	41	PHE
50	s	55	ARG
50	s	63	THR
50	s	66	MET
51	t	18	ARG
51	t	25	ARG

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Mol	Chain	Res	Type
51	t	28	MET
51	t	57	ILE
52	u	17	ARG
52	u	44	GLU
53	v	12	GLN
53	v	28	ASP
53	v	49	GLU
53	v	69	THR
53	v	70	LEU
53	v	80	VAL
53	v	95	THR
53	v	117	ARG
53	v	119	PHE
53	v	142	GLN
53	v	150	ARG
53	v	159	ARG
53	v	163	THR
53	v	167	GLU
53	v	202	VAL
53	v	238	ASP
53	v	240	ARG
53	v	254	VAL
53	v	262	ARG
53	v	273	GLN
53	v	285	ASP
53	v	295	LEU
53	v	310	MET
53	v	315	SER
53	v	323	ILE
53	v	337	ARG
53	v	338	THR
53	v	343	ARG
53	v	354	ASP
53	v	361	LEU
54	w	13	ASP
54	w	17	GLU
54	w	19	LEU
54	w	22	ASP
54	w	29	VAL
54	w	30	GLU
54	w	41	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such

sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
3	C	60	GLN
4	D	173	GLN
5	E	62	GLN
5	E	90	GLN
7	G	22	GLN
7	G	111	HIS
7	G	116	GLN
8	H	135	HIS
12	M	38	GLN
14	O	16	HIS
14	O	62	ASN
16	Q	3	ASN
17	R	20	GLN
17	R	72	ASN
18	S	12	HIS
18	S	18	GLN
19	T	15	GLN
19	T	61	ASN
21	V	40	ASN
21	V	46	GLN
22	W	44	HIS
22	W	49	ASN
25	Z	39	GLN
34	c	123	GLN
35	d	36	GLN
36	e	73	ASN
36	e	89	HIS
36	e	135	ASN
36	e	146	ASN
37	f	52	ASN
37	f	81	ASN
38	g	86	GLN
38	g	148	ASN
42	k	119	ASN
43	l	6	GLN
43	l	29	GLN
47	p	63	GLN
48	q	51	ASN
49	r	54	GLN
53	v	43	GLN
53	v	214	HIS

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Mol	Chain	Res	Type
53	v	253	HIS
53	v	283	ASN
53	v	286	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2903/2904 (99%)	855 (29%)	82 (2%)
2	B	117/118 (99%)	35 (29%)	1 (0%)
32	a	1529/1533 (99%)	490 (32%)	0
55	x	76/77 (98%)	22 (28%)	0
55	y	76/77 (98%)	18 (23%)	0
56	z	5/18 (27%)	1 (20%)	0
All	All	4706/4727 (99%)	1421 (30%)	83 (1%)

All (1421) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	13	A
1	A	14	A
1	A	23	G
1	A	27	G
1	A	34	U
1	A	35	G
1	A	39	G
1	A	43	G
1	A	45	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	55	G
1	A	60	G
1	A	61	C
1	A	63	A
1	A	69	C
1	A	71	A
1	A	73	A
1	A	74	A
1	A	75	G
1	A	83	A

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Mol	Chain	Res	Type
1	A	84	A
1	A	86	G
1	A	88	G
1	A	92	U
1	A	93	G
1	A	96	C
1	A	101	A
1	A	102	U
1	A	103	A
1	A	110	G
1	A	114	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	122	G
1	A	125	A
1	A	127	A
1	A	131	A
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	150	U
1	A	157	C
1	A	163	C
1	A	179	C
1	A	181	A
1	A	184	C
1	A	196	A
1	A	199	A
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	222	A
1	A	224	U
1	A	228	C
1	A	230	G
1	A	233	A
1	A	239	C
1	A	241	A

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Mol	Chain	Res	Type
1	A	248	G
1	A	249	C
1	A	252	G
1	A	261	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	271	G
1	A	272	A
1	A	276	U
1	A	278	A
1	A	279	A
1	A	285	G
1	A	291	G
1	A	295	G
1	A	302	C
1	A	311	A
1	A	312	G
1	A	313	G
1	A	318	C
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	331	C
1	A	346	A
1	A	352	A
1	A	353	C
1	A	356	G
1	A	361	G
1	A	362	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	399	U
1	A	402	A
1	A	403	U
1	A	404	A

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Mol	Chain	Res	Type
1	A	405	U
1	A	408	G
1	A	411	G
1	A	421	C
1	A	424	G
1	A	425	G
1	A	427	U
1	A	431	U
1	A	435	C
1	A	442	G
1	A	443	A
1	A	444	C
1	A	451	U
1	A	454	A
1	A	455	C
1	A	457	A
1	A	467	G
1	A	474	G
1	A	475	C
1	A	476	G
1	A	479	A
1	A	481	G
1	A	490	C
1	A	491	G
1	A	501	A
1	A	504	A
1	A	505	A
1	A	506	G
1	A	512	G
1	A	513	A
1	A	516	C
1	A	518	G
1	A	519	U
1	A	527	C
1	A	528	A
1	A	529	A
1	A	531	C
1	A	532	A
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G

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Mol	Chain	Res	Type
1	A	549	G
1	A	551	G
1	A	555	G
1	A	562	U
1	A	563	A
1	A	565	C
1	A	566	U
1	A	568	U
1	A	573	U
1	A	575	A
1	A	577	G
1	A	580	U
1	A	588	U
1	A	592	A
1	A	593	U
1	A	601	C
1	A	603	A
1	A	610	C
1	A	613	A
1	A	614	A
1	A	615	U
1	A	621	A
1	A	627	A
1	A	637	A
1	A	638	G
1	A	645	C
1	A	647	G
1	A	651	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	664	G
1	A	668	A
1	A	670	A
1	A	675	A
1	A	677	A
1	A	684	G
1	A	686	U
1	A	691	C
1	A	694	U
1	A	702	U

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Mol	Chain	Res	Type
1	A	710	U
1	A	717	C
1	A	726	G
1	A	728	G
1	A	729	G
1	A	730	A
1	A	731	C
1	A	734	A
1	A	738	G
1	A	742	A
1	A	743	A
1	A	746	PSU
1	A	747	5MU
1	A	757	G
1	A	763	G
1	A	764	A
1	A	765	C
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	788	A
1	A	792	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	821	A
1	A	827	U
1	A	828	U
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	850	U
1	A	856	G
1	A	858	G
1	A	859	G

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Mol	Chain	Res	Type
1	A	869	G
1	A	877	A
1	A	878	A
1	A	881	G
1	A	882	G
1	A	883	G
1	A	886	A
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	C
1	A	894	U
1	A	895	U
1	A	896	A
1	A	897	C
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	918	A
1	A	926	G
1	A	931	U
1	A	932	U
1	A	941	A
1	A	946	C
1	A	953	G
1	A	957	C
1	A	958	U
1	A	961	C
1	A	964	C
1	A	965	C
1	A	968	C
1	A	973	A
1	A	974	G
1	A	983	A
1	A	984	A
1	A	988	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	997	G

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Mol	Chain	Res	Type
1	A	1007	C
1	A	1008	A
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1017	G
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1034	G
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1051	G
1	A	1052	C
1	A	1054	A
1	A	1059	G
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	1073	A
1	A	1074	G
1	A	1075	C
1	A	1076	C
1	A	1077	A
1	A	1078	U
1	A	1080	A
1	A	1083	U
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1096	A
1	A	1097	U
1	A	1098	A

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Mol	Chain	Res	Type
1	A	1101	U
1	A	1102	C
1	A	1106	G
1	A	1111	A
1	A	1112	G
1	A	1118	C
1	A	1119	U
1	A	1121	C
1	A	1126	A
1	A	1127	A
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1136	G
1	A	1142	A
1	A	1143	A
1	A	1144	A
1	A	1151	A
1	A	1155	A
1	A	1156	A
1	A	1165	A
1	A	1170	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1179	G
1	A	1180	U
1	A	1182	G
1	A	1186	G
1	A	1187	G
1	A	1188	U
1	A	1195	G
1	A	1205	A
1	A	1206	G
1	A	1210	G
1	A	1212	G
1	A	1218	G
1	A	1223	G
1	A	1227	G

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Mol	Chain	Res	Type
1	A	1236	G
1	A	1238	G
1	A	1240	U
1	A	1244	A
1	A	1247	A
1	A	1248	G
1	A	1249	U
1	A	1252	G
1	A	1253	A
1	A	1256	G
1	A	1263	U
1	A	1265	A
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1277	G
1	A	1278	C
1	A	1288	G
1	A	1289	C
1	A	1294	U
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1306	C
1	A	1312	U
1	A	1313	U
1	A	1314	C
1	A	1315	C
1	A	1320	C
1	A	1321	A
1	A	1326	U
1	A	1329	U
1	A	1341	G
1	A	1344	U
1	A	1345	C
1	A	1352	U
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1371	G
1	A	1379	U

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Mol	Chain	Res	Type
1	A	1380	G
1	A	1383	A
1	A	1395	A
1	A	1398	C
1	A	1403	A
1	A	1404	C
1	A	1407	G
1	A	1408	G
1	A	1409	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1433	A
1	A	1434	A
1	A	1437	C
1	A	1438	U
1	A	1444	G
1	A	1449	G
1	A	1451	C
1	A	1453	A
1	A	1455	G
1	A	1456	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1466	U
1	A	1468	U
1	A	1471	G
1	A	1478	G
1	A	1482	G
1	A	1486	U
1	A	1488	C
1	A	1490	A
1	A	1492	G
1	A	1493	C
1	A	1494	A
1	A	1497	U

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Mol	Chain	Res	Type
1	A	1502	A
1	A	1503	A
1	A	1508	A
1	A	1515	A
1	A	1522	A
1	A	1523	U
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1550	C
1	A	1555	G
1	A	1558	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1580	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1592	C
1	A	1597	A
1	A	1599	U
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1613	G
1	A	1619	G
1	A	1627	G
1	A	1634	A
1	A	1638	C
1	A	1639	C
1	A	1643	G
1	A	1644	C
1	A	1646	C
1	A	1647	U

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Mol	Chain	Res	Type
1	A	1648	U
1	A	1649	G
1	A	1652	A
1	A	1654	A
1	A	1660	G
1	A	1664	A
1	A	1666	G
1	A	1667	G
1	A	1669	A
1	A	1674	G
1	A	1675	C
1	A	1695	G
1	A	1713	A
1	A	1715	G
1	A	1721	G
1	A	1724	G
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1733	G
1	A	1742	U
1	A	1758	U
1	A	1759	A
1	A	1764	C
1	A	1773	A
1	A	1782	U
1	A	1786	A
1	A	1791	A
1	A	1794	A
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1816	C
1	A	1821	A
1	A	1829	A
1	A	1835	2MG
1	A	1848	A
1	A	1864	U
1	A	1865	U
1	A	1866	A
1	A	1869	G

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Mol	Chain	Res	Type
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1882	U
1	A	1884	G
1	A	1885	A
1	A	1900	A
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1944	U
1	A	1955	U
1	A	1964	G
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1981	A
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2000	C
1	A	2002	G
1	A	2004	G
1	A	2006	C

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Mol	Chain	Res	Type
1	A	2016	U
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2030	A
1	A	2031	A
1	A	2034	U
1	A	2036	C
1	A	2043	C
1	A	2046	G
1	A	2049	G
1	A	2050	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2057	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	U
1	A	2069	G
1	A	2070	A
1	A	2072	C
1	A	2074	U
1	A	2075	U
1	A	2077	A
1	A	2080	A
1	A	2087	G
1	A	2093	G
1	A	2095	A
1	A	2101	A
1	A	2102	G
1	A	2107	G
1	A	2110	G
1	A	2111	U
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2117	A

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Mol	Chain	Res	Type
1	A	2118	U
1	A	2121	G
1	A	2122	U
1	A	2125	G
1	A	2130	U
1	A	2131	U
1	A	2132	U
1	A	2134	A
1	A	2139	U
1	A	2142	A
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2150	C
1	A	2154	A
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2160	C
1	A	2162	G
1	A	2164	C
1	A	2165	C
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2178	C
1	A	2182	U
1	A	2183	A
1	A	2189	U
1	A	2193	G
1	A	2194	U
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2214	C
1	A	2216	G
1	A	2221	G
1	A	2223	G
1	A	2225	A

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Mol	Chain	Res	Type
1	A	2226	C
1	A	2234	G
1	A	2238	G
1	A	2243	U
1	A	2249	U
1	A	2250	G
1	A	2266	A
1	A	2278	A
1	A	2279	G
1	A	2280	G
1	A	2282	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2292	U
1	A	2297	A
1	A	2301	C
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2311	A
1	A	2319	G
1	A	2322	A
1	A	2325	G
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2339	C
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2353	G
1	A	2354	C
1	A	2355	G
1	A	2357	G
1	A	2361	G
1	A	2376	A
1	A	2383	G
1	A	2384	U

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Mol	Chain	Res	Type
1	A	2385	C
1	A	2388	A
1	A	2391	G
1	A	2400	G
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2408	U
1	A	2409	G
1	A	2410	G
1	A	2419	U
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2432	A
1	A	2434	A
1	A	2435	A
1	A	2436	G
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2457	PSU
1	A	2464	G
1	A	2468	A
1	A	2469	A
1	A	2470	G
1	A	2476	A
1	A	2480	C
1	A	2484	G
1	A	2487	G
1	A	2490	G
1	A	2491	U
1	A	2492	U
1	A	2494	G
1	A	2498	OMC
1	A	2500	U

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Mol	Chain	Res	Type
1	A	2502	G
1	A	2503	A
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2511	U
1	A	2513	A
1	A	2517	C
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2528	U
1	A	2531	A
1	A	2535	G
1	A	2549	G
1	A	2554	U
1	A	2561	U
1	A	2562	U
1	A	2566	A
1	A	2567	G
1	A	2569	G
1	A	2573	C
1	A	2574	G
1	A	2578	G
1	A	2582	G
1	A	2585	U
1	A	2602	A
1	A	2603	G
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2621	G
1	A	2623	G
1	A	2629	U
1	A	2632	A
1	A	2634	A
1	A	2636	C
1	A	2639	A
1	A	2645	G
1	A	2646	C

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Mol	Chain	Res	Type
1	A	2647	U
1	A	2656	U
1	A	2658	C
1	A	2663	G
1	A	2665	A
1	A	2673	G
1	A	2682	A
1	A	2685	G
1	A	2689	U
1	A	2690	U
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2723	C
1	A	2725	A
1	A	2726	A
1	A	2728	U
1	A	2731	G
1	A	2732	G
1	A	2733	A
1	A	2735	G
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2750	A
1	A	2751	G
1	A	2752	C
1	A	2754	U
1	A	2756	U
1	A	2761	A
1	A	2762	C
1	A	2763	G
1	A	2765	A
1	A	2776	A
1	A	2777	G
1	A	2778	A
1	A	2780	G
1	A	2784	U
1	A	2791	G
1	A	2792	A
1	A	2793	C

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Mol	Chain	Res	Type
1	A	2794	C
1	A	2797	U
1	A	2800	A
1	A	2803	G
1	A	2805	C
1	A	2809	A
1	A	2813	A
1	A	2816	G
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2823	A
1	A	2824	C
1	A	2830	C
1	A	2833	U
1	A	2835	A
1	A	2836	U
1	A	2848	G
1	A	2849	U
1	A	2854	G
1	A	2867	G
1	A	2873	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2885	G
1	A	2886	A
1	A	2891	U
1	A	2892	G
1	A	2898	U
1	A	2899	A
1	A	2902	C
1	A	2903	U
1	A	2904	U
2	B	7	G
2	B	9	G
2	B	12	C
2	B	14	U
2	B	15	A
2	B	17	C
2	B	22	U
2	B	24	G

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Mol	Chain	Res	Type
2	B	29	A
2	B	30	C
2	B	34	A
2	B	35	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	47	C
2	B	56	G
2	B	58	A
2	B	64	G
2	B	66	A
2	B	68	C
2	B	83	G
2	B	86	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	99	A
2	B	105	G
2	B	108	A
2	B	109	A
2	B	117	G
2	B	118	C
2	B	119	A
32	a	3	A
32	a	4	U
32	a	6	G
32	a	9	G
32	a	11	G
32	a	13	U
32	a	18	C
32	a	22	G
32	a	25	C
32	a	32	A
32	a	33	A
32	a	43	C
32	a	47	C
32	a	48	C
32	a	50	A

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Mol	Chain	Res	Type
32	a	51	A
32	a	54	C
32	a	58	C
32	a	60	A
32	a	65	A
32	a	66	A
32	a	70	U
32	a	71	A
32	a	72	A
32	a	82	G
32	a	83	C
32	a	84	U
32	a	86	G
32	a	87	C
32	a	88	U
32	a	92	U
32	a	93	U
32	a	94	G
32	a	95	C
32	a	99	C
32	a	100	G
32	a	101	A
32	a	104	G
32	a	105	G
32	a	108	G
32	a	109	A
32	a	110	C
32	a	114	U
32	a	119	A
32	a	120	A
32	a	122	G
32	a	126	G
32	a	127	G
32	a	128	G
32	a	129	A
32	a	130	A
32	a	131	A
32	a	132	C
32	a	133	U
32	a	134	G
32	a	137	U
32	a	141	G

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Mol	Chain	Res	Type
32	a	142	G
32	a	144	G
32	a	145	G
32	a	146	G
32	a	149	A
32	a	158	G
32	a	161	A
32	a	163	C
32	a	164	G
32	a	165	G
32	a	168	G
32	a	169	C
32	a	171	A
32	a	173	U
32	a	182	A
32	a	184	G
32	a	187	G
32	a	191	G
32	a	195	A
32	a	197	A
32	a	202	G
32	a	203	G
32	a	204	G
32	a	205	A
32	a	207	C
32	a	209	U
32	a	210	C
32	a	211	G
32	a	212	G
32	a	213	G
32	a	214	C
32	a	217	C
32	a	219	U
32	a	226	G
32	a	231	U
32	a	232	G
32	a	235	C
32	a	240	G
32	a	245	U
32	a	247	G
32	a	251	G
32	a	253	A

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Mol	Chain	Res	Type
32	a	256	U
32	a	260	G
32	a	261	U
32	a	264	C
32	a	266	G
32	a	267	C
32	a	279	A
32	a	281	G
32	a	289	G
32	a	298	A
32	a	300	A
32	a	301	G
32	a	306	A
32	a	308	C
32	a	315	A
32	a	316	C
32	a	321	A
32	a	322	C
32	a	328	C
32	a	329	A
32	a	332	G
32	a	346	G
32	a	350	G
32	a	351	G
32	a	352	C
32	a	354	G
32	a	356	A
32	a	362	G
32	a	367	U
32	a	368	U
32	a	369	G
32	a	370	C
32	a	371	A
32	a	372	C
32	a	373	A
32	a	377	G
32	a	378	G
32	a	380	G
32	a	382	A
32	a	390	U
32	a	392	C
32	a	397	A

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Mol	Chain	Res	Type
32	a	398	U
32	a	406	G
32	a	408	A
32	a	412	A
32	a	413	G
32	a	414	A
32	a	421	U
32	a	422	C
32	a	423	G
32	a	424	G
32	a	425	G
32	a	426	U
32	a	429	U
32	a	434	U
32	a	436	C
32	a	437	U
32	a	439	U
32	a	449	G
32	a	451	A
32	a	454	G
32	a	456	A
32	a	458	U
32	a	463	U
32	a	464	U
32	a	465	A
32	a	467	U
32	a	469	C
32	a	474	G
32	a	476	U
32	a	478	A
32	a	481	G
32	a	482	A
32	a	484	G
32	a	485	U
32	a	488	C
32	a	495	A
32	a	497	G
32	a	499	A
32	a	503	C
32	a	507	C
32	a	508	U
32	a	509	A

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Mol	Chain	Res	Type
32	a	511	C
32	a	514	C
32	a	517	G
32	a	518	C
32	a	521	G
32	a	527	A
32	a	529	G
32	a	531	U
32	a	532	A
32	a	533	A
32	a	536	C
32	a	542	G
32	a	547	A
32	a	549	C
32	a	555	U
32	a	559	A
32	a	561	U
32	a	562	U
32	a	563	A
32	a	564	C
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	579	A
32	a	585	G
32	a	588	G
32	a	596	A
32	a	605	U
32	a	606	G
32	a	607	A
32	a	615	G
32	a	619	U
32	a	620	C
32	a	625	U
32	a	626	G
32	a	632	U
32	a	633	G
32	a	641	U
32	a	642	A
32	a	647	C

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Mol	Chain	Res	Type
32	a	653	U
32	a	654	G
32	a	656	G
32	a	661	G
32	a	665	A
32	a	667	G
32	a	671	G
32	a	672	U
32	a	687	A
32	a	688	G
32	a	701	U
32	a	702	A
32	a	703	G
32	a	707	U
32	a	712	A
32	a	713	G
32	a	720	C
32	a	721	G
32	a	723	U
32	a	724	G
32	a	729	A
32	a	731	G
32	a	733	G
32	a	734	G
32	a	744	C
32	a	747	A
32	a	748	G
32	a	752	G
32	a	753	A
32	a	755	G
32	a	760	G
32	a	772	U
32	a	774	G
32	a	787	A
32	a	790	A
32	a	793	U
32	a	794	A
32	a	799	G
32	a	809	G
32	a	812	G
32	a	813	U
32	a	814	A

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Mol	Chain	Res	Type
32	a	815	A
32	a	817	C
32	a	818	G
32	a	820	U
32	a	821	G
32	a	827	U
32	a	828	U
32	a	829	G
32	a	832	G
32	a	841	C
32	a	844	G
32	a	845	A
32	a	846	G
32	a	849	G
32	a	851	G
32	a	854	U
32	a	862	C
32	a	873	A
32	a	874	G
32	a	880	C
32	a	884	U
32	a	899	C
32	a	902	G
32	a	913	A
32	a	914	A
32	a	919	A
32	a	922	G
32	a	931	C
32	a	934	C
32	a	935	A
32	a	939	G
32	a	941	G
32	a	943	U
32	a	960	U
32	a	961	U
32	a	965	U
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	971	G
32	a	974	A

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Mol	Chain	Res	Type
32	a	975	A
32	a	976	G
32	a	977	A
32	a	983	A
32	a	986	U
32	a	990	C
32	a	992	U
32	a	993	G
32	a	994	A
32	a	996	A
32	a	999	C
32	a	1001	C
32	a	1004	A
32	a	1009	U
32	a	1017	U
32	a	1018	G
32	a	1023	U
32	a	1024	G
32	a	1026	G
32	a	1028	C
32	a	1029	U
32	a	1030	U
32	a	1031	C
32	a	1032	G
32	a	1033	G
32	a	1034	G
32	a	1036	A
32	a	1037	C
32	a	1043	G
32	a	1044	A
32	a	1046	A
32	a	1053	G
32	a	1054	C
32	a	1056	U
32	a	1061	G
32	a	1065	U
32	a	1070	U
32	a	1081	A
32	a	1082	A
32	a	1085	U
32	a	1087	G
32	a	1088	G

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Mol	Chain	Res	Type
32	a	1089	G
32	a	1094	G
32	a	1095	U
32	a	1100	C
32	a	1101	A
32	a	1110	A
32	a	1118	U
32	a	1119	C
32	a	1123	U
32	a	1124	G
32	a	1125	U
32	a	1127	G
32	a	1132	C
32	a	1136	C
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1140	C
32	a	1141	C
32	a	1142	G
32	a	1143	G
32	a	1145	A
32	a	1146	A
32	a	1148	U
32	a	1150	A
32	a	1151	A
32	a	1152	A
32	a	1157	A
32	a	1159	U
32	a	1160	G
32	a	1168	U
32	a	1169	A
32	a	1171	A
32	a	1174	G
32	a	1181	G
32	a	1184	G
32	a	1190	G
32	a	1191	A
32	a	1193	G
32	a	1194	U
32	a	1195	C
32	a	1196	A

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Mol	Chain	Res	Type
32	a	1197	A
32	a	1200	C
32	a	1201	A
32	a	1204	A
32	a	1207	2MG
32	a	1212	U
32	a	1213	A
32	a	1220	G
32	a	1221	G
32	a	1224	U
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1229	A
32	a	1236	A
32	a	1238	A
32	a	1239	A
32	a	1240	U
32	a	1256	A
32	a	1257	A
32	a	1258	G
32	a	1260	G
32	a	1261	A
32	a	1266	G
32	a	1267	C
32	a	1271	A
32	a	1275	A
32	a	1278	G
32	a	1280	A
32	a	1281	C
32	a	1282	C
32	a	1283	U
32	a	1286	U
32	a	1287	A
32	a	1298	U
32	a	1299	A
32	a	1300	G
32	a	1302	C
32	a	1305	G
32	a	1309	G
32	a	1314	C
32	a	1317	C

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Mol	Chain	Res	Type
32	a	1318	A
32	a	1322	C
32	a	1324	A
32	a	1327	C
32	a	1331	G
32	a	1332	A
32	a	1336	C
32	a	1346	A
32	a	1347	G
32	a	1348	U
32	a	1351	U
32	a	1359	C
32	a	1361	G
32	a	1362	A
32	a	1363	A
32	a	1366	C
32	a	1370	G
32	a	1374	A
32	a	1375	A
32	a	1379	G
32	a	1381	U
32	a	1389	C
32	a	1394	A
32	a	1395	C
32	a	1397	C
32	a	1404	C
32	a	1419	G
32	a	1422	G
32	a	1427	C
32	a	1428	A
32	a	1429	A
32	a	1432	G
32	a	1433	A
32	a	1436	U
32	a	1441	A
32	a	1446	A
32	a	1448	C
32	a	1452	C
32	a	1453	G
32	a	1455	G
32	a	1458	G
32	a	1491	G

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Mol	Chain	Res	Type
32	a	1492	A
32	a	1493	A
32	a	1494	G
32	a	1499	A
32	a	1502	A
32	a	1503	A
32	a	1506	U
32	a	1517	G
32	a	1520	C
32	a	1529	G
32	a	1530	G
32	a	1533	C
32	a	1534	A
55	x	5	G
55	x	7	U
55	x	8	G
55	x	12	C
55	x	15	C
55	x	17	U
55	x	18	G
55	x	19	G
55	x	20	U
55	x	21	A
55	x	22	G
55	x	26	G
55	x	35	A
55	x	36	U
55	x	47	U
55	x	48	C
55	x	49	G
55	x	50	U
55	x	52	G
55	x	59	A
55	x	60	U
55	x	76	A
55	y	4	G
55	y	5	G
55	y	15	C
55	y	16	C
55	y	18	G
55	y	20	U
55	y	21	A

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Mol	Chain	Res	Type
55	y	22	G
55	y	35	A
55	y	37	A
55	y	46	G
55	y	47	U
55	y	48	C
55	y	49	G
55	y	55	U
55	y	60	U
55	y	61	C
55	y	76	A
56	z	45	A

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	62	U
1	A	100	U
1	A	119	A
1	A	137	U
1	A	177	G
1	A	181	A
1	A	196	A
1	A	197	A
1	A	212	G
1	A	249	C
1	A	264	C
1	A	271	G
1	A	279	A
1	A	310	A
1	A	322	A
1	A	404	A
1	A	412	A
1	A	446	G
1	A	455	C
1	A	463	G
1	A	481	G
1	A	506	G
1	A	512	G
1	A	620	G
1	A	675	A

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Mol	Chain	Res	Type
1	A	728	G
1	A	733	G
1	A	762	U
1	A	764	A
1	A	784	G
1	A	830	G
1	A	884	U
1	A	896	A
1	A	913	U
1	A	974	G
1	A	984	A
1	A	1088	A
1	A	1126	A
1	A	1140	C
1	A	1141	U
1	A	1151	A
1	A	1190	G
1	A	1200	C
1	A	1224	U
1	A	1288	G
1	A	1311	G
1	A	1320	C
1	A	1344	U
1	A	1379	U
1	A	1602	U
1	A	1608	A
1	A	1730	C
1	A	1786	A
1	A	1857	G
1	A	1884	G
1	A	1918	A
1	A	1937	A
1	A	1939	5MU
1	A	2074	U
1	A	2146	C
1	A	2157	G
1	A	2182	U
1	A	2193	G
1	A	2225	A
1	A	2286	G
1	A	2324	U
1	A	2326	C

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Mol	Chain	Res	Type
1	A	2427	C
1	A	2458	G
1	A	2504	PSU
1	A	2517	C
1	A	2519	U
1	A	2581	G
1	A	2595	G
1	A	2602	A
1	A	2638	G
1	A	2645	G
1	A	2681	C
1	A	2790	U
1	A	2808	G
1	A	2893	A
2	B	40	U

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

28 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	2MG	A	1835	1	19,26,27	1.30	2 (10%)	20,38,41	2.42	7 (35%)
1	PSU	A	1911	1	16,21,22	1.15	1 (6%)	20,30,33	3.56	6 (30%)
1	PSU	A	1917	1	16,21,22	1.13	1 (6%)	20,30,33	3.66	8 (40%)
1	5MU	A	1939	1	14,22,23	0.96	1 (7%)	16,32,35	2.88	5 (31%)
1	5MC	A	1962	1	15,22,23	1.58	1 (6%)	17,32,35	1.00	0
1	OMG	A	2251	1,55	18,26,27	1.34	3 (16%)	22,38,41	2.00	6 (27%)
1	2MG	A	2445	1	19,26,27	1.30	2 (10%)	20,38,41	2.38	7 (35%)
1	PSU	A	2457	1	16,21,22	1.36	1 (6%)	20,30,33	3.69	7 (35%)
1	OMC	A	2498	1,57	15,22,23	0.84	1 (6%)	19,31,34	1.24	2 (10%)
1	PSU	A	2504	1	16,21,22	1.39	1 (6%)	20,30,33	3.68	9 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	A	2552	1	14,22,23	0.89	0	18,31,34	2.12	2 (11%)
1	PSU	A	2580	1	16,21,22	1.37	2 (12%)	20,30,33	3.52	8 (40%)
1	PSU	A	2605	1	16,21,22	1.23	1 (6%)	20,30,33	3.32	7 (35%)
1	1MG	A	745	1	18,26,27	1.44	3 (16%)	18,39,42	1.74	3 (16%)
1	PSU	A	746	1,57	16,21,22	1.29	1 (6%)	20,30,33	3.47	5 (25%)
1	5MU	A	747	1	14,22,23	0.87	1 (7%)	16,32,35	2.62	5 (31%)
1	PSU	A	955	1	16,21,22	1.13	1 (6%)	20,30,33	3.52	6 (30%)
32	2MG	a	1207	32	19,26,27	1.51	3 (15%)	20,38,41	2.51	8 (40%)
32	4OC	a	1402	32	16,23,24	0.77	0	19,32,35	1.20	3 (15%)
32	5MC	a	1407	32	15,22,23	1.62	2 (13%)	17,32,35	1.04	1 (5%)
32	UR3	a	1498	32	14,22,23	1.03	1 (7%)	16,32,35	0.99	1 (6%)
32	2MG	a	1516	32	19,26,27	1.36	2 (10%)	20,38,41	2.40	8 (40%)
32	MA6	a	1518	32	16,26,27	1.17	1 (6%)	18,38,41	2.69	5 (27%)
32	MA6	a	1519	32	16,26,27	1.19	1 (6%)	18,38,41	2.50	7 (38%)
32	PSU	a	516	32	16,21,22	1.06	1 (6%)	20,30,33	3.68	8 (40%)
32	2MG	a	966	32	19,26,27	1.47	3 (15%)	20,38,41	2.45	7 (35%)
32	5MC	a	967	32	15,22,23	1.64	1 (6%)	17,32,35	1.00	1 (5%)
53	MEQ	v	252	53	9,9,10	0.47	0	7,10,12	0.91	0

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
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/3/25/26	0/2/2/2
1	OMG	A	2251	1,55	-	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	-	0/5/27/28	0/3/3/3
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	1,57	-	0/5/27/28	0/2/2/2
1	PSU	A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	746	1,57	-	0/7/25/26	0/2/2/2
1	5MU	A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	-	0/5/27/28	0/3/3/3
32	4OC	a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	a	1498	32	-	0/3/25/26	0/2/2/2
32	2MG	a	1516	32	-	0/5/27/28	0/3/3/3
32	MA6	a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2
32	2MG	a	966	32	-	0/5/27/28	0/3/3/3
32	5MC	a	967	32	-	0/3/25/26	0/2/2/2
53	MEQ	v	252	53	-	0/7/9/11	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2504	PSU	C5-C1'	-4.42	1.48	1.52
1	A	2457	PSU	C5-C1'	-4.30	1.48	1.52
1	A	2580	PSU	C5-C1'	-3.91	1.48	1.52
1	A	746	PSU	C5-C1'	-3.76	1.49	1.52
1	A	2605	PSU	C5-C1'	-3.29	1.49	1.52
1	A	1911	PSU	C5-C1'	-3.25	1.49	1.52
1	A	955	PSU	C5-C1'	-3.22	1.49	1.52
1	A	1917	PSU	C5-C1'	-2.98	1.49	1.52
32	a	516	PSU	C5-C1'	-2.76	1.49	1.52
1	A	2580	PSU	C2-N3	-2.12	1.34	1.38
1	A	1939	5MU	C2-N3	-2.05	1.34	1.38
1	A	2251	OMG	O4'-C1'	2.05	1.44	1.41
32	a	1407	5MC	O4'-C1'	2.05	1.44	1.41
1	A	747	5MU	O4'-C1'	2.11	1.44	1.41
1	A	2498	OMC	O4'-C1'	2.18	1.44	1.41
32	a	966	2MG	C2-N2	2.35	1.36	1.34
32	a	1207	2MG	C2-N2	2.36	1.36	1.34
1	A	745	1MG	C6-N1	2.62	1.42	1.38
32	a	1498	UR3	C4-N3	2.78	1.42	1.38
1	A	2445	2MG	C5-C4	2.79	1.46	1.40
32	a	1516	2MG	C5-C4	2.95	1.47	1.40
1	A	1835	2MG	C5-C4	2.99	1.47	1.40
1	A	745	1MG	C5-C4	3.00	1.47	1.40
32	a	1518	MA6	C5-C4	3.04	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2251	OMG	C5-C4	3.09	1.47	1.40
32	a	1519	MA6	C5-C4	3.24	1.47	1.40
32	a	966	2MG	C5-C4	3.35	1.48	1.40
32	a	1207	2MG	C5-C4	3.40	1.48	1.40
1	A	745	1MG	C6-C5	3.61	1.47	1.41
1	A	2445	2MG	C6-C5	3.65	1.48	1.41
1	A	1835	2MG	C6-C5	3.76	1.48	1.41
1	A	2251	OMG	C6-C5	3.77	1.48	1.41
32	a	1516	2MG	C6-C5	3.97	1.48	1.41
32	a	966	2MG	C6-C5	4.03	1.49	1.41
32	a	1207	2MG	C6-C5	4.16	1.49	1.41
32	a	1407	5MC	C5-C4	5.46	1.49	1.41
1	A	1962	5MC	C5-C4	5.50	1.49	1.41
32	a	967	5MC	C5-C4	5.67	1.49	1.41

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1911	PSU	N1-C2-N3	-9.86	121.31	128.40
1	A	1917	PSU	N1-C2-N3	-9.85	121.32	128.40
32	a	516	PSU	N1-C2-N3	-9.66	121.45	128.40
1	A	955	PSU	N1-C2-N3	-9.13	121.83	128.40
1	A	746	PSU	N1-C2-N3	-9.02	121.91	128.40
1	A	2504	PSU	N1-C2-N3	-9.02	121.91	128.40
1	A	2457	PSU	N1-C2-N3	-8.81	122.06	128.40
1	A	2605	PSU	N1-C2-N3	-8.71	122.14	128.40
1	A	2457	PSU	C5-C4-N3	-8.63	118.35	125.43
1	A	2504	PSU	C5-C4-N3	-8.57	118.40	125.43
1	A	2580	PSU	N1-C2-N3	-8.51	122.28	128.40
1	A	2580	PSU	C5-C4-N3	-8.40	118.53	125.43
1	A	955	PSU	C5-C4-N3	-8.40	118.54	125.43
1	A	1917	PSU	C5-C4-N3	-8.28	118.63	125.43
1	A	746	PSU	C5-C4-N3	-8.25	118.66	125.43
32	a	516	PSU	C5-C4-N3	-8.22	118.69	125.43
1	A	1911	PSU	C5-C4-N3	-7.69	119.12	125.43
1	A	2605	PSU	C5-C4-N3	-6.73	119.91	125.43
1	A	747	5MU	C5-C4-N3	-6.20	118.40	125.24
32	a	1518	MA6	N3-C2-N1	-6.13	123.52	128.86
32	a	1519	MA6	N3-C2-N1	-6.01	123.62	128.86
1	A	1939	5MU	C5-C4-N3	-5.99	118.64	125.24
1	A	2457	PSU	C5-C1'-C2'	-5.15	106.67	115.55
32	a	1516	2MG	C6-C5-C4	-4.45	116.41	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1939	5MU	C4'-O4'-C1'	-4.39	105.10	109.77
1	A	1835	2MG	C6-C5-C4	-4.36	116.51	120.84
1	A	2445	2MG	C6-C5-C4	-4.34	116.52	120.84
1	A	2605	PSU	C5-C6-N1	-4.24	118.89	124.39
1	A	2605	PSU	C5-C1'-C2'	-4.09	108.50	115.55
32	a	1519	MA6	C4-C5-N7	-4.08	105.47	109.41
1	A	2504	PSU	C5-C6-N1	-4.08	119.10	124.39
1	A	746	PSU	C5-C6-N1	-4.01	119.19	124.39
1	A	2457	PSU	C5-C6-N1	-3.92	119.31	124.39
32	a	1207	2MG	C6-C5-C4	-3.80	117.06	120.84
32	a	1516	2MG	C5-C6-N1	-3.75	118.14	123.48
32	a	1207	2MG	C5-C6-N1	-3.71	118.19	123.48
1	A	2445	2MG	C5-C6-N1	-3.69	118.23	123.48
32	a	966	2MG	C6-C5-C4	-3.69	117.18	120.84
1	A	2580	PSU	C5-C6-N1	-3.64	119.66	124.39
32	a	966	2MG	C5-C6-N1	-3.62	118.33	123.48
1	A	955	PSU	C5-C6-N1	-3.47	119.89	124.39
1	A	2251	OMG	C5-C6-N1	-3.47	118.54	123.48
1	A	1911	PSU	C5-C6-N1	-3.42	119.96	124.39
1	A	2504	PSU	C5-C1'-C2'	-3.39	109.69	115.55
32	a	516	PSU	C5-C6-N1	-3.36	120.03	124.39
1	A	955	PSU	C5-C1'-C2'	-3.36	109.75	115.55
32	a	516	PSU	C5-C1'-C2'	-3.31	109.84	115.55
1	A	2251	OMG	C6-C5-C4	-3.30	117.57	120.84
1	A	1835	2MG	C5-C6-N1	-3.26	118.85	123.48
32	a	1516	2MG	C4-C5-N7	-3.18	106.34	109.41
32	a	1519	MA6	C10-N6-C9	-3.11	105.97	116.03
1	A	1911	PSU	C5-C1'-C2'	-3.06	110.26	115.55
1	A	2251	OMG	N3-C2-N1	-3.05	123.00	127.46
32	a	1207	2MG	N3-C2-N1	-3.01	121.68	126.23
32	a	966	2MG	N3-C2-N1	-2.91	121.83	126.23
1	A	2580	PSU	C5-C1'-C2'	-2.90	110.54	115.55
1	A	1917	PSU	C5-C6-N1	-2.85	120.69	124.39
1	A	2445	2MG	N3-C2-N1	-2.79	122.01	126.23
1	A	2445	2MG	C4-C5-N7	-2.73	106.77	109.41
1	A	1835	2MG	N3-C2-N1	-2.72	122.11	126.23
32	a	1207	2MG	C4-C5-N7	-2.70	106.80	109.41
1	A	1917	PSU	C5-C1'-C2'	-2.70	110.90	115.55
1	A	2251	OMG	C4-C5-N7	-2.61	106.89	109.41
32	a	1516	2MG	N3-C2-N1	-2.60	122.30	126.23
32	a	1519	MA6	C9-N6-C6	-2.58	111.69	119.51
32	a	1519	MA6	C10-N6-C6	-2.54	111.83	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1518	MA6	C9-N6-C6	-2.52	111.90	119.51
32	a	966	2MG	C4-C5-N7	-2.46	107.04	109.41
1	A	745	1MG	C4-C5-N7	-2.45	107.05	109.41
1	A	1939	5MU	C5-C6-N1	-2.45	119.50	122.15
1	A	1835	2MG	C4-C5-N7	-2.41	107.08	109.41
1	A	745	1MG	C6-C5-C4	-2.29	118.34	119.92
32	a	1518	MA6	C4-C5-N7	-2.29	107.20	109.41
32	a	1402	4OC	C5-C4-N3	-2.21	119.52	123.21
32	a	1516	2MG	CM2-N2-C2	-2.07	121.11	123.63
1	A	2552	OMU	C6-N1-C2	-2.05	117.95	121.28
32	a	1407	5MC	O4'-C1'-N1	2.00	112.09	108.08
32	a	1498	UR3	O3'-C3'-C4'	2.02	116.98	111.09
1	A	2504	PSU	C4'-O4'-C1'	2.07	111.87	109.48
1	A	747	5MU	C5M-C5-C4	2.10	122.59	120.17
1	A	1917	PSU	C4'-O4'-C1'	2.11	111.93	109.48
32	a	516	PSU	O4'-C1'-C5	2.19	113.32	109.93
1	A	2504	PSU	O4'-C1'-C2'	2.20	107.98	104.45
1	A	747	5MU	C4'-O4'-C1'	2.22	112.13	109.77
32	a	1402	4OC	N4-C4-N3	2.31	122.27	116.37
1	A	747	5MU	O4'-C1'-N1	2.33	112.74	108.08
1	A	2605	PSU	O4'-C1'-C5	2.41	113.66	109.93
1	A	2580	PSU	O4'-C1'-C2'	2.43	108.36	104.45
32	a	967	5MC	O4'-C1'-N1	2.44	112.96	108.08
1	A	2498	OMC	N4-C4-N3	2.45	120.77	116.64
32	a	1516	2MG	N2-C2-N1	2.48	119.36	116.95
1	A	2580	PSU	C3'-C2'-C1'	2.50	104.82	101.93
32	a	1207	2MG	C4'-O4'-C1'	2.56	112.50	109.77
1	A	2498	OMC	O4'-C1'-N1	2.64	113.36	108.08
32	a	1402	4OC	O4'-C1'-N1	2.69	113.47	108.08
1	A	2457	PSU	C3'-C2'-C1'	2.69	105.04	101.93
1	A	1917	PSU	C3'-C2'-C1'	2.75	105.11	101.93
32	a	516	PSU	C3'-C2'-C1'	2.87	105.24	101.93
1	A	1939	5MU	O4'-C1'-N1	2.94	113.97	108.08
1	A	2445	2MG	N2-C2-N1	2.98	119.85	116.95
32	a	1519	MA6	N1-C6-N6	3.18	120.38	117.00
1	A	2504	PSU	C3'-C2'-C1'	3.61	106.10	101.93
1	A	2251	OMG	C6-N1-C2	3.89	121.66	116.06
1	A	2580	PSU	C6-N1-C2	3.98	121.72	115.36
32	a	966	2MG	N2-C2-N3	4.02	120.86	116.95
32	a	1516	2MG	C6-N1-C2	4.03	122.39	115.18
1	A	1835	2MG	C6-N1-C2	4.03	122.39	115.18
1	A	2445	2MG	C6-N1-C2	4.06	122.44	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1917	PSU	C6-N1-C2	4.10	121.92	115.36
1	A	2457	PSU	C6-N1-C2	4.11	121.94	115.36
1	A	955	PSU	C6-N1-C2	4.13	121.97	115.36
32	a	966	2MG	C6-N1-C2	4.17	122.65	115.18
1	A	2504	PSU	C6-N1-C2	4.22	122.11	115.36
32	a	516	PSU	C6-N1-C2	4.26	122.18	115.36
32	a	1207	2MG	C6-N1-C2	4.31	122.90	115.18
1	A	746	PSU	C6-N1-C2	4.31	122.27	115.36
32	a	1518	MA6	C2-N1-C6	4.33	122.44	111.82
1	A	1911	PSU	C6-N1-C2	4.34	122.31	115.36
32	a	1207	2MG	N2-C2-N3	4.36	121.19	116.95
1	A	2605	PSU	C6-N1-C2	4.40	122.40	115.36
32	a	1519	MA6	C2-N1-C6	4.47	122.78	111.82
1	A	1835	2MG	N2-C2-N3	4.53	121.35	116.95
1	A	2605	PSU	C4-N3-C2	5.31	119.81	115.16
1	A	2251	OMG	C2-N3-C4	5.33	121.38	115.16
32	a	1516	2MG	C2-N3-C4	5.43	121.31	115.11
1	A	2445	2MG	C2-N3-C4	5.51	121.39	115.11
1	A	1835	2MG	C2-N3-C4	5.64	121.54	115.11
32	a	1207	2MG	C2-N3-C4	5.82	121.76	115.11
1	A	745	1MG	C2-N3-C4	5.89	122.03	115.16
32	a	966	2MG	C2-N3-C4	5.94	121.89	115.11
1	A	746	PSU	C4-N3-C2	6.23	120.61	115.16
1	A	2504	PSU	C4-N3-C2	6.27	120.64	115.16
1	A	2580	PSU	C4-N3-C2	6.44	120.79	115.16
1	A	955	PSU	C4-N3-C2	6.54	120.88	115.16
1	A	2457	PSU	C4-N3-C2	6.61	120.94	115.16
1	A	1911	PSU	C4-N3-C2	6.62	120.95	115.16
32	a	1518	MA6	N1-C6-N6	6.80	124.21	117.00
32	a	516	PSU	C4-N3-C2	6.81	121.12	115.16
1	A	1917	PSU	C4-N3-C2	7.02	121.30	115.16
1	A	1939	5MU	C4-N3-C2	7.06	121.33	115.16
1	A	747	5MU	C4-N3-C2	7.15	121.41	115.16
1	A	2552	OMU	C4-N3-C2	8.07	121.06	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1835	2MG	2	0
1	A	1939	5MU	1	0
1	A	1962	5MC	1	0
1	A	2504	PSU	14	0
1	A	2605	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 125 ligands modelled in this entry, 125 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.