



Full wwPDB EM Validation Report ⓘ

Nov 3, 2025 – 04:40 PM JST

PDB ID : 8ZFF / pdb_00008zff
EMDB ID : EMD-60059
Title : Structure of the Bacterial Ribosome without hypoxia-induced rRNA modifications
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Ito, T.; Suzuki, T.
Deposited on : 2024-05-07
Resolution : 2.59 Å(reported)
Based on initial model : 7K00

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

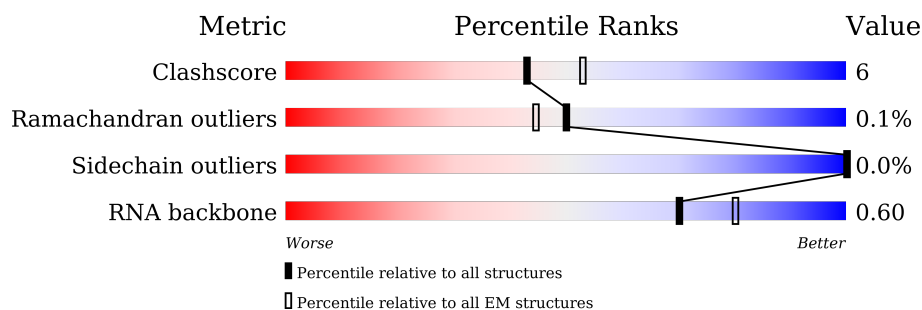
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	

















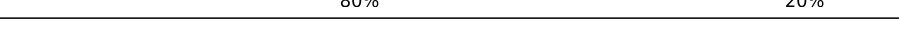
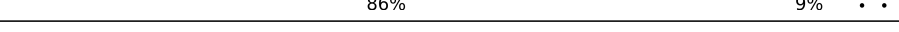
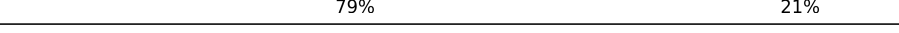


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Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	

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Mol	Chain	Length	Quality of chain
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	66	
54	Z	77	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MS6	1	82	X	-	-	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 140322 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32466	14487	5964	10503	1512		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2761	Total	C	N	O	P	0	0
			59301	26460	10925	19155	2761		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 42 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	6	Total	C	N	O	P	0	0
			130	58	25	41	6		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

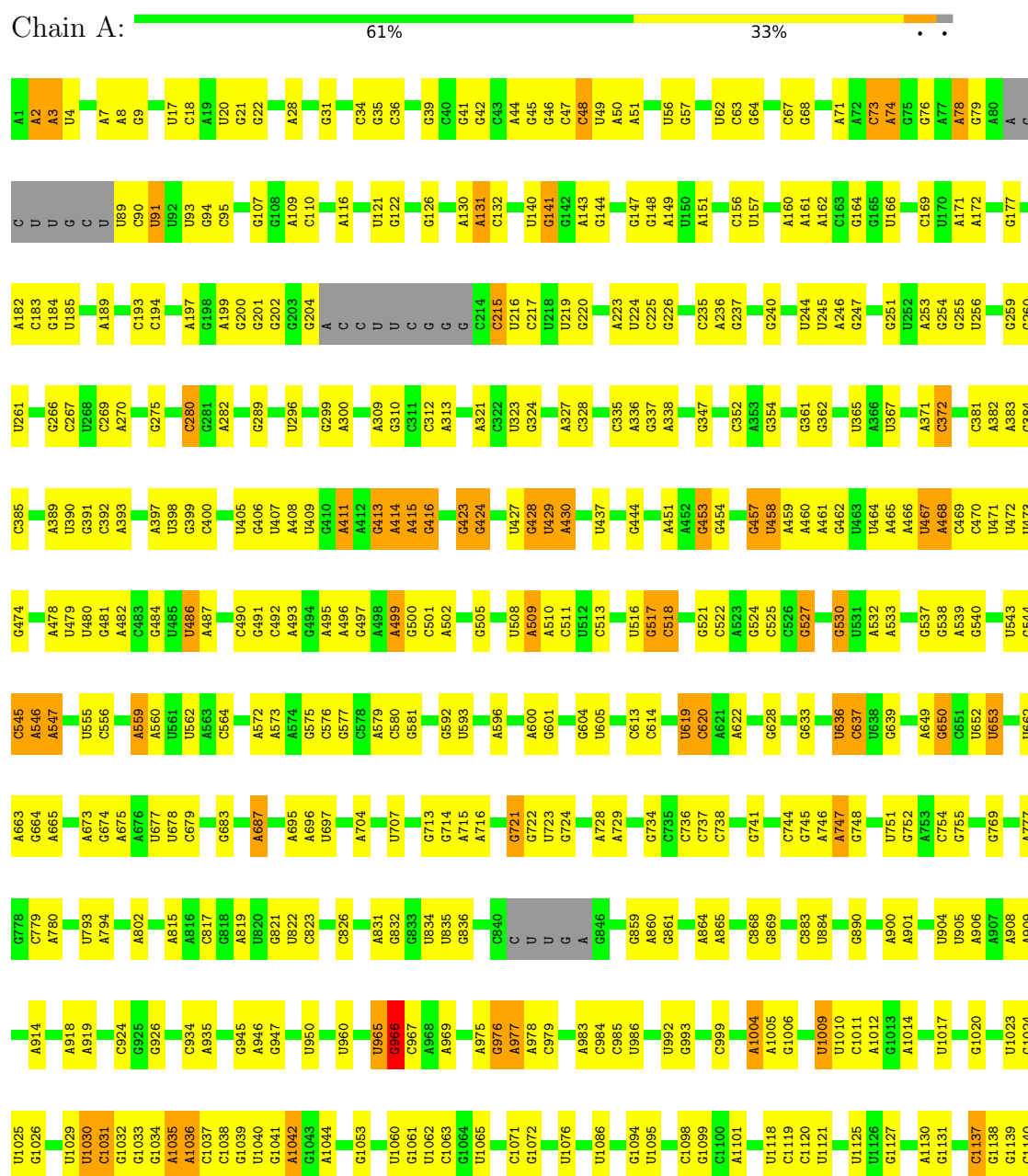
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

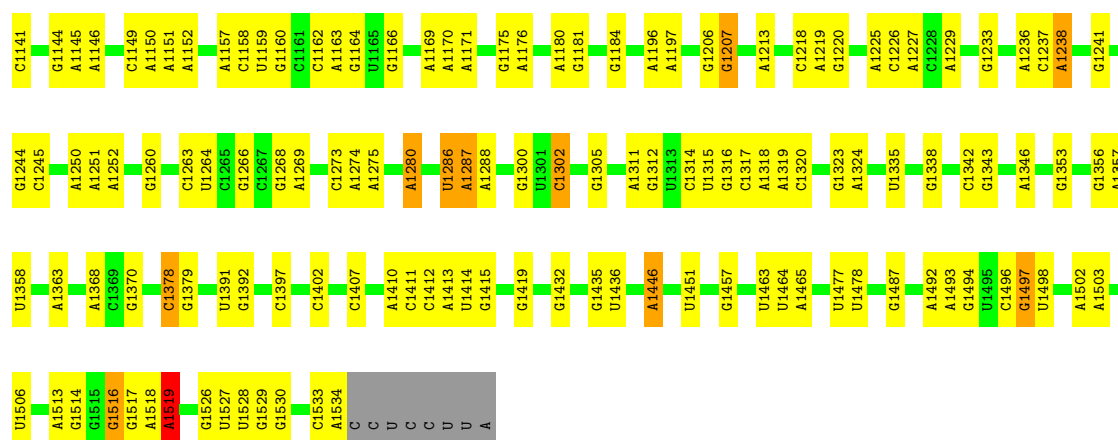
Mol	Chain	Residues	Atoms		AltConf
55	A	119	Total	Mg	0
			119	119	
55	a	328	Total	Mg	0
			328	328	
55	b	6	Total	Mg	0
			6	6	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	
55	Z	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

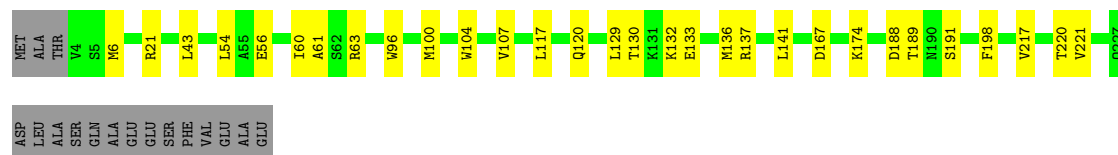
• Molecule 1: 16S rRNA





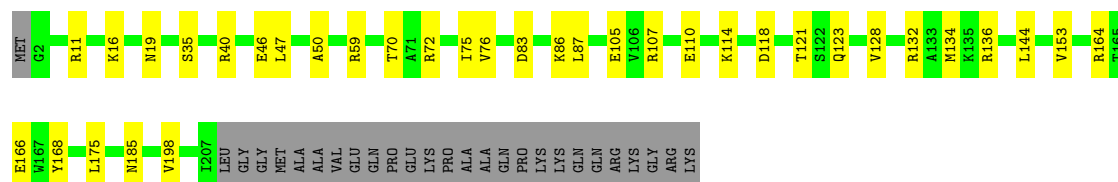
- Molecule 2: Small ribosomal subunit protein uS2

Chain B: 80% 12% 7%



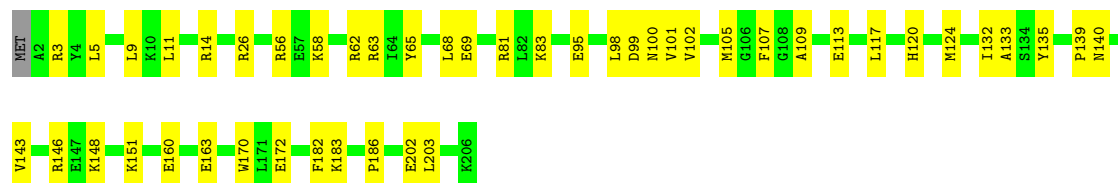
- Molecule 3: Small ribosomal subunit protein uS3

Chain C: 73% 15% 12%



- Molecule 4: Small ribosomal subunit protein uS4

Chain D: 77% 22%

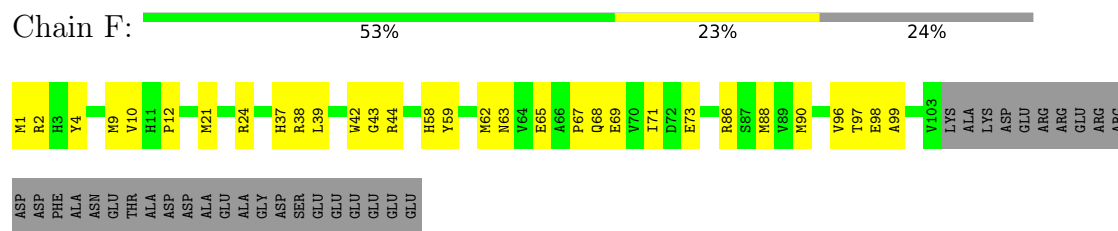


- Molecule 5: Small ribosomal subunit protein uS5

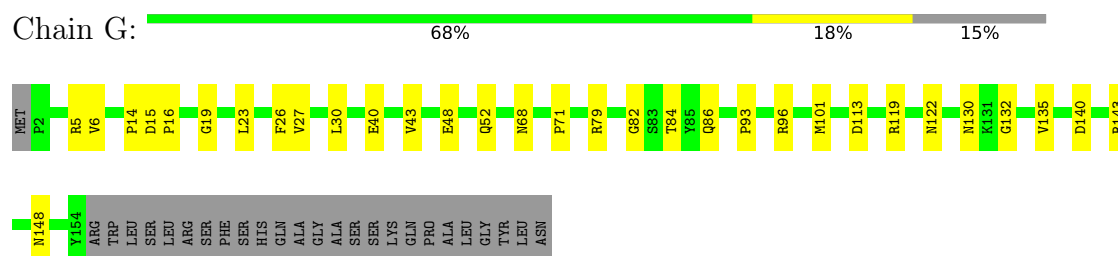
Chain E: 80% 13% 7%



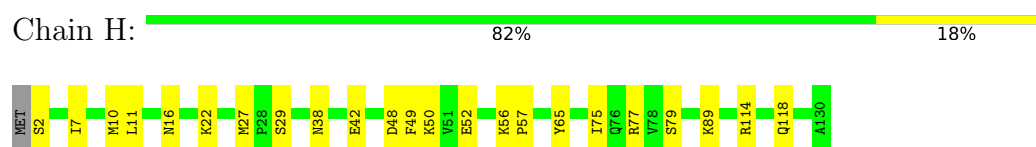
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



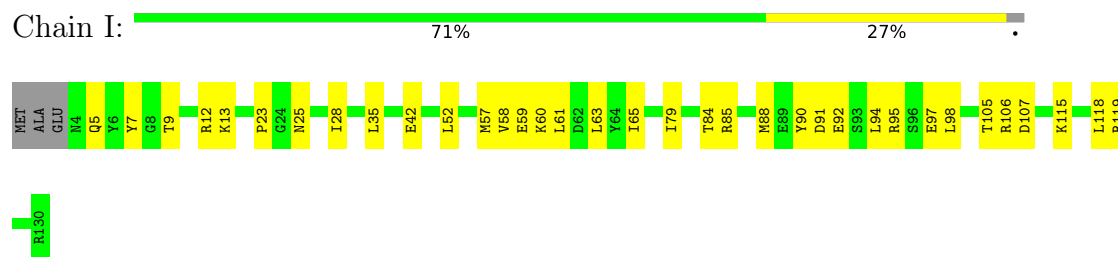
- Molecule 7: Small ribosomal subunit protein uS7



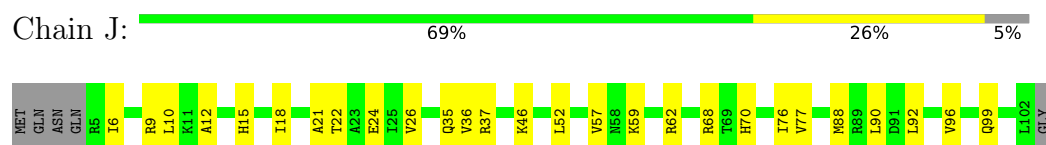
- Molecule 8: Small ribosomal subunit protein uS8



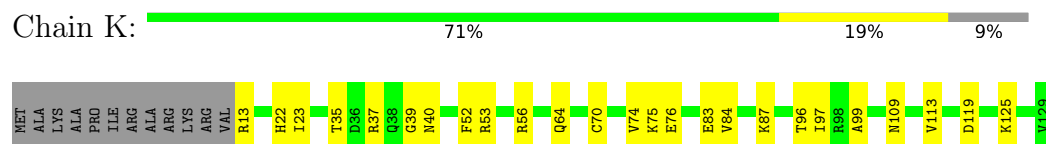
- Molecule 9: Small ribosomal subunit protein uS9




- Molecule 10: Small ribosomal subunit protein uS10



- Molecule 11: Small ribosomal subunit protein uS11



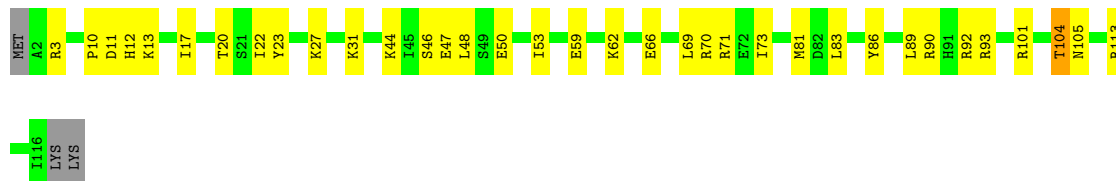
- Molecule 12: Small ribosomal subunit protein uS12

Chain L:  85% 15% .




- Molecule 13: Small ribosomal subunit protein uS13

Chain M:  68% 29% . .




- Molecule 14: Small ribosomal subunit protein uS14

Chain N:  79% 20% .



- Molecule 15: Small ribosomal subunit protein uS15

Chain O:  89% 10% .




- Molecule 16: Small ribosomal subunit protein bS16

Chain P:  76% 23% .



- Molecule 17: Small ribosomal subunit protein uS17

Chain Q:  80% 14% 6%



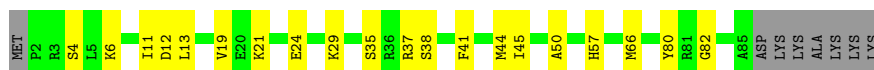
- Molecule 18: Small ribosomal subunit protein bS18

Chain R:  72% 16% 12%



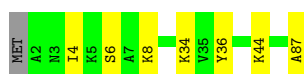
- Molecule 19: Small ribosomal subunit protein uS19

Chain S: 70% 22% 9%



- Molecule 20: Small ribosomal subunit protein bS20

Chain T: 91% 8%



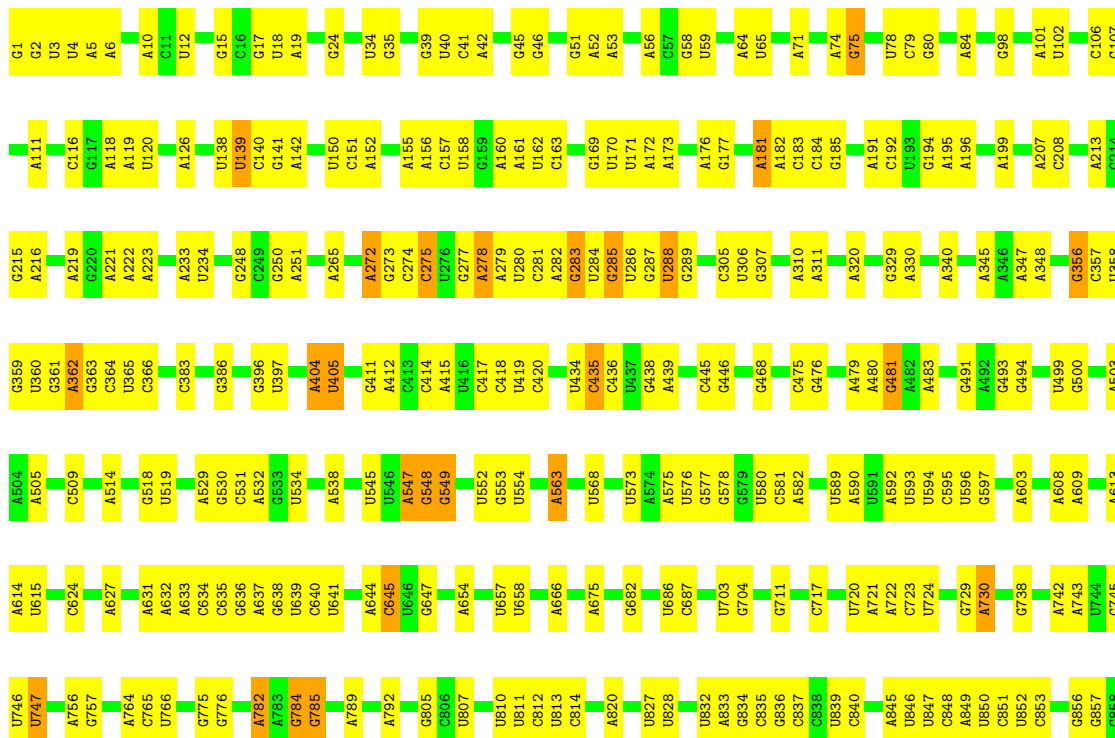
- Molecule 21: Small ribosomal subunit protein bS21

Chain U: 76% 23%

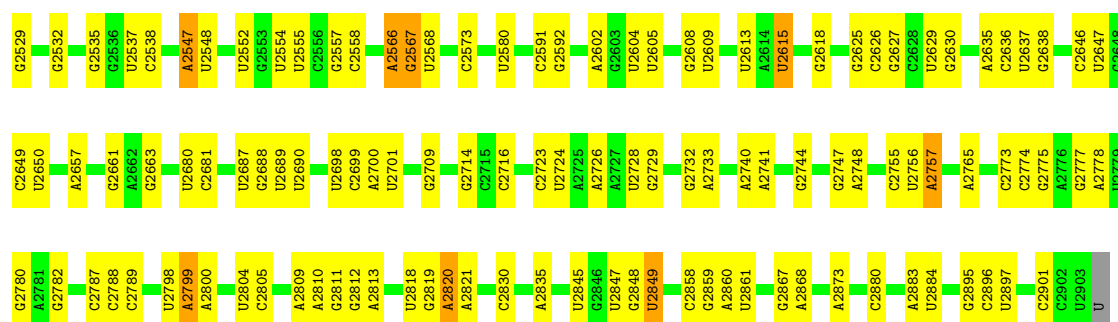


- Molecule 22: 23S rRNA

Chain a: 64% 28% 5%



G2410	U2305	U2189	C	A2052	C1914	G1797	C1646	G1537	C1437	U1340	U1181	G993	G859
U2419	G2308	G2190	U	C2055	3DI1915	U1796	U1647	G1538	U1438	G1941	G1182	C994	A863
C2420	U2312	G2193	U	G2056	U1916	G1799	G1649	U1539	A1430	A1942	U1183	C995	G864
C2313	U2313	U2194	G	A2060	U1917	C1800	A1544	A1544	G1441	U1344	U1184	A996	
G2316	G2316	A2198	A	G2061	G1929	A1802	A1654	G1546	U1442	C1349	G1197	A1000	U871
G2429	A2317	G2204	G	A2062	U1930	A1903	G1687	G1947	U1443	C1350	U1198	A1001	U872
A2430	U2329	G2204	U	G2063	U1931	A1932	G1674	A1549	G1444	C1351	U1199	A1001	G873
A2322	A2322	C2208	G	C2064	G1933	A1909	G1674	A1549	C1446	U1352	C1200	C1005	G874
A2435	A2322	C2208	U	C2065	A1937	A1937	A1677	U1554	G1448	A1354	U1203	C1006	A878
G2325	G2325	A2211	G	A1938	A1938	G1814	A1677	U1554	G1448	G1355	U1204	C1007	G880
C2326	C2326	A2211	A	U1939	A1815	A1815	A1678	C1558	G1452	G1361	U1206	U1012	G881
A2327	A2327	A2225	C	A2070	C1816	G1683	U1683	G1559	A1453	C1362	G1212	C1013	G882
A2328	A2328	G2228	G	A2071	G1684	C1685	G1684	U1560	G1453	C1363	G1026	U1013	G883
U2329	U2329	G2228	C	C2072	C1685	A1696	A1469	U1563	A1469	G1364	A1027	G1026	U894
G2330	G2330	U2229	C	C1962	C1696	A1696	A1470	U1564	A1470	A1365	A1028	A1029	
A2333	A2333	U2233	A	U2074	C1704	A1829	G1473	C1565	G1473	C1370	U1242	U1033	U887
A2336	A2336	G2234	G	U2075	A1705	G1831	U1474	A1566	U1474	G1371	A1243	A1039	C888
A2340	A2340	G2238	U	G2086	G1710	G1835	U1476	A1570	G1476	C1378	A1244	A1040	C889
U2343	U2343	G2239	C	G2087	A1711	G1842	U1477	A1571	A1477	U1379	G1245	A1041	C890
U2344	U2344	U2240	G	G2093	G1715	C1843	A1480	A1572	C1480	G1380	G1250	A1039	A892
A2346	A2346	A2241	A	A2094	G1980	G1843	U1481	C1575	U1481	C1251	G1251	G1041	U894
U2347	U2347	G2242	G	A2095	G1981	A1847	U1482	C1576	G1482	A1383	G1252	C1045	U895
C2348	C2348	U2244	U	C2096	U1982	A1848	U1483	C1577	A1483	A1253	A1254	A1046	A896
A2349	A2349	G2245	G	U2098	U1983	A1853	U1484	C1578	U1484	C1386	A1111	G1047	C897
C2350	C2350	U2246	A	U2099	U1984	A1854	U1485	U1578	U1485	A1387	G1112	A1047	A899
A2351	A2351	G2247	C	C2100	U1985	A1855	C1498	A1583	U1497	U1397	G1116	C1082	C903
U2352	U2352	C2248	C	A2101	U1986	A1856	C1499	U1584	U1498	C1398	G1117	C	G904
A2353	A2353	G2251	G	G2102	G1987	G1857	U1736	C1585	A1494	U1394	G1122	G	A909
C2354	C2354	G2251	A	C	C1987	A1858	G1737	A1586	U1495	A1395	G1125	A	A910
U2355	U2355	A2266	C	U	C2000	A1859	G1738	G1587	U1496	U1406	U1141	C	A911
A2356	A2356	A2267	U	U	G2012	G1862	A1744	A1590	C1498	U1405	U1132	U	C912
G2357	G2357	G2273	U	G	A2013	U1963	A1745	A1591	G1500	G1278	A1132	G	U931
C2374	C2374	A2274	G	A	A2014	U1964	U1746	A1597	A1508	G1280	A1134	U	A941
A2377	A2377	G2279	A	U	A2015	G1969	U1747	A1598	A1509	G1281	C1135	U	
U2378	U2378	U2283	A	U	A2020	C1870	C1760	U1599	G1510	U1282	U1141	C	C946
G2379	G2379	C2283	U	U	C2023	A1871	C1764	C1607	A1515	G1292	A1142	U	A947
C2380	C2380	A2287	C	A	G2024	A1872	A1773	A1608	G1519	C1293	G1149	A	C948
G2383	G2383	A2288	C	G	C2025	G1874	C1774	A1614	G1524	G1296	C1150	G	U955
U2384	U2384	U2291	A	A	U2026	G1875	A1774	A1614	G1524	G1300	A1156	A	A959
C2385	C2385	U2292	C	U	G2027	A1889	U1782	A1618	A1525	A1301	C1172	G	A960
A2389	A2389	G2293	C	A	A2030	A1890	A1786	A1618	G1526	C1428	U	C	C961
U2392	U2392	U2294	U	G	A2031	C1902	A1786	A1618	G1527	G1429	U	A	
C2394	C2394	G2294	U	U	G2032	C1905	G1790	G1622	A1528	G1430	A	G	
C2395	C2395	A2298	A	G	A2033	G1906	A1791	A1626	G1529	A1431	U	C	G966
A2396	A2396	U2299	A	C	A2033	G1906	A1791	A1626	G1529	G1432	G1319	C	G974
U2402	U2402	C2300	U	G	G2038	U1911	A1794	U1636	C1533	A1433	C1320	A	
C2403	C2403	U2302	G	A	U2039	A1912	A1794	A1637	U1534	A1434	G1177	U	A983
A2406	A2406		G	G	C2043	A1913	U1796	A1637	A1535	G1435	C1178	C	A984
			U2187	U2188							U1180	A	



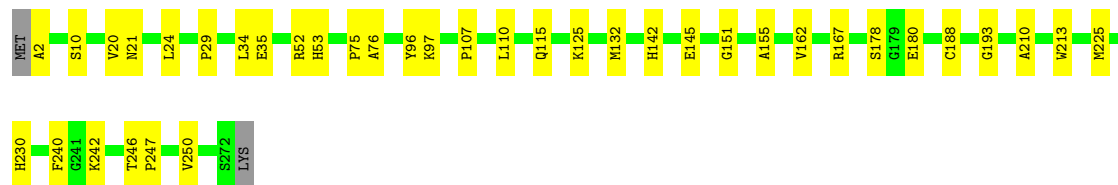
• Molecule 23: 5S rRNA

Chain b: 75% 23% ..



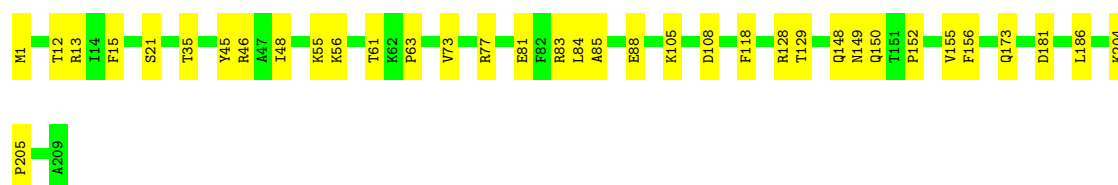
• Molecule 24: Large ribosomal subunit protein uL2

Chain c: 85% 14% .



• Molecule 25: Large ribosomal subunit protein uL3

Chain d: 83% 17%



• Molecule 26: Large ribosomal subunit protein uL4

Chain e: 91% 9%



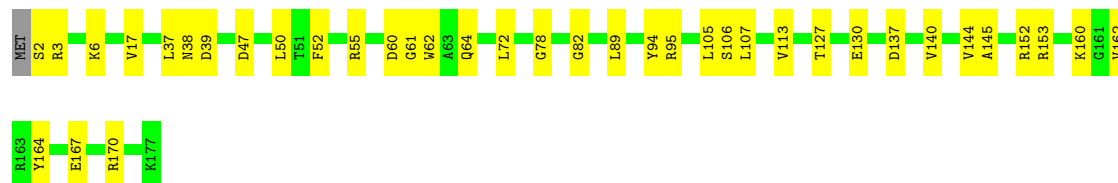
• Molecule 27: Large ribosomal subunit protein uL5

Chain f: 73% 26% .



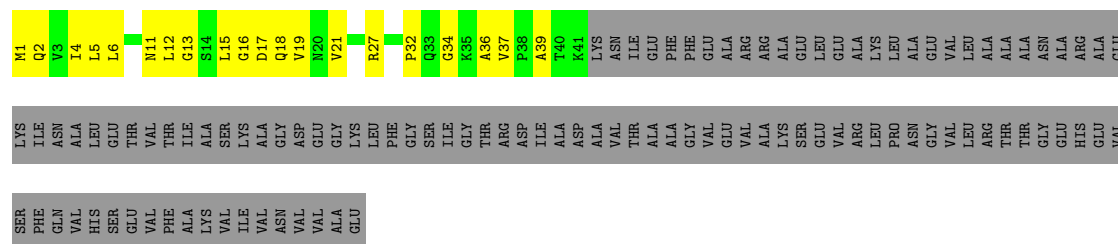
- Molecule 28: Large ribosomal subunit protein uL6

Chain g: 78% 21%



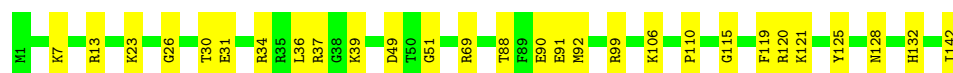
- Molecule 29: Large ribosomal subunit protein bL9

Chain h: 14% 13% 72%



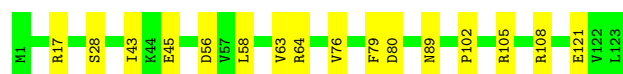
- Molecule 30: Large ribosomal subunit protein uL13

Chain i: 80% 20%



- Molecule 31: Large ribosomal subunit protein uL14

Chain j: 87% 13%

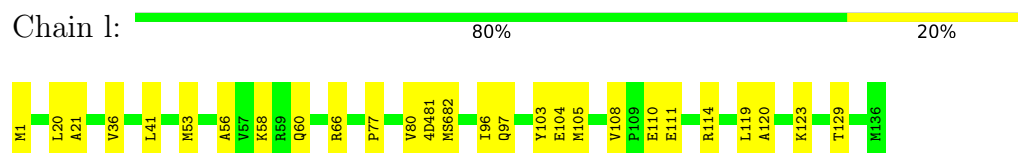


- Molecule 32: Large ribosomal subunit protein uL15

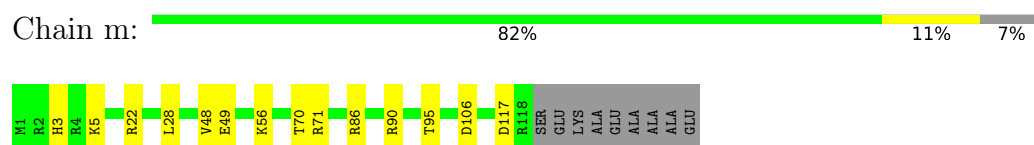
Chain k: 81% 19%



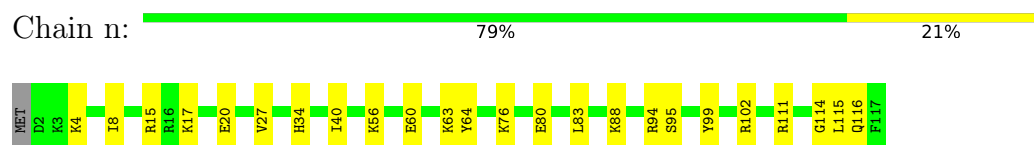
- Molecule 33: Large ribosomal subunit protein uL16



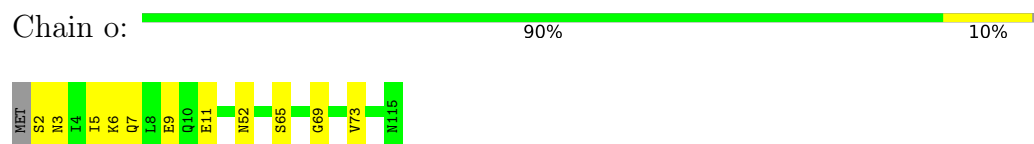
- Molecule 34: Large ribosomal subunit protein bL17



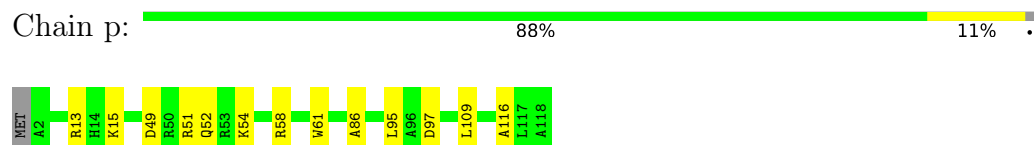
- Molecule 35: Large ribosomal subunit protein uL18



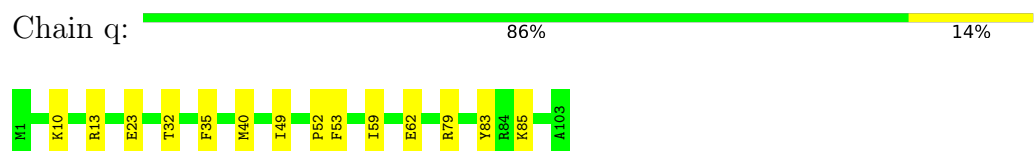
- Molecule 36: Large ribosomal subunit protein bL19



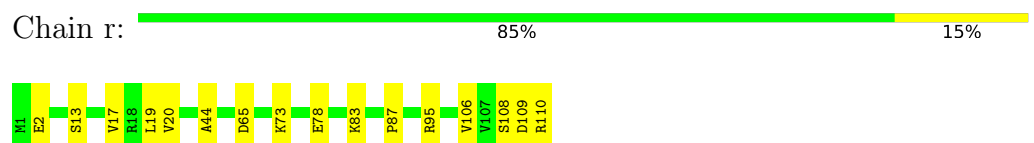
- Molecule 37: Large ribosomal subunit protein bL20




- Molecule 38: Large ribosomal subunit protein bL21



- Molecule 39: Large ribosomal subunit protein uL22




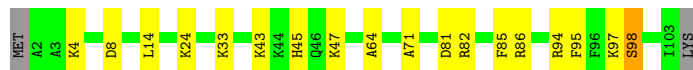
- Molecule 40: Large ribosomal subunit protein uL23

Chain s:  79% 14% 7%



- Molecule 41: Large ribosomal subunit protein uL24

Chain t:  81% 16% ..




- Molecule 42: Large ribosomal subunit protein bL25

Chain u:  86% 14%




- Molecule 43: Large ribosomal subunit protein bL27

Chain v:  80% 12% 8%




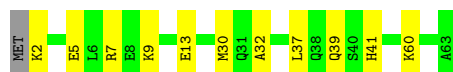
- Molecule 44: Large ribosomal subunit protein bL28

Chain w:  83% 15% .




- Molecule 45: Large ribosomal subunit protein uL29

Chain x:  81% 17% .



- Molecule 46: Large ribosomal subunit protein uL30

Chain y:  83% 15% .



- Molecule 47: Large ribosomal subunit protein bL32



- | |
|-----|
| MET |
| ALA |
| LYS |
| G4 |
| I5 |
| R6 |
| E7 |
| K8 |
| I9 |
| K10 |
| F20 |
| Y21 |
| T22 |
| K27 |
| R28 |
| T29 |
| K30 |
| E51 |
| A52 |
| K53 |
| I54 |
| LYS |

-
- ```

graph LR
 M1[M1] --> K2[K2]
 K2 --> R3[R3]
 R3 --> T4[T4]
 T4 --> M22[M22]
 M22 --> N26[N26]
 N26 --> G27[G27]
 G27 --> R28[R28]
 R28 --> K37[K37]
 K37 --> G38[G38]
 G38 --> R39[R39]
 R39 --> S45[S45]
 S45 --> K46[K46]

```

- 

- 
- | Node ID | Number of Nodes |
|---------|-----------------|
| M1      | 1               |
| R4      | 2               |
| I16     | 3               |
| V17     | 4               |
| K18     | 5               |
| G21     | 6               |
| V22     | 7               |
| I23     | 8               |
| R24     | 9               |
| V25     | 10              |
| P31     | 11              |
| Q35     | 12              |
| G38     | 13              |

- |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | I5 | K8 | Y9 | E10 | E11 | T12 | T13 | C16 | S17 | V20 | V21 | R25 | S26 | T27 | V28 | D31 | L32 | R33 | L34 | S38 | H41 | F44 | Q48 | ARG | ASP | VAL | ALA | THR | GLY | G55 | D68 | R69 | K62 | R63 | I66 | P60 | GLY | SER | TYR |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- A  
C  
U
- G G C A A C C U U A A A A C A C A A A U U U A A A A A G G A A A A U A G37 G42 U U C A A A G U C G A A A A A U C U A C U

- WORLDWIDE  
**PDB**  
PROTEIN DATA BANK





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 244856                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K3 (6k 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: 6MZ, 5MU, 4SU, MS6, OMC, 5MC, OMG, MEQ, OMU, D2T, 2MG, UR3, IAS, 4OC, H2U, G7M, 2MA, 1MG, PSU, 4D4, MG, 3TD, MA6

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  >5 | RMSZ        | # Z  >5  |
| 1   | A     | 0.35         | 0/36073 | 0.30        | 0/56264  |
| 2   | B     | 0.21         | 0/1784  | 0.32        | 0/2403   |
| 3   | C     | 0.26         | 0/1651  | 0.36        | 0/2225   |
| 4   | D     | 0.27         | 0/1665  | 0.37        | 0/2227   |
| 5   | E     | 0.30         | 0/1165  | 0.37        | 0/1568   |
| 6   | F     | 0.26         | 0/858   | 0.42        | 0/1160   |
| 7   | G     | 0.22         | 0/1219  | 0.36        | 0/1635   |
| 8   | H     | 0.31         | 0/989   | 0.38        | 0/1326   |
| 9   | I     | 0.27         | 0/1034  | 0.42        | 0/1375   |
| 10  | J     | 0.27         | 0/796   | 0.43        | 0/1077   |
| 11  | K     | 0.27         | 0/884   | 0.35        | 0/1191   |
| 12  | L     | 0.31         | 0/960   | 0.40        | 0/1286   |
| 13  | M     | 0.27         | 0/900   | 0.45        | 0/1204   |
| 14  | N     | 0.28         | 0/817   | 0.43        | 0/1088   |
| 15  | O     | 0.29         | 0/722   | 0.38        | 0/964    |
| 16  | P     | 0.31         | 0/653   | 0.39        | 0/877    |
| 17  | Q     | 0.28         | 0/650   | 0.36        | 0/871    |
| 18  | R     | 0.28         | 0/553   | 0.38        | 0/742    |
| 19  | S     | 0.24         | 0/685   | 0.39        | 0/922    |
| 20  | T     | 0.29         | 0/676   | 0.35        | 0/895    |
| 21  | U     | 0.19         | 0/597   | 0.35        | 0/792    |
| 22  | a     | 0.40         | 0/65842 | 0.31        | 0/102711 |
| 23  | b     | 0.33         | 0/2850  | 0.27        | 0/4444   |
| 24  | c     | 0.36         | 0/2121  | 0.39        | 0/2852   |
| 25  | d     | 0.36         | 0/1576  | 0.35        | 0/2119   |
| 26  | e     | 0.31         | 0/1571  | 0.35        | 0/2113   |
| 27  | f     | 0.27         | 0/1434  | 0.36        | 0/1926   |
| 28  | g     | 0.25         | 0/1343  | 0.42        | 0/1816   |
| 29  | h     | 0.23         | 0/306   | 0.40        | 0/413    |
| 30  | i     | 0.34         | 0/1152  | 0.35        | 0/1551   |
| 31  | j     | 0.35         | 0/955   | 0.36        | 0/1279   |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 32  | k     | 0.34         | 0/1062   | 0.39        | 0/1413          |
| 33  | l     | 0.34         | 0/1073   | 0.37        | 0/1433          |
| 34  | m     | 0.37         | 0/958    | 0.42        | 0/1281          |
| 35  | n     | 0.29         | 0/902    | 0.39        | 0/1209          |
| 36  | o     | 0.34         | 0/929    | 0.34        | 0/1242          |
| 37  | p     | 0.38         | 0/960    | 0.37        | 0/1278          |
| 38  | q     | 0.35         | 0/829    | 0.38        | 0/1107          |
| 39  | r     | 0.34         | 0/864    | 0.39        | 0/1156          |
| 40  | s     | 0.30         | 0/744    | 0.45        | 0/994           |
| 41  | t     | 0.28         | 0/787    | 0.49        | 2/1051 (0.2%)   |
| 42  | u     | 0.29         | 0/766    | 0.36        | 0/1025          |
| 43  | v     | 0.35         | 0/599    | 0.36        | 0/792           |
| 44  | w     | 0.34         | 0/635    | 0.40        | 0/848           |
| 45  | x     | 0.25         | 0/502    | 0.38        | 0/667           |
| 46  | y     | 0.33         | 0/453    | 0.36        | 0/605           |
| 47  | z     | 0.34         | 0/450    | 0.36        | 0/599           |
| 48  | 0     | 0.28         | 0/424    | 0.31        | 0/565           |
| 49  | 1     | 0.38         | 0/380    | 0.43        | 0/498           |
| 50  | 2     | 0.37         | 0/513    | 0.42        | 0/676           |
| 51  | 3     | 0.36         | 0/303    | 0.38        | 0/397           |
| 52  | 4     | 0.21         | 0/488    | 0.41        | 0/649           |
| 53  | X     | 0.29         | 0/145    | 0.26        | 0/224           |
| 54  | Z     | 0.28         | 0/1725   | 0.26        | 0/2687          |
| All | All   | 0.36         | 0/150972 | 0.33        | 2/225712 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 13  | M     | 0                   | 1                   |
| 33  | l     | 1                   | 0                   |
| 50  | 2     | 0                   | 1                   |
| All | All   | 1                   | 2                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 41  | t     | 98  | SER  | CA-C-N | 5.71 | 132.44      | 121.54   |
| 41  | t     | 98  | SER  | C-N-CA | 5.71 | 132.44      | 121.54   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 33  | l     | 82  | MS6  | C    |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 50  | 2     | 31  | HIS  | Peptide |
| 13  | M     | 104 | THR  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32466 | 0        | 16359    | 351     | 0            |
| 2   | B     | 1753  | 0        | 1780     | 19      | 0            |
| 3   | C     | 1624  | 0        | 1696     | 19      | 0            |
| 4   | D     | 1643  | 0        | 1707     | 36      | 0            |
| 5   | E     | 1152  | 0        | 1196     | 17      | 0            |
| 6   | F     | 839   | 0        | 833      | 24      | 0            |
| 7   | G     | 1203  | 0        | 1254     | 22      | 0            |
| 8   | H     | 979   | 0        | 1031     | 17      | 0            |
| 9   | I     | 1022  | 0        | 1070     | 30      | 0            |
| 10  | J     | 786   | 0        | 828      | 19      | 0            |
| 11  | K     | 877   | 0        | 884      | 16      | 0            |
| 12  | L     | 957   | 0        | 1017     | 17      | 0            |
| 13  | M     | 891   | 0        | 952      | 31      | 0            |
| 14  | N     | 805   | 0        | 844      | 12      | 0            |
| 15  | O     | 714   | 0        | 734      | 7       | 0            |
| 16  | P     | 643   | 0        | 661      | 11      | 0            |
| 17  | Q     | 641   | 0        | 682      | 9       | 0            |
| 18  | R     | 544   | 0        | 565      | 9       | 0            |
| 19  | S     | 668   | 0        | 693      | 15      | 0            |
| 20  | T     | 670   | 0        | 719      | 5       | 0            |
| 21  | U     | 589   | 0        | 629      | 10      | 0            |
| 22  | a     | 59301 | 0        | 29850    | 524     | 0            |
| 23  | b     | 2549  | 0        | 1291     | 15      | 0            |
| 24  | c     | 2082  | 0        | 2154     | 26      | 0            |
| 25  | d     | 1566  | 0        | 1618     | 26      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 26  | e     | 1552   | 0        | 1619     | 10      | 0            |
| 27  | f     | 1410   | 0        | 1444     | 37      | 0            |
| 28  | g     | 1323   | 0        | 1371     | 26      | 0            |
| 29  | h     | 303    | 0        | 327      | 15      | 0            |
| 30  | i     | 1129   | 0        | 1162     | 19      | 0            |
| 31  | j     | 946    | 0        | 1023     | 11      | 0            |
| 32  | k     | 1053   | 0        | 1129     | 21      | 0            |
| 33  | l     | 1075   | 0        | 1145     | 16      | 0            |
| 34  | m     | 945    | 0        | 989      | 9       | 0            |
| 35  | n     | 892    | 0        | 923      | 14      | 0            |
| 36  | o     | 917    | 0        | 962      | 8       | 0            |
| 37  | p     | 947    | 0        | 1019     | 12      | 0            |
| 38  | q     | 816    | 0        | 839      | 10      | 0            |
| 39  | r     | 857    | 0        | 922      | 10      | 0            |
| 40  | s     | 738    | 0        | 807      | 9       | 0            |
| 41  | t     | 779    | 0        | 831      | 14      | 0            |
| 42  | u     | 753    | 0        | 780      | 10      | 0            |
| 43  | v     | 592    | 0        | 607      | 6       | 0            |
| 44  | w     | 625    | 0        | 652      | 8       | 0            |
| 45  | x     | 501    | 0        | 531      | 7       | 0            |
| 46  | y     | 449    | 0        | 488      | 5       | 0            |
| 47  | z     | 444    | 0        | 458      | 9       | 0            |
| 48  | 0     | 417    | 0        | 451      | 8       | 0            |
| 49  | 1     | 377    | 0        | 418      | 9       | 0            |
| 50  | 2     | 504    | 0        | 572      | 7       | 0            |
| 51  | 3     | 302    | 0        | 343      | 6       | 0            |
| 52  | 4     | 480    | 0        | 482      | 18      | 0            |
| 53  | X     | 130    | 0        | 66       | 0       | 0            |
| 54  | Z     | 1645   | 0        | 842      | 16      | 0            |
| 55  | A     | 119    | 0        | 0        | 0       | 0            |
| 55  | Z     | 1      | 0        | 0        | 0       | 0            |
| 55  | a     | 328    | 0        | 0        | 0       | 0            |
| 55  | b     | 6      | 0        | 0        | 0       | 0            |
| 55  | c     | 1      | 0        | 0        | 0       | 0            |
| 55  | d     | 1      | 0        | 0        | 0       | 0            |
| 55  | z     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 140322 | 0        | 94249    | 1465    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1465) 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:414:A:HO2'    | 1:A:415:A:H8     | 0.99                     | 0.97              |
| 22:a:1047:G:HO2'  | 22:a:1110:G:H1   | 1.13                     | 0.97              |
| 1:A:76:G:H1       | 1:A:93:U:H3      | 1.11                     | 0.97              |
| 22:a:1870:C:HO2'  | 22:a:1871:A:H8   | 0.99                     | 0.95              |
| 22:a:2100:G:H1    | 22:a:2189:U:H3   | 0.95                     | 0.93              |
| 22:a:1534:U:H3    | 22:a:1537:G:H1   | 1.14                     | 0.91              |
| 25:d:61:THR:HG22  | 25:d:63:PRO:HD2  | 1.55                     | 0.89              |
| 1:A:42:G:H21      | 1:A:622:A:H8     | 1.21                     | 0.87              |
| 1:A:664:G:H22     | 1:A:741:G:H1     | 1.25                     | 0.83              |
| 1:A:437:U:HO2'    | 4:D:120:HIS:HD1  | 1.22                     | 0.83              |
| 28:g:38:ASN:ND2   | 28:g:64:GLN:OE1  | 2.12                     | 0.81              |
| 52:4:59:ARG:HA    | 52:4:62:LYS:HE2  | 1.61                     | 0.81              |
| 22:a:545:U:O2     | 22:a:548:G:O6    | 1.99                     | 0.80              |
| 1:A:509:A:H8      | 1:A:543:U:HO2'   | 1.30                     | 0.79              |
| 1:A:509:A:H8      | 1:A:543:U:O2'    | 1.65                     | 0.79              |
| 3:C:35:SER:OG     | 3:C:59:ARG:NH2   | 2.16                     | 0.78              |
| 1:A:677:U:H3      | 1:A:713:G:H22    | 1.32                     | 0.78              |
| 35:n:76:LYS:NZ    | 35:n:80:GLU:OE1  | 2.15                     | 0.78              |
| 1:A:8:A:N6        | 4:D:202:GLU:O    | 2.17                     | 0.78              |
| 22:a:1417:C:HO2'  | 22:a:1587:G:HO2' | 1.22                     | 0.77              |
| 27:f:158:THR:HG22 | 27:f:160:ALA:H   | 1.49                     | 0.77              |
| 13:M:12:HIS:O     | 13:M:44:LYS:NZ   | 2.17                     | 0.77              |
| 1:A:428:G:H1'     | 1:A:430:A:C8     | 2.19                     | 0.77              |
| 24:c:142:HIS:ND1  | 24:c:193:GLY:O   | 2.17                     | 0.76              |
| 16:P:14:ARG:HG3   | 16:P:42:ILE:HD11 | 1.67                     | 0.76              |
| 1:A:673:A:H2'     | 1:A:674:G:C8     | 2.21                     | 0.75              |
| 4:D:172:GLU:HG2   | 4:D:183:LYS:HD2  | 1.68                     | 0.74              |
| 7:G:68:ASN:ND2    | 7:G:130:ASN:OD1  | 2.21                     | 0.74              |
| 29:h:1:MET:N      | 29:h:21:VAL:O    | 2.21                     | 0.74              |
| 1:A:537:G:OP1     | 12:L:110:ARG:NH2 | 2.22                     | 0.73              |
| 26:e:173:THR:HA   | 26:e:199:MET:HE1 | 1.70                     | 0.72              |
| 9:I:106:ARG:NH1   | 9:I:107:ASP:O    | 2.23                     | 0.72              |
| 22:a:2100:G:O6    | 22:a:2189:U:O4   | 2.06                     | 0.72              |
| 32:k:91:ASP:OD1   | 32:k:92:LEU:N    | 2.21                     | 0.71              |
| 8:H:11:LEU:HD22   | 8:H:75:ILE:HD11  | 1.73                     | 0.71              |
| 22:a:2102:G:H1    | 22:a:2187:U:H3   | 0.79                     | 0.71              |
| 22:a:881:G:N1     | 22:a:895:U:N3    | 2.36                     | 0.71              |
| 3:C:110:GLU:HB2   | 3:C:144:LEU:HD22 | 1.71                     | 0.71              |
| 1:A:407:U:O2'     | 4:D:113:GLU:OE1  | 2.10                     | 0.70              |
| 22:a:881:G:H1     | 22:a:895:U:H3    | 1.35                     | 0.70              |
| 30:i:125:TYR:OH   | 30:i:132:HIS:NE2 | 2.24                     | 0.70              |
| 12:L:71:GLY:O     | 12:L:99:ARG:NH2  | 2.25                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:881:G:O6    | 22:a:895:U:O4    | 2.10                     | 0.69              |
| 35:n:99:TYR:OH   | 35:n:111:ARG:NH1 | 2.26                     | 0.69              |
| 1:A:1086:U:H3    | 1:A:1099:G:H22   | 1.39                     | 0.69              |
| 11:K:13:ARG:N    | 11:K:76:GLU:OE2  | 2.26                     | 0.69              |
| 28:g:39:ASP:O    | 28:g:55:ARG:NH1  | 2.25                     | 0.68              |
| 43:v:10:THR:HG22 | 43:v:12:ASN:H    | 1.56                     | 0.68              |
| 28:g:2:SER:OG    | 28:g:3:ARG:N     | 2.23                     | 0.68              |
| 3:C:128:VAL:HG13 | 3:C:132:ARG:HH21 | 1.59                     | 0.68              |
| 10:J:9:ARG:HB2   | 10:J:99:GLN:HB2  | 1.76                     | 0.68              |
| 10:J:10:LEU:HD13 | 10:J:22:THR:HG22 | 1.75                     | 0.68              |
| 22:a:1434:A:H2'  | 22:a:1435:G:C8   | 2.28                     | 0.68              |
| 13:M:23:TYR:HB3  | 13:M:66:GLU:HG3  | 1.76                     | 0.68              |
| 22:a:1434:A:H2'  | 22:a:1435:G:H8   | 1.58                     | 0.68              |
| 9:I:12:ARG:HG3   | 9:I:13:LYS:H     | 1.59                     | 0.68              |
| 4:D:124:MET:HG2  | 4:D:146:ARG:HG2  | 1.74                     | 0.67              |
| 19:S:50:ALA:HB1  | 19:S:57:HIS:HB3  | 1.75                     | 0.67              |
| 5:E:164:ILE:O    | 8:H:114:ARG:NH2  | 2.27                     | 0.67              |
| 24:c:2:ALA:N     | 24:c:20:VAL:O    | 2.28                     | 0.67              |
| 13:M:59:GLU:HA   | 13:M:62:LYS:HZ3  | 1.59                     | 0.67              |
| 48:0:7:GLU:OE2   | 48:0:27:LYS:NZ   | 2.23                     | 0.67              |
| 1:A:1026:G:O6    | 1:A:1035:A:N1    | 2.28                     | 0.67              |
| 22:a:1607:C:N4   | 22:a:1622:G:OP2  | 2.22                     | 0.67              |
| 22:a:639:U:H2'   | 22:a:640:C:C6    | 2.29                     | 0.67              |
| 11:K:37:ARG:NH1  | 11:K:83:GLU:OE2  | 2.28                     | 0.67              |
| 22:a:1007:C:OP1  | 30:i:37:ARG:NH2  | 2.28                     | 0.66              |
| 1:A:946:A:H2'    | 1:A:947:G:C8     | 2.30                     | 0.66              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8    | 2.30                     | 0.66              |
| 23:b:1:U:H2'     | 23:b:2:G:H8      | 1.60                     | 0.66              |
| 1:A:405:U:OP2    | 4:D:3:ARG:NH1    | 2.28                     | 0.66              |
| 1:A:544:G:OP1    | 4:D:56:ARG:NH2   | 2.27                     | 0.66              |
| 10:J:6:ILE:HB    | 10:J:76:ILE:HB   | 1.77                     | 0.66              |
| 22:a:1026:G:H2'  | 22:a:1027:A:H8   | 1.61                     | 0.66              |
| 4:D:98:LEU:HB2   | 4:D:135:TYR:HB3  | 1.77                     | 0.66              |
| 1:A:1137:C:O2    | 1:A:1138:G:N2    | 2.30                     | 0.65              |
| 19:S:29:LYS:HA   | 19:S:29:LYS:HE3  | 1.78                     | 0.65              |
| 7:G:113:ASP:OD2  | 7:G:122:ASN:ND2  | 2.29                     | 0.65              |
| 22:a:1534:U:O2   | 22:a:1537:G:O6   | 2.13                     | 0.65              |
| 1:A:1009:U:O2    | 1:A:1020:G:N2    | 2.19                     | 0.65              |
| 22:a:2102:G:N2   | 22:a:2187:U:O2   | 2.22                     | 0.65              |
| 22:a:2305:U:H5'' | 27:f:131:GLY:HA3 | 1.79                     | 0.65              |
| 22:a:2394:C:H5'' | 32:k:63:LYS:HE2  | 1.78                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:2:ARG:NH1    | 6:F:68:GLN:OE1    | 2.30                     | 0.65              |
| 38:q:10:LYS:NZ   | 38:q:23:GLU:OE1   | 2.27                     | 0.65              |
| 1:A:714:G:H2'    | 1:A:715:A:C8      | 2.32                     | 0.64              |
| 22:a:2299:U:OP1  | 27:f:72:LYS:NZ    | 2.30                     | 0.64              |
| 1:A:1006:G:O6    | 1:A:1023:U:O2     | 2.15                     | 0.64              |
| 22:a:139:U:H5''  | 22:a:140:C:H5     | 1.63                     | 0.64              |
| 22:a:1245:G:OP1  | 32:k:13:LYS:NZ    | 2.27                     | 0.64              |
| 24:c:107:PRO:HD2 | 24:c:110:LEU:HD22 | 1.79                     | 0.64              |
| 52:4:58:ASP:OD1  | 52:4:59:ARG:N     | 2.31                     | 0.64              |
| 1:A:147:G:H2'    | 1:A:148:G:C8      | 2.33                     | 0.64              |
| 18:R:16:GLU:HG3  | 18:R:18:VAL:HG23  | 1.78                     | 0.64              |
| 34:m:56:LYS:NZ   | 34:m:90:ARG:O     | 2.31                     | 0.64              |
| 22:a:1365:A:OP1  | 44:w:3:ARG:NH2    | 2.29                     | 0.64              |
| 22:a:782:A:N1    | 24:c:225:MET:HE2  | 2.13                     | 0.63              |
| 1:A:1397:C:OP2   | 5:E:29:ARG:NH2    | 2.31                     | 0.63              |
| 14:N:37:SER:OG   | 14:N:40:ASP:OD2   | 2.16                     | 0.63              |
| 31:j:43:ILE:HD12 | 31:j:56:ASP:HB2   | 1.80                     | 0.63              |
| 36:o:2:SER:OG    | 36:o:3:ASN:N      | 2.24                     | 0.63              |
| 1:A:427:U:H3'    | 1:A:428:G:H5''    | 1.80                     | 0.63              |
| 22:a:2328:A:H2'  | 22:a:2329:U:C6    | 2.34                     | 0.63              |
| 22:a:2313:C:O4'  | 27:f:37:ASN:ND2   | 2.31                     | 0.63              |
| 1:A:613:C:OP1    | 4:D:81:ARG:NH2    | 2.28                     | 0.63              |
| 18:R:37:GLY:O    | 18:R:63:ARG:NH2   | 2.29                     | 0.63              |
| 13:M:27:LYS:O    | 13:M:31:LYS:HG3   | 1.98                     | 0.63              |
| 22:a:284:U:O2    | 22:a:356:G:O6     | 2.16                     | 0.63              |
| 24:c:29:PRO:HG2  | 24:c:34:LEU:HD11  | 1.79                     | 0.63              |
| 16:P:36:VAL:HG11 | 16:P:57:ILE:HG13  | 1.80                     | 0.62              |
| 1:A:1311:A:OP1   | 52:4:59:ARG:NH1   | 2.32                     | 0.62              |
| 1:A:1378:C:OP1   | 7:G:5:ARG:NH1     | 2.32                     | 0.62              |
| 2:B:217:VAL:O    | 2:B:221:VAL:HG12  | 1.99                     | 0.62              |
| 13:M:11:ASP:OD2  | 13:M:46:SER:OG    | 2.15                     | 0.62              |
| 28:g:60:ASP:OD1  | 28:g:61:GLY:N     | 2.30                     | 0.62              |
| 22:a:1649:G:O2'  | 34:m:106:ASP:OD2  | 2.14                     | 0.62              |
| 22:a:2102:G:O6   | 22:a:2187:U:O4    | 2.18                     | 0.62              |
| 51:3:18:LYS:HE2  | 51:3:21:GLY:HA2   | 1.81                     | 0.62              |
| 22:a:2635:A:O2'  | 25:d:81:GLU:OE1   | 2.13                     | 0.62              |
| 43:v:59:LEU:HD12 | 43:v:80:ILE:HD12  | 1.82                     | 0.62              |
| 9:I:28:ILE:HG21  | 9:I:35:LEU:HD12   | 1.80                     | 0.62              |
| 1:A:1009:U:H3    | 1:A:1020:G:H1     | 0.72                     | 0.62              |
| 22:a:278:A:N1    | 22:a:361:G:O2'    | 2.32                     | 0.62              |
| 22:a:2298:A:OP1  | 27:f:71:ARG:NH2   | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:202:GLU:OE1  | 5:E:112:ARG:NH2  | 2.31                     | 0.61              |
| 1:A:1119:C:OP1   | 9:I:85:ARG:NH1   | 2.31                     | 0.61              |
| 1:A:398:U:H2'    | 1:A:399:G:H8     | 1.65                     | 0.61              |
| 2:B:117:LEU:HB3  | 2:B:141:LEU:HD12 | 1.82                     | 0.61              |
| 40:s:47:VAL:HG23 | 40:s:51:PHE:HD2  | 1.65                     | 0.61              |
| 1:A:413:G:H21    | 1:A:428:G:H2'    | 1.62                     | 0.61              |
| 1:A:1280:A:OP2   | 10:J:9:ARG:NH2   | 2.32                     | 0.61              |
| 1:A:413:G:N2     | 1:A:428:G:H2'    | 2.15                     | 0.61              |
| 1:A:76:G:O6      | 1:A:93:U:O4      | 2.18                     | 0.61              |
| 1:A:1130:A:H2'   | 1:A:1131:G:H8    | 1.64                     | 0.61              |
| 1:A:337:G:H2'    | 1:A:338:A:C8     | 2.36                     | 0.61              |
| 22:a:2547:A:H2'  | 22:a:2548:U:C6   | 2.35                     | 0.61              |
| 1:A:215:C:H1'    | 1:A:465:A:N6     | 2.16                     | 0.61              |
| 16:P:45:GLU:O    | 16:P:46:LYS:HG2  | 2.00                     | 0.61              |
| 22:a:320:A:N3    | 26:e:163:ASN:ND2 | 2.46                     | 0.61              |
| 1:A:1516:2MG:N1  | 1:A:1519:MA6:OP2 | 2.34                     | 0.61              |
| 47:z:54:VAL:HG23 | 47:z:55:ILE:HG12 | 1.83                     | 0.61              |
| 22:a:534:U:O2'   | 37:p:49:ASP:OD2  | 2.14                     | 0.60              |
| 22:a:1469:A:H2'  | 22:a:1470:A:C8   | 2.36                     | 0.60              |
| 22:a:2788:C:H2'  | 22:a:2789:C:C6   | 2.36                     | 0.60              |
| 1:A:492:C:H2'    | 1:A:493:A:C8     | 2.36                     | 0.60              |
| 3:C:46:GLU:HG2   | 3:C:87:LEU:HD21  | 1.84                     | 0.60              |
| 6:F:88:MET:HE2   | 6:F:90:MET:HE2   | 1.83                     | 0.60              |
| 14:N:3:LYS:HB2   | 14:N:6:MET:HG2   | 1.83                     | 0.60              |
| 8:H:29:SER:HB3   | 8:H:57:PRO:HB2   | 1.83                     | 0.60              |
| 22:a:1197:G:H2'  | 22:a:1198:U:H6   | 1.65                     | 0.60              |
| 33:l:53:MET:HG3  | 33:l:120:ALA:HB2 | 1.83                     | 0.60              |
| 26:e:176:ASP:OD1 | 26:e:179:SER:OG  | 2.18                     | 0.60              |
| 1:A:555:U:H2'    | 1:A:556:C:C6     | 2.36                     | 0.60              |
| 1:A:823:C:HO2'   | 8:H:2:SER:N      | 2.00                     | 0.60              |
| 1:A:1038:C:H2'   | 1:A:1039:G:H8    | 1.67                     | 0.60              |
| 1:A:1166:G:N1    | 1:A:1169:A:OP2   | 2.34                     | 0.60              |
| 22:a:1704:C:H2'  | 22:a:1705:A:H8   | 1.65                     | 0.60              |
| 1:A:202:G:H21    | 1:A:466:A:H61    | 1.48                     | 0.60              |
| 1:A:746:A:H2'    | 1:A:747:A:C8     | 2.37                     | 0.60              |
| 1:A:1009:U:O4    | 1:A:1020:G:O6    | 2.20                     | 0.60              |
| 26:e:111:GLU:OE2 | 26:e:115:GLN:NE2 | 2.35                     | 0.60              |
| 22:a:545:U:O2    | 22:a:548:G:C6    | 2.53                     | 0.60              |
| 30:i:13:ARG:NH1  | 30:i:49:ASP:O    | 2.34                     | 0.60              |
| 1:A:423:G:O2'    | 1:A:424:G:O4'    | 2.18                     | 0.60              |
| 19:S:11:ILE:HG13 | 19:S:38:SER:HB3  | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:a:1799:G:N7    | 24:c:178:SER:OG   | 2.31                     | 0.60              |
| 7:G:26:PHE:HD1    | 7:G:101:MET:HG2   | 1.66                     | 0.59              |
| 7:G:140:ASP:OD1   | 7:G:143:ARG:NH1   | 2.33                     | 0.59              |
| 1:A:1098:C:O2'    | 21:U:71:TYR:O     | 2.20                     | 0.59              |
| 1:A:1314:C:OP2    | 19:S:4:SER:OG     | 2.14                     | 0.59              |
| 13:M:104:THR:HG22 | 13:M:105:ASN:H    | 1.65                     | 0.59              |
| 22:a:1667:G:O2'   | 22:a:1991:U:O4    | 2.19                     | 0.59              |
| 33:l:53:MET:HE1   | 33:l:103:TYR:CD1  | 2.37                     | 0.59              |
| 1:A:1030:U:O2'    | 1:A:1031:C:O5'    | 2.18                     | 0.59              |
| 3:C:105:GLU:OE2   | 3:C:107:ARG:NH2   | 2.36                     | 0.59              |
| 7:G:93:PRO:HA     | 7:G:96:ARG:HD3    | 1.84                     | 0.59              |
| 22:a:1794:A:H2'   | 22:a:1795:C:C6    | 2.37                     | 0.59              |
| 27:f:29:PRO:HB2   | 27:f:169:LEU:HD22 | 1.84                     | 0.59              |
| 35:n:88:LYS:HE2   | 35:n:116:GLN:HE22 | 1.66                     | 0.59              |
| 27:f:106:ILE:HD12 | 52:4:34:LEU:HD21  | 1.84                     | 0.59              |
| 1:A:1218:C:H2'    | 1:A:1219:A:C8     | 2.38                     | 0.59              |
| 25:d:46:ARG:NH1   | 25:d:85:ALA:O     | 2.25                     | 0.59              |
| 21:U:31:GLU:OE2   | 21:U:35:ARG:NE    | 2.34                     | 0.59              |
| 22:a:284:U:H2'    | 22:a:285:G:H8     | 1.67                     | 0.59              |
| 22:a:2095:A:O5'   | 29:h:11:ASN:ND2   | 2.36                     | 0.59              |
| 42:u:9:ARG:HG2    | 42:u:41:GLU:HG3   | 1.84                     | 0.59              |
| 22:a:307:G:N1     | 22:a:310:A:OP2    | 2.31                     | 0.59              |
| 22:a:993:G:OP2    | 37:p:51:ARG:NH2   | 2.36                     | 0.59              |
| 22:a:1315:C:O2'   | 22:a:1392:A:N3    | 2.34                     | 0.58              |
| 33:l:41:LEU:HG    | 33:l:96:ILE:HG13  | 1.85                     | 0.58              |
| 15:O:18:ASP:OD2   | 15:O:20:ASN:N     | 2.29                     | 0.58              |
| 34:m:86:ARG:NE    | 34:m:117:ASP:OD2  | 2.33                     | 0.58              |
| 24:c:75:PRO:HG2   | 24:c:97:LYS:HG3   | 1.85                     | 0.58              |
| 33:l:105:MET:HE3  | 33:l:108:VAL:HG21 | 1.84                     | 0.58              |
| 1:A:545:C:H2'     | 1:A:546:A:H5'     | 1.86                     | 0.58              |
| 18:R:71:THR:HG23  | 18:R:73:ARG:H     | 1.68                     | 0.58              |
| 22:a:742:A:H2'    | 22:a:743:A:C8     | 2.38                     | 0.58              |
| 22:a:1548:A:H2'   | 22:a:1549:A:C8    | 2.38                     | 0.58              |
| 22:a:347:A:H2'    | 22:a:348:A:C8     | 2.39                     | 0.58              |
| 15:O:26:GLU:OE2   | 15:O:77:ARG:NH1   | 2.37                     | 0.58              |
| 1:A:950:U:O4      | 13:M:104:THR:HG21 | 2.04                     | 0.58              |
| 2:B:120:GLN:OE1   | 2:B:137:ARG:NH1   | 2.37                     | 0.58              |
| 1:A:539:A:H2'     | 1:A:540:G:C8      | 2.38                     | 0.57              |
| 22:a:499:U:H5''   | 41:t:43:LYS:HE2   | 1.86                     | 0.57              |
| 22:a:1636:U:H2'   | 22:a:1637:A:H8    | 1.68                     | 0.57              |
| 1:A:64:G:OP1      | 1:A:382:A:N6      | 2.37                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:201:G:O2'     | 1:A:469:C:O2'     | 2.20                     | 0.57              |
| 22:a:1047:G:O2'   | 22:a:1110:G:N1    | 2.22                     | 0.57              |
| 1:A:423:G:O2'     | 1:A:424:G:O5'     | 2.22                     | 0.57              |
| 22:a:2845:U:H5''  | 36:o:52:ASN:O     | 2.04                     | 0.57              |
| 22:a:414:C:H2'    | 22:a:415:A:C8     | 2.40                     | 0.57              |
| 27:f:80:ARG:HB2   | 27:f:83:TYR:HE2   | 1.70                     | 0.57              |
| 1:A:28:A:O2'      | 1:A:296:U:OP1     | 2.16                     | 0.57              |
| 22:a:631:A:OP2    | 50:2:23:LYS:NZ    | 2.37                     | 0.57              |
| 22:a:1386:C:H2'   | 22:a:1387:A:C8    | 2.39                     | 0.57              |
| 1:A:653:U:OP1     | 8:H:56:LYS:NZ     | 2.26                     | 0.57              |
| 12:L:99:ARG:NH1   | 12:L:104:CYS:SG   | 2.77                     | 0.57              |
| 32:k:132:ARG:HG3  | 32:k:142:ILE:HD12 | 1.86                     | 0.57              |
| 37:p:97:ASP:OD2   | 38:q:13:ARG:NH1   | 2.38                     | 0.57              |
| 22:a:2566:A:N1    | 31:j:28:SER:OG    | 2.35                     | 0.57              |
| 22:a:2799:A:O2'   | 22:a:2800:A:H5''  | 2.05                     | 0.57              |
| 10:J:26:VAL:HG23  | 10:J:36:VAL:HG21  | 1.85                     | 0.56              |
| 22:a:414:C:H2'    | 22:a:415:A:H8     | 1.71                     | 0.56              |
| 22:a:1720:U:H2'   | 22:a:1721:G:O4'   | 2.05                     | 0.56              |
| 1:A:131:A:H2'     | 1:A:132:C:C6      | 2.40                     | 0.56              |
| 1:A:1152:A:OP1    | 10:J:70:HIS:ND1   | 2.33                     | 0.56              |
| 4:D:11:LEU:HD13   | 4:D:63:ARG:HG2    | 1.88                     | 0.56              |
| 22:a:475:C:O2     | 22:a:479:A:N6     | 2.36                     | 0.56              |
| 22:a:639:U:H2'    | 22:a:640:C:H6     | 1.70                     | 0.56              |
| 22:a:1405:U:H2'   | 22:a:1406:U:C6    | 2.40                     | 0.56              |
| 22:a:1796:U:H2'   | 22:a:1797:G:H8    | 1.70                     | 0.56              |
| 29:h:6:LEU:HD11   | 29:h:37:VAL:HG13  | 1.85                     | 0.56              |
| 41:t:8:ASP:O      | 41:t:24:LYS:NZ    | 2.34                     | 0.56              |
| 13:M:10:PRO:HB2   | 13:M:13:LYS:HG3   | 1.87                     | 0.56              |
| 15:O:6:GLU:OE1    | 15:O:6:GLU:N      | 2.28                     | 0.56              |
| 7:G:113:ASP:HB2   | 7:G:119:ARG:HG3   | 1.87                     | 0.56              |
| 44:w:43:GLU:OE2   | 44:w:45:ARG:NH2   | 2.38                     | 0.56              |
| 48:0:9:ILE:HD12   | 48:0:51:GLU:HG3   | 1.87                     | 0.56              |
| 22:a:856:G:H2'    | 22:a:857:G:C8     | 2.41                     | 0.56              |
| 22:a:910:A:H2'    | 22:a:911:A:C8     | 2.40                     | 0.56              |
| 22:a:2316:G:H2'   | 22:a:2317:A:H8    | 1.70                     | 0.56              |
| 37:p:109:LEU:HD11 | 38:q:40:MET:HE1   | 1.86                     | 0.56              |
| 6:F:44:ARG:HG3    | 6:F:44:ARG:HH11   | 1.71                     | 0.56              |
| 13:M:59:GLU:HA    | 13:M:62:LYS:NZ    | 2.20                     | 0.56              |
| 19:S:19:VAL:HG21  | 19:S:44:MET:HG2   | 1.86                     | 0.56              |
| 30:i:88:THR:N     | 30:i:91:GLU:OE1   | 2.25                     | 0.56              |
| 34:m:22:ARG:HG3   | 34:m:70:THR:HA    | 1.87                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:390:U:H2'     | 1:A:391:G:C8     | 2.41                     | 0.56              |
| 22:a:1340:U:OP1   | 40:s:19:LYS:NZ   | 2.38                     | 0.56              |
| 1:A:390:U:H2'     | 1:A:391:G:H8     | 1.70                     | 0.56              |
| 1:A:713:G:H2'     | 1:A:714:G:C8     | 2.40                     | 0.56              |
| 3:C:19:ASN:O      | 3:C:40:ARG:NH2   | 2.38                     | 0.56              |
| 5:E:149:SER:OG    | 5:E:152:MET:HE3  | 2.05                     | 0.56              |
| 9:I:84:THR:HG23   | 9:I:98:LEU:HD13  | 1.88                     | 0.56              |
| 22:a:1636:U:H2'   | 22:a:1637:A:C8   | 2.41                     | 0.56              |
| 35:n:56:LYS:O     | 35:n:60:GLU:HG3  | 2.06                     | 0.56              |
| 13:M:104:THR:HG22 | 13:M:105:ASN:N   | 2.21                     | 0.55              |
| 1:A:546:A:H2'     | 4:D:68:LEU:HD21  | 1.87                     | 0.55              |
| 22:a:359:G:H2'    | 22:a:360:U:H6    | 1.71                     | 0.55              |
| 22:a:2883:A:OP2   | 47:z:50:ARG:NH1  | 2.39                     | 0.55              |
| 39:r:83:LYS:HG2   | 39:r:95:ARG:HD3  | 1.87                     | 0.55              |
| 1:A:399:G:H2'     | 1:A:400:C:C6     | 2.41                     | 0.55              |
| 1:A:414:A:O2'     | 1:A:415:A:O5'    | 2.24                     | 0.55              |
| 1:A:715:A:H2'     | 1:A:716:A:C8     | 2.41                     | 0.55              |
| 1:A:1144:G:N2     | 1:A:1146:A:H62   | 2.04                     | 0.55              |
| 6:F:88:MET:HE1    | 18:R:61:ARG:HG2  | 1.87                     | 0.55              |
| 22:a:284:U:H2'    | 22:a:285:G:C8    | 2.41                     | 0.55              |
| 22:a:360:U:H2'    | 22:a:361:G:O4'   | 2.07                     | 0.55              |
| 1:A:411:A:OP1     | 4:D:26:ARG:NH1   | 2.32                     | 0.55              |
| 1:A:1273:C:H2'    | 1:A:1274:A:O4'   | 2.07                     | 0.55              |
| 1:A:1356:G:H2'    | 1:A:1357:A:H8    | 1.70                     | 0.55              |
| 2:B:61:ALA:HB2    | 2:B:221:VAL:HG23 | 1.89                     | 0.55              |
| 22:a:2343:U:HO2'  | 22:a:2373:G:HO2' | 1.52                     | 0.55              |
| 1:A:1391:U:H2'    | 1:A:1392:G:C8    | 2.42                     | 0.55              |
| 1:A:744:C:H2'     | 1:A:745:G:H8     | 1.71                     | 0.55              |
| 22:a:84:A:N1      | 22:a:98:G:O2'    | 2.35                     | 0.55              |
| 22:a:2329:U:H2'   | 22:a:2330:G:C8   | 2.42                     | 0.55              |
| 1:A:1130:A:H2'    | 1:A:1131:G:C8    | 2.42                     | 0.55              |
| 5:E:13:GLU:OE2    | 5:E:68:ARG:NH1   | 2.39                     | 0.55              |
| 22:a:64:A:H2'     | 22:a:65:U:C6     | 2.42                     | 0.55              |
| 22:a:1252:G:OP2   | 37:p:13:ARG:NH1  | 2.31                     | 0.55              |
| 22:a:2291:U:H2'   | 22:a:2292:U:C6   | 2.42                     | 0.55              |
| 35:n:27:VAL:HG21  | 35:n:40:ILE:HD12 | 1.88                     | 0.55              |
| 22:a:191:A:H2'    | 22:a:192:C:C6    | 2.41                     | 0.55              |
| 22:a:1864:U:OP1   | 22:a:2410:G:O2'  | 2.19                     | 0.55              |
| 22:a:1869:G:N2    | 22:a:1872:A:OP2  | 2.38                     | 0.55              |
| 10:J:52:LEU:HD11  | 10:J:59:LYS:HD2  | 1.88                     | 0.55              |
| 27:f:116:GLY:HA3  | 27:f:178:ARG:HB3 | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:m:28:LEU:HD23 | 34:m:48:VAL:HG21 | 1.89                     | 0.55              |
| 1:A:78:A:H2'     | 1:A:79:G:H8      | 1.72                     | 0.54              |
| 22:a:365:U:H2'   | 22:a:366:C:C6    | 2.43                     | 0.54              |
| 22:a:1794:A:H2'  | 22:a:1795:C:H6   | 1.72                     | 0.54              |
| 1:A:1151:A:HO2'  | 1:A:1152:A:H8    | 1.53                     | 0.54              |
| 1:A:1323:G:H2'   | 1:A:1324:A:C8    | 2.41                     | 0.54              |
| 22:a:1816:C:N4   | 24:c:35:GLU:OE2  | 2.36                     | 0.54              |
| 23:b:66:A:N6     | 23:b:107:G:H2'   | 2.22                     | 0.54              |
| 21:U:39:GLU:OE1  | 21:U:47:ARG:NH1  | 2.41                     | 0.54              |
| 23:b:52:A:N7     | 35:n:64:TYR:OH   | 2.26                     | 0.54              |
| 1:A:1033:G:H2'   | 1:A:1034:G:C8    | 2.43                     | 0.54              |
| 16:P:36:VAL:HG13 | 16:P:53:ASP:HB3  | 1.90                     | 0.54              |
| 22:a:1156:A:C8   | 37:p:51:ARG:HG2  | 2.42                     | 0.54              |
| 22:a:2419:U:H4'  | 48:0:22:THR:HG21 | 1.90                     | 0.54              |
| 1:A:216:U:H2'    | 1:A:217:C:C6     | 2.42                     | 0.54              |
| 1:A:683:G:N2     | 11:K:39:GLY:O    | 2.40                     | 0.54              |
| 19:S:12:ASP:OD2  | 19:S:35:SER:OG   | 2.19                     | 0.54              |
| 22:a:172:A:H2'   | 22:a:173:A:C8    | 2.42                     | 0.54              |
| 22:a:1746:A:H2'  | 22:a:1747:U:C6   | 2.42                     | 0.54              |
| 32:k:77:ILE:HD11 | 32:k:108:ALA:HB1 | 1.90                     | 0.54              |
| 42:u:51:GLN:OE1  | 42:u:57:TYR:OH   | 2.23                     | 0.54              |
| 1:A:89:U:H2'     | 1:A:90:C:C6      | 2.43                     | 0.54              |
| 22:a:1266:G:O2'  | 22:a:2012:G:O6   | 2.25                     | 0.54              |
| 1:A:575:G:O2'    | 1:A:821:G:OP2    | 2.20                     | 0.54              |
| 9:I:88:MET:HE3   | 9:I:98:LEU:HD12  | 1.88                     | 0.54              |
| 22:a:126:A:OP1   | 49:1:45:SER:OG   | 2.26                     | 0.54              |
| 22:a:851:C:H2'   | 22:a:852:U:H6    | 1.73                     | 0.54              |
| 35:n:34:HIS:O    | 35:n:102:ARG:NH1 | 2.40                     | 0.54              |
| 1:A:78:A:H2'     | 1:A:79:G:C8      | 2.43                     | 0.54              |
| 27:f:80:ARG:HB2  | 27:f:83:TYR:CE2  | 2.42                     | 0.54              |
| 12:L:4:VAL:HG23  | 17:Q:34:TYR:HB3  | 1.90                     | 0.54              |
| 16:P:48:GLU:OE2  | 16:P:51:ARG:HB2  | 2.08                     | 0.54              |
| 33:l:1:MET:HE2   | 33:l:1:MET:HA    | 1.89                     | 0.54              |
| 1:A:1040:U:H2'   | 1:A:1041:G:C8    | 2.44                     | 0.53              |
| 6:F:37:HIS:HB3   | 6:F:97:THR:HG22  | 1.88                     | 0.53              |
| 10:J:24:GLU:HG3  | 10:J:90:LEU:HD21 | 1.90                     | 0.53              |
| 15:O:18:ASP:HB3  | 15:O:21:ASP:HB2  | 1.89                     | 0.53              |
| 22:a:721:A:H2'   | 22:a:722:A:C8    | 2.43                     | 0.53              |
| 22:a:1278:C:H2'  | 22:a:1279:G:H8   | 1.73                     | 0.53              |
| 23:b:1:U:H2'     | 23:b:2:G:C8      | 2.41                     | 0.53              |
| 1:A:45:G:H2'     | 1:A:46:G:H8      | 1.73                     | 0.53              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 22:a:568:U:H1'   | 22:a:2030:6MZ:H9C1 | 1.90                     | 0.53              |
| 22:a:636:G:OP1   | 32:k:129:LYS:NZ    | 2.41                     | 0.53              |
| 22:a:881:G:N2    | 22:a:895:U:O2      | 2.39                     | 0.53              |
| 25:d:1:MET:SD    | 25:d:205:PRO:HG2   | 2.47                     | 0.53              |
| 1:A:499:A:H61    | 1:A:547:A:H5''     | 1.73                     | 0.53              |
| 1:A:1120:C:H2'   | 1:A:1121:U:H6      | 1.73                     | 0.53              |
| 8:H:50:LYS:HG3   | 8:H:52:GLU:OE2     | 2.09                     | 0.53              |
| 14:N:29:ALA:O    | 14:N:33:ASP:HB2    | 2.08                     | 0.53              |
| 22:a:729:G:H5''  | 22:a:730:A:H5''    | 1.89                     | 0.53              |
| 22:a:1796:U:H2'  | 22:a:1797:G:C8     | 2.44                     | 0.53              |
| 22:a:2243:U:H2'  | 22:a:2244:U:C6     | 2.44                     | 0.53              |
| 1:A:1040:U:H2'   | 1:A:1041:G:H8      | 1.72                     | 0.53              |
| 3:C:123:GLN:OE1  | 3:C:136:ARG:NH2    | 2.42                     | 0.53              |
| 22:a:807:U:OP2   | 32:k:41:ARG:NH1    | 2.42                     | 0.53              |
| 22:a:1509:A:HO2' | 22:a:1510:G:H8     | 1.55                     | 0.53              |
| 41:t:4:LYS:O     | 41:t:94:ARG:NH2    | 2.41                     | 0.53              |
| 22:a:851:C:H2'   | 22:a:852:U:C6      | 2.44                     | 0.53              |
| 22:a:2848:G:O2'  | 22:a:2867:G:N2     | 2.33                     | 0.53              |
| 25:d:13:ARG:HD3  | 25:d:21:SER:OG     | 2.07                     | 0.53              |
| 1:A:17:U:H2'     | 1:A:18:C:C6        | 2.43                     | 0.53              |
| 1:A:201:G:HO2'   | 1:A:469:C:HO2'     | 1.55                     | 0.53              |
| 22:a:1570:A:H2'  | 22:a:1571:A:C8     | 2.42                     | 0.53              |
| 22:a:2430:A:N3   | 22:a:2430:A:H2'    | 2.23                     | 0.53              |
| 1:A:382:A:H2'    | 1:A:383:A:C8       | 2.44                     | 0.53              |
| 1:A:636:U:O2'    | 1:A:637:C:H5'      | 2.08                     | 0.53              |
| 6:F:96:VAL:HG12  | 6:F:96:VAL:O       | 2.09                     | 0.53              |
| 22:a:468:G:OP2   | 49:l:37:LYS:NZ     | 2.42                     | 0.53              |
| 23:b:66:A:H61    | 23:b:107:G:H2'     | 1.74                     | 0.53              |
| 1:A:148:G:O2'    | 1:A:1446:A:N3      | 2.40                     | 0.53              |
| 1:A:524:G:H2'    | 1:A:525:C:C6       | 2.44                     | 0.53              |
| 24:c:21:ASN:HB3  | 24:c:24:LEU:HG     | 1.89                     | 0.53              |
| 1:A:508:U:H1'    | 1:A:509:A:H2       | 1.74                     | 0.53              |
| 1:A:1010:U:H2'   | 1:A:1011:C:C6      | 2.43                     | 0.53              |
| 10:J:18:ILE:O    | 10:J:22:THR:HG23   | 2.07                     | 0.53              |
| 13:M:70:ARG:HE   | 27:f:112:ARG:HH12  | 1.57                     | 0.53              |
| 22:a:138:U:O2'   | 22:a:141:G:O6      | 2.26                     | 0.53              |
| 22:a:221:A:N1    | 22:a:265:A:O2'     | 2.41                     | 0.53              |
| 22:a:1141:U:H4'  | 22:a:1142:A:O4'    | 2.09                     | 0.53              |
| 25:d:181:ASP:HB3 | 25:d:186:LEU:HB2   | 1.91                     | 0.53              |
| 1:A:754:C:O5'    | 15:O:72:ARG:NH2    | 2.42                     | 0.52              |
| 22:a:1028:A:H2'  | 22:a:1029:A:C8     | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 44:w:6:GLN:O     | 44:w:74:ARG:NH1  | 2.42                     | 0.52              |
| 1:A:202:G:O2'    | 1:A:468:A:N3     | 2.40                     | 0.52              |
| 1:A:362:G:N2     | 1:A:365:U:OP2    | 2.39                     | 0.52              |
| 22:a:892:A:H2'   | 22:a:893:C:C6    | 2.44                     | 0.52              |
| 22:a:1292:G:H2'  | 22:a:1293:C:C6   | 2.45                     | 0.52              |
| 22:a:1856:U:H2'  | 22:a:1857:G:O4'  | 2.09                     | 0.52              |
| 1:A:530:G:H2'    | 1:A:530:G:N3     | 2.24                     | 0.52              |
| 22:a:2591:C:H2'  | 22:a:2592:G:C8   | 2.43                     | 0.52              |
| 22:a:476:G:N1    | 22:a:479:A:OP2   | 2.37                     | 0.52              |
| 11:K:75:LYS:HZ3  | 11:K:75:LYS:HB2  | 1.73                     | 0.52              |
| 22:a:359:G:H2'   | 22:a:360:U:C6    | 2.44                     | 0.52              |
| 22:a:640:C:H2'   | 22:a:641:U:C6    | 2.44                     | 0.52              |
| 22:a:742:A:H2'   | 22:a:743:A:H8    | 1.75                     | 0.52              |
| 22:a:363:G:H2'   | 22:a:364:C:H6    | 1.75                     | 0.52              |
| 22:a:879:G:H2'   | 22:a:880:G:C8    | 2.45                     | 0.52              |
| 37:p:86:ALA:HB2  | 37:p:116:ALA:HB2 | 1.92                     | 0.52              |
| 54:Z:22:A:H61    | 54:Z:47:A:H2'    | 1.73                     | 0.52              |
| 1:A:415:A:H2'    | 1:A:416:G:H8     | 1.75                     | 0.52              |
| 1:A:459:A:H2'    | 1:A:460:A:C8     | 2.45                     | 0.52              |
| 22:a:720:U:H2'   | 22:a:721:A:C8    | 2.45                     | 0.52              |
| 22:a:1149:G:H2'  | 22:a:1150:C:C6   | 2.45                     | 0.52              |
| 22:a:1548:A:H2'  | 22:a:1549:A:H8   | 1.75                     | 0.52              |
| 22:a:2327:A:H2'  | 22:a:2328:A:C8   | 2.44                     | 0.52              |
| 27:f:98:GLU:OE2  | 52:4:25:ARG:NE   | 2.37                     | 0.52              |
| 32:k:57:LEU:HD22 | 50:2:54:ASP:HB3  | 1.91                     | 0.52              |
| 32:k:81:ASP:HA   | 32:k:84:LYS:HD2  | 1.91                     | 0.52              |
| 35:n:83:LEU:HD11 | 35:n:114:GLY:HA3 | 1.92                     | 0.52              |
| 1:A:151:A:OP2    | 1:A:169:C:N4     | 2.42                     | 0.52              |
| 22:a:3:U:H2'     | 22:a:4:U:C6      | 2.45                     | 0.52              |
| 22:a:2101:A:H2'  | 22:a:2102:G:H8   | 1.75                     | 0.52              |
| 54:Z:24:C:H2'    | 54:Z:25:U:C6     | 2.45                     | 0.52              |
| 1:A:517:G:O2'    | 1:A:518:C:O5'    | 2.27                     | 0.52              |
| 5:E:151:GLU:OE2  | 5:E:151:GLU:N    | 2.41                     | 0.52              |
| 22:a:1:G:H2'     | 22:a:2:G:H8      | 1.75                     | 0.52              |
| 22:a:1484:U:H2'  | 22:a:1485:U:C6   | 2.45                     | 0.52              |
| 22:a:2483:C:N3   | 33:l:123:LYS:NZ  | 2.58                     | 0.52              |
| 27:f:140:GLU:HA  | 52:4:28:VAL:HG22 | 1.92                     | 0.52              |
| 51:3:16:ILE:HD13 | 51:3:25:VAL:HG22 | 1.92                     | 0.52              |
| 1:A:601:G:OP1    | 8:H:89:LYS:NZ    | 2.31                     | 0.52              |
| 1:A:769:G:H4'    | 1:A:1513:A:H4'   | 1.92                     | 0.52              |
| 16:P:40:ASN:HB3  | 16:P:43:ALA:HB2  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:903:C:H2'   | 22:a:904:G:H8     | 1.74                     | 0.52              |
| 22:a:1802:A:H2'  | 22:a:1803:A:C8    | 2.44                     | 0.52              |
| 28:g:107:LEU:HB3 | 28:g:152:ARG:HG3  | 1.92                     | 0.52              |
| 29:h:4:ILE:HG22  | 29:h:18:GLN:HG2   | 1.92                     | 0.52              |
| 29:h:6:LEU:HD21  | 29:h:37:VAL:HG22  | 1.92                     | 0.52              |
| 1:A:696:A:H2'    | 1:A:697:U:H6      | 1.75                     | 0.51              |
| 2:B:104:TRP:HA   | 2:B:107:VAL:HG22  | 1.92                     | 0.51              |
| 22:a:1386:C:H2'  | 22:a:1387:A:H8    | 1.75                     | 0.51              |
| 33:l:77:PRO:HG2  | 33:l:80:VAL:HG21  | 1.91                     | 0.51              |
| 1:A:224:U:H2'    | 1:A:225:C:C6      | 2.45                     | 0.51              |
| 1:A:451:A:N6     | 1:A:480:U:O2'     | 2.41                     | 0.51              |
| 4:D:58:LYS:HD3   | 4:D:203:LEU:HD11  | 1.91                     | 0.51              |
| 22:a:1902:C:H4'  | 24:c:242:LYS:O    | 2.11                     | 0.51              |
| 22:a:2266:A:H4'  | 22:a:2267:A:N3    | 2.25                     | 0.51              |
| 1:A:1062:U:H2'   | 1:A:1063:C:C6     | 2.44                     | 0.51              |
| 1:A:1314:C:H2'   | 1:A:1315:U:C6     | 2.45                     | 0.51              |
| 22:a:288:U:H2'   | 22:a:289:G:C8     | 2.45                     | 0.51              |
| 22:a:1597:A:H5'' | 22:a:1598:A:H5'   | 1.93                     | 0.51              |
| 25:d:108:ASP:OD2 | 25:d:173:GLN:HA   | 2.11                     | 0.51              |
| 45:x:39:GLN:OE1  | 45:x:41:HIS:HE1   | 1.94                     | 0.51              |
| 7:G:15:ASP:OD2   | 7:G:19:GLY:N      | 2.43                     | 0.51              |
| 9:I:7:TYR:HH     | 9:I:9:THR:HG1     | 1.58                     | 0.51              |
| 22:a:552:U:H2'   | 22:a:553:G:H8     | 1.76                     | 0.51              |
| 22:a:644:A:H2'   | 22:a:645:C:O4'    | 2.10                     | 0.51              |
| 22:a:1526:C:H2'  | 22:a:1527:G:O4'   | 2.10                     | 0.51              |
| 4:D:99:ASP:OD2   | 4:D:100:ASN:N     | 2.44                     | 0.51              |
| 22:a:2618:G:H21  | 25:d:155:VAL:HG21 | 1.75                     | 0.51              |
| 22:a:2698:U:H2'  | 22:a:2699:C:C6    | 2.46                     | 0.51              |
| 1:A:945:G:C2     | 1:A:946:A:C8      | 2.98                     | 0.51              |
| 13:M:86:TYR:O    | 13:M:90:ARG:HG2   | 2.10                     | 0.51              |
| 22:a:277:G:H4'   | 22:a:278:A:O5'    | 2.11                     | 0.51              |
| 22:a:347:A:H2'   | 22:a:348:A:H8     | 1.75                     | 0.51              |
| 1:A:269:C:H2'    | 1:A:270:A:C8      | 2.45                     | 0.51              |
| 1:A:464:U:N3     | 1:A:467:U:OP2     | 2.30                     | 0.51              |
| 1:A:900:A:H2'    | 1:A:901:A:C8      | 2.45                     | 0.51              |
| 4:D:101:VAL:HG12 | 4:D:105:MET:HE2   | 1.91                     | 0.51              |
| 22:a:2246:G:H2'  | 22:a:2247:A:C8    | 2.46                     | 0.51              |
| 41:t:86:ARG:HG3  | 41:t:95:PHE:CE1   | 2.46                     | 0.51              |
| 1:A:2:A:H4'      | 4:D:83:LYS:NZ     | 2.26                     | 0.51              |
| 10:J:24:GLU:OE2  | 10:J:92:LEU:HD13  | 2.11                     | 0.51              |
| 13:M:59:GLU:OE2  | 13:M:62:LYS:NZ    | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:183:C:H42   | 22:a:213:A:H61   | 1.59                     | 0.51              |
| 38:q:40:MET:HE2  | 38:q:49:ILE:HG12 | 1.92                     | 0.51              |
| 41:t:33:LYS:HB3  | 41:t:64:ALA:HB1  | 1.93                     | 0.51              |
| 3:C:164:ARG:NH1  | 3:C:166:GLU:OE2  | 2.44                     | 0.51              |
| 13:M:92:ARG:HD3  | 22:a:888:C:C5    | 2.46                     | 0.51              |
| 22:a:581:C:H2'   | 22:a:582:A:C8    | 2.46                     | 0.51              |
| 22:a:703:U:H2'   | 22:a:704:G:O4'   | 2.11                     | 0.51              |
| 22:a:879:G:H2'   | 22:a:880:G:H8    | 1.76                     | 0.51              |
| 22:a:995:C:OP2   | 37:p:54:LYS:NZ   | 2.39                     | 0.51              |
| 25:d:55:LYS:HE2  | 25:d:77:ARG:HA   | 1.92                     | 0.51              |
| 29:h:34:GLY:O    | 29:h:36:ALA:N    | 2.44                     | 0.51              |
| 7:G:16:PRO:HB2   | 9:I:42:GLU:HG3   | 1.93                     | 0.50              |
| 7:G:68:ASN:HD22  | 7:G:130:ASN:CG   | 2.18                     | 0.50              |
| 8:H:22:LYS:O     | 8:H:65:TYR:OH    | 2.26                     | 0.50              |
| 13:M:89:LEU:HD22 | 13:M:93:ARG:HH12 | 1.76                     | 0.50              |
| 22:a:306:U:H2'   | 22:a:307:G:O4'   | 2.11                     | 0.50              |
| 22:a:2273:A:H2'  | 22:a:2274:A:C8   | 2.46                     | 0.50              |
| 1:A:509:A:O2'    | 1:A:510:A:N3     | 2.35                     | 0.50              |
| 6:F:1:MET:HG3    | 6:F:65:GLU:HG2   | 1.92                     | 0.50              |
| 22:a:1197:G:H2'  | 22:a:1198:U:C6   | 2.46                     | 0.50              |
| 36:o:5:ILE:HG22  | 36:o:9:GLU:OE1   | 2.10                     | 0.50              |
| 1:A:1229:A:OP2   | 13:M:113:ARG:NH1 | 2.44                     | 0.50              |
| 3:C:47:LEU:HD21  | 3:C:87:LEU:HD11  | 1.93                     | 0.50              |
| 10:J:88:MET:HE3  | 10:J:88:MET:HA   | 1.94                     | 0.50              |
| 22:a:1242:U:H2'  | 22:a:1243:C:C6   | 2.47                     | 0.50              |
| 22:a:1930:G:O2'  | 22:a:1968:G:O6   | 2.28                     | 0.50              |
| 48:O:10:LYS:HD2  | 48:O:20:PHE:CD2  | 2.46                     | 0.50              |
| 9:I:57:MET:HE1   | 9:I:90:TYR:CE1   | 2.47                     | 0.50              |
| 1:A:1477:U:H2'   | 1:A:1478:U:C6    | 2.47                     | 0.50              |
| 22:a:849:A:H2'   | 22:a:850:U:C6    | 2.47                     | 0.50              |
| 22:a:2074:U:H2'  | 22:a:2075:U:C6   | 2.47                     | 0.50              |
| 22:a:2469:A:N6   | 22:a:2481:G:O2'  | 2.39                     | 0.50              |
| 1:A:539:A:OP1    | 12:L:111:LYS:HD2 | 2.12                     | 0.50              |
| 1:A:1010:U:H2'   | 1:A:1011:C:H6    | 1.77                     | 0.50              |
| 7:G:48:GLU:O     | 7:G:52:GLN:HG2   | 2.12                     | 0.50              |
| 8:H:10:MET:HG3   | 8:H:27:MET:SD    | 2.52                     | 0.50              |
| 22:a:24:G:O2'    | 39:r:78:GLU:O    | 2.30                     | 0.50              |
| 22:a:2680:U:O2'  | 22:a:2681:C:H5'  | 2.12                     | 0.50              |
| 25:d:13:ARG:HD2  | 25:d:15:PHE:CZ   | 2.46                     | 0.50              |
| 39:r:2:GLU:HA    | 39:r:108:SER:HB3 | 1.92                     | 0.50              |
| 2:B:54:LEU:HG    | 2:B:220:THR:HG21 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:72:ILE:HD12  | 5:E:145:GLU:HG3  | 1.93                     | 0.50              |
| 22:a:721:A:H2'   | 22:a:722:A:H8    | 1.77                     | 0.50              |
| 22:a:1980:G:O2'  | 22:a:1982:U:OP2  | 2.29                     | 0.50              |
| 42:u:48:MET:HE3  | 42:u:51:GLN:NE2  | 2.27                     | 0.50              |
| 1:A:728:A:H2'    | 1:A:729:A:C8     | 2.47                     | 0.50              |
| 4:D:140:ASN:N    | 4:D:182:PHE:O    | 2.40                     | 0.50              |
| 7:G:15:ASP:OD1   | 7:G:23:LEU:HB3   | 2.12                     | 0.50              |
| 22:a:468:G:N7    | 49:1:39:ARG:NH2  | 2.56                     | 0.50              |
| 22:a:820:A:H4'   | 22:a:836:G:H22   | 1.77                     | 0.50              |
| 22:a:848:C:H2'   | 22:a:849:A:C8    | 2.47                     | 0.50              |
| 22:a:898:C:H2'   | 22:a:899:A:O4'   | 2.12                     | 0.50              |
| 1:A:653:U:H5'    | 8:H:56:LYS:NZ    | 2.27                     | 0.50              |
| 13:M:3:ARG:HH21  | 27:f:110:ARG:HG2 | 1.76                     | 0.50              |
| 31:j:63:VAL:HG23 | 31:j:64:ARG:HG3  | 1.93                     | 0.50              |
| 2:B:96:TRP:CZ2   | 2:B:100:MET:HB3  | 2.47                     | 0.49              |
| 23:b:42:C:C6     | 27:f:66:LEU:HB2  | 2.47                     | 0.49              |
| 1:A:486:U:H2'    | 1:A:487:A:H8     | 1.78                     | 0.49              |
| 1:A:1004:A:C5    | 1:A:1026:G:H1'   | 2.46                     | 0.49              |
| 20:T:44:LYS:HZ3  | 20:T:87:ALA:HB2  | 1.76                     | 0.49              |
| 22:a:833:A:H2'   | 22:a:834:G:C8    | 2.47                     | 0.49              |
| 22:a:1182:G:H2'  | 22:a:1183:U:O4'  | 2.11                     | 0.49              |
| 1:A:235:C:H2'    | 1:A:236:A:C8     | 2.47                     | 0.49              |
| 1:A:501:C:H2'    | 1:A:502:A:C8     | 2.47                     | 0.49              |
| 22:a:397:U:OP2   | 44:w:10:LYS:NZ   | 2.33                     | 0.49              |
| 22:a:638:G:H2'   | 22:a:639:U:C6    | 2.47                     | 0.49              |
| 22:a:657:U:H2'   | 22:a:658:U:C6    | 2.47                     | 0.49              |
| 22:a:1590:A:H2'  | 22:a:1591:A:C8   | 2.48                     | 0.49              |
| 22:a:1614:A:H8   | 22:a:1614:A:P    | 2.35                     | 0.49              |
| 22:a:2537:U:H2'  | 22:a:2538:C:C6   | 2.47                     | 0.49              |
| 28:g:2:SER:O     | 28:g:6:LYS:HG2   | 2.13                     | 0.49              |
| 28:g:52:PHE:CE2  | 28:g:72:LEU:HD22 | 2.48                     | 0.49              |
| 52:4:8:LYS:NZ    | 52:4:10:GLU:HB3  | 2.27                     | 0.49              |
| 4:D:102:VAL:HG13 | 4:D:107:PHE:HB2  | 1.94                     | 0.49              |
| 22:a:593:U:H2'   | 22:a:594:U:C6    | 2.47                     | 0.49              |
| 22:a:871:U:H2'   | 22:a:872:U:C6    | 2.47                     | 0.49              |
| 22:a:1704:C:H2'  | 22:a:1705:A:C8   | 2.46                     | 0.49              |
| 9:I:58:VAL:HG13  | 9:I:59:GLU:OE1   | 2.13                     | 0.49              |
| 22:a:894:U:H2'   | 22:a:895:U:C6    | 2.46                     | 0.49              |
| 22:a:1438:U:H2'  | 22:a:1439:A:H8   | 1.78                     | 0.49              |
| 22:a:2646:C:OP2  | 22:a:2732:G:O2'  | 2.31                     | 0.49              |
| 46:y:58:GLU:HG2  | 46:y:58:GLU:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1038:C:H2'   | 1:A:1039:G:C8    | 2.45                     | 0.49              |
| 7:G:30:LEU:HD22  | 7:G:43:VAL:HG23  | 1.94                     | 0.49              |
| 22:a:594:U:H2'   | 22:a:595:C:C6    | 2.48                     | 0.49              |
| 22:a:1026:G:H2'  | 22:a:1027:A:C8   | 2.45                     | 0.49              |
| 22:a:1296:G:OP1  | 22:a:2709:G:O2'  | 2.21                     | 0.49              |
| 22:a:2395:C:H2'  | 22:a:2396:G:O4'  | 2.12                     | 0.49              |
| 1:A:1118:U:H2'   | 1:A:1119:C:H6    | 1.78                     | 0.49              |
| 1:A:1314:C:H2'   | 1:A:1315:U:H6    | 1.78                     | 0.49              |
| 6:F:88:MET:HG2   | 6:F:90:MET:HE2   | 1.93                     | 0.49              |
| 10:J:12:ALA:HB2  | 10:J:96:VAL:HG22 | 1.94                     | 0.49              |
| 12:L:111:LYS:HA  | 12:L:114:ARG:CG  | 2.43                     | 0.49              |
| 22:a:577:G:O2'   | 22:a:1254:A:OP1  | 2.30                     | 0.49              |
| 22:a:2637:U:H5'' | 25:d:83:ARG:HH11 | 1.78                     | 0.49              |
| 22:a:2830:C:O3'  | 25:d:56:LYS:NZ   | 2.45                     | 0.49              |
| 32:k:77:ILE:CD1  | 32:k:108:ALA:HB1 | 2.43                     | 0.49              |
| 33:l:66:ARG:NH1  | 33:l:104:GLU:OE1 | 2.46                     | 0.49              |
| 1:A:389:A:H3'    | 1:A:390:U:H6     | 1.76                     | 0.49              |
| 1:A:459:A:H2'    | 1:A:460:A:H8     | 1.76                     | 0.49              |
| 1:A:744:C:H2'    | 1:A:745:G:C8     | 2.47                     | 0.49              |
| 22:a:2:G:H2'     | 22:a:3:U:C6      | 2.48                     | 0.49              |
| 22:a:116:C:O2'   | 22:a:126:A:N3    | 2.38                     | 0.49              |
| 22:a:848:C:H2'   | 22:a:849:A:H8    | 1.78                     | 0.49              |
| 22:a:1853:A:H2'  | 22:a:1854:A:C8   | 2.48                     | 0.49              |
| 22:a:2030:6MZ:C2 | 22:a:2499:C:H5'' | 2.43                     | 0.49              |
| 26:e:58:LYS:NZ   | 26:e:70:SER:O    | 2.36                     | 0.49              |
| 28:g:94:TYR:HA   | 28:g:106:SER:O   | 2.13                     | 0.49              |
| 30:i:69:ARG:NH1  | 30:i:90:GLU:OE2  | 2.42                     | 0.49              |
| 1:A:215:C:H2'    | 1:A:216:U:C6     | 2.48                     | 0.49              |
| 1:A:600:A:H5''   | 8:H:89:LYS:HD3   | 1.94                     | 0.49              |
| 1:A:663:A:H5'    | 1:A:836:G:OP1    | 2.13                     | 0.49              |
| 1:A:868:C:H2'    | 1:A:869:G:O4'    | 2.13                     | 0.49              |
| 14:N:19:LYS:HD2  | 14:N:20:TYR:CE1  | 2.48                     | 0.49              |
| 22:a:363:G:H2'   | 22:a:364:C:C6    | 2.48                     | 0.49              |
| 22:a:500:G:N1    | 22:a:503:A:OP2   | 2.42                     | 0.49              |
| 22:a:1533:C:O2   | 22:a:1539:U:N3   | 2.45                     | 0.49              |
| 28:g:153:ARG:HB2 | 28:g:153:ARG:CZ  | 2.43                     | 0.49              |
| 2:B:60:ILE:HA    | 2:B:63:ARG:NH1   | 2.28                     | 0.49              |
| 6:F:21:MET:HA    | 6:F:24:ARG:HG2   | 1.95                     | 0.49              |
| 22:a:5:A:H2'     | 22:a:6:A:C8      | 2.48                     | 0.49              |
| 22:a:106:C:H2'   | 22:a:107:G:H8    | 1.78                     | 0.49              |
| 22:a:2312:U:H5'  | 27:f:85:ILE:HD11 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 33:l:58:LYS:O    | 33:l:60:GLN:NE2   | 2.45                     | 0.49              |
| 21:U:4:ILE:HG13  | 21:U:19:PHE:HA    | 1.94                     | 0.48              |
| 22:a:219:A:N3    | 22:a:234:U:O2'    | 2.40                     | 0.48              |
| 22:a:278:A:C6    | 22:a:362:A:C8     | 3.01                     | 0.48              |
| 25:d:48:ILE:HG23 | 25:d:84:LEU:HD11  | 1.95                     | 0.48              |
| 1:A:45:G:H2'     | 1:A:46:G:C8       | 2.48                     | 0.48              |
| 1:A:415:A:H2'    | 1:A:416:G:C8      | 2.48                     | 0.48              |
| 3:C:11:ARG:NH2   | 3:C:175:LEU:O     | 2.46                     | 0.48              |
| 5:E:113:ALA:O    | 5:E:117:VAL:HG22  | 2.14                     | 0.48              |
| 14:N:49:GLN:OE1  | 19:S:13:LEU:N     | 2.29                     | 0.48              |
| 22:a:172:A:H2'   | 22:a:173:A:H8     | 1.79                     | 0.48              |
| 22:a:1342:A:O2'  | 22:a:1344:U:OP2   | 2.27                     | 0.48              |
| 22:a:1494:A:H2'  | 22:a:1495:A:C8    | 2.48                     | 0.48              |
| 22:a:2532:G:O2'  | 22:a:2657:A:N1    | 2.45                     | 0.48              |
| 24:c:145:GLU:HG2 | 24:c:151:GLY:C    | 2.38                     | 0.48              |
| 25:d:12:THR:OG1  | 25:d:13:ARG:N     | 2.46                     | 0.48              |
| 27:f:68:THR:N    | 27:f:86:GLY:O     | 2.41                     | 0.48              |
| 30:i:110:PRO:O   | 30:i:115:GLY:HA3  | 2.13                     | 0.48              |
| 1:A:518:C:H2'    | 1:A:530:G:C8      | 2.48                     | 0.48              |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8     | 2.48                     | 0.48              |
| 2:B:129:LEU:HD23 | 2:B:133:GLU:HB3   | 1.95                     | 0.48              |
| 22:a:1000:A:H2'  | 22:a:1001:A:C8    | 2.48                     | 0.48              |
| 22:a:2101:A:H2'  | 22:a:2102:G:C8    | 2.48                     | 0.48              |
| 33:l:21:ALA:HB2  | 33:l:97:GLN:HB2   | 1.96                     | 0.48              |
| 1:A:460:A:H2'    | 1:A:461:A:C8      | 2.48                     | 0.48              |
| 1:A:460:A:H2'    | 1:A:461:A:H8      | 1.78                     | 0.48              |
| 1:A:1029:U:H2'   | 1:A:1030:U:O4'    | 2.12                     | 0.48              |
| 9:I:115:LYS:HB2  | 9:I:118:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:471:U:H2'    | 1:A:472:U:C6      | 2.49                     | 0.48              |
| 1:A:1004:A:H2'   | 1:A:1005:A:O4'    | 2.12                     | 0.48              |
| 2:B:130:THR:C    | 2:B:132:LYS:H     | 2.21                     | 0.48              |
| 22:a:1527:G:N1   | 22:a:1544:A:OP2   | 2.38                     | 0.48              |
| 22:a:2025:C:H2'  | 22:a:2026:U:C6    | 2.48                     | 0.48              |
| 1:A:223:A:H2'    | 1:A:224:U:C6      | 2.49                     | 0.48              |
| 13:M:17:ILE:O    | 13:M:20:THR:OG1   | 2.32                     | 0.48              |
| 22:a:1932:A:H2'  | 22:a:1933:G:O4'   | 2.13                     | 0.48              |
| 22:a:2228:G:H2'  | 22:a:2229:U:C6    | 2.49                     | 0.48              |
| 22:a:2287:A:OP1  | 48:O:30:LYS:NZ    | 2.40                     | 0.48              |
| 22:a:2392:A:OP2  | 50:2:31:HIS:NE2   | 2.47                     | 0.48              |
| 28:g:95:ARG:HB2  | 28:g:95:ARG:NH1   | 2.28                     | 0.48              |
| 33:l:36:VAL:HG21 | 33:l:129:THR:HG23 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:312:C:H2'    | 1:A:313:A:C8     | 2.49                     | 0.48              |
| 28:g:47:ASP:N    | 28:g:47:ASP:OD1  | 2.46                     | 0.48              |
| 1:A:407:U:H2'    | 1:A:408:A:H8     | 1.79                     | 0.48              |
| 10:J:35:GLN:HG2  | 10:J:77:VAL:HG23 | 1.96                     | 0.48              |
| 13:M:44:LYS:HB2  | 13:M:47:GLU:OE1  | 2.13                     | 0.48              |
| 22:a:171:U:H2'   | 22:a:172:A:H8    | 1.79                     | 0.48              |
| 24:c:115:GLN:O   | 24:c:125:LYS:NZ  | 2.44                     | 0.48              |
| 39:r:65:ASP:OD2  | 39:r:65:ASP:N    | 2.46                     | 0.48              |
| 22:a:58:G:H2'    | 22:a:59:U:C6     | 2.49                     | 0.48              |
| 1:A:324:G:N1     | 1:A:327:A:OP2    | 2.44                     | 0.48              |
| 22:a:250:G:H2'   | 22:a:251:A:C8    | 2.49                     | 0.48              |
| 22:a:1534:U:C4   | 22:a:1535:A:H1'  | 2.49                     | 0.48              |
| 27:f:16:LEU:HD12 | 27:f:28:VAL:HG13 | 1.94                     | 0.48              |
| 27:f:62:GLY:O    | 27:f:95:ARG:NH1  | 2.44                     | 0.48              |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.49                     | 0.47              |
| 1:A:429:U:H5'    | 4:D:9:LEU:HD12   | 1.96                     | 0.47              |
| 12:L:99:ARG:HD2  | 12:L:104:CYS:SG  | 2.54                     | 0.47              |
| 22:a:2246:G:H2'  | 22:a:2247:A:H8   | 1.79                     | 0.47              |
| 22:a:2392:A:C2   | 32:k:55:MET:HE3  | 2.48                     | 0.47              |
| 27:f:37:ASN:OD1  | 27:f:38:MET:N    | 2.48                     | 0.47              |
| 29:h:27:ARG:NH1  | 44:w:60:ASP:OD2  | 2.36                     | 0.47              |
| 40:s:43:ILE:O    | 40:s:47:VAL:HG12 | 2.14                     | 0.47              |
| 1:A:831:A:H5''   | 2:B:21:ARG:HE    | 1.79                     | 0.47              |
| 22:a:150:U:H2'   | 22:a:151:C:C6    | 2.50                     | 0.47              |
| 22:a:2340:A:H5'  | 23:b:41:G:H21    | 1.79                     | 0.47              |
| 22:a:2740:A:H2'  | 22:a:2741:A:C8   | 2.49                     | 0.47              |
| 22:a:2773:C:H2'  | 22:a:2774:C:H6   | 1.78                     | 0.47              |
| 1:A:604:G:H2'    | 1:A:605:U:O4'    | 2.15                     | 0.47              |
| 17:Q:60:GLU:OE2  | 17:Q:76:VAL:HB   | 2.14                     | 0.47              |
| 22:a:2377:A:H2'  | 22:a:2378:A:C8   | 2.49                     | 0.47              |
| 23:b:106:G:H2'   | 23:b:107:G:O4'   | 2.14                     | 0.47              |
| 1:A:161:A:H2'    | 1:A:162:A:C8     | 2.49                     | 0.47              |
| 1:A:259:G:OP1    | 20:T:36:TYR:OH   | 2.22                     | 0.47              |
| 1:A:299:G:H2'    | 1:A:300:A:C8     | 2.50                     | 0.47              |
| 22:a:563:A:OP2   | 38:q:79:ARG:NH2  | 2.39                     | 0.47              |
| 22:a:1179:G:H2'  | 22:a:1180:U:C6   | 2.50                     | 0.47              |
| 22:a:2554:U:H2'  | 22:a:2555:U:C6   | 2.50                     | 0.47              |
| 28:g:38:ASN:OD1  | 28:g:39:ASP:N    | 2.46                     | 0.47              |
| 29:h:32:PRO:HA   | 44:w:39:TRP:CD1  | 2.49                     | 0.47              |
| 1:A:580:C:H2'    | 1:A:581:G:O4'    | 2.15                     | 0.47              |
| 1:A:1039:G:H2'   | 1:A:1040:U:C6    | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:364:C:H2'   | 22:a:365:U:C6    | 2.49                     | 0.47              |
| 22:a:547:A:H3'   | 22:a:548:G:C8    | 2.50                     | 0.47              |
| 22:a:2567:G:H2'  | 22:a:2568:U:C6   | 2.49                     | 0.47              |
| 1:A:335:C:H2'    | 1:A:336:A:H8     | 1.80                     | 0.47              |
| 1:A:398:U:H2'    | 1:A:399:G:C8     | 2.47                     | 0.47              |
| 13:M:50:GLU:HA   | 13:M:53:ILE:HG22 | 1.97                     | 0.47              |
| 22:a:1428:C:C5   | 22:a:1569:A:H5'' | 2.48                     | 0.47              |
| 32:k:30:THR:HG21 | 32:k:34:GLY:O    | 2.13                     | 0.47              |
| 1:A:219:U:H2'    | 1:A:220:G:H8     | 1.79                     | 0.47              |
| 1:A:393:A:OP2    | 16:P:12:LYS:NZ   | 2.37                     | 0.47              |
| 1:A:662:U:H2'    | 1:A:663:A:C8     | 2.49                     | 0.47              |
| 1:A:1071:C:H2'   | 1:A:1072:G:H8    | 1.79                     | 0.47              |
| 1:A:1140:C:H2'   | 1:A:1141:C:H6    | 1.79                     | 0.47              |
| 1:A:1268:G:H2'   | 1:A:1269:A:C8    | 2.49                     | 0.47              |
| 1:A:1527:U:H2'   | 1:A:1528:U:C6    | 2.49                     | 0.47              |
| 1:A:1533:C:H4'   | 1:A:1534:A:C8    | 2.50                     | 0.47              |
| 2:B:6:MET:HG3    | 2:B:43:LEU:HD23  | 1.97                     | 0.47              |
| 9:I:65:ILE:HD13  | 9:I:79:ILE:HG23  | 1.97                     | 0.47              |
| 9:I:88:MET:CE    | 9:I:98:LEU:HD12  | 2.44                     | 0.47              |
| 9:I:92:GLU:OE2   | 9:I:95:ARG:NE    | 2.35                     | 0.47              |
| 22:a:675:A:N3    | 22:a:2443:C:O2'  | 2.45                     | 0.47              |
| 22:a:720:U:H2'   | 22:a:721:A:H8    | 1.80                     | 0.47              |
| 22:a:1378:A:O2'  | 22:a:1380:G:N7   | 2.47                     | 0.47              |
| 22:a:2097:A:H2'  | 22:a:2098:U:C6   | 2.49                     | 0.47              |
| 23:b:2:G:H2'     | 23:b:3:C:C6      | 2.50                     | 0.47              |
| 36:o:7:GLN:NE2   | 36:o:11:GLU:OE2  | 2.42                     | 0.47              |
| 40:s:71:GLY:O    | 40:s:72:GLN:NE2  | 2.48                     | 0.47              |
| 45:x:5:GLU:O     | 45:x:9:LYS:NZ    | 2.48                     | 0.47              |
| 50:2:62:LEU:HB3  | 50:2:65:ALA:HB2  | 1.97                     | 0.47              |
| 1:A:736:C:OP1    | 18:R:61:ARG:NH1  | 2.48                     | 0.47              |
| 1:A:1238:A:OP1   | 1:A:1335:U:O2'   | 2.25                     | 0.47              |
| 22:a:580:U:H2'   | 22:a:581:C:C6    | 2.50                     | 0.47              |
| 22:a:832:U:H2'   | 22:a:833:A:C8    | 2.50                     | 0.47              |
| 22:a:1536:C:O2   | 22:a:1537:G:N2   | 2.48                     | 0.47              |
| 22:a:1585:C:H2'  | 22:a:1586:A:O4'  | 2.14                     | 0.47              |
| 22:a:2233:U:H2'  | 22:a:2234:G:C8   | 2.49                     | 0.47              |
| 40:s:3:ARG:HB3   | 40:s:5:GLU:OE1   | 2.14                     | 0.47              |
| 54:Z:16:C:OP1    | 54:Z:17:C:N4     | 2.42                     | 0.47              |
| 1:A:470:C:H2'    | 1:A:471:U:H6     | 1.80                     | 0.47              |
| 1:A:918:A:H2'    | 1:A:919:A:C8     | 2.50                     | 0.47              |
| 1:A:1302:C:C5    | 13:M:17:ILE:HG13 | 2.50                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:46:LEU:HD22 | 19:S:13:LEU:HD13  | 1.97                     | 0.47              |
| 19:S:45:ILE:HD12 | 19:S:45:ILE:H     | 1.79                     | 0.47              |
| 22:a:2086:U:H2'  | 22:a:2087:G:C8    | 2.50                     | 0.47              |
| 24:c:155:ALA:HB2 | 24:c:162:VAL:HG23 | 1.97                     | 0.47              |
| 28:g:78:GLY:HA2  | 28:g:82:GLY:HA2   | 1.97                     | 0.47              |
| 31:j:76:VAL:HG12 | 36:o:73:VAL:HB    | 1.97                     | 0.47              |
| 1:A:107:G:N1     | 20:T:6:SER:OG     | 2.36                     | 0.47              |
| 1:A:337:G:H2'    | 1:A:338:A:H8      | 1.77                     | 0.47              |
| 1:A:500:G:H2'    | 1:A:501:C:C6      | 2.50                     | 0.47              |
| 1:A:652:U:O4     | 1:A:752:G:O2'     | 2.33                     | 0.47              |
| 22:a:272:A:H2'   | 22:a:273:G:C8     | 2.50                     | 0.47              |
| 22:a:2780:G:OP2  | 30:i:120:ARG:HD3  | 2.15                     | 0.47              |
| 22:a:2809:A:H2'  | 22:a:2810:A:C8    | 2.50                     | 0.47              |
| 31:j:79:PHE:HE2  | 31:j:102:PRO:HG2  | 1.79                     | 0.47              |
| 1:A:235:C:H2'    | 1:A:236:A:H8      | 1.81                     | 0.46              |
| 7:G:79:ARG:HA    | 7:G:84:THR:HA     | 1.97                     | 0.46              |
| 9:I:28:ILE:HA    | 9:I:63:LEU:HB2    | 1.98                     | 0.46              |
| 11:K:23:ILE:HG21 | 11:K:96:THR:HG21  | 1.96                     | 0.46              |
| 12:L:36:ARG:HG2  | 12:L:38:TYR:CD1   | 2.49                     | 0.46              |
| 22:a:2052:A:H4'  | 25:d:148:GLN:O    | 2.15                     | 0.46              |
| 1:A:140:U:H2'    | 1:A:141:G:O4'     | 2.15                     | 0.46              |
| 1:A:1011:C:H2'   | 1:A:1012:A:C8     | 2.51                     | 0.46              |
| 4:D:99:ASP:OD1   | 4:D:133:ALA:HB1   | 2.15                     | 0.46              |
| 8:H:7:ILE:O      | 8:H:11:LEU:HG     | 2.15                     | 0.46              |
| 10:J:59:LYS:HE2  | 10:J:62:ARG:HH22  | 1.80                     | 0.46              |
| 19:S:41:PHE:H    | 19:S:44:MET:HE2   | 1.80                     | 0.46              |
| 22:a:1203:U:OP2  | 22:a:1204:A:O2'   | 2.27                     | 0.46              |
| 22:a:2014:A:H2'  | 22:a:2015:A:C8    | 2.50                     | 0.46              |
| 1:A:428:G:O2'    | 1:A:429:U:O5'     | 2.27                     | 0.46              |
| 1:A:1036:A:H2'   | 1:A:1037:C:O4'    | 2.15                     | 0.46              |
| 1:A:1120:C:H2'   | 1:A:1121:U:C6     | 2.49                     | 0.46              |
| 22:a:837:C:N3    | 22:a:941:A:N6     | 2.61                     | 0.46              |
| 22:a:2071:A:H2'  | 22:a:2072:C:C6    | 2.50                     | 0.46              |
| 41:t:85:PHE:HE1  | 41:t:94:ARG:HG2   | 1.80                     | 0.46              |
| 1:A:126:G:OP1    | 1:A:605:U:O2'     | 2.24                     | 0.46              |
| 1:A:999:C:N3     | 1:A:1042:A:N6     | 2.64                     | 0.46              |
| 2:B:6:MET:HE3    | 2:B:43:LEU:HB3    | 1.98                     | 0.46              |
| 5:E:61:GLN:O     | 5:E:65:GLU:HG2    | 2.15                     | 0.46              |
| 22:a:3:U:H2'     | 22:a:4:U:H6       | 1.81                     | 0.46              |
| 22:a:274:C:C4    | 22:a:275:C:N3     | 2.84                     | 0.46              |
| 41:t:86:ARG:HG3  | 41:t:95:PHE:CD1   | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 45:x:32:ALA:HB2  | 45:x:37:LEU:HD23 | 1.97                     | 0.46              |
| 52:4:20:ASN:OD1  | 52:4:21:VAL:N    | 2.48                     | 0.46              |
| 54:Z:22:A:N6     | 54:Z:47:A:H2'    | 2.31                     | 0.46              |
| 1:A:834:U:H2'    | 1:A:835:U:C6     | 2.51                     | 0.46              |
| 17:Q:77:ARG:HH12 | 17:Q:79:VAL:HA   | 1.80                     | 0.46              |
| 22:a:613:A:H2'   | 22:a:614:A:O4'   | 2.15                     | 0.46              |
| 22:a:881:G:O6    | 22:a:895:U:C4    | 2.69                     | 0.46              |
| 22:a:1842:G:H2'  | 22:a:1843:C:C6   | 2.51                     | 0.46              |
| 22:a:2100:G:N2   | 22:a:2189:U:O2   | 2.36                     | 0.46              |
| 52:4:16:CYS:HA   | 52:4:34:LEU:HB2  | 1.97                     | 0.46              |
| 1:A:860:A:H2'    | 1:A:861:G:O4'    | 2.15                     | 0.46              |
| 1:A:1225:A:H2'   | 1:A:1226:C:C5    | 2.51                     | 0.46              |
| 9:I:28:ILE:HG12  | 9:I:63:LEU:HB2   | 1.98                     | 0.46              |
| 10:J:36:VAL:HG12 | 10:J:76:ILE:HD13 | 1.96                     | 0.46              |
| 22:a:897:C:H2'   | 22:a:898:C:C6    | 2.51                     | 0.46              |
| 22:a:1199:U:H2'  | 22:a:1200:C:C6   | 2.51                     | 0.46              |
| 22:a:1684:G:H2'  | 22:a:1685:C:C6   | 2.51                     | 0.46              |
| 22:a:2477:U:O2   | 51:3:4:ARG:NH2   | 2.48                     | 0.46              |
| 22:a:2522:U:O2'  | 22:a:2647:U:OP1  | 2.22                     | 0.46              |
| 22:a:2557:G:H2'  | 22:a:2558:C:C6   | 2.50                     | 0.46              |
| 40:s:6:ARG:O     | 40:s:10:VAL:HG13 | 2.15                     | 0.46              |
| 43:v:50:ASN:HB2  | 43:v:82:ILE:HB   | 1.98                     | 0.46              |
| 1:A:579:A:H2'    | 1:A:580:C:C6     | 2.51                     | 0.46              |
| 1:A:946:A:H2'    | 1:A:947:G:H8     | 1.75                     | 0.46              |
| 1:A:1410:A:H2'   | 1:A:1411:C:C6    | 2.51                     | 0.46              |
| 7:G:14:PRO:HB2   | 7:G:19:GLY:HA2   | 1.97                     | 0.46              |
| 32:k:29:LYS:O    | 32:k:29:LYS:HG2  | 2.15                     | 0.46              |
| 1:A:309:A:H2'    | 1:A:310:G:H8     | 1.81                     | 0.46              |
| 1:A:323:U:H2'    | 1:A:324:G:O4'    | 2.15                     | 0.46              |
| 11:K:52:PHE:O    | 11:K:53:ARG:HD2  | 2.16                     | 0.46              |
| 11:K:64:GLN:HB2  | 11:K:99:ALA:HB2  | 1.98                     | 0.46              |
| 22:a:581:C:H2'   | 22:a:582:A:H8    | 1.81                     | 0.46              |
| 22:a:613:A:H8    | 22:a:613:A:OP1   | 1.98                     | 0.46              |
| 22:a:836:G:C5    | 22:a:837:C:C5    | 3.03                     | 0.46              |
| 22:a:888:C:H2'   | 22:a:889:C:C6    | 2.51                     | 0.46              |
| 26:e:191:ASP:O   | 26:e:195:GLN:HG3 | 2.15                     | 0.46              |
| 44:w:17:ASN:HB2  | 44:w:25:THR:OG1  | 2.16                     | 0.46              |
| 1:A:405:U:C5     | 4:D:5:LEU:HD11   | 2.50                     | 0.46              |
| 1:A:501:C:H2'    | 1:A:502:A:H8     | 1.81                     | 0.46              |
| 1:A:1030:U:O2'   | 1:A:1031:C:O2    | 2.33                     | 0.46              |
| 22:a:279:A:N6    | 22:a:361:G:H1'   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:1039:A:H2'  | 22:a:1040:A:O4'  | 2.16                     | 0.46              |
| 22:a:1563:U:H2'  | 22:a:1564:C:C6   | 2.51                     | 0.46              |
| 27:f:58:ALA:HB2  | 27:f:65:PRO:HD3  | 1.98                     | 0.46              |
| 54:Z:29:C:H2'    | 54:Z:30:G:H8     | 1.81                     | 0.46              |
| 1:A:90:C:H2'     | 1:A:91:U:C6      | 2.50                     | 0.46              |
| 1:A:371:A:H2'    | 1:A:372:C:O4'    | 2.16                     | 0.46              |
| 1:A:470:C:H2'    | 1:A:471:U:C6     | 2.50                     | 0.46              |
| 2:B:188:ASP:OD1  | 2:B:189:THR:N    | 2.46                     | 0.46              |
| 22:a:1363:C:O2'  | 22:a:1809:A:N3   | 2.44                     | 0.46              |
| 22:a:2532:G:N2   | 22:a:2663:G:O2'  | 2.49                     | 0.46              |
| 42:u:75:GLN:HB3  | 42:u:90:ASP:HB3  | 1.98                     | 0.46              |
| 1:A:864:A:H4'    | 5:E:90:THR:HG23  | 1.97                     | 0.45              |
| 22:a:160:A:N3    | 22:a:2208:C:O2'  | 2.44                     | 0.45              |
| 22:a:184:C:H2'   | 22:a:185:G:H8    | 1.80                     | 0.45              |
| 22:a:1394:U:H2'  | 22:a:1395:A:O4'  | 2.17                     | 0.45              |
| 22:a:2064:C:H2'  | 22:a:2065:C:C6   | 2.51                     | 0.45              |
| 22:a:2294:G:P    | 35:n:94:ARG:HH12 | 2.38                     | 0.45              |
| 22:a:2515:C:H2'  | 22:a:2516:A:H8   | 1.81                     | 0.45              |
| 22:a:2849:U:H4'  | 22:a:2868:A:C2   | 2.50                     | 0.45              |
| 1:A:269:C:H2'    | 1:A:270:A:H8     | 1.81                     | 0.45              |
| 21:U:51:SER:O    | 21:U:55:ARG:HG3  | 2.16                     | 0.45              |
| 22:a:419:U:H2'   | 22:a:420:C:C6    | 2.50                     | 0.45              |
| 22:a:518:G:H2'   | 22:a:519:U:C6    | 2.51                     | 0.45              |
| 22:a:1412:U:H2'  | 22:a:1413:A:C8   | 2.50                     | 0.45              |
| 27:f:147:ASP:OD1 | 27:f:150:ARG:NH1 | 2.49                     | 0.45              |
| 28:g:17:VAL:HG11 | 28:g:50:LEU:HD11 | 1.97                     | 0.45              |
| 39:r:109:ASP:OD2 | 39:r:110:ARG:HG2 | 2.17                     | 0.45              |
| 1:A:539:A:P      | 12:L:111:LYS:HD2 | 2.56                     | 0.45              |
| 22:a:39:G:H2'    | 22:a:40:U:C6     | 2.52                     | 0.45              |
| 22:a:56:A:H5''   | 49:1:46:LYS:HE3  | 1.97                     | 0.45              |
| 22:a:641:U:O2'   | 22:a:2350:C:OP1  | 2.32                     | 0.45              |
| 22:a:1842:G:H2'  | 22:a:1843:C:H6   | 1.81                     | 0.45              |
| 22:a:2514:U:H2'  | 22:a:2515:C:C6   | 2.52                     | 0.45              |
| 1:A:1014:A:C2    | 1:A:1219:A:H1'   | 2.51                     | 0.45              |
| 1:A:1033:G:H2'   | 1:A:1034:G:H8    | 1.81                     | 0.45              |
| 19:S:21:LYS:O    | 19:S:24:GLU:HG3  | 2.16                     | 0.45              |
| 22:a:279:A:H61   | 22:a:361:G:H1'   | 1.81                     | 0.45              |
| 22:a:1496:A:H2'  | 22:a:1498:C:C5   | 2.52                     | 0.45              |
| 27:f:144:ASP:OD1 | 27:f:144:ASP:N   | 2.44                     | 0.45              |
| 1:A:414:A:C4     | 1:A:415:A:C8     | 3.05                     | 0.45              |
| 1:A:1169:A:H2'   | 1:A:1170:A:C8    | 2.51                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1463:U:H2'  | 1:A:1464:U:C6    | 2.51                     | 0.45              |
| 22:a:277:G:OP2  | 22:a:277:G:H8    | 1.99                     | 0.45              |
| 22:a:538:A:H5'' | 30:i:7:LYS:HE3   | 1.99                     | 0.45              |
| 22:a:722:A:H2'  | 22:a:723:C:C6    | 2.51                     | 0.45              |
| 22:a:1447:C:H2' | 22:a:1448:G:H8   | 1.82                     | 0.45              |
| 22:a:1476:U:H2' | 22:a:1477:A:H8   | 1.81                     | 0.45              |
| 22:a:2649:C:H2' | 22:a:2650:U:C6   | 2.52                     | 0.45              |
| 31:j:58:LEU:HA  | 31:j:89:ASN:OD1  | 2.16                     | 0.45              |
| 47:z:52:ARG:CZ  | 47:z:54:VAL:HG12 | 2.46                     | 0.45              |
| 49:1:22:MET:O   | 49:1:28:ARG:NH1  | 2.49                     | 0.45              |
| 1:A:56:U:H2'    | 1:A:57:G:C8      | 2.52                     | 0.45              |
| 13:M:70:ARG:HE  | 27:f:112:ARG:NH1 | 2.15                     | 0.45              |
| 22:a:155:A:H2'  | 22:a:156:A:C8    | 2.52                     | 0.45              |
| 22:a:2615:U:C2  | 47:z:4:GLN:HA    | 2.51                     | 0.45              |
| 22:a:2812:G:H2' | 22:a:2813:A:C8   | 2.51                     | 0.45              |
| 23:b:14:U:OP2   | 23:b:70:C:O2'    | 2.35                     | 0.45              |
| 24:c:132:MET:O  | 24:c:167:ARG:NH2 | 2.50                     | 0.45              |
| 27:f:15:LYS:HE2 | 27:f:15:LYS:HB3  | 1.84                     | 0.45              |
| 27:f:170:LEU:O  | 27:f:175:PHE:HB2 | 2.16                     | 0.45              |
| 5:E:26:LYS:HB3  | 5:E:26:LYS:HE2   | 1.81                     | 0.45              |
| 13:M:66:GLU:HB3 | 27:f:112:ARG:NH1 | 2.32                     | 0.45              |
| 13:M:101:ARG:HE | 13:M:104:THR:HB  | 1.82                     | 0.45              |
| 22:a:272:A:H2'  | 22:a:273:G:H8    | 1.82                     | 0.45              |
| 22:a:687:C:H1'  | 49:1:4:THR:HG22  | 1.97                     | 0.45              |
| 22:a:874:G:C6   | 22:a:904:G:C6    | 3.05                     | 0.45              |
| 22:a:1183:U:H2' | 22:a:1184:U:C6   | 2.52                     | 0.45              |
| 22:a:1590:A:H2' | 22:a:1591:A:H8   | 1.80                     | 0.45              |
| 22:a:1599:U:H2' | 22:a:1600:C:C6   | 2.52                     | 0.45              |
| 22:a:2636:C:H2' | 22:a:2637:U:C6   | 2.52                     | 0.45              |
| 24:c:240:PHE:O  | 24:c:242:LYS:NZ  | 2.45                     | 0.45              |
| 35:n:4:LYS:O    | 35:n:8:ILE:HG12  | 2.16                     | 0.45              |
| 38:q:52:PRO:HG2 | 38:q:53:PHE:CD2  | 2.51                     | 0.45              |
| 1:A:1071:C:H2'  | 1:A:1072:G:C8    | 2.52                     | 0.45              |
| 4:D:58:LYS:NZ   | 4:D:69:GLU:OE1   | 2.49                     | 0.45              |
| 22:a:2:G:H2'    | 22:a:3:U:H6      | 1.82                     | 0.45              |
| 22:a:784:G:H5'  | 22:a:785:G:OP1   | 2.15                     | 0.45              |
| 40:s:56:GLU:N   | 40:s:56:GLU:OE1  | 2.50                     | 0.45              |
| 1:A:73:C:O2'    | 1:A:74:A:H8      | 1.99                     | 0.45              |
| 1:A:384:G:H2'   | 1:A:385:C:C6     | 2.52                     | 0.45              |
| 1:A:407:U:H2'   | 1:A:408:A:C8     | 2.52                     | 0.45              |
| 22:a:483:A:C8   | 41:t:45:HIS:HD2  | 2.35                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:568:U:OP1   | 32:k:36:LYS:HE2  | 2.17                     | 0.45              |
| 46:y:3:LYS:HE2   | 46:y:40:ASP:HB3  | 1.98                     | 0.45              |
| 1:A:592:G:H2'    | 1:A:593:U:C6     | 2.52                     | 0.45              |
| 1:A:1314:C:OP1   | 19:S:6:LYS:NZ    | 2.32                     | 0.45              |
| 1:A:1496:C:H2'   | 1:A:1497:G:O4'   | 2.17                     | 0.45              |
| 22:a:1432:G:H2'  | 22:a:1433:A:C8   | 2.52                     | 0.45              |
| 28:g:160:LYS:HB3 | 28:g:160:LYS:HE2 | 1.77                     | 0.45              |
| 35:n:15:ARG:NH2  | 35:n:95:SER:OG   | 2.50                     | 0.45              |
| 38:q:32:THR:HA   | 38:q:62:GLU:HA   | 1.99                     | 0.45              |
| 38:q:83:TYR:OH   | 38:q:85:LYS:HE3  | 2.17                     | 0.45              |
| 1:A:780:A:H5''   | 11:K:125:LYS:HD3 | 1.99                     | 0.44              |
| 3:C:83:ASP:HA    | 3:C:86:LYS:HD2   | 1.98                     | 0.44              |
| 7:G:86:GLN:HB2   | 7:G:148:ASN:OD1  | 2.16                     | 0.44              |
| 16:P:8:ARG:CZ    | 16:P:15:PRO:HB3  | 2.47                     | 0.44              |
| 22:a:608:A:H2'   | 22:a:609:A:C8    | 2.52                     | 0.44              |
| 22:a:813:U:H2'   | 22:a:814:C:C6    | 2.53                     | 0.44              |
| 22:a:1397:U:OP2  | 22:a:1398:C:N4   | 2.35                     | 0.44              |
| 25:d:108:ASP:N   | 25:d:204:LYS:O   | 2.34                     | 0.44              |
| 37:p:15:LYS:HB3  | 37:p:15:LYS:HE2  | 1.83                     | 0.44              |
| 38:q:35:PHE:HB2  | 38:q:59:ILE:HB   | 1.99                     | 0.44              |
| 41:t:97:LYS:O    | 41:t:98:SER:OG   | 2.34                     | 0.44              |
| 42:u:48:MET:O    | 42:u:51:GLN:HG3  | 2.17                     | 0.44              |
| 1:A:381:C:H2'    | 1:A:382:A:O4'    | 2.16                     | 0.44              |
| 1:A:751:U:H2'    | 1:A:752:G:O4'    | 2.16                     | 0.44              |
| 9:I:91:ASP:HB3   | 9:I:94:LEU:HD23  | 1.99                     | 0.44              |
| 17:Q:14:SER:HB2  | 17:Q:22:VAL:HG12 | 1.98                     | 0.44              |
| 22:a:5:A:H2'     | 22:a:6:A:H8      | 1.82                     | 0.44              |
| 22:a:577:G:H2'   | 22:a:578:G:C8    | 2.52                     | 0.44              |
| 22:a:2649:C:H2'  | 22:a:2650:U:H6   | 1.82                     | 0.44              |
| 33:l:111:GLU:H   | 33:l:111:GLU:CD  | 2.26                     | 0.44              |
| 46:y:4:THR:HB    | 46:y:37:GLU:HG2  | 2.00                     | 0.44              |
| 1:A:965:U:H5''   | 1:A:966:2MG:OP1  | 2.17                     | 0.44              |
| 1:A:1414:U:H2'   | 1:A:1415:G:H8    | 1.82                     | 0.44              |
| 4:D:170:TRP:CD2  | 4:D:186:PRO:HB3  | 2.52                     | 0.44              |
| 9:I:52:LEU:HD11  | 9:I:63:LEU:HD21  | 2.00                     | 0.44              |
| 22:a:1028:A:N3   | 22:a:2486:C:O2'  | 2.40                     | 0.44              |
| 22:a:1045:C:O2   | 22:a:1111:A:N6   | 2.50                     | 0.44              |
| 22:a:2420:C:H4'  | 48:O:54:ILE:HG21 | 1.99                     | 0.44              |
| 22:a:2818:U:H2'  | 22:a:2819:G:H8   | 1.81                     | 0.44              |
| 24:c:76:ALA:HB2  | 24:c:96:TYR:CD1  | 2.52                     | 0.44              |
| 25:d:35:THR:HG22 | 25:d:73:VAL:HG21 | 1.98                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:g:89:LEU:CD2  | 28:g:162:VAL:HG22 | 2.48                     | 0.44              |
| 41:t:85:PHE:CE1  | 41:t:94:ARG:HG2   | 2.52                     | 0.44              |
| 1:A:335:C:H2'    | 1:A:336:A:C8      | 2.52                     | 0.44              |
| 1:A:687:A:C2     | 1:A:704:A:C5      | 3.05                     | 0.44              |
| 1:A:1025:U:H4'   | 1:A:1026:G:O4'    | 2.18                     | 0.44              |
| 11:K:83:GLU:HG2  | 11:K:109:ASN:HD22 | 1.83                     | 0.44              |
| 21:U:39:GLU:HG2  | 21:U:43:THR:HB    | 2.00                     | 0.44              |
| 22:a:139:U:H5''  | 22:a:140:C:C5     | 2.47                     | 0.44              |
| 22:a:948:C:H1'   | 22:a:984:A:C8     | 2.52                     | 0.44              |
| 22:a:1799:G:O2'  | 24:c:180:GLU:OE2  | 2.17                     | 0.44              |
| 22:a:1937:A:O2'  | 22:a:1939:5MU:OP2 | 2.33                     | 0.44              |
| 22:a:2455:G:H2'  | 22:a:2456:C:C6    | 2.53                     | 0.44              |
| 37:p:49:ASP:HA   | 37:p:52:GLN:HB2   | 1.98                     | 0.44              |
| 43:v:25:ARG:HH11 | 43:v:31:VAL:HG12  | 1.83                     | 0.44              |
| 1:A:275:G:H5'    | 17:Q:16:LYS:HE2   | 1.98                     | 0.44              |
| 5:E:65:GLU:OE1   | 5:E:68:ARG:NH2    | 2.51                     | 0.44              |
| 11:K:52:PHE:HD1  | 11:K:56:ARG:HE    | 1.66                     | 0.44              |
| 11:K:84:VAL:HG11 | 11:K:97:ILE:HG12  | 1.99                     | 0.44              |
| 15:O:17:ARG:H    | 15:O:17:ARG:HD3   | 1.81                     | 0.44              |
| 22:a:909:A:H2'   | 22:a:912:C:H5     | 1.81                     | 0.44              |
| 22:a:1199:U:H2'  | 22:a:1200:C:H6    | 1.83                     | 0.44              |
| 22:a:2038:G:H2'  | 22:a:2039:U:O4'   | 2.16                     | 0.44              |
| 32:k:62:PRO:HG2  | 50:2:25:LYS:HB3   | 1.99                     | 0.44              |
| 1:A:1219:A:H2'   | 1:A:1220:G:C8     | 2.53                     | 0.44              |
| 1:A:1457:G:OP1   | 20:T:34:LYS:NZ    | 2.41                     | 0.44              |
| 5:E:134:ILE:HD12 | 5:E:134:ILE:H     | 1.82                     | 0.44              |
| 6:F:88:MET:HE2   | 6:F:90:MET:CE     | 2.48                     | 0.44              |
| 22:a:183:C:N4    | 22:a:213:A:H61    | 2.16                     | 0.44              |
| 22:a:624:C:O2'   | 22:a:657:U:OP1    | 2.33                     | 0.44              |
| 22:a:2591:C:H2'  | 22:a:2592:G:H8    | 1.83                     | 0.44              |
| 1:A:544:G:OP2    | 4:D:63:ARG:NH2    | 2.51                     | 0.44              |
| 1:A:883:C:O2'    | 1:A:884:U:H5'     | 2.18                     | 0.44              |
| 6:F:43:GLY:HA2   | 6:F:58:HIS:CE1    | 2.52                     | 0.44              |
| 18:R:68:LEU:HD23 | 18:R:68:LEU:HA    | 1.85                     | 0.44              |
| 22:a:364:C:H2'   | 22:a:365:U:H6     | 1.81                     | 0.44              |
| 22:a:1441:G:H2'  | 22:a:1442:U:C6    | 2.52                     | 0.44              |
| 22:a:2000:C:OP1  | 34:m:5:LYS:NZ     | 2.43                     | 0.44              |
| 22:a:2895:G:H2'  | 22:a:2896:C:C6    | 2.53                     | 0.44              |
| 24:c:145:GLU:HB2 | 24:c:188:CYS:HB3  | 1.99                     | 0.44              |
| 25:d:46:ARG:NH2  | 25:d:88:GLU:O     | 2.49                     | 0.44              |
| 30:i:36:LEU:O    | 30:i:51:GLY:HA3   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 34:m:49:GLU:OE2  | 34:m:95:THR:OG1 | 2.35                     | 0.44              |
| 52:4:31:ASP:OD1  | 52:4:32:LEU:N   | 2.50                     | 0.44              |
| 1:A:109:A:H5'    | 1:A:110:C:C5    | 2.52                     | 0.44              |
| 1:A:826:C:O2     | 8:H:16:ASN:ND2  | 2.51                     | 0.44              |
| 9:I:12:ARG:O     | 9:I:13:LYS:C    | 2.61                     | 0.44              |
| 16:P:44:SER:N    | 16:P:47:GLU:OE1 | 2.42                     | 0.44              |
| 22:a:305:C:H2'   | 22:a:306:U:C6   | 2.53                     | 0.44              |
| 22:a:548:G:H5''  | 22:a:549:G:OP2  | 2.18                     | 0.44              |
| 22:a:895:U:H2'   | 22:a:897:C:C6   | 2.52                     | 0.44              |
| 22:a:1412:U:H2'  | 22:a:1413:A:H8  | 1.81                     | 0.44              |
| 22:a:1447:C:H2'  | 22:a:1448:G:C8  | 2.53                     | 0.44              |
| 22:a:2189:U:H1'  | 22:a:2190:G:H5' | 2.00                     | 0.44              |
| 22:a:2636:C:O2'  | 25:d:45:TYR:OH  | 2.34                     | 0.44              |
| 27:f:64:LYS:HD3  | 52:4:5:ILE:HD12 | 2.00                     | 0.44              |
| 31:j:121:GLU:OE2 | 36:o:65:SER:OG  | 2.36                     | 0.44              |
| 48:0:10:LYS:O    | 48:0:52:ALA:N   | 2.44                     | 0.44              |
| 49:1:3:ARG:HA    | 49:1:3:ARG:HD3  | 1.77                     | 0.44              |
| 1:A:49:U:C2      | 1:A:361:G:N2    | 2.86                     | 0.44              |
| 1:A:236:A:H2'    | 1:A:237:G:C8    | 2.52                     | 0.44              |
| 1:A:399:G:H2'    | 1:A:400:C:H6    | 1.82                     | 0.44              |
| 1:A:461:A:H2'    | 1:A:462:G:H8    | 1.82                     | 0.44              |
| 1:A:555:U:H2'    | 1:A:556:C:H6    | 1.83                     | 0.44              |
| 1:A:721:G:H4'    | 1:A:722:G:O4'   | 2.18                     | 0.44              |
| 1:A:1151:A:O2'   | 1:A:1152:A:H8   | 2.01                     | 0.44              |
| 4:D:160:GLU:O    | 4:D:163:GLU:HG2 | 2.17                     | 0.44              |
| 6:F:12:PRO:O     | 6:F:44:ARG:NH2  | 2.51                     | 0.44              |
| 22:a:279:A:H2'   | 22:a:280:U:O4'  | 2.17                     | 0.44              |
| 22:a:479:A:N3    | 22:a:481:G:H5'' | 2.32                     | 0.44              |
| 22:a:576:U:H2'   | 22:a:577:G:C8   | 2.52                     | 0.44              |
| 22:a:897:C:H2'   | 22:a:898:C:H6   | 1.83                     | 0.44              |
| 22:a:1370:C:H2'  | 22:a:1371:G:O4' | 2.18                     | 0.44              |
| 43:v:38:VAL:HG12 | 43:v:59:LEU:HB2 | 1.98                     | 0.44              |
| 1:A:674:G:H2'    | 1:A:675:A:H8    | 1.83                     | 0.43              |
| 6:F:44:ARG:HG3   | 6:F:44:ARG:NH1  | 2.30                     | 0.43              |
| 8:H:77:ARG:NE    | 8:H:79:SER:O    | 2.51                     | 0.43              |
| 14:N:22:ALA:O    | 14:N:26:GLU:OE1 | 2.36                     | 0.43              |
| 21:U:7:ARG:N     | 21:U:10:GLU:OE2 | 2.40                     | 0.43              |
| 22:a:878:A:N6    | 22:a:899:A:O2'  | 2.50                     | 0.43              |
| 23:b:45:A:C4     | 23:b:46:A:C8    | 3.06                     | 0.43              |
| 24:c:132:MET:HG3 | 24:c:188:CYS:O  | 2.17                     | 0.43              |
| 28:g:37:LEU:HD23 | 28:g:37:LEU:HA  | 1.83                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1118:U:H2'    | 1:A:1119:C:C6    | 2.53                     | 0.43              |
| 22:a:182:A:H2'    | 22:a:183:C:H6    | 1.83                     | 0.43              |
| 22:a:207:A:H2'    | 22:a:208:C:O4'   | 2.19                     | 0.43              |
| 22:a:634:C:H2'    | 22:a:635:C:C6    | 2.53                     | 0.43              |
| 22:a:639:U:C2     | 22:a:640:C:C5    | 3.07                     | 0.43              |
| 22:a:895:U:H2'    | 22:a:897:C:H6    | 1.84                     | 0.43              |
| 22:a:1319:C:O2'   | 22:a:1320:C:H5'  | 2.18                     | 0.43              |
| 22:a:1437:C:H2'   | 22:a:1438:U:C6   | 2.53                     | 0.43              |
| 22:a:2247:A:H2'   | 22:a:2248:C:H6   | 1.83                     | 0.43              |
| 24:c:246:THR:HG23 | 24:c:250:VAL:O   | 2.18                     | 0.43              |
| 29:h:5:LEU:HD21   | 29:h:12:LEU:HD11 | 2.00                     | 0.43              |
| 46:y:41:THR:HG22  | 46:y:43:ALA:H    | 1.83                     | 0.43              |
| 1:A:908:A:H2'     | 1:A:909:A:C8     | 2.53                     | 0.43              |
| 1:A:1236:A:H2'    | 1:A:1237:C:C6    | 2.53                     | 0.43              |
| 12:L:31:ARG:O     | 12:L:58:THR:HG23 | 2.18                     | 0.43              |
| 26:e:190:ALA:O    | 26:e:194:LYS:HG2 | 2.18                     | 0.43              |
| 29:h:17:ASP:N     | 29:h:17:ASP:OD1  | 2.50                     | 0.43              |
| 39:r:20:VAL:HG11  | 39:r:44:ALA:HA   | 2.00                     | 0.43              |
| 46:y:45:ARG:HH12  | 46:y:59:GLU:CD   | 2.27                     | 0.43              |
| 50:2:32:ILE:O     | 50:2:32:ILE:HG13 | 2.17                     | 0.43              |
| 18:R:12:ARG:O     | 18:R:16:GLU:HG2  | 2.18                     | 0.43              |
| 22:a:514:A:N3     | 22:a:581:C:O2'   | 2.42                     | 0.43              |
| 22:a:1683:U:H2'   | 22:a:1684:G:H8   | 1.84                     | 0.43              |
| 22:a:1869:G:N2    | 22:a:1871:A:H3'  | 2.32                     | 0.43              |
| 22:a:2820:A:H4'   | 34:m:3:HIS:CD2   | 2.54                     | 0.43              |
| 27:f:153:ASP:OD1  | 27:f:153:ASP:N   | 2.50                     | 0.43              |
| 30:i:125:TYR:HH   | 30:i:132:HIS:CD2 | 2.34                     | 0.43              |
| 36:o:3:ASN:HA     | 36:o:6:LYS:HG2   | 2.01                     | 0.43              |
| 54:Z:19:G:H1'     | 54:Z:59:A:C2     | 2.53                     | 0.43              |
| 1:A:34:C:H2'      | 1:A:35:G:H8      | 1.82                     | 0.43              |
| 1:A:678:U:H2'     | 1:A:679:C:H6     | 1.84                     | 0.43              |
| 1:A:736:C:H2'     | 1:A:737:C:C6     | 2.53                     | 0.43              |
| 1:A:977:A:O2'     | 1:A:979:C:OP2    | 2.33                     | 0.43              |
| 1:A:1144:G:H21    | 1:A:1146:A:H62   | 1.66                     | 0.43              |
| 6:F:98:GLU:HG2    | 6:F:99:ALA:N     | 2.33                     | 0.43              |
| 8:H:48:ASP:OD2    | 8:H:49:PHE:N     | 2.47                     | 0.43              |
| 22:a:1212:G:H1'   | 22:a:1237:A:N6   | 2.33                     | 0.43              |
| 22:a:2096:C:H2'   | 22:a:2097:A:H8   | 1.84                     | 0.43              |
| 22:a:2193:G:H2'   | 22:a:2194:U:C6   | 2.54                     | 0.43              |
| 28:g:60:ASP:O     | 28:g:62:TRP:N    | 2.50                     | 0.43              |
| 28:g:145:ALA:HB1  | 28:g:164:TYR:HE1 | 1.84                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:h:12:LEU:HD13 | 29:h:19:VAL:HG11  | 2.00                     | 0.43              |
| 32:k:10:GLU:OE1  | 32:k:11:GLY:N     | 2.52                     | 0.43              |
| 33:l:20:LEU:HD13 | 42:u:81:PRO:HG2   | 2.01                     | 0.43              |
| 42:u:72:VAL:HG12 | 42:u:93:ARG:HA    | 2.01                     | 0.43              |
| 1:A:41:G:H2'     | 1:A:42:G:C8       | 2.53                     | 0.43              |
| 1:A:613:C:H2'    | 1:A:614:C:C6      | 2.54                     | 0.43              |
| 3:C:70:THR:HG21  | 3:C:76:VAL:HG21   | 1.98                     | 0.43              |
| 9:I:98:LEU:HD23  | 9:I:98:LEU:HA     | 1.78                     | 0.43              |
| 21:U:3:VAL:O     | 21:U:4:ILE:HD13   | 2.18                     | 0.43              |
| 22:a:17:G:H2'    | 22:a:18:U:C6      | 2.53                     | 0.43              |
| 22:a:171:U:H2'   | 22:a:172:A:C8     | 2.53                     | 0.43              |
| 22:a:479:A:H1'   | 22:a:480:A:H5''   | 2.01                     | 0.43              |
| 22:a:1484:U:H2'  | 22:a:1485:U:H6    | 1.82                     | 0.43              |
| 22:a:1509:A:O2'  | 22:a:1510:G:H8    | 2.01                     | 0.43              |
| 22:a:2700:A:H2'  | 22:a:2701:U:C6    | 2.54                     | 0.43              |
| 23:b:2:G:H2'     | 23:b:3:C:H6       | 1.83                     | 0.43              |
| 28:g:105:LEU:HB2 | 28:g:113:VAL:HG13 | 1.99                     | 0.43              |
| 30:i:99:ARG:HA   | 30:i:99:ARG:HD2   | 1.78                     | 0.43              |
| 1:A:156:C:H2'    | 1:A:157:U:O4'     | 2.18                     | 0.43              |
| 1:A:1180:A:OP1   | 9:I:105:THR:OG1   | 2.24                     | 0.43              |
| 4:D:148:LYS:O    | 4:D:151:LYS:NZ    | 2.52                     | 0.43              |
| 6:F:98:GLU:HG2   | 6:F:99:ALA:H      | 1.84                     | 0.43              |
| 22:a:589:U:H2'   | 22:a:590:A:C8     | 2.54                     | 0.43              |
| 34:m:71:ARG:HD2  | 34:m:71:ARG:HA    | 1.66                     | 0.43              |
| 40:s:48:GLN:HE21 | 40:s:55:VAL:H     | 1.67                     | 0.43              |
| 1:A:20:U:H2'     | 1:A:21:G:O4'      | 2.19                     | 0.43              |
| 1:A:649:A:H2'    | 1:A:650:G:O4'     | 2.19                     | 0.43              |
| 1:A:904:U:H2'    | 1:A:905:U:C6      | 2.53                     | 0.43              |
| 1:A:1011:C:H2'   | 1:A:1012:A:H8     | 1.84                     | 0.43              |
| 1:A:1175:G:H2'   | 1:A:1176:A:H8     | 1.84                     | 0.43              |
| 1:A:1238:A:H2    | 1:A:1241:G:N3     | 2.17                     | 0.43              |
| 9:I:57:MET:HA    | 9:I:60:LYS:NZ     | 2.33                     | 0.43              |
| 9:I:94:LEU:HD13  | 9:I:97:GLU:OE2    | 2.19                     | 0.43              |
| 22:a:891:G:C2    | 22:a:892:A:N7     | 2.87                     | 0.43              |
| 22:a:1558:C:O4'  | 22:a:1560:G:C8    | 2.72                     | 0.43              |
| 22:a:2072:C:H2'  | 22:a:2073:C:H6    | 1.83                     | 0.43              |
| 22:a:2300:C:H2'  | 22:a:2301:C:H6    | 1.83                     | 0.43              |
| 22:a:2687:U:H2'  | 22:a:2688:G:O4'   | 2.18                     | 0.43              |
| 1:A:538:G:H2'    | 1:A:539:A:H8      | 1.82                     | 0.43              |
| 1:A:1004:A:O2'   | 1:A:1036:A:N6     | 2.38                     | 0.43              |
| 1:A:1251:A:H2'   | 1:A:1252:A:C8     | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:9:MET:SD     | 6:F:86:ARG:HB3   | 2.58                     | 0.43              |
| 6:F:42:TRP:HB2   | 6:F:59:TYR:HB2   | 2.01                     | 0.43              |
| 18:R:21:ILE:HG21 | 18:R:55:LEU:HD12 | 2.01                     | 0.43              |
| 22:a:666:A:H4'   | 32:k:48:ARG:HD3  | 2.01                     | 0.43              |
| 22:a:1212:G:O2'  | 22:a:1236:G:N2   | 2.42                     | 0.43              |
| 22:a:1786:A:H1'  | 22:a:1938:A:N6   | 2.34                     | 0.43              |
| 22:a:2756:U:H1'  | 22:a:2757:A:H5'' | 2.00                     | 0.43              |
| 42:u:48:MET:SD   | 42:u:86:LEU:HD13 | 2.58                     | 0.43              |
| 48:0:5:ILE:HG23  | 48:0:28:ARG:NH1  | 2.34                     | 0.43              |
| 1:A:193:C:H2'    | 1:A:194:C:C6     | 2.53                     | 0.43              |
| 1:A:216:U:H2'    | 1:A:217:C:H6     | 1.83                     | 0.43              |
| 1:A:517:G:HO2'   | 1:A:518:C:P      | 2.42                     | 0.43              |
| 3:C:118:ASP:HA   | 3:C:121:THR:OG1  | 2.19                     | 0.43              |
| 9:I:9:THR:O      | 9:I:85:ARG:HD2   | 2.18                     | 0.43              |
| 22:a:273:G:H2'   | 22:a:274:C:C6    | 2.54                     | 0.43              |
| 22:a:499:U:H2'   | 22:a:500:G:O4'   | 2.19                     | 0.43              |
| 22:a:863:A:H2'   | 22:a:864:G:H8    | 1.83                     | 0.43              |
| 22:a:1586:A:H3'  | 22:a:1587:G:H8   | 1.83                     | 0.43              |
| 22:a:1914:C:H2'  | 22:a:1915:3TD:H6 | 2.01                     | 0.43              |
| 22:a:2329:U:H2'  | 22:a:2330:G:H8   | 1.84                     | 0.43              |
| 22:a:2637:U:C2   | 22:a:2782:G:N2   | 2.87                     | 0.43              |
| 22:a:2804:U:H2'  | 22:a:2805:C:C6   | 2.54                     | 0.43              |
| 27:f:17:MET:SD   | 27:f:22:TYR:HB2  | 2.59                     | 0.43              |
| 39:r:73:LYS:HB3  | 39:r:106:VAL:HB  | 2.00                     | 0.43              |
| 1:A:62:U:OP1     | 1:A:385:C:O2'    | 2.31                     | 0.42              |
| 7:G:132:GLY:O    | 7:G:135:VAL:HG22 | 2.19                     | 0.42              |
| 17:Q:9:GLN:NE2   | 17:Q:79:VAL:HG21 | 2.33                     | 0.42              |
| 22:a:1198:U:H2'  | 22:a:1199:U:C6   | 2.54                     | 0.42              |
| 22:a:1774:C:O2   | 22:a:1774:C:H2'  | 2.19                     | 0.42              |
| 22:a:1782:U:O2   | 22:a:2608:G:O2'  | 2.23                     | 0.42              |
| 22:a:1790:C:H2'  | 22:a:1791:A:C8   | 2.53                     | 0.42              |
| 22:a:1824:G:O3'  | 24:c:247:PRO:HD3 | 2.19                     | 0.42              |
| 22:a:2747:G:O6   | 22:a:2755:C:H5'' | 2.18                     | 0.42              |
| 40:s:14:PRO:HD3  | 45:x:30:MET:SD   | 2.59                     | 0.42              |
| 45:x:2:LYS:HA    | 45:x:5:GLU:OE2   | 2.19                     | 0.42              |
| 47:z:11:SER:O    | 47:z:15:MET:HG3  | 2.19                     | 0.42              |
| 1:A:89:U:H2'     | 1:A:90:C:H6      | 1.84                     | 0.42              |
| 1:A:444:G:C6     | 1:A:491:G:C6     | 3.07                     | 0.42              |
| 1:A:619:U:O2     | 1:A:619:U:H2'    | 2.19                     | 0.42              |
| 1:A:976:G:OP2    | 1:A:1358:U:O2'   | 2.35                     | 0.42              |
| 1:A:1030:U:O2'   | 1:A:1031:C:P     | 2.77                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1149:C:H2'   | 1:A:1150:A:C8    | 2.53                     | 0.42              |
| 3:C:47:LEU:HB3   | 3:C:50:ALA:HB3   | 2.00                     | 0.42              |
| 3:C:153:VAL:HG22 | 3:C:198:VAL:HG22 | 2.01                     | 0.42              |
| 4:D:139:PRO:HA   | 4:D:182:PHE:HD2  | 1.84                     | 0.42              |
| 14:N:47:LYS:HD2  | 14:N:47:LYS:HA   | 1.85                     | 0.42              |
| 22:a:64:A:H2'    | 22:a:65:U:H6     | 1.81                     | 0.42              |
| 22:a:1181:U:H2'  | 22:a:1182:G:C8   | 2.54                     | 0.42              |
| 22:a:1599:U:H2'  | 22:a:1600:C:H6   | 1.84                     | 0.42              |
| 51:3:25:VAL:HB   | 51:3:35:GLN:HB2  | 2.01                     | 0.42              |
| 1:A:171:A:H2'    | 1:A:172:A:C8     | 2.54                     | 0.42              |
| 1:A:246:A:C2     | 1:A:282:A:C5     | 3.06                     | 0.42              |
| 1:A:522:C:H41    | 12:L:50:ARG:NH2  | 2.17                     | 0.42              |
| 1:A:1318:A:H1'   | 19:S:37:ARG:HH11 | 1.84                     | 0.42              |
| 2:B:56:GLU:HG3   | 2:B:198:PHE:CE2  | 2.54                     | 0.42              |
| 6:F:38:ARG:NH2   | 6:F:63:ASN:OD1   | 2.49                     | 0.42              |
| 7:G:6:VAL:HG12   | 7:G:6:VAL:O      | 2.20                     | 0.42              |
| 8:H:118:GLN:OE1  | 8:H:118:GLN:HA   | 2.19                     | 0.42              |
| 22:a:711:G:C6    | 22:a:721:A:C6    | 3.06                     | 0.42              |
| 22:a:2723:C:H2'  | 22:a:2724:U:O4'  | 2.20                     | 0.42              |
| 22:a:2847:U:H2'  | 22:a:2848:G:O4'  | 2.19                     | 0.42              |
| 30:i:34:ARG:HG3  | 30:i:39:LYS:HB2  | 2.00                     | 0.42              |
| 51:3:18:LYS:HG3  | 51:3:23:ILE:HD13 | 2.02                     | 0.42              |
| 54:Z:26:C:C2     | 54:Z:27:G:C8     | 3.08                     | 0.42              |
| 1:A:280:C:N3     | 17:Q:41:THR:HG22 | 2.34                     | 0.42              |
| 1:A:559:A:H4'    | 1:A:560:A:H3'    | 2.02                     | 0.42              |
| 1:A:1162:C:H2'   | 1:A:1163:A:H8    | 1.83                     | 0.42              |
| 1:A:1315:U:H2'   | 1:A:1316:G:O4'   | 2.20                     | 0.42              |
| 22:a:1773:A:C8   | 22:a:1829:A:C8   | 3.07                     | 0.42              |
| 22:a:1997:C:OP2  | 25:d:129:THR:OG1 | 2.30                     | 0.42              |
| 22:a:2461:A:H2'  | 22:a:2462:C:C6   | 2.54                     | 0.42              |
| 23:b:42:C:N3     | 27:f:90:THR:HG22 | 2.34                     | 0.42              |
| 27:f:176:PRO:HG3 | 52:4:44:PHE:CE2  | 2.54                     | 0.42              |
| 32:k:93:ASN:OD1  | 32:k:94:THR:N    | 2.53                     | 0.42              |
| 35:n:63:LYS:HG3  | 35:n:64:TYR:N    | 2.34                     | 0.42              |
| 42:u:86:LEU:HD23 | 42:u:89:ILE:HD11 | 2.02                     | 0.42              |
| 1:A:1342:C:H2'   | 1:A:1343:G:C8    | 2.55                     | 0.42              |
| 13:M:83:LEU:HD11 | 19:S:66:MET:HG2  | 2.00                     | 0.42              |
| 22:a:1281:G:H2'  | 22:a:1282:U:C6   | 2.55                     | 0.42              |
| 22:a:1349:C:C2   | 22:a:1350:C:C5   | 3.08                     | 0.42              |
| 22:a:1499:C:C2   | 22:a:1500:G:C8   | 3.08                     | 0.42              |
| 33:l:110:GLU:O   | 33:l:114:ARG:HG3 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 38:q:62:GLU:N    | 38:q:62:GLU:OE1   | 2.53                     | 0.42              |
| 54:Z:55:5MU:H2'  | 54:Z:56:PSU:O4'   | 2.20                     | 0.42              |
| 1:A:562:U:H1'    | 12:L:12:ARG:HB3   | 2.01                     | 0.42              |
| 1:A:636:U:OP1    | 17:Q:6:ARG:NE     | 2.52                     | 0.42              |
| 9:I:5:GLN:OE1    | 9:I:5:GLN:N       | 2.53                     | 0.42              |
| 22:a:404:A:H1'   | 22:a:405:U:OP2    | 2.19                     | 0.42              |
| 22:a:538:A:H4'   | 30:i:7:LYS:HG2    | 2.02                     | 0.42              |
| 27:f:105:THR:HA  | 52:4:38:SER:HB2   | 2.01                     | 0.42              |
| 28:g:164:TYR:HB2 | 28:g:167:GLU:HB2  | 2.02                     | 0.42              |
| 30:i:31:GLU:OE1  | 30:i:34:ARG:NH1   | 2.52                     | 0.42              |
| 42:u:75:GLN:HB2  | 42:u:92:VAL:HG23  | 2.00                     | 0.42              |
| 54:Z:51:U:H2'    | 54:Z:52:C:C6      | 2.55                     | 0.42              |
| 1:A:1125:U:OP1   | 10:J:37:ARG:NE    | 2.52                     | 0.42              |
| 1:A:1312:G:OP2   | 52:4:63:ARG:NH2   | 2.49                     | 0.42              |
| 13:M:81:MET:HE3  | 22:a:888:C:C2     | 2.55                     | 0.42              |
| 14:N:24:ARG:NH1  | 14:N:55:SER:OG    | 2.53                     | 0.42              |
| 14:N:73:PHE:CZ   | 14:N:78:GLY:HA2   | 2.55                     | 0.42              |
| 15:O:3:LEU:HD23  | 15:O:3:LEU:HA     | 1.93                     | 0.42              |
| 22:a:18:U:H2'    | 22:a:19:A:C8      | 2.55                     | 0.42              |
| 22:a:191:A:H2'   | 22:a:192:C:H6     | 1.85                     | 0.42              |
| 22:a:756:A:H2'   | 22:a:757:G:O4'    | 2.20                     | 0.42              |
| 22:a:881:G:H2'   | 22:a:882:G:H8     | 1.85                     | 0.42              |
| 22:a:1039:A:H2   | 22:a:1116:G:H22   | 1.68                     | 0.42              |
| 22:a:1830:C:H2'  | 22:a:1831:G:H8    | 1.85                     | 0.42              |
| 22:a:2266:A:H4'  | 22:a:2267:A:C2    | 2.55                     | 0.42              |
| 22:a:2896:C:H2'  | 22:a:2897:U:C6    | 2.54                     | 0.42              |
| 43:v:37:ILE:HG21 | 43:v:80:ILE:HG21  | 2.01                     | 0.42              |
| 44:w:71:LEU:HG   | 44:w:76:GLU:OE2   | 2.20                     | 0.42              |
| 1:A:62:U:H2'     | 1:A:63:C:C6       | 2.54                     | 0.42              |
| 1:A:312:C:H2'    | 1:A:313:A:H8      | 1.85                     | 0.42              |
| 1:A:864:A:H2'    | 1:A:865:A:C8      | 2.54                     | 0.42              |
| 7:G:79:ARG:HH21  | 7:G:82:GLY:HA2    | 1.85                     | 0.42              |
| 11:K:87:LYS:HB2  | 11:K:113:VAL:HG23 | 2.00                     | 0.42              |
| 19:S:80:TYR:CZ   | 19:S:82:GLY:HA2   | 2.54                     | 0.42              |
| 22:a:75:G:H22    | 22:a:111:A:H2     | 1.67                     | 0.42              |
| 22:a:2328:A:H2'  | 22:a:2329:U:H6    | 1.78                     | 0.42              |
| 25:d:128:ARG:HA  | 25:d:128:ARG:HD3  | 1.80                     | 0.42              |
| 27:f:65:PRO:HA   | 27:f:89:VAL:HG12  | 2.01                     | 0.42              |
| 35:n:111:ARG:HA  | 35:n:115:LEU:O    | 2.20                     | 0.42              |
| 1:A:620:C:C2     | 4:D:132:ILE:HD13  | 2.55                     | 0.42              |
| 1:A:779:C:H2'    | 1:A:780:A:O4'     | 2.20                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1157:A:C2     | 1:A:1181:G:C4    | 3.08                     | 0.42              |
| 1:A:1244:G:H2'    | 1:A:1245:C:C6    | 2.55                     | 0.42              |
| 1:A:1250:A:H2'    | 1:A:1251:A:C8    | 2.54                     | 0.42              |
| 1:A:1286:U:H2'    | 1:A:1287:A:H5'   | 2.01                     | 0.42              |
| 1:A:1526:G:H2'    | 1:A:1527:U:C6    | 2.54                     | 0.42              |
| 3:C:16:LYS:HA     | 3:C:16:LYS:HD3   | 1.83                     | 0.42              |
| 13:M:92:ARG:NH1   | 22:a:887:U:H5''  | 2.35                     | 0.42              |
| 21:U:58:LYS:HG3   | 21:U:59:LYS:N    | 2.35                     | 0.42              |
| 22:a:45:G:H5''    | 22:a:46:G:O5'    | 2.19                     | 0.42              |
| 22:a:445:C:H2'    | 22:a:446:G:O4'   | 2.20                     | 0.42              |
| 22:a:632:A:H2'    | 22:a:633:A:C8    | 2.55                     | 0.42              |
| 22:a:1476:U:H2'   | 22:a:1477:A:C8   | 2.55                     | 0.42              |
| 29:h:34:GLY:C     | 29:h:36:ALA:H    | 2.28                     | 0.42              |
| 30:i:92:MET:HE3   | 30:i:92:MET:HB3  | 1.90                     | 0.42              |
| 31:j:105:ARG:HH11 | 31:j:108:ARG:NH1 | 2.17                     | 0.42              |
| 1:A:678:U:H2'     | 1:A:679:C:C6     | 2.55                     | 0.42              |
| 10:J:21:ALA:HB1   | 10:J:92:LEU:HD12 | 2.01                     | 0.42              |
| 22:a:2096:C:H2'   | 22:a:2097:A:C8   | 2.55                     | 0.42              |
| 27:f:121:SER:HB2  | 27:f:128:TYR:CE1 | 2.55                     | 0.42              |
| 28:g:127:THR:HB   | 28:g:130:GLU:OE1 | 2.19                     | 0.42              |
| 52:4:41:HIS:HB3   | 52:4:44:PHE:CD1  | 2.55                     | 0.42              |
| 1:A:408:A:H2'     | 1:A:409:U:C6     | 2.54                     | 0.41              |
| 1:A:983:A:H5'     | 1:A:984:C:OP2    | 2.20                     | 0.41              |
| 1:A:1513:A:H2'    | 1:A:1514:G:C8    | 2.55                     | 0.41              |
| 1:A:1526:G:H2'    | 1:A:1527:U:H6    | 1.85                     | 0.41              |
| 4:D:65:TYR:OH     | 4:D:95:GLU:OE2   | 2.26                     | 0.41              |
| 10:J:15:HIS:HB3   | 10:J:70:HIS:CE1  | 2.55                     | 0.41              |
| 22:a:723:C:H2'    | 22:a:724:U:O4'   | 2.20                     | 0.41              |
| 22:a:959:A:H2'    | 22:a:960:A:C8    | 2.55                     | 0.41              |
| 22:a:966:G:C1'    | 22:a:2267:A:H62  | 2.33                     | 0.41              |
| 22:a:1545:A:H2'   | 22:a:1546:G:O4'  | 2.20                     | 0.41              |
| 22:a:1790:C:H2'   | 22:a:1791:A:C5   | 2.55                     | 0.41              |
| 22:a:1814:G:OP2   | 22:a:1815:A:O2'  | 2.23                     | 0.41              |
| 22:a:2100:G:H2'   | 22:a:2101:A:C8   | 2.54                     | 0.41              |
| 22:a:2241:A:H2'   | 22:a:2242:G:C8   | 2.55                     | 0.41              |
| 22:a:2804:U:H2'   | 22:a:2805:C:H6   | 1.84                     | 0.41              |
| 28:g:137:ASP:HB3  | 28:g:140:VAL:HB  | 2.02                     | 0.41              |
| 41:t:81:ASP:OD1   | 41:t:82:ARG:N    | 2.52                     | 0.41              |
| 54:Z:11:A:H2'     | 54:Z:12:G:C8     | 2.54                     | 0.41              |
| 1:A:543:U:OP1     | 4:D:14:ARG:HD2   | 2.20                     | 0.41              |
| 1:A:737:C:H2'     | 1:A:738:C:H6     | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:985:C:H2'     | 1:A:986:U:C6      | 2.54                     | 0.41              |
| 3:C:114:LYS:HB2   | 3:C:185:ASN:HD22  | 1.85                     | 0.41              |
| 10:J:46:LYS:HG2   | 10:J:68:ARG:HG2   | 2.02                     | 0.41              |
| 14:N:79:LEU:HB2   | 14:N:84:VAL:HG23  | 2.02                     | 0.41              |
| 22:a:181:A:H1'    | 22:a:435:C:H5'    | 2.02                     | 0.41              |
| 22:a:434:U:O2     | 22:a:436:C:N4     | 2.53                     | 0.41              |
| 22:a:1473:G:H2'   | 22:a:1474:U:C6    | 2.54                     | 0.41              |
| 22:a:1736:U:H2'   | 22:a:1737:G:O4'   | 2.20                     | 0.41              |
| 22:a:1889:A:H2'   | 22:a:1890:A:C8    | 2.55                     | 0.41              |
| 22:a:2193:G:H2'   | 22:a:2194:U:H6    | 1.85                     | 0.41              |
| 22:a:2291:U:OP1   | 22:a:2380:C:O2'   | 2.38                     | 0.41              |
| 24:c:225:MET:SD   | 24:c:230:HIS:HB2  | 2.60                     | 0.41              |
| 28:g:105:LEU:HB3  | 28:g:107:LEU:HG   | 2.02                     | 0.41              |
| 30:i:49:ASP:OD1   | 30:i:121:LYS:NZ   | 2.46                     | 0.41              |
| 1:A:90:C:H2'      | 1:A:91:U:H6       | 1.85                     | 0.41              |
| 1:A:1039:G:H2'    | 1:A:1040:U:H6     | 1.85                     | 0.41              |
| 1:A:1263:C:H2'    | 1:A:1264:U:H6     | 1.85                     | 0.41              |
| 6:F:39:LEU:HD13   | 6:F:62:MET:HG2    | 2.02                     | 0.41              |
| 22:a:52:A:H2'     | 22:a:53:A:C8      | 2.56                     | 0.41              |
| 22:a:2020:A:H5'   | 47:z:9:THR:CG2    | 2.50                     | 0.41              |
| 22:a:2787:C:H1'   | 25:d:63:PRO:HG3   | 2.03                     | 0.41              |
| 24:c:210:ALA:HA   | 24:c:213:TRP:CE3  | 2.55                     | 0.41              |
| 28:g:170:ARG:HH12 | 51:3:31:PRO:HD3   | 1.86                     | 0.41              |
| 30:i:23:LYS:NZ    | 30:i:142:ILE:OXT  | 2.43                     | 0.41              |
| 31:j:80:ASP:OD2   | 36:o:69:GLY:HA3   | 2.20                     | 0.41              |
| 31:j:105:ARG:HH11 | 31:j:108:ARG:HH12 | 1.69                     | 0.41              |
| 52:4:12:ILE:HG13  | 52:4:13:THR:N     | 2.35                     | 0.41              |
| 1:A:184:G:H2'     | 1:A:185:U:C6      | 2.55                     | 0.41              |
| 1:A:508:U:C1'     | 1:A:509:A:H2      | 2.33                     | 0.41              |
| 1:A:821:G:H2'     | 1:A:822:U:C6      | 2.55                     | 0.41              |
| 6:F:69:GLU:O      | 6:F:73:GLU:OE1    | 2.38                     | 0.41              |
| 9:I:94:LEU:HA     | 9:I:97:GLU:OE2    | 2.21                     | 0.41              |
| 11:K:35:THR:HG1   | 11:K:40:ASN:C     | 2.27                     | 0.41              |
| 22:a:596:U:H2'    | 22:a:597:G:H8     | 1.86                     | 0.41              |
| 22:a:1654:A:O2'   | 25:d:118:PHE:O    | 2.37                     | 0.41              |
| 22:a:2100:G:O6    | 22:a:2189:U:C4    | 2.72                     | 0.41              |
| 22:a:2773:C:H2'   | 22:a:2774:C:C6    | 2.56                     | 0.41              |
| 1:A:592:G:H2'     | 1:A:593:U:H6      | 1.85                     | 0.41              |
| 1:A:695:A:H2'     | 1:A:696:A:C8      | 2.56                     | 0.41              |
| 1:A:859:G:H2'     | 1:A:860:A:C8      | 2.56                     | 0.41              |
| 1:A:978:A:C2      | 1:A:1319:A:C4     | 3.09                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1076:U:OP1   | 2:B:174:LYS:NZ   | 2.30                     | 0.41              |
| 1:A:1464:U:H2'   | 1:A:1465:A:H8    | 1.85                     | 0.41              |
| 4:D:105:MET:HE1  | 4:D:143:VAL:HB   | 2.02                     | 0.41              |
| 22:a:169:G:H2'   | 22:a:170:U:C6    | 2.55                     | 0.41              |
| 22:a:417:C:H2'   | 22:a:418:C:C6    | 2.55                     | 0.41              |
| 22:a:483:A:H5''  | 41:t:47:LYS:HD2  | 2.00                     | 0.41              |
| 22:a:820:A:H4'   | 22:a:836:G:N2    | 2.36                     | 0.41              |
| 22:a:1744:A:H3'  | 22:a:1745:A:H8   | 1.86                     | 0.41              |
| 22:a:2098:U:H2'  | 22:a:2099:U:O4'  | 2.21                     | 0.41              |
| 22:a:2627:G:N2   | 22:a:2777:G:OP2  | 2.53                     | 0.41              |
| 41:t:14:LEU:HD11 | 41:t:71:ALA:HB2  | 2.01                     | 0.41              |
| 54:Z:1:C:H2'     | 54:Z:2:G:H8      | 1.86                     | 0.41              |
| 1:A:110:C:O2'    | 16:P:25:ARG:O    | 2.32                     | 0.41              |
| 1:A:255:G:H2'    | 1:A:256:U:C6     | 2.55                     | 0.41              |
| 7:G:27:VAL:HG11  | 7:G:40:GLU:HG3   | 2.03                     | 0.41              |
| 9:I:25:ASN:OD1   | 9:I:25:ASN:N     | 2.54                     | 0.41              |
| 11:K:97:ILE:HG22 | 21:U:12:PHE:HZ   | 1.86                     | 0.41              |
| 12:L:106:GLY:O   | 12:L:108:LYS:NZ  | 2.54                     | 0.41              |
| 13:M:48:LEU:HD23 | 13:M:48:LEU:HA   | 1.86                     | 0.41              |
| 17:Q:58:VAL:HG12 | 17:Q:79:VAL:HB   | 2.03                     | 0.41              |
| 22:a:553:G:H2'   | 22:a:554:U:H6    | 1.86                     | 0.41              |
| 22:a:832:U:H2'   | 22:a:833:A:H8    | 1.86                     | 0.41              |
| 22:a:1429:G:H2'  | 22:a:1430:G:H8   | 1.85                     | 0.41              |
| 22:a:1637:A:H5'  | 22:a:1760:C:O2'  | 2.21                     | 0.41              |
| 22:a:2100:G:N1   | 22:a:2189:U:N3   | 2.33                     | 0.41              |
| 30:i:26:GLY:O    | 30:i:30:THR:HG23 | 2.20                     | 0.41              |
| 41:t:98:SER:OG   | 41:t:98:SER:O    | 2.33                     | 0.41              |
| 49:1:22:MET:HE3  | 49:1:22:MET:HB3  | 1.86                     | 0.41              |
| 1:A:2:A:H4'      | 4:D:83:LYS:HZ2   | 1.85                     | 0.41              |
| 1:A:1163:A:H2'   | 1:A:1164:G:C8    | 2.55                     | 0.41              |
| 7:G:71:PRO:O     | 7:G:96:ARG:HG2   | 2.21                     | 0.41              |
| 22:a:170:U:H2'   | 22:a:171:U:C6    | 2.56                     | 0.41              |
| 22:a:194:G:H2'   | 22:a:195:A:O4'   | 2.20                     | 0.41              |
| 22:a:438:G:H2'   | 22:a:439:A:C8    | 2.55                     | 0.41              |
| 26:e:3:LEU:O     | 26:e:12:LEU:N    | 2.48                     | 0.41              |
| 27:f:46:ASP:HB3  | 27:f:49:LEU:HG   | 2.02                     | 0.41              |
| 29:h:2:GLN:HB3   | 29:h:39:ALA:HB3  | 2.03                     | 0.41              |
| 29:h:12:LEU:HD12 | 29:h:13:GLY:N    | 2.36                     | 0.41              |
| 32:k:19:LEU:HD13 | 32:k:31:GLY:HA3  | 2.02                     | 0.41              |
| 1:A:219:U:H2'    | 1:A:220:G:C8     | 2.55                     | 0.41              |
| 1:A:457:G:H3'    | 1:A:458:U:H6     | 1.86                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1412:C:H2'   | 1:A:1413:A:C8     | 2.55                     | 0.41              |
| 3:C:72:ARG:HB3   | 3:C:75:ILE:HD12   | 2.02                     | 0.41              |
| 6:F:10:VAL:HB    | 6:F:58:HIS:HB3    | 2.03                     | 0.41              |
| 6:F:90:MET:HE1   | 18:R:23:TYR:OH    | 2.21                     | 0.41              |
| 22:a:151:C:H2'   | 22:a:152:A:H8     | 1.85                     | 0.41              |
| 22:a:273:G:H2'   | 22:a:274:C:H6     | 1.86                     | 0.41              |
| 22:a:286:U:H2'   | 22:a:287:G:H8     | 1.85                     | 0.41              |
| 22:a:835:C:C2    | 22:a:836:G:C8     | 3.08                     | 0.41              |
| 22:a:852:U:H2'   | 22:a:853:C:C6     | 2.56                     | 0.41              |
| 22:a:1361:G:H2'  | 22:a:1362:C:C6    | 2.56                     | 0.41              |
| 22:a:1446:C:H2'  | 22:a:1447:C:C6    | 2.56                     | 0.41              |
| 22:a:1614:A:C6   | 39:r:87:PRO:HB3   | 2.56                     | 0.41              |
| 22:a:2700:A:H2'  | 22:a:2701:U:H6    | 1.86                     | 0.41              |
| 24:c:240:PHE:O   | 24:c:242:LYS:HG3  | 2.21                     | 0.41              |
| 25:d:152:PRO:HG3 | 25:d:156:PHE:CZ   | 2.56                     | 0.41              |
| 33:l:56:ALA:HB2  | 33:l:119:LEU:HD12 | 2.03                     | 0.41              |
| 47:z:43:ILE:HG22 | 47:z:49:TYR:HB2   | 2.02                     | 0.41              |
| 1:A:31:G:O2'     | 1:A:48:C:N4       | 2.54                     | 0.41              |
| 1:A:160:A:H2'    | 1:A:161:A:O4'     | 2.20                     | 0.41              |
| 1:A:486:U:H2'    | 1:A:487:A:C8      | 2.56                     | 0.41              |
| 1:A:707:U:H4'    | 11:K:22:HIS:CD2   | 2.56                     | 0.41              |
| 1:A:1125:U:C2    | 1:A:1127:G:C8     | 3.09                     | 0.41              |
| 1:A:1206:G:H2'   | 1:A:1207:2MG:O4'  | 2.20                     | 0.41              |
| 1:A:1233:G:OP1   | 9:I:119:ARG:NH1   | 2.53                     | 0.41              |
| 1:A:1266:G:N2    | 1:A:1269:A:OP2    | 2.43                     | 0.41              |
| 2:B:167:ASP:HB2  | 2:B:191:SER:HB2   | 2.03                     | 0.41              |
| 5:E:89:HIS:O     | 5:E:90:THR:C      | 2.64                     | 0.41              |
| 9:I:23:PRO:HA    | 9:I:61:LEU:HD23   | 2.02                     | 0.41              |
| 12:L:10:LYS:HB3  | 12:L:10:LYS:HE3   | 1.71                     | 0.41              |
| 12:L:108:LYS:HA  | 12:L:108:LYS:HD3  | 1.90                     | 0.41              |
| 13:M:69:LEU:O    | 13:M:73:ILE:HG12  | 2.21                     | 0.41              |
| 22:a:176:A:O2'   | 22:a:177:G:H5'    | 2.21                     | 0.41              |
| 22:a:184:C:H2'   | 22:a:185:G:C8     | 2.56                     | 0.41              |
| 22:a:283:G:H2'   | 22:a:284:U:O4'    | 2.21                     | 0.41              |
| 22:a:288:U:H2'   | 22:a:289:G:H8     | 1.85                     | 0.41              |
| 22:a:839:U:H2'   | 22:a:840:C:C6     | 2.56                     | 0.41              |
| 22:a:1028:A:N6   | 22:a:1125:G:H2'   | 2.36                     | 0.41              |
| 22:a:1315:C:H2'  | 22:a:1316:U:C6    | 2.56                     | 0.41              |
| 22:a:1354:A:H2'  | 22:a:1355:G:O4'   | 2.21                     | 0.41              |
| 22:a:1473:G:C6   | 22:a:1519:G:C6    | 3.08                     | 0.41              |
| 22:a:1710:G:H2'  | 22:a:1711:A:C8    | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:a:2625:G:H2'  | 22:a:2626:C:O4'  | 2.20                     | 0.41              |
| 22:a:2811:G:H5'' | 25:d:61:THR:HG23 | 2.03                     | 0.41              |
| 22:a:2820:A:N3   | 22:a:2820:A:H2'  | 2.35                     | 0.41              |
| 23:b:39:A:H2'    | 23:b:40:U:C6     | 2.56                     | 0.41              |
| 37:p:58:ARG:HA   | 37:p:61:TRP:CE3  | 2.55                     | 0.41              |
| 39:r:19:LEU:HD23 | 39:r:19:LEU:HA   | 1.89                     | 0.41              |
| 52:4:16:CYS:SG   | 52:4:17:SER:N    | 2.94                     | 0.41              |
| 54:Z:10:G:N2     | 54:Z:27:G:H1'    | 2.36                     | 0.41              |
| 54:Z:44:A:H2'    | 54:Z:45:A:C8     | 2.56                     | 0.41              |
| 1:A:3:A:N1       | 1:A:628:G:O2'    | 2.40                     | 0.41              |
| 1:A:453:G:C4     | 1:A:454:G:C8     | 3.09                     | 0.41              |
| 1:A:472:U:H2'    | 1:A:473:U:C6     | 2.56                     | 0.41              |
| 1:A:696:A:H2'    | 1:A:697:U:C6     | 2.54                     | 0.41              |
| 1:A:1060:U:H2'   | 1:A:1061:G:H8    | 1.85                     | 0.41              |
| 1:A:1144:G:O6    | 1:A:1145:A:N6    | 2.54                     | 0.41              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6    | 2.56                     | 0.41              |
| 5:E:13:GLU:HG2   | 5:E:39:VAL:HG12  | 2.02                     | 0.41              |
| 6:F:67:PRO:HB2   | 6:F:69:GLU:CD    | 2.46                     | 0.41              |
| 22:a:2373:G:H2'  | 22:a:2374:C:C6   | 2.56                     | 0.41              |
| 31:j:17:ARG:HB2  | 31:j:45:GLU:HG3  | 2.03                     | 0.41              |
| 32:k:78:ARG:HG2  | 32:k:113:ALA:HB3 | 2.03                     | 0.41              |
| 37:p:95:LEU:HD23 | 37:p:95:LEU:HA   | 1.93                     | 0.41              |
| 47:z:38:HIS:ND1  | 47:z:39:LEU:O    | 2.53                     | 0.41              |
| 50:2:55:LEU:HD23 | 50:2:55:LEU:HA   | 1.93                     | 0.41              |
| 1:A:67:C:H2'     | 1:A:68:G:C8      | 2.56                     | 0.40              |
| 1:A:184:G:H2'    | 1:A:185:U:H6     | 1.85                     | 0.40              |
| 1:A:619:U:H2'    | 1:A:619:U:OP1    | 2.21                     | 0.40              |
| 4:D:62:ARG:HE    | 4:D:62:ARG:HB3   | 1.76                     | 0.40              |
| 16:P:52:LEU:HD12 | 16:P:78:VAL:HG11 | 2.03                     | 0.40              |
| 20:T:4:ILE:O     | 20:T:8:LYS:HG3   | 2.21                     | 0.40              |
| 22:a:40:U:H2'    | 22:a:41:C:C6     | 2.55                     | 0.40              |
| 22:a:78:U:H2'    | 22:a:79:C:C6     | 2.57                     | 0.40              |
| 22:a:765:C:H2'   | 22:a:766:U:C6    | 2.56                     | 0.40              |
| 22:a:810:U:C4    | 32:k:29:LYS:O    | 2.74                     | 0.40              |
| 22:a:1575:C:H2'  | 22:a:1576:U:O4'  | 2.22                     | 0.40              |
| 22:a:1685:C:H2'  | 22:a:1686:C:H6   | 1.87                     | 0.40              |
| 22:a:2301:C:H2'  | 22:a:2302:U:C6   | 2.56                     | 0.40              |
| 22:a:2859:G:H2'  | 22:a:2860:A:C8   | 2.56                     | 0.40              |
| 26:e:7:ASP:OD1   | 26:e:8:ALA:N     | 2.53                     | 0.40              |
| 30:i:106:LYS:HG2 | 30:i:119:PHE:CD1 | 2.56                     | 0.40              |
| 47:z:12:LYS:HB3  | 47:z:12:LYS:HE3  | 1.58                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 52:4:26:SER:OG   | 52:4:28:VAL:HG23 | 2.20                     | 0.40              |
| 1:A:924:C:O2'    | 1:A:1502:A:N1    | 2.51                     | 0.40              |
| 2:B:130:THR:O    | 2:B:132:LYS:N    | 2.54                     | 0.40              |
| 3:C:134:MET:HE2  | 3:C:168:TYR:HD2  | 1.86                     | 0.40              |
| 4:D:102:VAL:HG11 | 4:D:117:LEU:HD11 | 2.03                     | 0.40              |
| 8:H:38:ASN:O     | 8:H:42:GLU:HG3   | 2.21                     | 0.40              |
| 9:I:88:MET:HE1   | 9:I:95:ARG:HA    | 2.03                     | 0.40              |
| 11:K:70:CYS:O    | 11:K:74:VAL:HG22 | 2.20                     | 0.40              |
| 12:L:99:ARG:HB3  | 12:L:117:TYR:HA  | 2.02                     | 0.40              |
| 13:M:71:ARG:NH2  | 27:f:113:ASP:OD2 | 2.54                     | 0.40              |
| 14:N:83:LYS:HA   | 14:N:83:LYS:HD3  | 1.77                     | 0.40              |
| 22:a:12:U:O2     | 22:a:2626:C:H4'  | 2.21                     | 0.40              |
| 22:a:161:A:OP2   | 22:a:162:U:O2'   | 2.29                     | 0.40              |
| 22:a:357:C:H2'   | 22:a:358:U:C6    | 2.57                     | 0.40              |
| 22:a:1480:C:H2'  | 22:a:1481:U:O4'  | 2.22                     | 0.40              |
| 22:a:1684:G:H2'  | 22:a:1685:C:H6   | 1.85                     | 0.40              |
| 22:a:2364:C:H2'  | 22:a:2365:G:O4'  | 2.21                     | 0.40              |
| 22:a:2818:U:H2'  | 22:a:2819:G:C8   | 2.56                     | 0.40              |
| 33:l:53:MET:HE3  | 33:l:53:MET:HB2  | 1.97                     | 0.40              |
| 54:Z:15:G:N2     | 54:Z:22:A:N3     | 2.70                     | 0.40              |
| 1:A:244:U:O4     | 1:A:906:A:H1'    | 2.21                     | 0.40              |
| 1:A:1158:C:C4    | 1:A:1160:G:C8    | 3.10                     | 0.40              |
| 1:A:1263:C:H2'   | 1:A:1264:U:C6    | 2.56                     | 0.40              |
| 5:E:81:LEU:HB2   | 5:E:98:PRO:HG3   | 2.02                     | 0.40              |
| 13:M:22:ILE:HG23 | 13:M:66:GLU:OE2  | 2.21                     | 0.40              |
| 22:a:896:A:N7    | 22:a:897:C:H1'   | 2.36                     | 0.40              |
| 22:a:903:C:H2'   | 22:a:904:G:C8    | 2.54                     | 0.40              |
| 22:a:1046:A:H5'  | 22:a:1047:G:H5'' | 2.04                     | 0.40              |
| 22:a:1444:G:C4   | 22:a:1445:G:C8   | 3.09                     | 0.40              |
| 22:a:1571:A:H2'  | 22:a:1572:A:C8   | 2.55                     | 0.40              |
| 22:a:1874:C:H2'  | 22:a:1875:G:O4'  | 2.21                     | 0.40              |
| 22:a:2292:U:H2'  | 22:a:2293:G:C8   | 2.56                     | 0.40              |
| 22:a:2638:G:O2'  | 22:a:2775:G:N2   | 2.50                     | 0.40              |
| 25:d:105:LYS:HA  | 25:d:105:LYS:HD3 | 1.70                     | 0.40              |
| 39:r:13:SER:O    | 39:r:17:VAL:HG23 | 2.21                     | 0.40              |
| 54:Z:20:G:H3'    | 54:Z:21:H2U:N3   | 2.37                     | 0.40              |
| 1:A:41:G:H2'     | 1:A:42:G:H8      | 1.87                     | 0.40              |
| 1:A:253:A:H2'    | 1:A:254:G:C8     | 2.57                     | 0.40              |
| 1:A:490:C:H2'    | 1:A:491:G:H8     | 1.85                     | 0.40              |
| 5:E:160:SER:O    | 5:E:164:ILE:HG12 | 2.21                     | 0.40              |
| 7:G:113:ASP:HB2  | 7:G:119:ARG:CG   | 2.51                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:a:18:U:H2'    | 22:a:19:A:H8      | 1.86                     | 0.40              |
| 22:a:157:C:H2'   | 22:a:158:U:O4'    | 2.22                     | 0.40              |
| 22:a:340:A:O2'   | 26:e:162:ARG:NH1  | 2.54                     | 0.40              |
| 22:a:493:G:H2'   | 22:a:494:G:O4'    | 2.21                     | 0.40              |
| 22:a:729:G:OP1   | 24:c:10:SER:OG    | 2.35                     | 0.40              |
| 22:a:1535:A:O2'  | 22:a:1537:G:N1    | 2.55                     | 0.40              |
| 22:a:1683:U:H2'  | 22:a:1684:G:C8    | 2.56                     | 0.40              |
| 22:a:1710:G:H4'  | 22:a:2858:C:O2    | 2.21                     | 0.40              |
| 22:a:2728:U:HO2' | 22:a:2729:G:H8    | 1.70                     | 0.40              |
| 22:a:2728:U:O2'  | 22:a:2729:G:H8    | 2.05                     | 0.40              |
| 23:b:48:U:H2'    | 23:b:49:C:C6      | 2.57                     | 0.40              |
| 29:h:15:LEU:HD23 | 29:h:16:GLY:N     | 2.36                     | 0.40              |
| 35:n:17:LYS:O    | 35:n:20:GLU:HG2   | 2.21                     | 0.40              |
| 45:x:9:LYS:HB3   | 45:x:13:GLU:HB2   | 2.03                     | 0.40              |
| 1:A:260:G:H2'    | 1:A:261:U:C6      | 2.56                     | 0.40              |
| 1:A:538:G:H2'    | 1:A:539:A:C8      | 2.56                     | 0.40              |
| 1:A:1037:C:H2'   | 1:A:1038:C:H6     | 1.86                     | 0.40              |
| 2:B:136:MET:HE2  | 2:B:136:MET:HB3   | 2.00                     | 0.40              |
| 4:D:109:ALA:H    | 4:D:113:GLU:HG2   | 1.85                     | 0.40              |
| 6:F:4:TYR:CE2    | 6:F:71:ILE:HG13   | 2.56                     | 0.40              |
| 12:L:36:ARG:HG2  | 12:L:38:TYR:HD1   | 1.87                     | 0.40              |
| 22:a:287:G:H2'   | 22:a:288:U:C6     | 2.56                     | 0.40              |
| 22:a:682:G:H5'   | 49:1:26:ASN:ND2   | 2.36                     | 0.40              |
| 22:a:1495:A:H2'  | 22:a:1496:A:C8    | 2.57                     | 0.40              |
| 22:a:1677:A:H2'  | 22:a:1678:A:C8    | 2.56                     | 0.40              |
| 24:c:52:ARG:O    | 24:c:53:HIS:HB2   | 2.21                     | 0.40              |
| 28:g:140:VAL:O   | 28:g:144:VAL:HG23 | 2.21                     | 0.40              |
| 45:x:7:ARG:O     | 45:x:60:LYS:NZ    | 2.48                     | 0.40              |
| 54:Z:17:C:H5'    | 54:Z:62:C:OP1     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | B     | 222/241 (92%) | 211 (95%) | 11 (5%) | 0        | 100         | 100 |
| 3   | C     | 204/233 (88%) | 197 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 4   | D     | 203/206 (98%) | 199 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 5   | E     | 154/167 (92%) | 147 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 6   | F     | 101/135 (75%) | 95 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 7   | G     | 151/179 (84%) | 139 (92%) | 12 (8%) | 0        | 100         | 100 |
| 8   | H     | 127/130 (98%) | 122 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 9   | I     | 125/130 (96%) | 120 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 10  | J     | 96/103 (93%)  | 91 (95%)  | 4 (4%)  | 1 (1%)   | 13          | 29  |
| 11  | K     | 113/129 (88%) | 105 (93%) | 8 (7%)  | 0        | 100         | 100 |
| 12  | L     | 120/124 (97%) | 111 (92%) | 9 (8%)  | 0        | 100         | 100 |
| 13  | M     | 113/118 (96%) | 108 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 14  | N     | 98/101 (97%)  | 94 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 15  | O     | 86/89 (97%)   | 84 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 16  | P     | 79/82 (96%)   | 75 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 17  | Q     | 77/84 (92%)   | 77 (100%) | 0       | 0        | 100         | 100 |
| 18  | R     | 64/75 (85%)   | 60 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| 19  | S     | 82/92 (89%)   | 82 (100%) | 0       | 0        | 100         | 100 |
| 20  | T     | 84/87 (97%)   | 83 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 21  | U     | 68/71 (96%)   | 67 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 24  | c     | 269/273 (98%) | 261 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 25  | d     | 206/209 (99%) | 202 (98%) | 3 (2%)  | 1 (0%)   | 25          | 47  |
| 26  | e     | 199/201 (99%) | 196 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 27  | f     | 175/179 (98%) | 166 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 28  | g     | 174/177 (98%) | 165 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 29  | h     | 39/149 (26%)  | 35 (90%)  | 4 (10%) | 0        | 100         | 100 |
| 30  | i     | 140/142 (99%) | 138 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 31  | j     | 121/123 (98%) | 118 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 32  | k     | 142/144 (99%) | 138 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 33  | l     | 132/136 (97%) | 131 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 34  | m     | 116/127 (91%) | 111 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 35  | n     | 114/117 (97%) | 109 (96%) | 5 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 36  | o     | 112/115 (97%)   | 108 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 37  | p     | 115/118 (98%)   | 115 (100%) | 0        | 0        | 100         | 100 |
| 38  | q     | 101/103 (98%)   | 95 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 39  | r     | 108/110 (98%)   | 108 (100%) | 0        | 0        | 100         | 100 |
| 40  | s     | 91/100 (91%)    | 87 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 41  | t     | 100/104 (96%)   | 91 (91%)   | 9 (9%)   | 0        | 100         | 100 |
| 42  | u     | 92/94 (98%)     | 89 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 43  | v     | 76/85 (89%)     | 73 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 44  | w     | 75/78 (96%)     | 73 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 45  | x     | 60/63 (95%)     | 56 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 46  | y     | 56/59 (95%)     | 54 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 47  | z     | 54/57 (95%)     | 54 (100%)  | 0        | 0        | 100         | 100 |
| 48  | 0     | 49/55 (89%)     | 49 (100%)  | 0        | 0        | 100         | 100 |
| 49  | 1     | 44/46 (96%)     | 44 (100%)  | 0        | 0        | 100         | 100 |
| 50  | 2     | 62/65 (95%)     | 59 (95%)   | 2 (3%)   | 1 (2%)   | 8           | 17  |
| 51  | 3     | 36/38 (95%)     | 36 (100%)  | 0        | 0        | 100         | 100 |
| 52  | 4     | 56/70 (80%)     | 53 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| All | All   | 5481/5913 (93%) | 5281 (96%) | 197 (4%) | 3 (0%)   | 50          | 71  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | d     | 149 | ASN  |
| 10  | J     | 57  | VAL  |
| 50  | 2     | 32  | ILE  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | B     | 186/199 (94%)  | 186 (100%) | 0        | 100         | 100 |
| 3   | C     | 170/190 (90%)  | 170 (100%) | 0        | 100         | 100 |
| 4   | D     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 5   | E     | 119/126 (94%)  | 119 (100%) | 0        | 100         | 100 |
| 6   | F     | 90/116 (78%)   | 90 (100%)  | 0        | 100         | 100 |
| 7   | G     | 126/147 (86%)  | 126 (100%) | 0        | 100         | 100 |
| 8   | H     | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 9   | I     | 105/107 (98%)  | 105 (100%) | 0        | 100         | 100 |
| 10  | J     | 86/90 (96%)    | 86 (100%)  | 0        | 100         | 100 |
| 11  | K     | 89/98 (91%)    | 89 (100%)  | 0        | 100         | 100 |
| 12  | L     | 102/103 (99%)  | 102 (100%) | 0        | 100         | 100 |
| 13  | M     | 93/96 (97%)    | 93 (100%)  | 0        | 100         | 100 |
| 14  | N     | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 15  | O     | 76/77 (99%)    | 76 (100%)  | 0        | 100         | 100 |
| 16  | P     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 17  | Q     | 73/78 (94%)    | 73 (100%)  | 0        | 100         | 100 |
| 18  | R     | 57/65 (88%)    | 57 (100%)  | 0        | 100         | 100 |
| 19  | S     | 72/79 (91%)    | 72 (100%)  | 0        | 100         | 100 |
| 20  | T     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 21  | U     | 60/61 (98%)    | 60 (100%)  | 0        | 100         | 100 |
| 24  | c     | 216/218 (99%)  | 216 (100%) | 0        | 100         | 100 |
| 25  | d     | 163/163 (100%) | 163 (100%) | 0        | 100         | 100 |
| 26  | e     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 27  | f     | 148/150 (99%)  | 148 (100%) | 0        | 100         | 100 |
| 28  | g     | 137/138 (99%)  | 137 (100%) | 0        | 100         | 100 |
| 29  | h     | 32/114 (28%)   | 32 (100%)  | 0        | 100         | 100 |
| 30  | i     | 116/116 (100%) | 115 (99%)  | 1 (1%)   | 75          | 90  |
| 31  | j     | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 32  | k     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 33  | l     | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 34  | m     | 98/103 (95%)   | 98 (100%)  | 0        | 100         | 100 |
| 35  | n     | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 36  | o     | 99/100 (99%)    | 99 (100%)   | 0        | 100         | 100 |
| 37  | p     | 89/90 (99%)     | 89 (100%)   | 0        | 100         | 100 |
| 38  | q     | 84/84 (100%)    | 84 (100%)   | 0        | 100         | 100 |
| 39  | r     | 93/93 (100%)    | 93 (100%)   | 0        | 100         | 100 |
| 40  | s     | 80/84 (95%)     | 80 (100%)   | 0        | 100         | 100 |
| 41  | t     | 83/85 (98%)     | 83 (100%)   | 0        | 100         | 100 |
| 42  | u     | 78/78 (100%)    | 78 (100%)   | 0        | 100         | 100 |
| 43  | v     | 59/63 (94%)     | 59 (100%)   | 0        | 100         | 100 |
| 44  | w     | 67/68 (98%)     | 67 (100%)   | 0        | 100         | 100 |
| 45  | x     | 54/55 (98%)     | 54 (100%)   | 0        | 100         | 100 |
| 46  | y     | 48/49 (98%)     | 48 (100%)   | 0        | 100         | 100 |
| 47  | z     | 47/48 (98%)     | 47 (100%)   | 0        | 100         | 100 |
| 48  | 0     | 46/49 (94%)     | 46 (100%)   | 0        | 100         | 100 |
| 49  | 1     | 38/38 (100%)    | 38 (100%)   | 0        | 100         | 100 |
| 50  | 2     | 51/52 (98%)     | 51 (100%)   | 0        | 100         | 100 |
| 51  | 3     | 34/34 (100%)    | 34 (100%)   | 0        | 100         | 100 |
| 52  | 4     | 55/62 (89%)     | 55 (100%)   | 0        | 100         | 100 |
| All | All   | 4573/4825 (95%) | 4572 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | i     | 128 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 69  | HIS  |
| 4   | D     | 36  | GLN  |
| 4   | D     | 136 | GLN  |
| 5   | E     | 97  | GLN  |
| 5   | E     | 121 | HIS  |
| 5   | E     | 122 | ASN  |
| 5   | E     | 132 | ASN  |
| 7   | G     | 68  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 130 | ASN  |
| 8   | H     | 18  | GLN  |
| 8   | H     | 38  | ASN  |
| 9   | I     | 4   | ASN  |
| 9   | I     | 37  | GLN  |
| 11  | K     | 109 | ASN  |
| 13  | M     | 8   | ASN  |
| 13  | M     | 12  | HIS  |
| 14  | N     | 4   | GLN  |
| 16  | P     | 79  | ASN  |
| 17  | Q     | 9   | GLN  |
| 20  | T     | 48  | GLN  |
| 24  | c     | 90  | ASN  |
| 24  | c     | 115 | GLN  |
| 24  | c     | 134 | ASN  |
| 25  | d     | 173 | GLN  |
| 26  | e     | 9   | GLN  |
| 26  | e     | 62  | GLN  |
| 26  | e     | 115 | GLN  |
| 28  | g     | 22  | GLN  |
| 28  | g     | 73  | ASN  |
| 28  | g     | 88  | GLN  |
| 29  | h     | 11  | ASN  |
| 31  | j     | 93  | GLN  |
| 33  | l     | 13  | HIS  |
| 33  | l     | 97  | GLN  |
| 35  | n     | 98  | GLN  |
| 36  | o     | 66  | ASN  |
| 40  | s     | 48  | GLN  |
| 40  | s     | 70  | HIS  |
| 40  | s     | 72  | GLN  |
| 41  | t     | 74  | ASN  |
| 43  | v     | 12  | ASN  |
| 44  | w     | 36  | HIS  |
| 45  | x     | 15  | ASN  |
| 45  | x     | 45  | GLN  |
| 49  | 1     | 26  | ASN  |
| 52  | 4     | 30  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1508/1542 (97%) | 201 (13%)         | 6 (0%)          |
| 22  | a     | 2757/2904 (94%) | 301 (10%)         | 0               |
| 23  | b     | 118/120 (98%)   | 13 (11%)          | 0               |
| 53  | X     | 5/66 (7%)       | 0                 | 0               |
| 54  | Z     | 76/77 (98%)     | 10 (13%)          | 0               |
| All | All   | 4464/4709 (94%) | 525 (11%)         | 6 (0%)          |

All (525) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | A    |
| 1   | A     | 3   | A    |
| 1   | A     | 4   | U    |
| 1   | A     | 7   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 22  | G    |
| 1   | A     | 39  | G    |
| 1   | A     | 44  | A    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 71  | A    |
| 1   | A     | 73  | C    |
| 1   | A     | 74  | A    |
| 1   | A     | 78  | A    |
| 1   | A     | 91  | U    |
| 1   | A     | 94  | G    |
| 1   | A     | 95  | C    |
| 1   | A     | 116 | A    |
| 1   | A     | 121 | U    |
| 1   | A     | 122 | G    |
| 1   | A     | 130 | A    |
| 1   | A     | 131 | A    |
| 1   | A     | 141 | G    |
| 1   | A     | 143 | A    |
| 1   | A     | 144 | G    |
| 1   | A     | 149 | A    |
| 1   | A     | 164 | G    |
| 1   | A     | 166 | U    |
| 1   | A     | 177 | G    |
| 1   | A     | 182 | A    |
| 1   | A     | 183 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 189 | A    |
| 1   | A     | 197 | A    |
| 1   | A     | 199 | A    |
| 1   | A     | 200 | G    |
| 1   | A     | 204 | G    |
| 1   | A     | 215 | C    |
| 1   | A     | 226 | G    |
| 1   | A     | 240 | G    |
| 1   | A     | 245 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 280 | C    |
| 1   | A     | 289 | G    |
| 1   | A     | 321 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 347 | G    |
| 1   | A     | 352 | C    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 372 | C    |
| 1   | A     | 392 | C    |
| 1   | A     | 397 | A    |
| 1   | A     | 406 | G    |
| 1   | A     | 411 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 415 | A    |
| 1   | A     | 416 | G    |
| 1   | A     | 423 | G    |
| 1   | A     | 424 | G    |
| 1   | A     | 428 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 453 | G    |
| 1   | A     | 457 | G    |
| 1   | A     | 458 | U    |
| 1   | A     | 467 | U    |
| 1   | A     | 468 | A    |
| 1   | A     | 474 | G    |
| 1   | A     | 478 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 479 | U    |
| 1   | A     | 481 | G    |
| 1   | A     | 482 | A    |
| 1   | A     | 484 | G    |
| 1   | A     | 486 | U    |
| 1   | A     | 495 | A    |
| 1   | A     | 496 | A    |
| 1   | A     | 497 | G    |
| 1   | A     | 499 | A    |
| 1   | A     | 505 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 513 | C    |
| 1   | A     | 517 | G    |
| 1   | A     | 518 | C    |
| 1   | A     | 521 | G    |
| 1   | A     | 527 | G7M  |
| 1   | A     | 530 | G    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 545 | C    |
| 1   | A     | 546 | A    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 564 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 576 | C    |
| 1   | A     | 577 | G    |
| 1   | A     | 596 | A    |
| 1   | A     | 619 | U    |
| 1   | A     | 620 | C    |
| 1   | A     | 633 | G    |
| 1   | A     | 637 | C    |
| 1   | A     | 639 | G    |
| 1   | A     | 650 | G    |
| 1   | A     | 653 | U    |
| 1   | A     | 665 | A    |
| 1   | A     | 687 | A    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 734  | G    |
| 1   | A     | 747  | A    |
| 1   | A     | 748  | G    |
| 1   | A     | 755  | G    |
| 1   | A     | 777  | A    |
| 1   | A     | 793  | U    |
| 1   | A     | 794  | A    |
| 1   | A     | 802  | A    |
| 1   | A     | 815  | A    |
| 1   | A     | 817  | C    |
| 1   | A     | 819  | A    |
| 1   | A     | 832  | G    |
| 1   | A     | 890  | G    |
| 1   | A     | 914  | A    |
| 1   | A     | 926  | G    |
| 1   | A     | 934  | C    |
| 1   | A     | 935  | A    |
| 1   | A     | 960  | U    |
| 1   | A     | 965  | U    |
| 1   | A     | 966  | 2MG  |
| 1   | A     | 969  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1009 | U    |
| 1   | A     | 1017 | U    |
| 1   | A     | 1024 | G    |
| 1   | A     | 1031 | C    |
| 1   | A     | 1032 | G    |
| 1   | A     | 1035 | A    |
| 1   | A     | 1036 | A    |
| 1   | A     | 1042 | A    |
| 1   | A     | 1044 | A    |
| 1   | A     | 1053 | G    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1137 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1139 | G    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1171 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1196 | A    |
| 1   | A     | 1197 | A    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1260 | G    |
| 1   | A     | 1275 | A    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1286 | U    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1302 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1368 | A    |
| 1   | A     | 1370 | G    |
| 1   | A     | 1378 | C    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1419 | G    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1451 | U    |
| 1   | A     | 1487 | G    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1493 | A    |
| 1   | A     | 1494 | G    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1519 | MA6  |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | a     | 10  | A    |
| 22  | a     | 15  | G    |
| 22  | a     | 34  | U    |
| 22  | a     | 35  | G    |
| 22  | a     | 42  | A    |
| 22  | a     | 51  | G    |
| 22  | a     | 71  | A    |
| 22  | a     | 74  | A    |
| 22  | a     | 75  | G    |
| 22  | a     | 80  | G    |
| 22  | a     | 101 | A    |
| 22  | a     | 102 | U    |
| 22  | a     | 118 | A    |
| 22  | a     | 119 | A    |
| 22  | a     | 120 | U    |
| 22  | a     | 139 | U    |
| 22  | a     | 142 | A    |
| 22  | a     | 163 | C    |
| 22  | a     | 181 | A    |
| 22  | a     | 196 | A    |
| 22  | a     | 199 | A    |
| 22  | a     | 215 | G    |
| 22  | a     | 216 | A    |
| 22  | a     | 222 | A    |
| 22  | a     | 223 | A    |
| 22  | a     | 233 | A    |
| 22  | a     | 248 | G    |
| 22  | a     | 272 | A    |
| 22  | a     | 275 | C    |
| 22  | a     | 278 | A    |
| 22  | a     | 281 | C    |
| 22  | a     | 282 | A    |
| 22  | a     | 283 | G    |
| 22  | a     | 285 | G    |
| 22  | a     | 288 | U    |
| 22  | a     | 311 | A    |
| 22  | a     | 329 | G    |
| 22  | a     | 330 | A    |
| 22  | a     | 345 | A    |
| 22  | a     | 356 | G    |
| 22  | a     | 362 | A    |
| 22  | a     | 383 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | a     | 386 | G    |
| 22  | a     | 396 | G    |
| 22  | a     | 404 | A    |
| 22  | a     | 405 | U    |
| 22  | a     | 411 | G    |
| 22  | a     | 412 | A    |
| 22  | a     | 435 | C    |
| 22  | a     | 481 | G    |
| 22  | a     | 491 | G    |
| 22  | a     | 505 | A    |
| 22  | a     | 509 | C    |
| 22  | a     | 529 | A    |
| 22  | a     | 530 | G    |
| 22  | a     | 531 | C    |
| 22  | a     | 532 | A    |
| 22  | a     | 547 | A    |
| 22  | a     | 548 | G    |
| 22  | a     | 549 | G    |
| 22  | a     | 563 | A    |
| 22  | a     | 573 | U    |
| 22  | a     | 575 | A    |
| 22  | a     | 592 | A    |
| 22  | a     | 603 | A    |
| 22  | a     | 615 | U    |
| 22  | a     | 627 | A    |
| 22  | a     | 637 | A    |
| 22  | a     | 645 | C    |
| 22  | a     | 647 | G    |
| 22  | a     | 654 | A    |
| 22  | a     | 686 | U    |
| 22  | a     | 717 | C    |
| 22  | a     | 730 | A    |
| 22  | a     | 738 | G    |
| 22  | a     | 747 | 5MU  |
| 22  | a     | 764 | A    |
| 22  | a     | 775 | G    |
| 22  | a     | 776 | G    |
| 22  | a     | 782 | A    |
| 22  | a     | 784 | G    |
| 22  | a     | 785 | G    |
| 22  | a     | 789 | A    |
| 22  | a     | 792 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 805  | G    |
| 22  | a     | 811  | U    |
| 22  | a     | 812  | C    |
| 22  | a     | 827  | U    |
| 22  | a     | 828  | U    |
| 22  | a     | 845  | A    |
| 22  | a     | 846  | U    |
| 22  | a     | 847  | U    |
| 22  | a     | 859  | G    |
| 22  | a     | 883  | G    |
| 22  | a     | 884  | U    |
| 22  | a     | 888  | C    |
| 22  | a     | 890  | C    |
| 22  | a     | 891  | G    |
| 22  | a     | 893  | C    |
| 22  | a     | 895  | U    |
| 22  | a     | 896  | A    |
| 22  | a     | 897  | C    |
| 22  | a     | 910  | A    |
| 22  | a     | 931  | U    |
| 22  | a     | 946  | C    |
| 22  | a     | 961  | C    |
| 22  | a     | 974  | G    |
| 22  | a     | 983  | A    |
| 22  | a     | 996  | A    |
| 22  | a     | 1005 | C    |
| 22  | a     | 1012 | U    |
| 22  | a     | 1013 | C    |
| 22  | a     | 1033 | U    |
| 22  | a     | 1041 | G    |
| 22  | a     | 1045 | C    |
| 22  | a     | 1046 | A    |
| 22  | a     | 1047 | G    |
| 22  | a     | 1111 | A    |
| 22  | a     | 1112 | G    |
| 22  | a     | 1122 | G    |
| 22  | a     | 1132 | U    |
| 22  | a     | 1133 | A    |
| 22  | a     | 1135 | C    |
| 22  | a     | 1142 | A    |
| 22  | a     | 1206 | G    |
| 22  | a     | 1212 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 1250 | G    |
| 22  | a     | 1253 | A    |
| 22  | a     | 1256 | G    |
| 22  | a     | 1271 | G    |
| 22  | a     | 1272 | A    |
| 22  | a     | 1293 | C    |
| 22  | a     | 1300 | G    |
| 22  | a     | 1301 | A    |
| 22  | a     | 1329 | U    |
| 22  | a     | 1352 | U    |
| 22  | a     | 1365 | A    |
| 22  | a     | 1379 | U    |
| 22  | a     | 1383 | A    |
| 22  | a     | 1411 | U    |
| 22  | a     | 1416 | G    |
| 22  | a     | 1427 | A    |
| 22  | a     | 1428 | C    |
| 22  | a     | 1452 | G    |
| 22  | a     | 1453 | A    |
| 22  | a     | 1475 | G    |
| 22  | a     | 1482 | G    |
| 22  | a     | 1493 | C    |
| 22  | a     | 1508 | A    |
| 22  | a     | 1509 | A    |
| 22  | a     | 1510 | G    |
| 22  | a     | 1515 | A    |
| 22  | a     | 1524 | G    |
| 22  | a     | 1529 | G    |
| 22  | a     | 1535 | A    |
| 22  | a     | 1537 | G    |
| 22  | a     | 1539 | U    |
| 22  | a     | 1554 | U    |
| 22  | a     | 1566 | A    |
| 22  | a     | 1569 | A    |
| 22  | a     | 1578 | U    |
| 22  | a     | 1583 | A    |
| 22  | a     | 1584 | U    |
| 22  | a     | 1585 | C    |
| 22  | a     | 1608 | A    |
| 22  | a     | 1626 | A    |
| 22  | a     | 1646 | C    |
| 22  | a     | 1647 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 1648 | U    |
| 22  | a     | 1649 | G    |
| 22  | a     | 1674 | G    |
| 22  | a     | 1715 | G    |
| 22  | a     | 1729 | U    |
| 22  | a     | 1730 | C    |
| 22  | a     | 1731 | G    |
| 22  | a     | 1738 | G    |
| 22  | a     | 1764 | C    |
| 22  | a     | 1773 | A    |
| 22  | a     | 1786 | A    |
| 22  | a     | 1800 | C    |
| 22  | a     | 1801 | A    |
| 22  | a     | 1807 | G    |
| 22  | a     | 1808 | A    |
| 22  | a     | 1816 | C    |
| 22  | a     | 1829 | A    |
| 22  | a     | 1847 | A    |
| 22  | a     | 1848 | A    |
| 22  | a     | 1858 | A    |
| 22  | a     | 1862 | G    |
| 22  | a     | 1870 | C    |
| 22  | a     | 1871 | A    |
| 22  | a     | 1872 | A    |
| 22  | a     | 1905 | C    |
| 22  | a     | 1906 | G    |
| 22  | a     | 1913 | A    |
| 22  | a     | 1914 | C    |
| 22  | a     | 1915 | 3TD  |
| 22  | a     | 1929 | G    |
| 22  | a     | 1930 | G    |
| 22  | a     | 1937 | A    |
| 22  | a     | 1955 | U    |
| 22  | a     | 1967 | C    |
| 22  | a     | 1970 | A    |
| 22  | a     | 1971 | U    |
| 22  | a     | 1972 | G    |
| 22  | a     | 1991 | U    |
| 22  | a     | 1993 | U    |
| 22  | a     | 2020 | A    |
| 22  | a     | 2023 | C    |
| 22  | a     | 2027 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 2031 | A    |
| 22  | a     | 2033 | A    |
| 22  | a     | 2043 | C    |
| 22  | a     | 2055 | C    |
| 22  | a     | 2056 | G    |
| 22  | a     | 2060 | A    |
| 22  | a     | 2061 | G    |
| 22  | a     | 2062 | A    |
| 22  | a     | 2069 | G7M  |
| 22  | a     | 2093 | G    |
| 22  | a     | 2189 | U    |
| 22  | a     | 2190 | G    |
| 22  | a     | 2198 | A    |
| 22  | a     | 2204 | G    |
| 22  | a     | 2211 | A    |
| 22  | a     | 2225 | A    |
| 22  | a     | 2238 | G    |
| 22  | a     | 2239 | G    |
| 22  | a     | 2279 | G    |
| 22  | a     | 2283 | C    |
| 22  | a     | 2287 | A    |
| 22  | a     | 2288 | A    |
| 22  | a     | 2305 | U    |
| 22  | a     | 2308 | G    |
| 22  | a     | 2322 | A    |
| 22  | a     | 2325 | G    |
| 22  | a     | 2333 | A    |
| 22  | a     | 2336 | A    |
| 22  | a     | 2345 | G    |
| 22  | a     | 2347 | C    |
| 22  | a     | 2350 | C    |
| 22  | a     | 2361 | G    |
| 22  | a     | 2377 | A    |
| 22  | a     | 2383 | G    |
| 22  | a     | 2385 | C    |
| 22  | a     | 2396 | G    |
| 22  | a     | 2402 | U    |
| 22  | a     | 2403 | C    |
| 22  | a     | 2406 | A    |
| 22  | a     | 2425 | A    |
| 22  | a     | 2429 | G    |
| 22  | a     | 2430 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 2435 | A    |
| 22  | a     | 2441 | U    |
| 22  | a     | 2445 | 2MG  |
| 22  | a     | 2448 | A    |
| 22  | a     | 2469 | A    |
| 22  | a     | 2475 | C    |
| 22  | a     | 2476 | A    |
| 22  | a     | 2478 | A    |
| 22  | a     | 2491 | U    |
| 22  | a     | 2498 | OMC  |
| 22  | a     | 2502 | G    |
| 22  | a     | 2503 | 2MA  |
| 22  | a     | 2505 | G    |
| 22  | a     | 2518 | A    |
| 22  | a     | 2529 | G    |
| 22  | a     | 2535 | G    |
| 22  | a     | 2547 | A    |
| 22  | a     | 2566 | A    |
| 22  | a     | 2567 | G    |
| 22  | a     | 2573 | C    |
| 22  | a     | 2602 | A    |
| 22  | a     | 2609 | U    |
| 22  | a     | 2613 | U    |
| 22  | a     | 2615 | U    |
| 22  | a     | 2629 | U    |
| 22  | a     | 2630 | G    |
| 22  | a     | 2661 | G    |
| 22  | a     | 2689 | U    |
| 22  | a     | 2690 | U    |
| 22  | a     | 2714 | G    |
| 22  | a     | 2716 | C    |
| 22  | a     | 2726 | A    |
| 22  | a     | 2733 | A    |
| 22  | a     | 2744 | G    |
| 22  | a     | 2748 | A    |
| 22  | a     | 2757 | A    |
| 22  | a     | 2765 | A    |
| 22  | a     | 2778 | A    |
| 22  | a     | 2798 | U    |
| 22  | a     | 2799 | A    |
| 22  | a     | 2820 | A    |
| 22  | a     | 2821 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | a     | 2835 | A    |
| 22  | a     | 2849 | U    |
| 22  | a     | 2861 | U    |
| 22  | a     | 2873 | A    |
| 22  | a     | 2880 | C    |
| 22  | a     | 2884 | U    |
| 22  | a     | 2901 | C    |
| 23  | b     | 9    | G    |
| 23  | b     | 13   | G    |
| 23  | b     | 24   | G    |
| 23  | b     | 35   | C    |
| 23  | b     | 36   | C    |
| 23  | b     | 42   | C    |
| 23  | b     | 44   | G    |
| 23  | b     | 56   | G    |
| 23  | b     | 67   | G    |
| 23  | b     | 89   | U    |
| 23  | b     | 90   | C    |
| 23  | b     | 99   | A    |
| 23  | b     | 109  | A    |
| 54  | Z     | 8    | 4SU  |
| 54  | Z     | 9    | G    |
| 54  | Z     | 18   | U    |
| 54  | Z     | 19   | G    |
| 54  | Z     | 20   | G    |
| 54  | Z     | 21   | H2U  |
| 54  | Z     | 22   | A    |
| 54  | Z     | 23   | G    |
| 54  | Z     | 48   | U    |
| 54  | Z     | 77   | A    |

All (6) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 429  | U    |
| 1   | A     | 517  | G    |
| 1   | A     | 532  | A    |
| 1   | A     | 636  | U    |
| 1   | A     | 1030 | U    |
| 1   | A     | 1035 | A    |

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

45 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     | 1516 | 1     | 18,26,27     | 2.07 | 6 (33%)  | 16,38,41    | 1.49 | 4 (25%)  |
| 22  | PSU  | a     | 1917 | 22    | 18,21,22     | 1.01 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 54  | PSU  | Z     | 56   | 54    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 22  | 3TD  | a     | 1915 | 22    | 18,22,23     | 4.06 | 6 (33%)  | 22,32,35    | 1.74 | 3 (13%)  |
| 22  | 5MC  | a     | 1962 | 22    | 18,22,23     | 3.54 | 7 (38%)  | 26,32,35    | 1.09 | 2 (7%)   |
| 22  | G7M  | a     | 2069 | 22,55 | 20,26,27     | 2.57 | 7 (35%)  | 17,39,42    | 1.13 | 1 (5%)   |
| 22  | OMU  | a     | 2552 | 22    | 19,22,23     | 2.69 | 6 (31%)  | 26,31,34    | 1.82 | 5 (19%)  |
| 22  | PSU  | a     | 746  | 22,55 | 18,21,22     | 1.07 | 2 (11%)  | 22,30,33    | 1.71 | 3 (13%)  |
| 1   | 2MG  | A     | 1207 | 1     | 18,26,27     | 2.13 | 6 (33%)  | 16,38,41    | 1.46 | 4 (25%)  |
| 22  | 2MA  | a     | 2503 | 22,55 | 19,25,26     | 3.24 | 8 (42%)  | 21,37,40    | 2.74 | 3 (14%)  |
| 22  | OMG  | a     | 2251 | 22,54 | 18,26,27     | 2.66 | 8 (44%)  | 19,38,41    | 1.49 | 4 (21%)  |
| 22  | 6MZ  | a     | 1618 | 22    | 18,25,26     | 1.94 | 3 (16%)  | 16,36,39    | 2.10 | 3 (18%)  |
| 33  | MS6  | l     | 82   | 33    | 7,7,8        | 4.42 | 2 (28%)  | 6,7,9       | 2.29 | 2 (33%)  |
| 1   | G7M  | A     | 527  | 1     | 20,26,27     | 2.64 | 7 (35%)  | 17,39,42    | 1.07 | 1 (5%)   |
| 54  | H2U  | Z     | 21   | 54    | 18,21,22     | 1.05 | 2 (11%)  | 21,30,33    | 0.74 | 0        |
| 11  | IAS  | K     | 119  | 11    | 6,7,8        | 1.02 | 0        | 6,8,10      | 1.26 | 1 (16%)  |
| 33  | 4D4  | l     | 81   | 33    | 9,11,12      | 1.51 | 2 (22%)  | 8,13,15     | 2.04 | 3 (37%)  |
| 22  | H2U  | a     | 2449 | 22    | 18,21,22     | 1.29 | 3 (16%)  | 21,30,33    | 1.03 | 1 (4%)   |
| 22  | PSU  | a     | 2580 | 22    | 18,21,22     | 1.11 | 3 (16%)  | 22,30,33    | 2.09 | 6 (27%)  |
| 12  | D2T  | L     | 89   | 12    | 7,9,10       | 1.40 | 0        | 6,11,13     | 2.06 | 3 (50%)  |
| 22  | PSU  | a     | 2604 | 22    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.86 | 4 (18%)  |
| 22  | PSU  | a     | 2504 | 22    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 1   | 2MG  | A     | 966  | 1     | 18,26,27     | 2.11 | 6 (33%)  | 16,38,41    | 1.49 | 3 (18%)  |
| 1   | PSU  | A     | 516  | 1,55  | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.68 | 5 (22%)  |
| 1   | 4OC  | A     | 1402 | 1,55  | 20,23,24     | 2.93 | 8 (40%)  | 26,32,35    | 1.01 | 2 (7%)   |
| 54  | 5MU  | Z     | 55   | 54    | 19,22,23     | 4.64 | 6 (31%)  | 28,32,35    | 3.67 | 9 (32%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5MC  | A     | 967  | 1     | 18,22,23     | 3.68 | 8 (44%)  | 26,32,35    | 1.02 | 1 (3%)   |
| 54  | 4SU  | Z     | 8    | 54    | 18,21,22     | 4.10 | 8 (44%)  | 26,30,33    | 2.27 | 4 (15%)  |
| 22  | 5MU  | a     | 1939 | 22    | 19,22,23     | 4.51 | 7 (36%)  | 28,32,35    | 3.82 | 10 (35%) |
| 22  | 5MU  | a     | 747  | 22    | 19,22,23     | 4.54 | 7 (36%)  | 28,32,35    | 3.79 | 10 (35%) |
| 1   | 5MC  | A     | 1407 | 1     | 18,22,23     | 3.54 | 8 (44%)  | 26,32,35    | 1.02 | 2 (7%)   |
| 1   | UR3  | A     | 1498 | 1     | 19,22,23     | 2.60 | 7 (36%)  | 26,32,35    | 1.33 | 1 (3%)   |
| 22  | OMC  | a     | 2498 | 22,55 | 19,22,23     | 2.75 | 8 (42%)  | 26,31,34    | 0.86 | 0        |
| 22  | 1MG  | a     | 745  | 22    | 18,26,27     | 2.51 | 5 (27%)  | 19,39,42    | 1.43 | 3 (15%)  |
| 22  | 2MG  | a     | 2445 | 22    | 18,26,27     | 2.06 | 6 (33%)  | 16,38,41    | 1.52 | 4 (25%)  |
| 22  | PSU  | a     | 2457 | 22    | 18,21,22     | 1.08 | 2 (11%)  | 22,30,33    | 2.02 | 6 (27%)  |
| 54  | OMC  | Z     | 33   | 54    | 19,22,23     | 2.84 | 8 (42%)  | 26,31,34    | 0.75 | 0        |
| 25  | MEQ  | d     | 150  | 25    | 8,9,10       | 1.10 | 0        | 5,10,12     | 1.50 | 2 (40%)  |
| 1   | MA6  | A     | 1518 | 1     | 18,26,27     | 1.09 | 1 (5%)   | 19,38,41    | 1.63 | 3 (15%)  |
| 22  | PSU  | a     | 955  | 22    | 18,21,22     | 1.08 | 2 (11%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 22  | PSU  | a     | 2605 | 22    | 18,21,22     | 1.02 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 22  | 6MZ  | a     | 2030 | 22    | 18,25,26     | 1.91 | 2 (11%)  | 16,36,39    | 2.40 | 3 (18%)  |
| 1   | MA6  | A     | 1519 | 1     | 18,26,27     | 1.06 | 1 (5%)   | 19,38,41    | 1.69 | 3 (15%)  |
| 22  | 2MG  | a     | 1835 | 22    | 18,26,27     | 2.04 | 6 (33%)  | 16,38,41    | 1.49 | 4 (25%)  |
| 22  | PSU  | a     | 1911 | 22    | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.84 | 3 (13%)  |

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     | 1516 | 1     | -       | 0/5/27/28 | 0/3/3/3 |
| 22  | PSU  | a     | 1917 | 22    | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | PSU  | Z     | 56   | 54    | -       | 0/7/25/26 | 0/2/2/2 |
| 22  | 3TD  | a     | 1915 | 22    | -       | 2/7/25/26 | 0/2/2/2 |
| 22  | 5MC  | a     | 1962 | 22    | -       | 0/7/25/26 | 0/2/2/2 |
| 22  | G7M  | a     | 2069 | 22,55 | -       | 1/3/25/26 | 0/3/3/3 |
| 22  | OMU  | a     | 2552 | 22    | -       | 1/9/27/28 | 0/2/2/2 |
| 22  | PSU  | a     | 746  | 22,55 | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | 2MG  | A     | 1207 | 1     | -       | 0/5/27/28 | 0/3/3/3 |
| 22  | 2MA  | a     | 2503 | 22,55 | -       | 1/3/25/26 | 0/3/3/3 |
| 22  | OMG  | a     | 2251 | 22,54 | -       | 1/5/27/28 | 0/3/3/3 |
| 22  | 6MZ  | a     | 1618 | 22    | -       | 0/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 33  | MS6  | l     | 82   | 33    | 1/1/1/2 | 1/4/6/8    | -       |
| 1   | G7M  | A     | 527  | 1     | -       | 3/3/25/26  | 0/3/3/3 |
| 54  | H2U  | Z     | 21   | 54    | -       | 7/7/38/39  | 0/2/2/2 |
| 11  | IAS  | K     | 119  | 11    | -       | 0/7/7/8    | -       |
| 33  | 4D4  | l     | 81   | 33    | -       | 3/11/12/14 | -       |
| 22  | H2U  | a     | 2449 | 22    | -       | 0/7/38/39  | 0/2/2/2 |
| 22  | PSU  | a     | 2580 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 12  | D2T  | L     | 89   | 12    | -       | 3/7/12/14  | -       |
| 22  | PSU  | a     | 2604 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | PSU  | a     | 2504 | 22    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | A     | 966  | 1     | -       | 2/5/27/28  | 0/3/3/3 |
| 1   | PSU  | A     | 516  | 1,55  | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | A     | 1402 | 1,55  | -       | 1/9/29/30  | 0/2/2/2 |
| 54  | 5MU  | Z     | 55   | 54    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 967  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 4SU  | Z     | 8    | 54    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | a     | 1939 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | a     | 747  | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | A     | 1407 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | UR3  | A     | 1498 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | OMC  | a     | 2498 | 22,55 | -       | 0/9/27/28  | 0/2/2/2 |
| 22  | 1MG  | a     | 745  | 22    | -       | 0/3/25/26  | 0/3/3/3 |
| 22  | 2MG  | a     | 2445 | 22    | -       | 2/5/27/28  | 0/3/3/3 |
| 22  | PSU  | a     | 2457 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | OMC  | Z     | 33   | 54    | -       | 0/9/27/28  | 0/2/2/2 |
| 25  | MEQ  | d     | 150  | 25    | -       | 2/8/9/11   | -       |
| 1   | MA6  | A     | 1518 | 1     | -       | 0/7/29/30  | 0/3/3/3 |
| 22  | PSU  | a     | 955  | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | PSU  | a     | 2605 | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 6MZ  | a     | 2030 | 22    | -       | 2/5/27/28  | 0/3/3/3 |
| 1   | MA6  | A     | 1519 | 1     | -       | 2/7/29/30  | 0/3/3/3 |
| 22  | 2MG  | a     | 1835 | 22    | -       | 0/5/27/28  | 0/3/3/3 |
| 22  | PSU  | a     | 1911 | 22    | -       | 0/7/25/26  | 0/2/2/2 |

All (192) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 22  | a     | 1915 | 3TD  | C6-C5 | 12.17  | 1.49        | 1.35     |
| 33  | l     | 82   | MS6  | C-S   | -11.34 | 1.57        | 1.81     |
| 54  | Z     | 55   | 5MU  | C6-N1 | 10.58  | 1.56        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | Z     | 55   | 5MU  | C2-N1 | 10.35 | 1.55        | 1.38     |
| 22  | a     | 747  | 5MU  | C6-N1 | 10.25 | 1.55        | 1.38     |
| 22  | a     | 1939 | 5MU  | C6-N1 | 10.04 | 1.55        | 1.38     |
| 22  | a     | 747  | 5MU  | C2-N1 | 10.02 | 1.54        | 1.38     |
| 22  | a     | 1939 | 5MU  | C2-N1 | 9.79  | 1.54        | 1.38     |
| 54  | Z     | 8    | 4SU  | C4-N3 | 9.33  | 1.47        | 1.37     |
| 1   | A     | 967  | 5MC  | C6-C5 | 9.27  | 1.49        | 1.34     |
| 54  | Z     | 55   | 5MU  | C4-C5 | 9.15  | 1.60        | 1.44     |
| 1   | A     | 1407 | 5MC  | C6-C5 | 9.06  | 1.49        | 1.34     |
| 22  | a     | 1962 | 5MC  | C6-C5 | 8.83  | 1.49        | 1.34     |
| 22  | a     | 747  | 5MU  | C4-C5 | 8.73  | 1.59        | 1.44     |
| 22  | a     | 1939 | 5MU  | C4-C5 | 8.71  | 1.59        | 1.44     |
| 22  | a     | 1915 | 3TD  | C2-N1 | 8.57  | 1.48        | 1.37     |
| 22  | a     | 2503 | 2MA  | C4-N3 | 8.26  | 1.48        | 1.35     |
| 22  | a     | 1939 | 5MU  | C4-N3 | -7.85 | 1.24        | 1.38     |
| 22  | a     | 747  | 5MU  | C4-N3 | -7.67 | 1.24        | 1.38     |
| 54  | Z     | 8    | 4SU  | C2-N1 | 7.62  | 1.50        | 1.38     |
| 54  | Z     | 55   | 5MU  | C4-N3 | -7.40 | 1.25        | 1.38     |
| 1   | A     | 967  | 5MC  | C4-N3 | 7.08  | 1.46        | 1.34     |
| 22  | a     | 2503 | 2MA  | C2-N3 | 6.97  | 1.46        | 1.34     |
| 22  | a     | 1962 | 5MC  | C4-N3 | 6.91  | 1.45        | 1.34     |
| 22  | a     | 1618 | 6MZ  | C6-N6 | 6.88  | 1.46        | 1.35     |
| 22  | a     | 2030 | 6MZ  | C6-N6 | 6.74  | 1.46        | 1.35     |
| 1   | A     | 1407 | 5MC  | C4-N3 | 6.61  | 1.45        | 1.34     |
| 54  | Z     | 8    | 4SU  | C2-N3 | 6.47  | 1.49        | 1.38     |
| 1   | A     | 1498 | UR3  | C2-N1 | 6.46  | 1.47        | 1.38     |
| 54  | Z     | 55   | 5MU  | C6-C5 | 6.42  | 1.45        | 1.34     |
| 1   | A     | 1402 | 4OC  | C4-N3 | 6.36  | 1.43        | 1.32     |
| 1   | A     | 527  | G7M  | C2-N2 | 6.35  | 1.49        | 1.34     |
| 1   | A     | 967  | 5MC  | C2-N3 | 6.33  | 1.49        | 1.36     |
| 22  | a     | 2069 | G7M  | C2-N2 | 6.21  | 1.48        | 1.34     |
| 22  | a     | 747  | 5MU  | C6-C5 | 6.17  | 1.44        | 1.34     |
| 22  | a     | 1962 | 5MC  | C2-N3 | 6.13  | 1.48        | 1.36     |
| 22  | a     | 1939 | 5MU  | C6-C5 | 6.10  | 1.44        | 1.34     |
| 54  | Z     | 33   | OMC  | C2-N3 | 6.00  | 1.48        | 1.36     |
| 22  | a     | 2552 | OMU  | C2-N1 | 6.00  | 1.48        | 1.38     |
| 1   | A     | 1402 | 4OC  | C6-C5 | 6.00  | 1.49        | 1.35     |
| 22  | a     | 2552 | OMU  | C2-N3 | 5.97  | 1.48        | 1.38     |
| 1   | A     | 1407 | 5MC  | C2-N3 | 5.95  | 1.48        | 1.36     |
| 22  | a     | 745  | 1MG  | C2-N3 | 5.94  | 1.45        | 1.34     |
| 22  | a     | 2503 | 2MA  | C2-N1 | 5.93  | 1.44        | 1.34     |
| 54  | Z     | 8    | 4SU  | C6-C5 | 5.91  | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1498 | UR3  | C6-C5 | 5.87  | 1.48        | 1.35     |
| 22  | a     | 745  | 1MG  | C2-N2 | 5.78  | 1.44        | 1.34     |
| 22  | a     | 1915 | 3TD  | C6-N1 | 5.76  | 1.45        | 1.36     |
| 22  | a     | 2498 | OMC  | C2-N3 | 5.74  | 1.48        | 1.36     |
| 54  | Z     | 33   | OMC  | C6-C5 | 5.72  | 1.48        | 1.35     |
| 22  | a     | 2498 | OMC  | C6-C5 | 5.57  | 1.48        | 1.35     |
| 22  | a     | 2552 | OMU  | C6-C5 | 5.56  | 1.48        | 1.35     |
| 22  | a     | 2251 | OMG  | C4-N3 | 5.52  | 1.50        | 1.37     |
| 54  | Z     | 8    | 4SU  | C4-S4 | -5.47 | 1.58        | 1.68     |
| 1   | A     | 1402 | 4OC  | C2-N3 | 5.47  | 1.47        | 1.36     |
| 54  | Z     | 8    | 4SU  | C5-C4 | 5.38  | 1.49        | 1.42     |
| 1   | A     | 527  | G7M  | C2-N3 | 5.37  | 1.46        | 1.33     |
| 22  | a     | 2069 | G7M  | C2-N3 | 5.11  | 1.45        | 1.33     |
| 22  | a     | 2251 | OMG  | C2-N3 | 4.99  | 1.45        | 1.33     |
| 1   | A     | 966  | 2MG  | C4-N3 | 4.98  | 1.49        | 1.37     |
| 1   | A     | 967  | 5MC  | C6-N1 | 4.92  | 1.46        | 1.38     |
| 1   | A     | 1207 | 2MG  | C4-N3 | 4.90  | 1.49        | 1.37     |
| 22  | a     | 1835 | 2MG  | C4-N3 | 4.85  | 1.49        | 1.37     |
| 1   | A     | 966  | 2MG  | C2-N1 | 4.84  | 1.44        | 1.36     |
| 22  | a     | 2251 | OMG  | C2-N2 | 4.83  | 1.45        | 1.34     |
| 1   | A     | 1207 | 2MG  | C2-N1 | 4.80  | 1.44        | 1.36     |
| 1   | A     | 527  | G7M  | C4-N3 | 4.79  | 1.49        | 1.37     |
| 54  | Z     | 33   | OMC  | C4-N3 | 4.77  | 1.44        | 1.34     |
| 1   | A     | 1516 | 2MG  | C4-N3 | 4.75  | 1.48        | 1.37     |
| 54  | Z     | 33   | OMC  | C4-N4 | 4.72  | 1.45        | 1.33     |
| 1   | A     | 1407 | 5MC  | C6-N1 | 4.70  | 1.46        | 1.38     |
| 22  | a     | 2445 | 2MG  | C4-N3 | 4.70  | 1.48        | 1.37     |
| 1   | A     | 1498 | UR3  | C2-N3 | 4.68  | 1.48        | 1.39     |
| 22  | a     | 2069 | G7M  | C4-N3 | 4.64  | 1.48        | 1.37     |
| 22  | a     | 1962 | 5MC  | C6-N1 | 4.58  | 1.45        | 1.38     |
| 22  | a     | 2498 | OMC  | C4-N4 | 4.57  | 1.44        | 1.33     |
| 22  | a     | 745  | 1MG  | C4-N3 | 4.52  | 1.48        | 1.37     |
| 1   | A     | 1516 | 2MG  | C2-N1 | 4.46  | 1.43        | 1.36     |
| 22  | a     | 1835 | 2MG  | C2-N1 | 4.46  | 1.43        | 1.36     |
| 22  | a     | 2498 | OMC  | C4-N3 | 4.45  | 1.43        | 1.34     |
| 22  | a     | 1915 | 3TD  | C2-N3 | 4.35  | 1.48        | 1.38     |
| 22  | a     | 2445 | 2MG  | C2-N1 | 4.35  | 1.43        | 1.36     |
| 1   | A     | 1402 | 4OC  | C4-N4 | 4.20  | 1.44        | 1.35     |
| 54  | Z     | 33   | OMC  | C2-N1 | 4.06  | 1.48        | 1.40     |
| 1   | A     | 967  | 5MC  | C4-N4 | 4.01  | 1.44        | 1.34     |
| 22  | a     | 2498 | OMC  | C2-N1 | 3.94  | 1.48        | 1.40     |
| 1   | A     | 967  | 5MC  | C2-N1 | 3.92  | 1.48        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1407 | 5MC  | C4-N4 | 3.91  | 1.44        | 1.34     |
| 1   | A     | 527  | G7M  | C6-N1 | 3.91  | 1.43        | 1.37     |
| 22  | a     | 1962 | 5MC  | C4-N4 | 3.89  | 1.44        | 1.34     |
| 22  | a     | 2069 | G7M  | C6-N1 | 3.79  | 1.43        | 1.37     |
| 1   | A     | 1402 | 4OC  | C2-N1 | 3.73  | 1.48        | 1.40     |
| 22  | a     | 1962 | 5MC  | C2-N1 | 3.69  | 1.48        | 1.40     |
| 1   | A     | 1402 | 4OC  | C5-C4 | 3.61  | 1.48        | 1.40     |
| 1   | A     | 1407 | 5MC  | C2-N1 | 3.59  | 1.47        | 1.40     |
| 22  | a     | 2251 | OMG  | C5-C4 | -3.56 | 1.34        | 1.43     |
| 22  | a     | 2503 | 2MA  | C6-N6 | -3.41 | 1.21        | 1.34     |
| 1   | A     | 1207 | 2MG  | C6-N1 | 3.31  | 1.42        | 1.37     |
| 1   | A     | 966  | 2MG  | C6-N1 | 3.30  | 1.42        | 1.37     |
| 22  | a     | 2251 | OMG  | C6-N1 | 3.30  | 1.42        | 1.37     |
| 22  | a     | 2251 | OMG  | C5-C6 | 3.27  | 1.54        | 1.47     |
| 1   | A     | 1402 | 4OC  | O2-C2 | -3.25 | 1.17        | 1.23     |
| 22  | a     | 2552 | OMU  | O2-C2 | -3.21 | 1.17        | 1.23     |
| 54  | Z     | 56   | PSU  | C6-C5 | 3.20  | 1.39        | 1.35     |
| 22  | a     | 2449 | H2U  | C2-N3 | -3.20 | 1.32        | 1.38     |
| 54  | Z     | 8    | 4SU  | O2-C2 | -3.20 | 1.17        | 1.23     |
| 22  | a     | 2498 | OMC  | O2-C2 | -3.14 | 1.17        | 1.23     |
| 22  | a     | 2503 | 2MA  | C6-C5 | 3.14  | 1.54        | 1.43     |
| 22  | a     | 2449 | H2U  | C4-N3 | -3.13 | 1.32        | 1.37     |
| 22  | a     | 2503 | 2MA  | C6-N1 | 3.13  | 1.39        | 1.33     |
| 1   | A     | 1516 | 2MG  | C6-N1 | 3.12  | 1.42        | 1.37     |
| 22  | a     | 745  | 1MG  | C5-C4 | -3.08 | 1.35        | 1.43     |
| 54  | Z     | 8    | 4SU  | C6-N1 | 3.08  | 1.45        | 1.38     |
| 1   | A     | 1519 | MA6  | C5-C4 | -3.05 | 1.32        | 1.40     |
| 22  | a     | 2552 | OMU  | O4-C4 | -3.04 | 1.18        | 1.24     |
| 1   | A     | 527  | G7M  | C5-C6 | 3.02  | 1.53        | 1.45     |
| 22  | a     | 2445 | 2MG  | C5-C4 | -3.02 | 1.35        | 1.43     |
| 1   | A     | 1518 | MA6  | C5-C4 | -3.02 | 1.32        | 1.40     |
| 1   | A     | 1207 | 2MG  | C5-C6 | 3.02  | 1.53        | 1.47     |
| 22  | a     | 2445 | 2MG  | C6-N1 | 3.01  | 1.42        | 1.37     |
| 22  | a     | 2030 | 6MZ  | C5-C4 | -3.01 | 1.33        | 1.40     |
| 22  | a     | 2069 | G7M  | C5-C6 | 2.98  | 1.53        | 1.45     |
| 1   | A     | 1516 | 2MG  | C5-C4 | -2.93 | 1.35        | 1.43     |
| 54  | Z     | 33   | OMC  | O2-C2 | -2.93 | 1.18        | 1.23     |
| 1   | A     | 1516 | 2MG  | C5-C6 | 2.92  | 1.53        | 1.47     |
| 22  | a     | 1835 | 2MG  | C6-N1 | 2.92  | 1.42        | 1.37     |
| 1   | A     | 966  | 2MG  | C5-C6 | 2.88  | 1.53        | 1.47     |
| 22  | a     | 2445 | 2MG  | C5-C6 | 2.87  | 1.53        | 1.47     |
| 22  | a     | 1618 | 6MZ  | C5-C4 | -2.87 | 1.33        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | a     | 1835 | 2MG  | C5-C4   | -2.87 | 1.35        | 1.43     |
| 1   | A     | 516  | PSU  | C6-C5   | 2.83  | 1.38        | 1.35     |
| 33  | l     | 81   | 4D4  | OB-CB   | -2.83 | 1.37        | 1.43     |
| 54  | Z     | 33   | OMC  | C6-N1   | 2.81  | 1.44        | 1.38     |
| 1   | A     | 1402 | 4OC  | C6-N1   | 2.80  | 1.44        | 1.38     |
| 22  | a     | 2552 | OMU  | C4-N3   | 2.77  | 1.43        | 1.38     |
| 1   | A     | 1207 | 2MG  | C5-C4   | -2.76 | 1.36        | 1.43     |
| 22  | a     | 2251 | OMG  | O6-C6   | -2.76 | 1.17        | 1.23     |
| 1   | A     | 527  | G7M  | C2-N1   | 2.75  | 1.44        | 1.37     |
| 1   | A     | 1498 | UR3  | C6-N1   | 2.75  | 1.44        | 1.38     |
| 1   | A     | 1407 | 5MC  | O2-C2   | -2.74 | 1.18        | 1.23     |
| 54  | Z     | 21   | H2U  | C2-N3   | -2.73 | 1.33        | 1.38     |
| 22  | a     | 2504 | PSU  | C6-C5   | 2.71  | 1.38        | 1.35     |
| 22  | a     | 1911 | PSU  | C6-C5   | 2.71  | 1.38        | 1.35     |
| 22  | a     | 746  | PSU  | C6-C5   | 2.68  | 1.38        | 1.35     |
| 22  | a     | 2457 | PSU  | C6-C5   | 2.67  | 1.38        | 1.35     |
| 22  | a     | 2604 | PSU  | C6-C5   | 2.67  | 1.38        | 1.35     |
| 22  | a     | 1917 | PSU  | C6-C5   | 2.66  | 1.38        | 1.35     |
| 22  | a     | 1835 | 2MG  | C5-C6   | 2.66  | 1.52        | 1.47     |
| 22  | a     | 2069 | G7M  | C2-N1   | 2.63  | 1.44        | 1.37     |
| 22  | a     | 2498 | OMC  | C6-N1   | 2.59  | 1.44        | 1.38     |
| 54  | Z     | 21   | H2U  | C4-N3   | -2.58 | 1.33        | 1.37     |
| 1   | A     | 966  | 2MG  | C5-C4   | -2.57 | 1.36        | 1.43     |
| 22  | a     | 2069 | G7M  | O6-C6   | -2.57 | 1.18        | 1.23     |
| 22  | a     | 955  | PSU  | C6-C5   | 2.57  | 1.38        | 1.35     |
| 22  | a     | 1962 | 5MC  | O2-C2   | -2.55 | 1.19        | 1.23     |
| 22  | a     | 1939 | 5MU  | O2-C2   | -2.54 | 1.18        | 1.23     |
| 33  | l     | 82   | MS6  | CB-CA   | 2.52  | 1.56        | 1.53     |
| 22  | a     | 1915 | 3TD  | C4-N3   | 2.50  | 1.45        | 1.40     |
| 22  | a     | 2605 | PSU  | C6-C5   | 2.49  | 1.38        | 1.35     |
| 33  | l     | 81   | 4D4  | CZ-NE   | 2.48  | 1.38        | 1.33     |
| 1   | A     | 967  | 5MC  | O2-C2   | -2.46 | 1.19        | 1.23     |
| 1   | A     | 1498 | UR3  | O2-C2   | -2.46 | 1.18        | 1.22     |
| 1   | A     | 1498 | UR3  | O4-C4   | -2.45 | 1.18        | 1.23     |
| 1   | A     | 527  | G7M  | O6-C6   | -2.44 | 1.18        | 1.23     |
| 22  | a     | 2580 | PSU  | C6-C5   | 2.44  | 1.38        | 1.35     |
| 22  | a     | 747  | 5MU  | O2-C2   | -2.42 | 1.18        | 1.23     |
| 22  | a     | 2445 | 2MG  | O6-C6   | -2.33 | 1.18        | 1.23     |
| 22  | a     | 2449 | H2U  | C2-N1   | -2.33 | 1.32        | 1.35     |
| 22  | a     | 1835 | 2MG  | O6-C6   | -2.32 | 1.18        | 1.23     |
| 22  | a     | 745  | 1MG  | O6-C6   | -2.31 | 1.18        | 1.22     |
| 22  | a     | 2580 | PSU  | O4'-C1' | -2.31 | 1.40        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 22  | a     | 1915 | 3TD  | O4-C4  | -2.31 | 1.18        | 1.23     |
| 1   | A     | 1516 | 2MG  | O6-C6  | -2.27 | 1.18        | 1.23     |
| 22  | a     | 1939 | 5MU  | O4-C4  | -2.19 | 1.19        | 1.23     |
| 22  | a     | 2580 | PSU  | C4-C5  | -2.18 | 1.37        | 1.44     |
| 22  | a     | 1618 | 6MZ  | C2-N3  | 2.17  | 1.35        | 1.32     |
| 1   | A     | 967  | 5MC  | CM5-C5 | 2.15  | 1.56        | 1.50     |
| 54  | Z     | 33   | OMC  | C5-C4  | 2.13  | 1.47        | 1.42     |
| 1   | A     | 1207 | 2MG  | O6-C6  | -2.13 | 1.19        | 1.23     |
| 22  | a     | 2503 | 2MA  | CM2-C2 | 2.13  | 1.55        | 1.49     |
| 22  | a     | 2503 | 2MA  | C5-C4  | -2.13 | 1.35        | 1.40     |
| 22  | a     | 746  | PSU  | C4-C5  | -2.12 | 1.38        | 1.44     |
| 22  | a     | 955  | PSU  | C4-C5  | -2.11 | 1.38        | 1.44     |
| 22  | a     | 2251 | OMG  | C2-N1  | 2.11  | 1.42        | 1.37     |
| 1   | A     | 966  | 2MG  | O6-C6  | -2.08 | 1.19        | 1.23     |
| 22  | a     | 2605 | PSU  | C4-C5  | -2.07 | 1.38        | 1.44     |
| 1   | A     | 1498 | UR3  | C5-C4  | 2.06  | 1.49        | 1.43     |
| 54  | Z     | 55   | 5MU  | O2-C2  | -2.06 | 1.19        | 1.23     |
| 22  | a     | 747  | 5MU  | O4-C4  | -2.04 | 1.19        | 1.23     |
| 22  | a     | 2457 | PSU  | C4-C5  | -2.03 | 1.38        | 1.44     |
| 1   | A     | 1407 | 5MC  | CM5-C5 | 2.02  | 1.55        | 1.50     |
| 22  | a     | 2498 | OMC  | C5-C4  | 2.01  | 1.47        | 1.42     |

All (153) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 22  | a     | 747  | 5MU  | C5-C4-N3  | 12.47  | 125.95      | 115.31   |
| 22  | a     | 1939 | 5MU  | C5-C4-N3  | 12.46  | 125.95      | 115.31   |
| 54  | Z     | 55   | 5MU  | C5-C4-N3  | 12.28  | 125.79      | 115.31   |
| 22  | a     | 1939 | 5MU  | C5-C6-N1  | -10.87 | 112.16      | 123.34   |
| 22  | a     | 747  | 5MU  | C5-C6-N1  | -10.71 | 112.33      | 123.34   |
| 54  | Z     | 55   | 5MU  | C5-C6-N1  | -10.21 | 112.83      | 123.34   |
| 22  | a     | 2503 | 2MA  | C1'-N9-C4 | -9.01  | 110.80      | 126.64   |
| 54  | Z     | 8    | 4SU  | C4-N3-C2  | -7.92  | 119.64      | 127.34   |
| 22  | a     | 2503 | 2MA  | C2-N3-C4  | 7.36   | 121.50      | 115.52   |
| 22  | a     | 2030 | 6MZ  | C9-N6-C6  | -5.95  | 117.75      | 122.87   |
| 1   | A     | 1518 | MA6  | N3-C2-N1  | -5.89  | 119.47      | 128.68   |
| 1   | A     | 1519 | MA6  | N3-C2-N1  | -5.83  | 119.56      | 128.68   |
| 22  | a     | 2552 | OMU  | C4-N3-C2  | -5.70  | 119.07      | 126.58   |
| 54  | Z     | 8    | 4SU  | C5-C4-N3  | 5.65   | 119.93      | 114.69   |
| 22  | a     | 1915 | 3TD  | N1-C2-N3  | 5.62   | 120.57      | 116.14   |
| 22  | a     | 2030 | 6MZ  | N3-C2-N1  | -5.59  | 119.93      | 128.68   |
| 22  | a     | 1618 | 6MZ  | N3-C2-N1  | -5.52  | 120.05      | 128.68   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22  | a     | 1939 | 5MU  | C4-N3-C2  | -5.33 | 120.45      | 127.35   |
| 22  | a     | 2457 | PSU  | N1-C2-N3  | 5.28  | 121.11      | 115.13   |
| 22  | a     | 2580 | PSU  | N1-C2-N3  | 5.25  | 121.07      | 115.13   |
| 22  | a     | 747  | 5MU  | C4-N3-C2  | -5.24 | 120.57      | 127.35   |
| 22  | a     | 747  | 5MU  | O4-C4-C5  | -5.15 | 118.93      | 124.90   |
| 1   | A     | 1498 | UR3  | C4-N3-C2  | -5.14 | 119.72      | 124.56   |
| 22  | a     | 2605 | PSU  | C4-N3-C2  | -5.02 | 119.10      | 126.34   |
| 22  | a     | 1939 | 5MU  | O4-C4-C5  | -5.00 | 119.11      | 124.90   |
| 22  | a     | 2457 | PSU  | C4-N3-C2  | -4.98 | 119.16      | 126.34   |
| 22  | a     | 955  | PSU  | N1-C2-N3  | 4.96  | 120.75      | 115.13   |
| 22  | a     | 955  | PSU  | C4-N3-C2  | -4.96 | 119.20      | 126.34   |
| 22  | a     | 2580 | PSU  | C4-N3-C2  | -4.94 | 119.22      | 126.34   |
| 22  | a     | 1911 | PSU  | C4-N3-C2  | -4.92 | 119.25      | 126.34   |
| 54  | Z     | 55   | 5MU  | O4-C4-C5  | -4.90 | 119.22      | 124.90   |
| 22  | a     | 2604 | PSU  | C4-N3-C2  | -4.88 | 119.30      | 126.34   |
| 54  | Z     | 55   | 5MU  | C4-N3-C2  | -4.88 | 121.03      | 127.35   |
| 22  | a     | 1917 | PSU  | C4-N3-C2  | -4.87 | 119.32      | 126.34   |
| 22  | a     | 746  | PSU  | C4-N3-C2  | -4.83 | 119.38      | 126.34   |
| 22  | a     | 2605 | PSU  | N1-C2-N3  | 4.80  | 120.57      | 115.13   |
| 22  | a     | 2504 | PSU  | N1-C2-N3  | 4.78  | 120.54      | 115.13   |
| 22  | a     | 1618 | 6MZ  | C9-N6-C6  | -4.77 | 118.76      | 122.87   |
| 22  | a     | 2504 | PSU  | C4-N3-C2  | -4.74 | 119.51      | 126.34   |
| 54  | Z     | 56   | PSU  | C4-N3-C2  | -4.70 | 119.56      | 126.34   |
| 22  | a     | 1939 | 5MU  | N3-C2-N1  | 4.67  | 121.09      | 114.89   |
| 22  | a     | 2604 | PSU  | N1-C2-N3  | 4.66  | 120.41      | 115.13   |
| 22  | a     | 1917 | PSU  | N1-C2-N3  | 4.66  | 120.41      | 115.13   |
| 54  | Z     | 56   | PSU  | N1-C2-N3  | 4.66  | 120.41      | 115.13   |
| 33  | l     | 82   | MS6  | CA-C-S    | 4.64  | 124.36      | 114.47   |
| 22  | a     | 747  | 5MU  | N3-C2-N1  | 4.57  | 120.95      | 114.89   |
| 22  | a     | 1911 | PSU  | N1-C2-N3  | 4.56  | 120.30      | 115.13   |
| 22  | a     | 2552 | OMU  | N3-C2-N1  | 4.41  | 120.75      | 114.89   |
| 1   | A     | 516  | PSU  | C4-N3-C2  | -4.37 | 120.04      | 126.34   |
| 54  | Z     | 55   | 5MU  | N3-C2-N1  | 4.35  | 120.67      | 114.89   |
| 22  | a     | 746  | PSU  | N1-C2-N3  | 4.32  | 120.02      | 115.13   |
| 22  | a     | 1939 | 5MU  | C5M-C5-C6 | -4.30 | 117.11      | 122.85   |
| 22  | a     | 745  | 1MG  | C5-C6-N1  | 4.24  | 120.28      | 113.90   |
| 22  | a     | 747  | 5MU  | C5M-C5-C6 | -4.22 | 117.21      | 122.85   |
| 1   | A     | 516  | PSU  | N1-C2-N3  | 4.12  | 119.79      | 115.13   |
| 22  | a     | 1915 | 3TD  | C4-N3-C2  | -4.11 | 120.14      | 124.61   |
| 54  | Z     | 55   | 5MU  | C5M-C5-C6 | -4.10 | 117.38      | 122.85   |
| 54  | Z     | 55   | 5MU  | C5M-C5-C4 | 4.07  | 123.24      | 118.77   |
| 22  | a     | 1939 | 5MU  | C5M-C5-C4 | 3.93  | 123.09      | 118.77   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22  | a     | 2030 | 6MZ  | C2-N1-C6  | 3.91  | 119.94      | 116.59   |
| 22  | a     | 747  | 5MU  | C5M-C5-C4 | 3.89  | 123.05      | 118.77   |
| 22  | a     | 2445 | 2MG  | C5-C6-N1  | 3.73  | 120.54      | 113.95   |
| 22  | a     | 1835 | 2MG  | C5-C6-N1  | 3.70  | 120.49      | 113.95   |
| 54  | Z     | 8    | 4SU  | N3-C2-N1  | 3.69  | 119.79      | 114.89   |
| 54  | Z     | 8    | 4SU  | C5-C4-S4  | -3.68 | 119.72      | 124.47   |
| 33  | l     | 81   | 4D4  | NE-CZ-NH2 | 3.64  | 127.09      | 120.70   |
| 1   | A     | 1516 | 2MG  | C5-C6-N1  | 3.60  | 120.31      | 113.95   |
| 1   | A     | 1207 | 2MG  | C5-C6-N1  | 3.60  | 120.30      | 113.95   |
| 1   | A     | 966  | 2MG  | C5-C6-N1  | 3.59  | 120.28      | 113.95   |
| 22  | a     | 2251 | OMG  | C5-C6-N1  | 3.54  | 120.21      | 113.95   |
| 22  | a     | 1962 | 5MC  | C5-C6-N1  | -3.54 | 119.70      | 123.34   |
| 22  | a     | 1618 | 6MZ  | C2-N1-C6  | 3.50  | 119.59      | 116.59   |
| 1   | A     | 1407 | 5MC  | C5-C6-N1  | -3.50 | 119.74      | 123.34   |
| 22  | a     | 2552 | OMU  | C5-C4-N3  | 3.41  | 119.94      | 114.84   |
| 22  | a     | 2580 | PSU  | O2-C2-N1  | -3.28 | 119.18      | 122.79   |
| 22  | a     | 2251 | OMG  | C2-N1-C6  | -3.26 | 119.09      | 125.10   |
| 12  | L     | 89   | D2T  | OD2-CG-CB | 3.21  | 120.09      | 113.15   |
| 22  | a     | 2503 | 2MA  | N3-C2-N1  | -3.06 | 120.14      | 125.73   |
| 1   | A     | 967  | 5MC  | C5-C6-N1  | -3.04 | 120.21      | 123.34   |
| 1   | A     | 527  | G7M  | C2-N1-C6  | -3.00 | 119.57      | 125.10   |
| 22  | a     | 2069 | G7M  | C2-N1-C6  | -3.00 | 119.57      | 125.10   |
| 12  | L     | 89   | D2T  | OD1-CG-CB | -2.93 | 116.31      | 122.44   |
| 54  | Z     | 56   | PSU  | O2-C2-N1  | -2.89 | 119.61      | 122.79   |
| 1   | A     | 1516 | 2MG  | C8-N7-C5  | 2.89  | 108.50      | 102.99   |
| 22  | a     | 2457 | PSU  | O2-C2-N1  | -2.87 | 119.64      | 122.79   |
| 33  | l     | 82   | MS6  | CE-SD-CG  | 2.86  | 110.23      | 100.40   |
| 22  | a     | 2449 | H2U  | C4-N3-C2  | -2.81 | 123.46      | 125.79   |
| 22  | a     | 2445 | 2MG  | C8-N7-C5  | 2.81  | 108.33      | 102.99   |
| 33  | l     | 81   | 4D4  | CB-CA-C   | -2.77 | 107.34      | 111.77   |
| 1   | A     | 1207 | 2MG  | C8-N7-C5  | 2.76  | 108.26      | 102.99   |
| 22  | a     | 2580 | PSU  | C6-N1-C2  | -2.75 | 119.88      | 122.68   |
| 22  | a     | 1939 | 5MU  | O2-C2-N1  | -2.72 | 119.17      | 122.79   |
| 22  | a     | 2251 | OMG  | C8-N7-C5  | 2.72  | 108.17      | 102.99   |
| 22  | a     | 1939 | 5MU  | O4-C4-N3  | -2.70 | 114.94      | 120.12   |
| 22  | a     | 2580 | PSU  | C6-C5-C4  | 2.70  | 120.08      | 118.20   |
| 22  | a     | 1835 | 2MG  | C8-N7-C5  | 2.68  | 108.10      | 102.99   |
| 22  | a     | 745  | 1MG  | C8-N7-C5  | 2.68  | 108.09      | 102.99   |
| 54  | Z     | 55   | 5MU  | O4-C4-N3  | -2.67 | 114.99      | 120.12   |
| 22  | a     | 2457 | PSU  | C6-C5-C4  | 2.66  | 120.06      | 118.20   |
| 1   | A     | 966  | 2MG  | C8-N7-C5  | 2.62  | 107.98      | 102.99   |
| 22  | a     | 747  | 5MU  | O4-C4-N3  | -2.61 | 115.12      | 120.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1519 | MA6  | N1-C6-N6    | -2.61 | 114.31      | 117.06   |
| 22  | a     | 1911 | PSU  | O2-C2-N1    | -2.60 | 119.93      | 122.79   |
| 22  | a     | 2552 | OMU  | O4-C4-C5    | -2.59 | 120.61      | 125.16   |
| 25  | d     | 150  | MEQ  | OE1-CD-CG   | 2.58  | 126.74      | 122.02   |
| 22  | a     | 2580 | PSU  | O4'-C1'-C2' | 2.58  | 108.78      | 105.14   |
| 22  | a     | 2457 | PSU  | C6-N1-C2    | -2.58 | 120.05      | 122.68   |
| 22  | a     | 2445 | 2MG  | CM2-N2-C2   | -2.58 | 118.17      | 123.86   |
| 1   | A     | 966  | 2MG  | O6-C6-C5    | -2.57 | 119.35      | 124.37   |
| 22  | a     | 1835 | 2MG  | O6-C6-C5    | -2.52 | 119.45      | 124.37   |
| 22  | a     | 955  | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 1   | A     | 516  | PSU  | O2-C2-N1    | -2.51 | 120.02      | 122.79   |
| 22  | a     | 2552 | OMU  | O2-C2-N1    | -2.51 | 119.45      | 122.79   |
| 1   | A     | 1518 | MA6  | N1-C6-N6    | -2.50 | 114.42      | 117.06   |
| 22  | a     | 2604 | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 22  | a     | 747  | 5MU  | O2-C2-N1    | -2.49 | 119.47      | 122.79   |
| 22  | a     | 2504 | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 22  | a     | 1917 | PSU  | O2-C2-N1    | -2.44 | 120.10      | 122.79   |
| 12  | L     | 89   | D2T  | O-C-CA      | -2.44 | 118.38      | 124.78   |
| 1   | A     | 1402 | 4OC  | C6-C5-C4    | 2.43  | 119.94      | 116.96   |
| 1   | A     | 1519 | MA6  | C4-C5-N7    | -2.42 | 106.88      | 109.40   |
| 33  | l     | 81   | 4D4  | O-C-CA      | -2.41 | 118.47      | 124.78   |
| 1   | A     | 1207 | 2MG  | O6-C6-C5    | -2.40 | 119.68      | 124.37   |
| 54  | Z     | 55   | 5MU  | O2-C2-N1    | -2.36 | 119.65      | 122.79   |
| 22  | a     | 1835 | 2MG  | CM2-N2-C2   | -2.32 | 118.74      | 123.86   |
| 22  | a     | 955  | PSU  | C6-N1-C2    | -2.32 | 120.31      | 122.68   |
| 22  | a     | 2504 | PSU  | C6-N1-C2    | -2.31 | 120.32      | 122.68   |
| 22  | a     | 2445 | 2MG  | O6-C6-C5    | -2.30 | 119.88      | 124.37   |
| 54  | Z     | 56   | PSU  | C6-N1-C2    | -2.26 | 120.37      | 122.68   |
| 22  | a     | 2605 | PSU  | O2-C2-N1    | -2.26 | 120.30      | 122.79   |
| 22  | a     | 1915 | 3TD  | C6-C5-C4    | 2.26  | 119.78      | 118.22   |
| 22  | a     | 2251 | OMG  | O6-C6-C5    | -2.24 | 119.99      | 124.37   |
| 54  | Z     | 56   | PSU  | C6-C5-C4    | 2.22  | 119.75      | 118.20   |
| 22  | a     | 1917 | PSU  | C6-C5-C4    | 2.20  | 119.74      | 118.20   |
| 1   | A     | 1407 | 5MC  | CM5-C5-C6   | -2.17 | 119.95      | 122.85   |
| 1   | A     | 1516 | 2MG  | O6-C6-C5    | -2.15 | 120.17      | 124.37   |
| 1   | A     | 1207 | 2MG  | CM2-N2-C2   | -2.15 | 119.12      | 123.86   |
| 22  | a     | 746  | PSU  | O2-C2-N1    | -2.13 | 120.44      | 122.79   |
| 1   | A     | 516  | PSU  | C6-N1-C2    | -2.13 | 120.50      | 122.68   |
| 1   | A     | 516  | PSU  | O4'-C1'-C2' | 2.13  | 108.14      | 105.14   |
| 22  | a     | 955  | PSU  | C6-C5-C4    | 2.12  | 119.68      | 118.20   |
| 1   | A     | 1516 | 2MG  | CM2-N2-C2   | -2.12 | 119.18      | 123.86   |
| 22  | a     | 1939 | 5MU  | C6-C5-C4    | 2.12  | 119.80      | 118.03   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1518 | MA6  | C4-C5-N7    | -2.11 | 107.20      | 109.40   |
| 22  | a     | 745  | 1MG  | O6-C6-C5    | -2.09 | 120.50      | 124.19   |
| 25  | d     | 150  | MEQ  | CG-CD-NE2   | -2.06 | 113.42      | 116.29   |
| 22  | a     | 747  | 5MU  | C6-C5-C4    | 2.05  | 119.74      | 118.03   |
| 22  | a     | 1962 | 5MC  | CM5-C5-C6   | -2.05 | 120.11      | 122.85   |
| 22  | a     | 2457 | PSU  | O4'-C1'-C2' | 2.03  | 108.00      | 105.14   |
| 11  | K     | 119  | IAS  | OXT-C-CA    | 2.03  | 120.29      | 113.38   |
| 22  | a     | 1917 | PSU  | C6-N1-C2    | -2.02 | 120.62      | 122.68   |
| 22  | a     | 2604 | PSU  | C6-N1-C2    | -2.02 | 120.62      | 122.68   |
| 1   | A     | 1402 | 4OC  | O2-C2-N3    | -2.01 | 119.06      | 122.33   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 33  | l     | 82  | MS6  | C    |

All (41) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A     | 966  | 2MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 54  | Z     | 21   | H2U  | O4'-C4'-C5'-O5' |
| 54  | Z     | 21   | H2U  | C3'-C4'-C5'-O5' |
| 54  | Z     | 21   | H2U  | O4'-C1'-N1-C6   |
| 54  | Z     | 21   | H2U  | C2'-C1'-N1-C6   |
| 22  | a     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 22  | a     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 22  | a     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 22  | a     | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 22  | a     | 2445 | 2MG  | C3'-C4'-C5'-O5' |
| 54  | Z     | 21   | H2U  | O4'-C1'-N1-C2   |
| 54  | Z     | 21   | H2U  | C2'-C1'-N1-C2   |
| 1   | A     | 516  | PSU  | C3'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 1   | A     | 516  | PSU  | O4'-C4'-C5'-O5' |
| 1   | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 22  | a     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 25  | d     | 150  | MEQ  | NE2-CD-CG-CB    |
| 25  | d     | 150  | MEQ  | OE1-CD-CG-CB    |
| 22  | a     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 1   | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 54  | Z     | 55   | 5MU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | a     | 2445 | 2MG  | O4'-C4'-C5'-O5' |
| 54  | Z     | 55   | 5MU  | C3'-C4'-C5'-O5' |
| 1   | A     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 12  | L     | 89   | D2T  | CG-CB-SB-CB1    |
| 12  | L     | 89   | D2T  | SB-CB-CG-OD1    |
| 22  | a     | 2552 | OMU  | C3'-C2'-O2'-CM2 |
| 33  | l     | 82   | MS6  | CB-CG-SD-CE     |
| 33  | l     | 81   | 4D4  | NE-CD-CG-CB     |
| 54  | Z     | 21   | H2U  | C4'-C5'-O5'-P   |
| 22  | a     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 1   | A     | 527  | G7M  | C4'-C5'-O5'-P   |
| 33  | l     | 81   | 4D4  | CG-CD-NE-CZ     |
| 22  | a     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 12  | L     | 89   | D2T  | SB-CB-CG-OD2    |
| 1   | A     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 22  | a     | 746  | PSU  | O4'-C1'-C5-C6   |
| 22  | a     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 33  | l     | 81   | 4D4  | O-C-CA-CB       |

There are no ring outliers.

10 monomers are involved in 9 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A     | 1516 | 2MG  | 1       | 0            |
| 54  | Z     | 56   | PSU  | 1       | 0            |
| 22  | a     | 1915 | 3TD  | 1       | 0            |
| 1   | A     | 1207 | 2MG  | 1       | 0            |
| 54  | Z     | 21   | H2U  | 1       | 0            |
| 1   | A     | 966  | 2MG  | 1       | 0            |
| 54  | Z     | 55   | 5MU  | 1       | 0            |
| 22  | a     | 1939 | 5MU  | 1       | 0            |
| 22  | a     | 2030 | 6MZ  | 2       | 0            |
| 1   | A     | 1519 | MA6  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 457 ligands modelled in this entry, 457 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.