Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 08:24 PM EDT

PDB ID	:	6OT3 / pdb_00006ot3
EMDB ID	:	EMD-20193
Title	:	RF2 accommodated state bound Release complex 70S at 24 ms
Authors	:	Fu, Z.; Indrisiunaite, G.; Kaledhonkar, S.; Shah, B.; Sun, M.; Chen, B.; Grassucci, R.A.; Ehrenberg, M.; Frank, J.
Deposited on	:	2019-05-02
Resolution	:	3.90 Å(reported)

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:

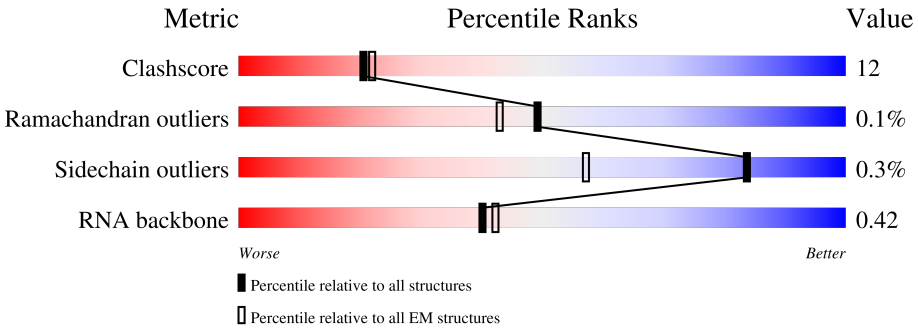
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

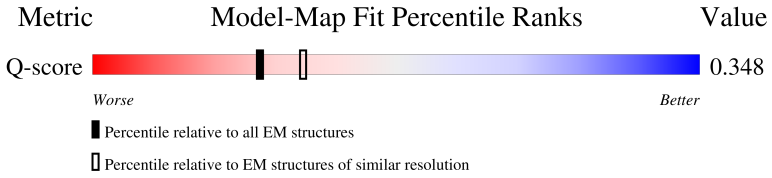
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	2903	54% 36% 10%
2	2	1534	51% 40% 8%
3	3	120	61% 32% 8%

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Mol	Chain	Length	Quality of chain
4	4	9	78% 11% 11%
5	B	271	75% 25%
6	C	209	75% 24%
7	D	201	78% 22%
8	E	177	74% 26%
9	F	175	79% 21%
10	G	149	70% 30%
11	J	142	89% 11%
12	K	123	78% 22%
13	L	144	83% 17%
14	M	136	82% 18%
15	N	119	65% 34%
16	O	116	77% 23%
17	P	114	76% 24%
18	Q	117	76% 24%
19	R	103	67% 31%
20	S	110	81% 19%
21	T	94	78% 22%
22	U	103	75% 25%
23	V	94	73% 27%
24	W	76	74% 26%
25	X	77	71% 29%
26	Y	62	77% 23%
27	Z	58	72% 28%
28	a	66	73% 27%

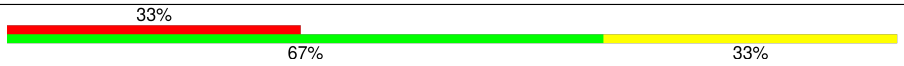
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Mol	Chain	Length	Quality of chain
29	b	56	70% 30%
30	c	52	73% 27%
31	d	46	74% 26%
32	e	64	88% 9%
33	f	38	82% 18%
34	g	225	79% 20%
35	h	208	74% 26%
36	i	205	76% 24%
37	j	156	76% 24%
38	k	104	66% 34%
39	l	151	74% 26%
40	m	129	81% 19%
41	n	127	76% 24%
42	o	99	78% 22%
43	p	117	82% 18%
44	q	87	82% 18%
45	r	116	80% 20%
46	s	100	78% 22%
47	t	88	57% 33% 8%
48	u	82	68% 32%
49	v	80	79% 21%
50	w	66	77% 23%
51	x	83	70% 30%
52	y	86	91% 9%
53	z	70	91% 9%

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Mol	Chain	Length	Quality of chain
54	5	76	
55	A	357	
56	6	3	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 146899 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	9	184	83	26	66	9	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

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

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

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

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	87	Total	C	N	O	S	0	0
			673	417	137	116	3		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	66	Total 544	C 344	N 102	O 97	S 1	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	83	Total 663	C 424	N 126	O 111	S 2	0	0

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	86	Total 669	C 414	N 138	O 114	S 3	0	0

- Molecule 53 is a protein called 30S ribosomal protein S21.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
54	5	76	Total 1627	C 727	N 296	O 527	P 76	S 1	0	0

- Molecule 55 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	A	357	Total 2833	C 1742	N 498	O 583	S 10	0	0

- Molecule 56 is a protein called FME-PHE-PHE.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	3	Total	C	N	O	S	0	0
			32	24	3	4	1		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	1	2	Total	Mg	0
			2	2	
57	2	1	Total	Mg	0
			1	1	
57	3	8	Total	Mg	0
			8	8	
57	i	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	a	1	Total	Zn	0
			1	1	
58	f	1	Total	Zn	0
			1	1	

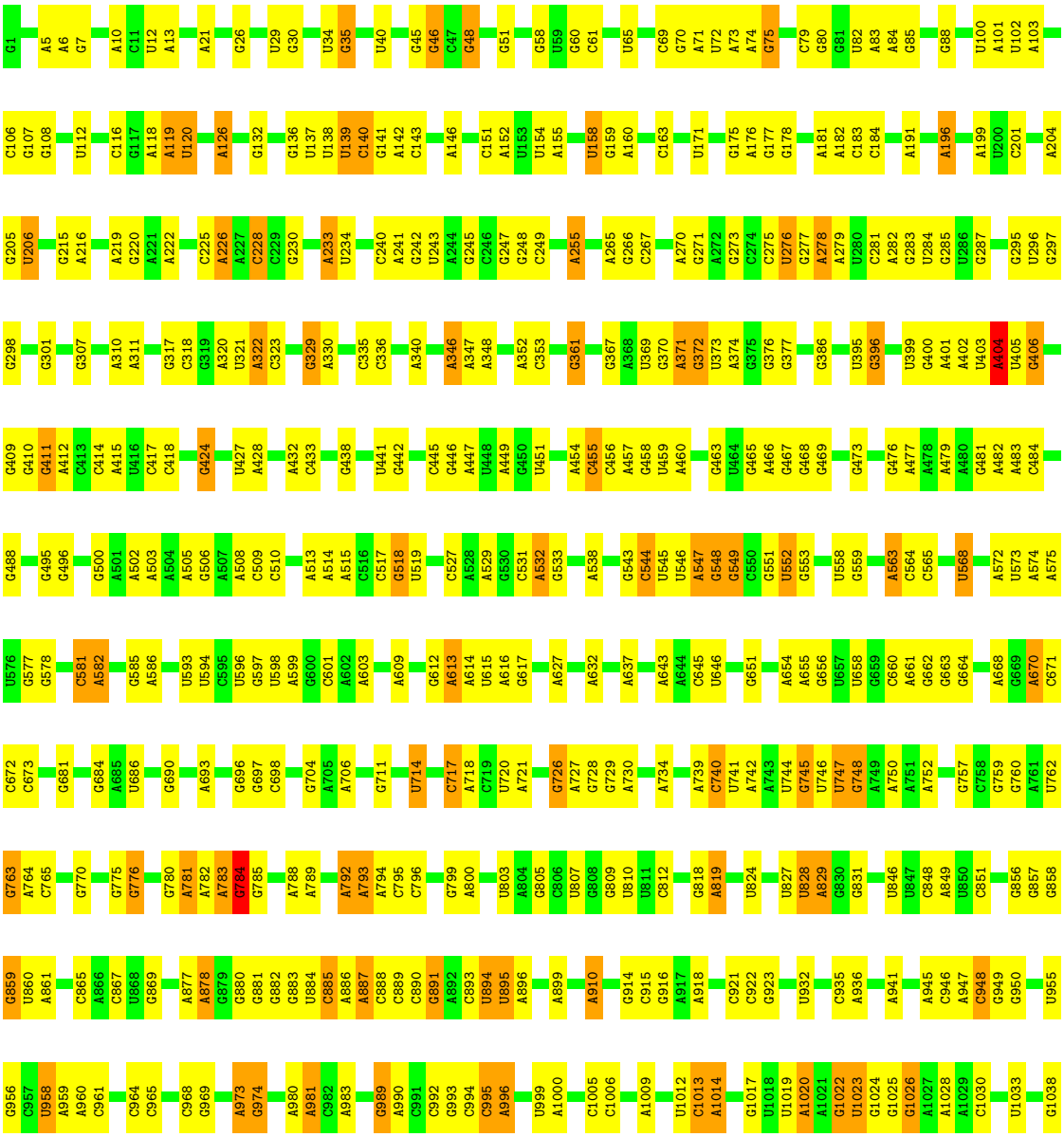
3 Residue-property plots (i)

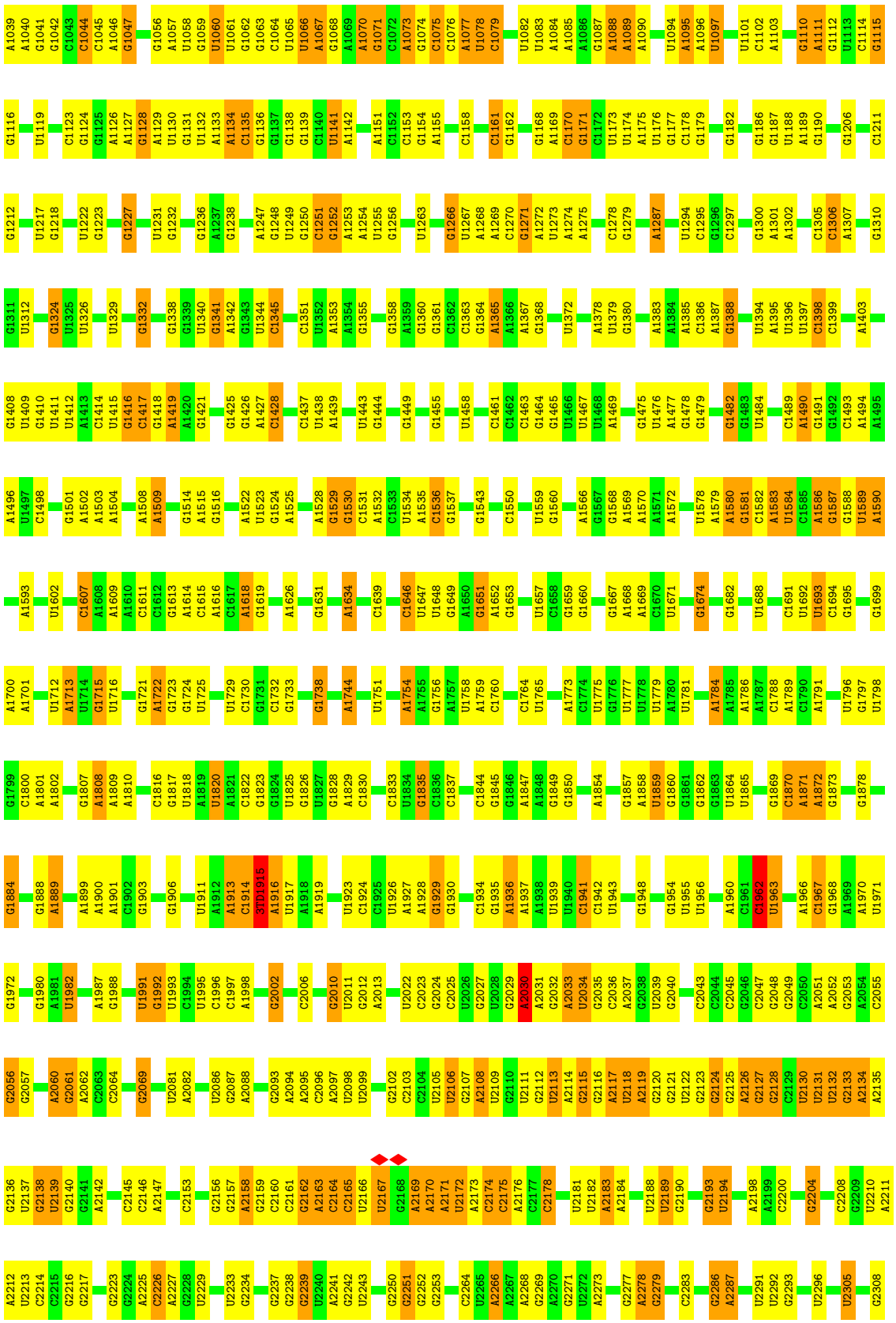
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

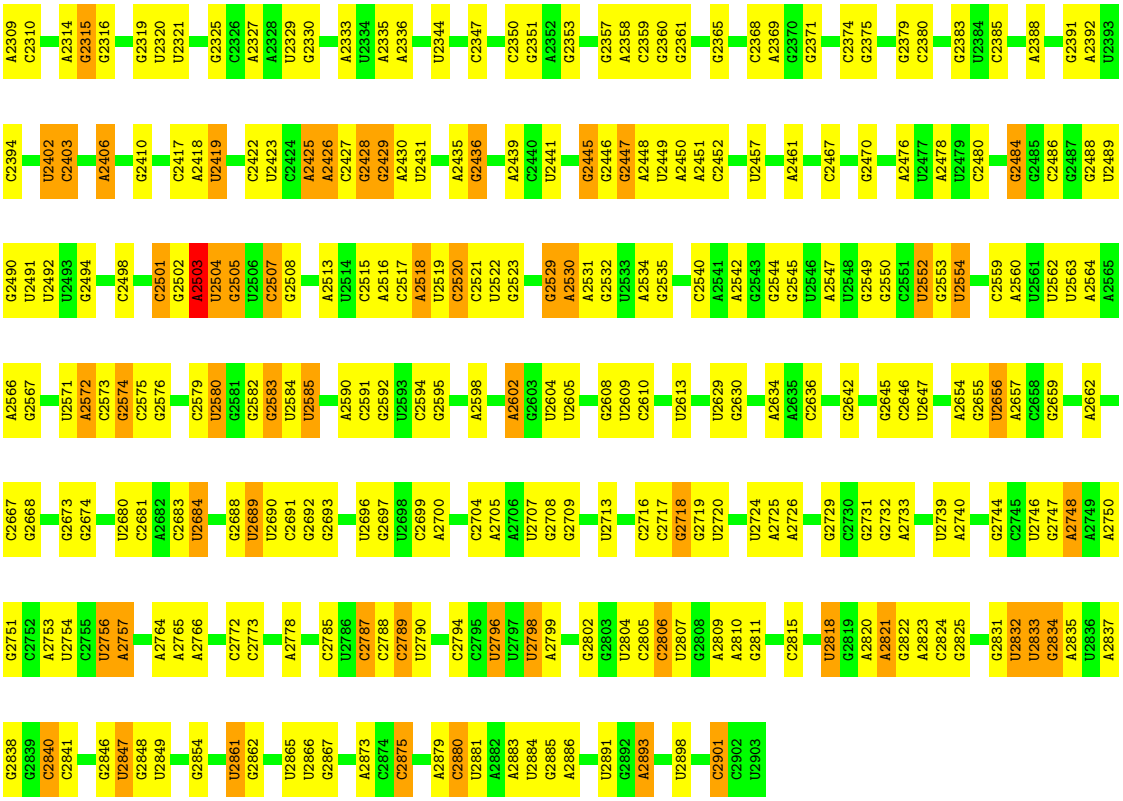
- Molecule 1: 23S ribosomal RNA

Chain 1:





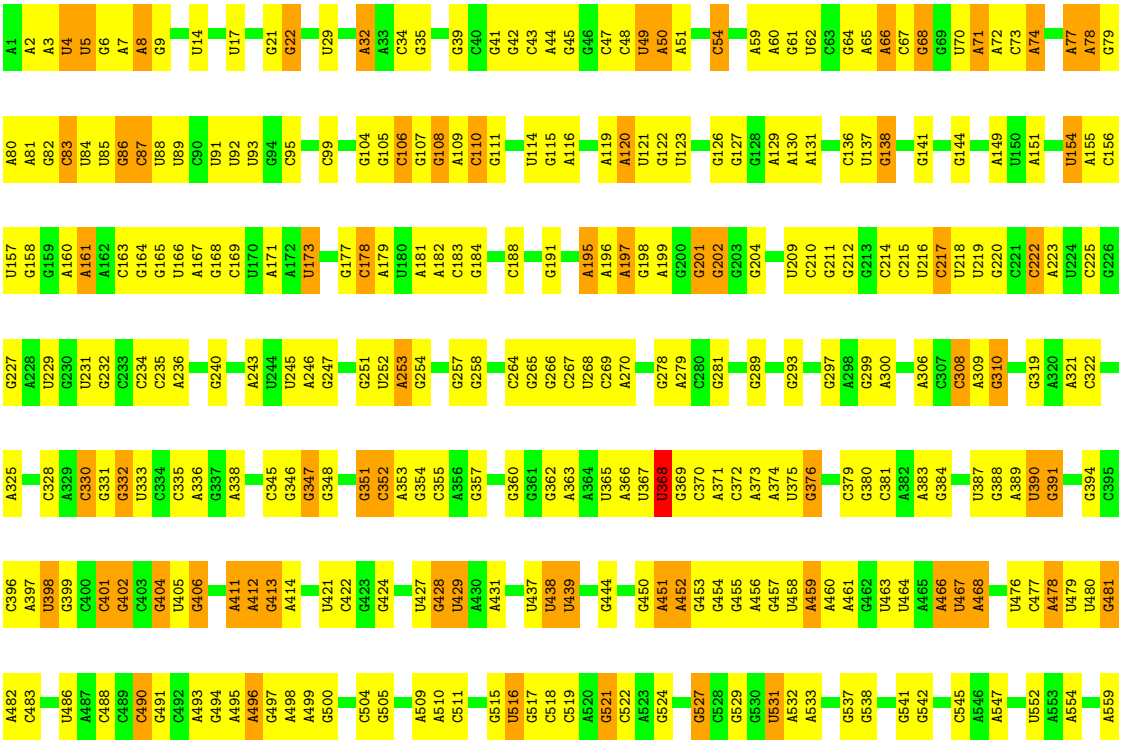

A1039 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 U1094 A1095 A1096 U1097 U1101 C1102 A1103 G1110 A1111 G1112 U1113 C1114 G1115
G1116 U1119 C1123 G1124 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1137 G1138 G1139 C1140 U1141 A1142 A1151 C1152 C1153 G1154 A1155 C1158 C1161 G1162 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 G1182 G1186 G1187 U1188 A1189 G1190 G1206 C1211
G1212 U1217 G1218 U1222 G1223 G1227 U1231 G1232 G1236 A1237 G1238 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 U1263 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 C1278 G1279 A1287 U1294 C1295 G1296 C1297 G1300 A1301 A1302 C1305 C1306 A1307 G1310
G1311 U1312 G1324 U1325 U1326 U1329 G1332 G1338 G1339 U1340 G1341 A1342 G1343 U1344 C1345 C1351 U1352 A1353 A1354 G1355 G1358 A1359 G1360 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 U1372 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1387 G1388 U1394 A1395 U1396 U1397 C1398 C1399 A1403
G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1425 G1426 A1427 C1428 C1437 U1438 A1439 U1443 G1444 G1449 G1455 U1458 C1461 C1462 C1463 G1464 G1465 U1466 U1467 U1468 A1469 G1475 U1476 A1477 G1478 G1479 G1482 G1483 U1484 C1489 A1490 G1491 G1492 C1493 A1494 A1495
A1496 U1497 C1498 G1501 A1502 A1503 A1504 A1508 A1509 G1514 A1515 G1516 A1522 U1523 G1524 A1525 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1543 C1550 U1559 G1560 A1566 G1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590
A1593 U1602 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1619 A1626 G1631 A1634 C1639 C1646 U1647 U1648 G1649 A1650 G1651 A1652 G1653 U1657 C1658 G1659 G1660 G1667 A1668 A1669 C1670 U1671 G1674 G1682 U1688 C1691 U1692 U1693 C1694 G1695 G1699
A1700 A1701 U1712 A1713 U1714 G1715 U1716 G1721 A1722 G1723 G1724 U1725 U1729 C1730 C1731 C1732 G1733 G1738 A1744 U1751 A1754 A1755 G1756 A1757 U1758 A1759 C1760 C1764 U1765 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 U1781 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 U1796 G1797 U1798
G1799 C1800 A1801 A1802 G1807 A1808 A1809 A1810 C1816 G1817 U1818 A1819 U1820 A1821 C1822 G1823 G1824 U1825 G1826 U1827 G1828 A1829 C1830 C1833 U1834 G1835 C1836 C1837 C1844 G1845 G1846 A1847 A1848 G1849 G1850 A1854 G1857 A1858 U1859 G1860 G1861 G1862 G1863 U1864 U1865 G1869 C1870 A1871 A1872 G1873 G1878
G1884 G1888 A1889 A1899 A1900 A1901 C1902 G1903 G1906 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 G1948 G1954 U1955 U1956 A1960 C1961 C1962 U1963 A1966 C1967 G1968 A1969 A1970 U1971
G1972 G1980 A1981 U1982 A1987 G1988 U1991 G1992 U1993 C1994 U1995 C1996 C1997 A1998 G2002 C2006 G2010 U2011 G2012 A2013 U2022 C2023 G2024 C2025 U2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 A2037 G2038 U2039 G2040 C2043 C2044 C2045 G2046 C2047 G2048 G2049 C2050 A2051 A2052 G2053 A2054 C2055
G2056 G2057 A2060 G2061 A2062 C2063 C2064 G2069 U2081 A2082 U2086 G2087 A2088 G2093 A2094 A2095 C2096 A2097 U2098 U2099 G2102 C2103 C2104 U2105 U2106 C2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135
G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2145 C2146 A2147 C2153 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 U2181 U2182 A2183 A2184 U2188 U2189 G2190 G2193 U2194 A2198 A2199 C2200 G2204 C2208 G2209 U2210 A2211
A2212 U2213 C2214 C2215 G2216 G2217 G2223 G2224 A2225 C2226 A2227 G2228 U2229 U2233 G2234 G2237 G2238 G2239 U2240 A2241 G2242 U2243 G2250 G2251 G2252 G2253 C2264 U2265 A2266 A2267 A2268 G2269 A2270 G2271 U2272 A2273 G2277 A2278 G2279 C2283 G2286 A2287 U2291 U2292 G2293 U2296 U2305 G2308

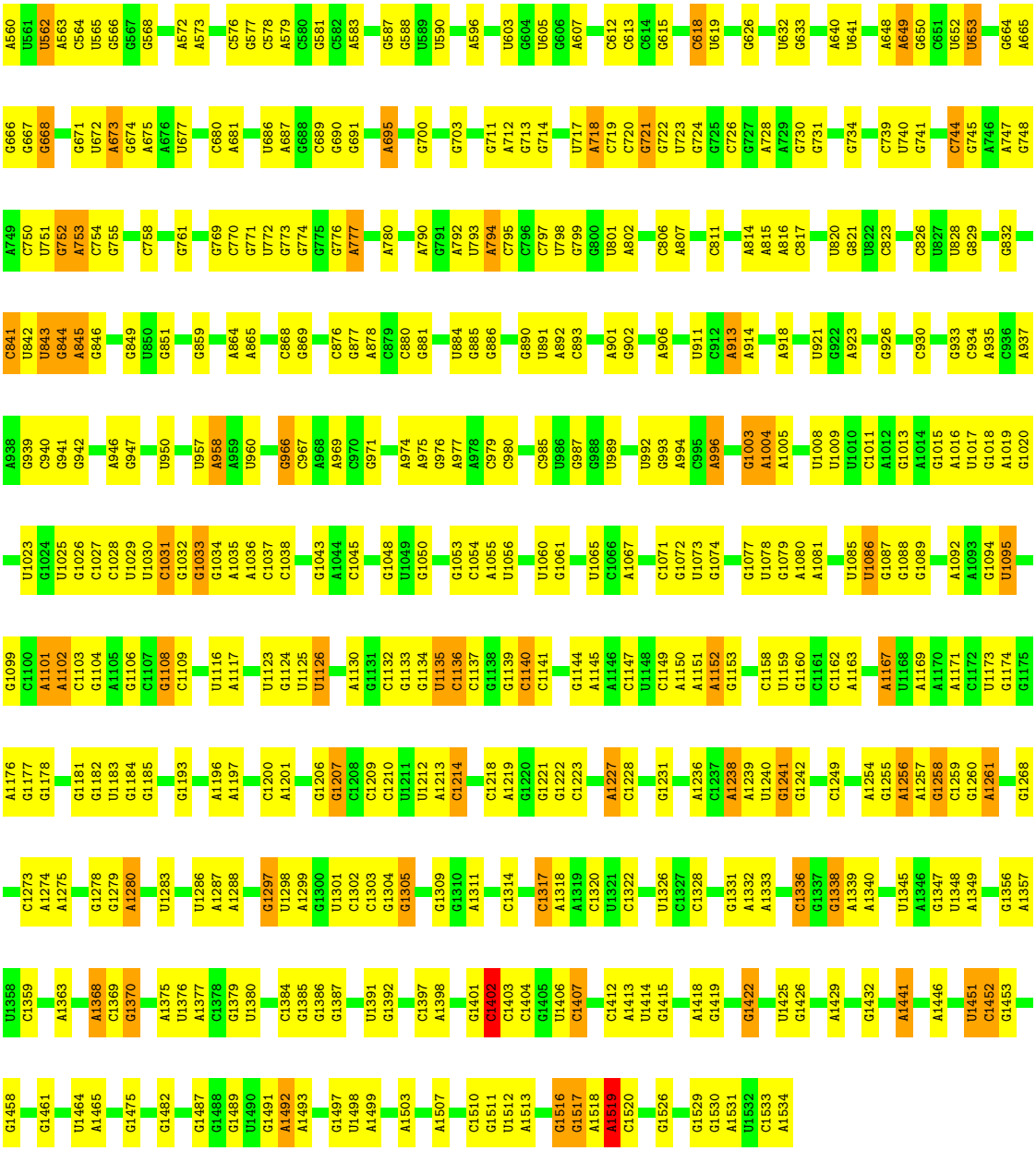


• Molecule 2: 16S ribosomal RNA

Chain 2:



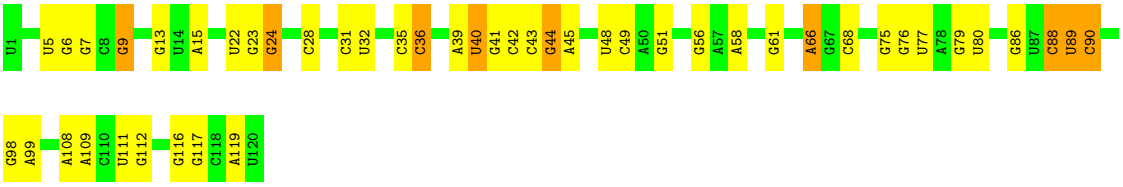




• Molecule 3: 5S ribosomal RNA

Chain 3:





• Molecule 4: mRNA

Chain 4:

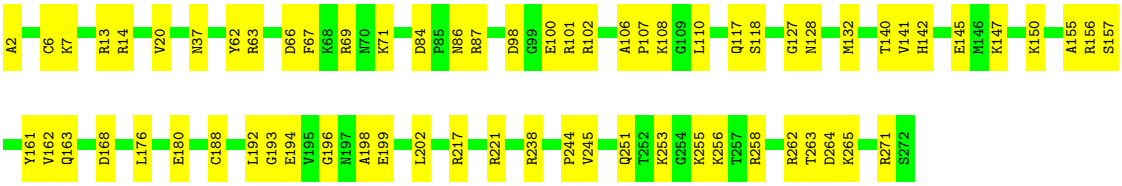




• Molecule 5: 50S ribosomal protein L2

Chain B:

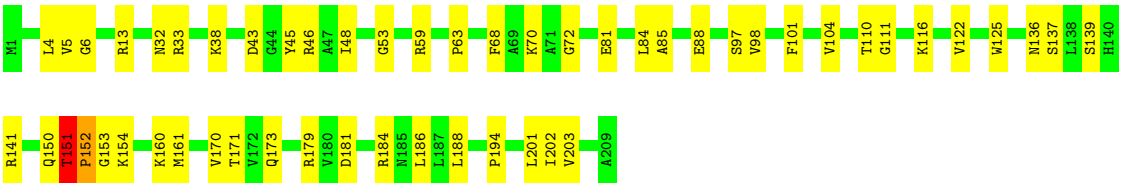




• Molecule 6: 50S ribosomal protein L3

Chain C:

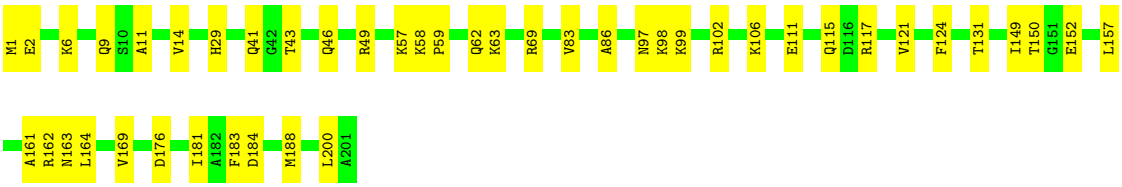




• Molecule 7: 50S ribosomal protein L4

Chain D:

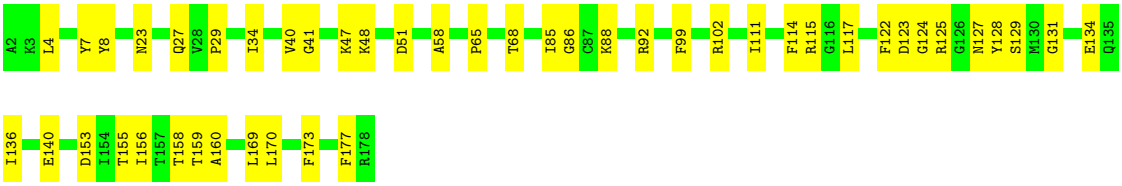




• Molecule 8: 50S ribosomal protein L5

Chain E:





• Molecule 9: 50S ribosomal protein L6

Chain F:





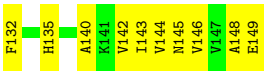


• Molecule 10: 50S ribosomal protein L9

Chain G:



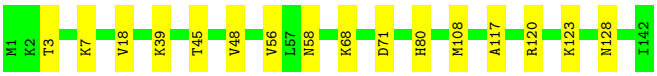




• Molecule 11: 50S ribosomal protein L13

Chain J:

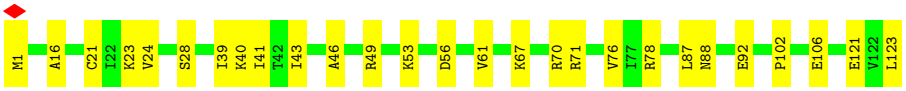




• Molecule 12: 50S ribosomal protein L14

Chain K:

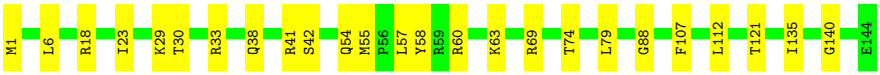




• Molecule 13: 50S ribosomal protein L15

Chain L:





• Molecule 14: 50S ribosomal protein L16

Chain M:

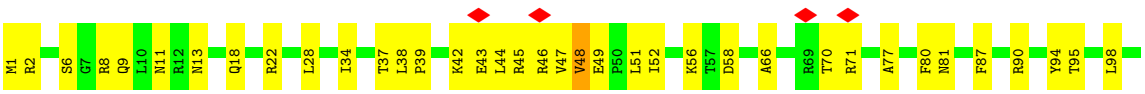


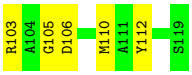


• Molecule 15: 50S ribosomal protein L17

Chain N:



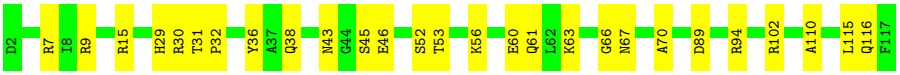




• Molecule 16: 50S ribosomal protein L18

Chain O:

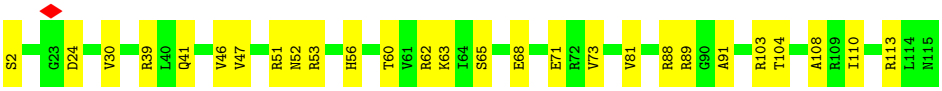




• Molecule 17: 50S ribosomal protein L19

Chain P:

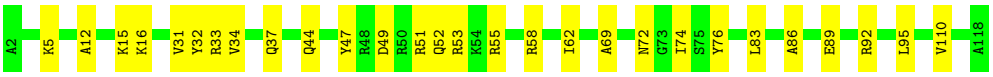




• Molecule 18: 50S ribosomal protein L20

Chain Q:

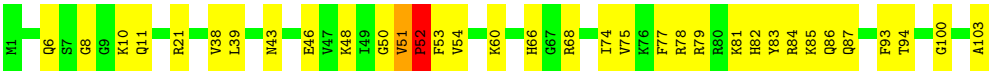




• Molecule 19: 50S ribosomal protein L21

Chain R:

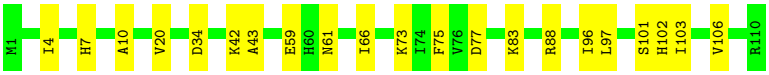




• Molecule 20: 50S ribosomal protein L22

Chain S:

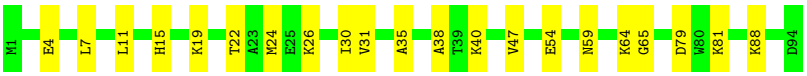




• Molecule 21: 50S ribosomal protein L23

Chain T:

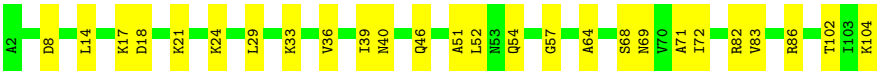




• Molecule 22: 50S ribosomal protein L24

Chain U:

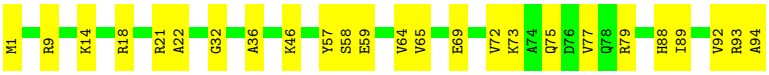




• Molecule 23: 50S ribosomal protein L25

Chain V:





• Molecule 24: 50S ribosomal protein L27

Chain W:

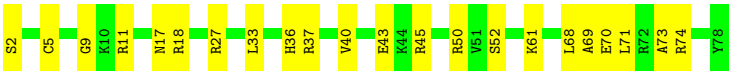




• Molecule 25: 50S ribosomal protein L28

Chain X:

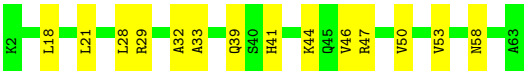




• Molecule 26: 50S ribosomal protein L29

Chain Y:





• Molecule 27: 50S ribosomal protein L30

Chain Z:

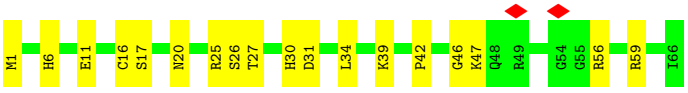




• Molecule 28: 50S ribosomal protein L31

Chain a:

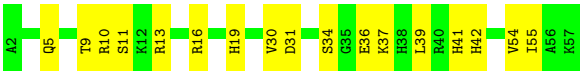




• Molecule 29: 50S ribosomal protein L32

Chain b:

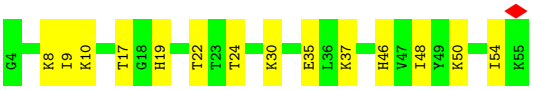




• Molecule 30: 50S ribosomal protein L33

Chain c:

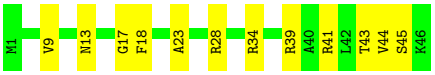




• Molecule 31: 50S ribosomal protein L34

Chain d:

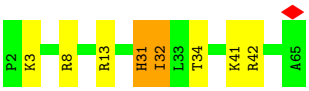




• Molecule 32: 50S ribosomal protein L35

Chain e:





• Molecule 33: 50S ribosomal protein L36

Chain f:

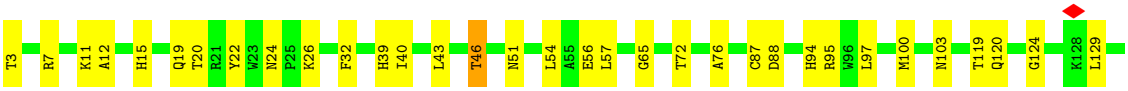


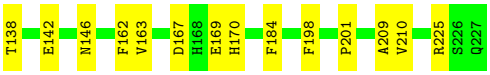


• Molecule 34: 30S ribosomal protein S2

Chain g:



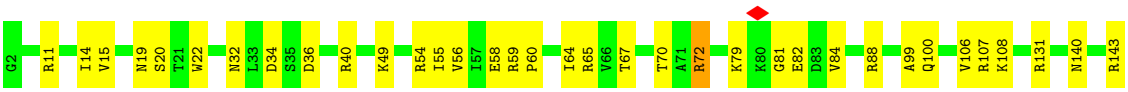




• Molecule 35: 30S ribosomal protein S3

Chain h:



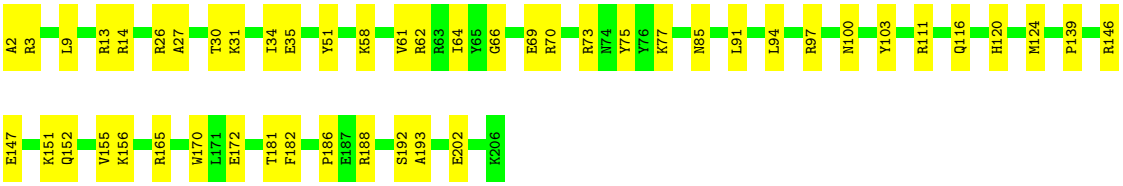




• Molecule 36: 30S ribosomal protein S4

Chain i:

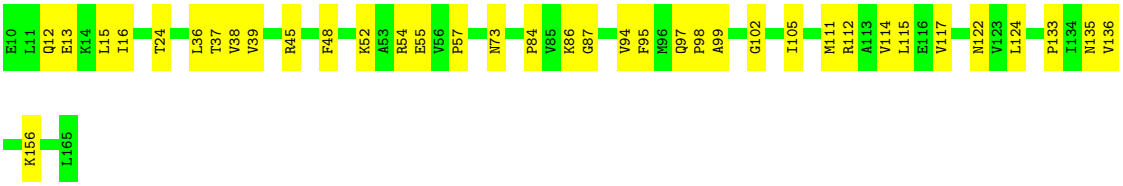




• Molecule 37: 30S ribosomal protein S5

Chain j:





• Molecule 38: 30S ribosomal protein S6

Chain k:

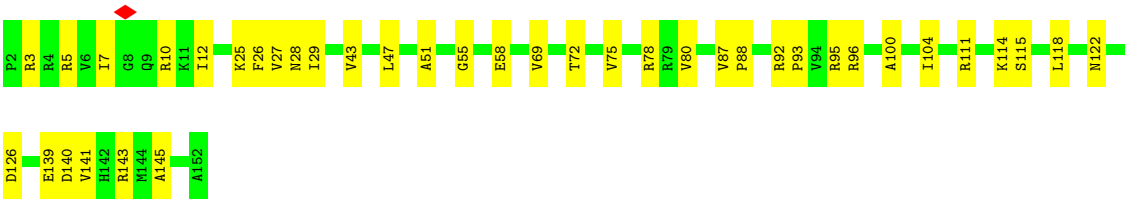




• Molecule 39: 30S ribosomal protein S7

Chain l:

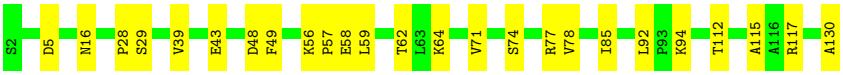




• Molecule 40: 30S ribosomal protein S8

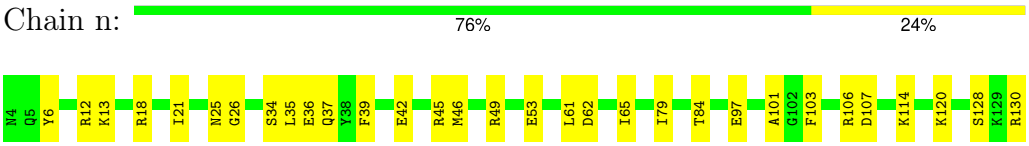
Chain m:





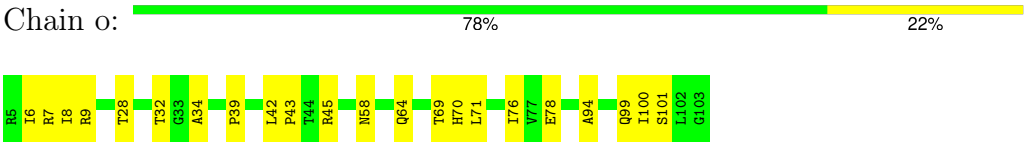
• Molecule 41: 30S ribosomal protein S9

Chain n:



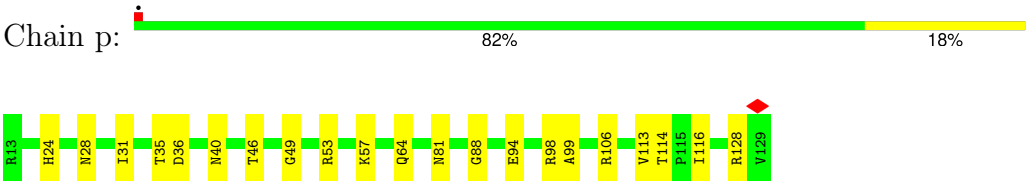
• Molecule 42: 30S ribosomal protein S10

Chain o:



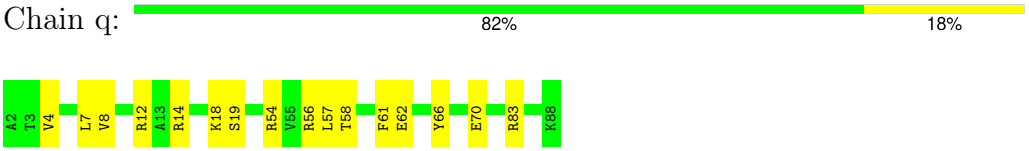
• Molecule 43: 30S ribosomal protein S11

Chain p:



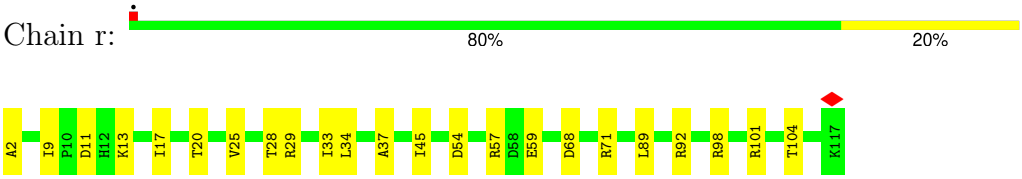
• Molecule 44: 30S ribosomal protein S12

Chain q:



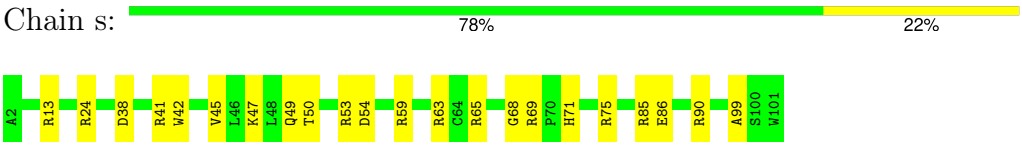
• Molecule 45: 30S ribosomal protein S13

Chain r:



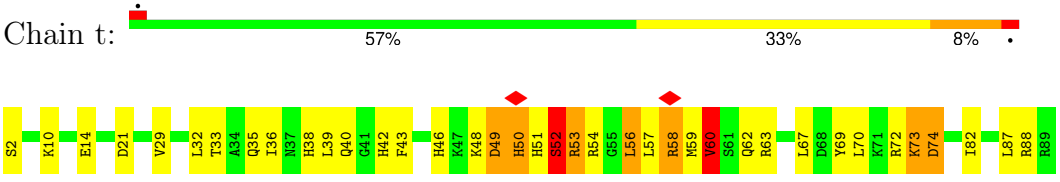
• Molecule 46: 30S ribosomal protein S14

Chain s:



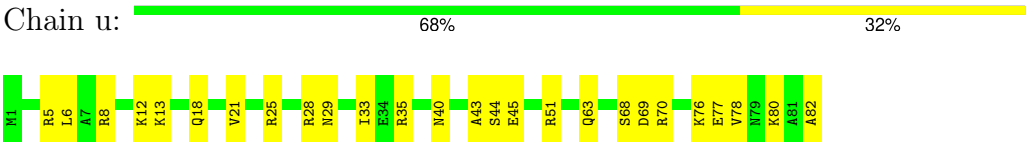
• Molecule 47: 30S ribosomal protein S15

Chain t:



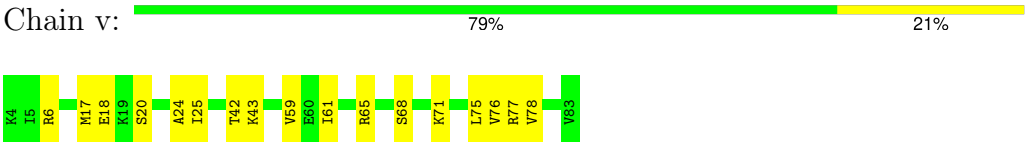
• Molecule 48: 30S ribosomal protein S16

Chain u:



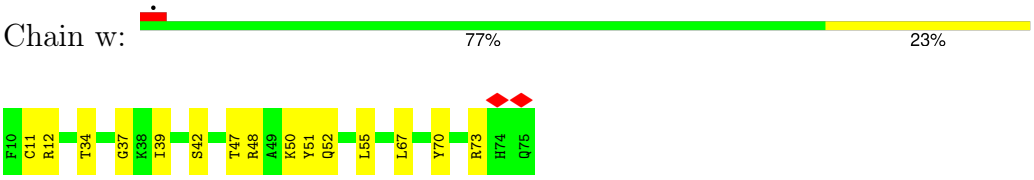
• Molecule 49: 30S ribosomal protein S17

Chain v:



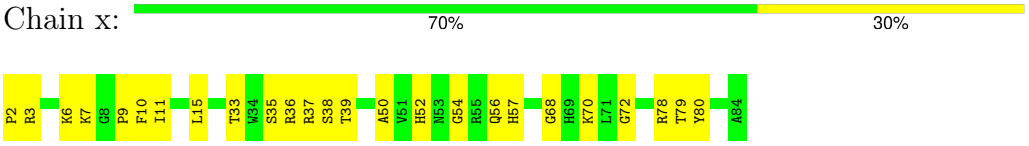
• Molecule 50: 30S ribosomal protein S18

Chain w:



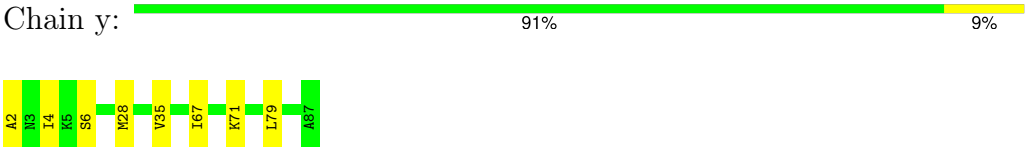
• Molecule 51: 30S ribosomal protein S19

Chain x:



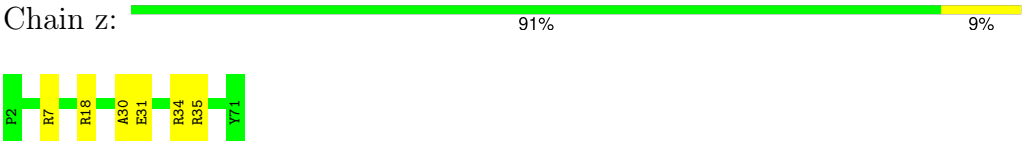
• Molecule 52: 30S ribosomal protein S20

Chain y:



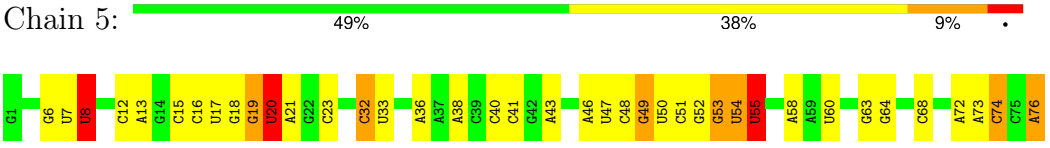
• Molecule 53: 30S ribosomal protein S21

Chain z:



• Molecule 54: P-tRNA

Chain 5:



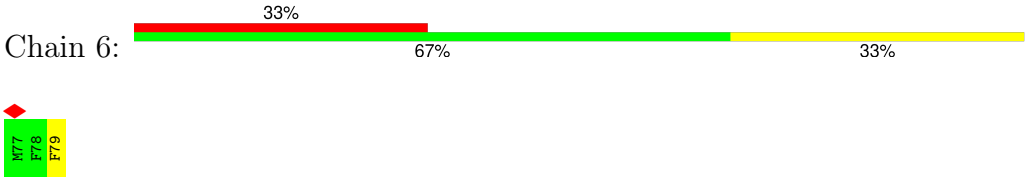
• Molecule 55: Peptide chain release factor 2

Chain A:



• Molecule 56: FME-PHE-PHE

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, OMU, OMC, 4OC, 5MC, 1MG, G7M, 2MA, 6MZ, 2MG, MA6, H2U, UR3, 3TD, PSU, OMG, 4SU, FME, ZN

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	1	0.36	0/69286	0.37	4/108087 (0.0%)
2	2	0.35	0/36590	0.37	1/57074 (0.0%)
3	3	0.33	0/2872	0.34	0/4478
4	4	0.29	0/203	0.36	0/312
5	B	0.36	0/2121	0.60	0/2852
6	C	0.38	0/1586	0.65	1/2134 (0.0%)
7	D	0.34	0/1571	0.56	0/2113
8	E	0.33	0/1434	0.57	0/1926
9	F	0.31	0/1333	0.52	0/1805
10	G	0.28	0/1122	0.62	1/1515 (0.1%)
11	J	0.34	0/1152	0.57	0/1551
12	K	0.34	0/955	0.61	0/1279
13	L	0.33	0/1062	0.59	0/1413
14	M	0.34	0/1093	0.57	0/1460
15	N	0.38	0/964	0.79	0/1289
16	O	0.30	0/902	0.56	0/1209
17	P	0.38	0/929	0.66	0/1242
18	Q	0.35	0/960	0.57	0/1278
19	R	0.43	1/829 (0.1%)	0.65	1/1107 (0.1%)
20	S	0.34	0/864	0.58	0/1156
21	T	0.33	0/752	0.57	0/1005
22	U	0.36	0/796	0.63	0/1062
23	V	0.32	0/766	0.51	0/1025
24	W	0.33	0/589	0.51	0/779
25	X	0.39	0/635	0.56	0/848
26	Y	0.32	0/502	0.57	0/667
27	Z	0.30	0/452	0.55	0/605
28	a	0.31	0/531	0.58	0/709
29	b	0.34	0/450	0.57	0/599
30	c	0.30	0/433	0.56	0/576
31	d	0.37	0/380	0.62	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.41	0/513	0.67	1/676 (0.1%)
33	f	0.30	0/303	0.60	0/397
34	g	0.32	0/1791	0.66	2/2413 (0.1%)
35	h	0.32	0/1663	0.59	0/2241
36	i	0.30	0/1665	0.55	0/2227
37	j	0.35	0/1165	0.61	0/1568
38	k	0.33	0/867	0.63	0/1171
39	l	0.29	0/1195	0.56	0/1602
40	m	0.32	0/989	0.55	0/1326
41	n	0.29	0/1034	0.61	0/1375
42	o	0.29	0/800	0.59	0/1082
43	p	0.31	0/893	0.53	0/1205
44	q	0.33	0/682	0.57	0/918
45	r	0.31	0/909	0.63	0/1215
46	s	0.30	0/817	0.53	0/1088
47	t	0.38	0/722	0.95	4/964 (0.4%)
48	u	0.33	0/659	0.66	0/884
49	v	0.32	0/657	0.64	0/881
50	w	0.30	0/553	0.54	0/743
51	x	0.29	0/680	0.55	0/915
52	y	0.34	0/675	0.54	0/895
53	z	0.29	0/597	0.56	0/792
54	5	0.32	0/1704	0.35	0/2654
55	A	0.32	0/2873	0.65	4/3870 (0.1%)
56	6	0.43	0/23	0.44	0/29
All	All	0.35	1/158543 (0.0%)	0.45	19/236784 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	52	PRO	N-CA	-6.09	1.39	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	t	52	SER	N-CA-C	-8.02	101.31	112.45
47	t	60	VAL	N-CA-C	-7.78	103.27	110.82
47	t	58	ARG	N-CA-C	-7.00	103.64	111.28
32	e	31	HIS	O-C-N	6.44	130.59	123.25
1	1	784	G	C4'-C3'-O3'	5.80	121.70	113.00
1	1	404	A	C4'-C3'-O3'	5.79	118.09	109.40
34	g	46	THR	CA-C-N	5.79	125.99	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	g	46	THR	C-N-CA	5.79	125.99	120.43
1	1	784	G	C2'-C3'-O3'	-5.56	105.37	113.70
55	A	338	THR	CA-C-N	5.54	131.67	121.70
55	A	338	THR	C-N-CA	5.54	131.67	121.70
1	1	2847	U	C4'-C3'-O3'	-5.47	104.80	113.00
6	C	152	PRO	N-CA-C	-5.32	101.40	112.36
10	G	13	GLY	N-CA-C	5.27	117.55	110.43
19	R	52	PRO	N-CA-C	-5.25	101.66	112.47
47	t	56	LEU	N-CA-C	-5.04	105.87	111.36
55	A	227	ASP	CA-C-N	5.03	131.16	121.54
55	A	227	ASP	C-N-CA	5.03	131.16	121.54
2	2	368	U	C2'-C3'-O3'	-5.00	106.20	113.70

There are no chirality outliers.

There are no planarity outliers.

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	1	62336	0	31370	692	0
2	2	32929	0	16587	369	0
3	3	2569	0	1301	34	0
4	4	184	0	95	1	0
5	B	2082	0	2154	51	0
6	C	1565	0	1616	50	0
7	D	1552	0	1619	32	0
8	E	1410	0	1444	34	0
9	F	1313	0	1358	23	0
10	G	1111	0	1148	28	0
11	J	1129	0	1162	12	0
12	K	946	0	1023	20	0
13	L	1053	0	1129	21	0
14	M	1074	0	1157	17	0
15	N	951	0	994	36	0
16	O	892	0	923	21	0
17	P	917	0	962	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	947	0	1019	22	0
19	R	816	0	839	36	0
20	S	857	0	922	18	0
21	T	746	0	811	14	0
22	U	788	0	844	19	0
23	V	753	0	780	18	0
24	W	582	0	599	13	0
25	X	625	0	652	18	0
26	Y	501	0	531	9	0
27	Z	448	0	488	9	0
28	a	522	0	520	14	0
29	b	444	0	458	14	0
30	c	426	0	464	10	0
31	d	377	0	418	8	0
32	e	504	0	572	10	0
33	f	302	0	340	6	0
34	g	1760	0	1787	27	0
35	h	1636	0	1710	34	0
36	i	1643	0	1707	37	0
37	j	1152	0	1196	27	0
38	k	848	0	846	25	0
39	l	1181	0	1238	27	0
40	m	979	0	1031	15	0
41	n	1022	0	1070	21	0
42	o	790	0	831	17	0
43	p	877	0	887	13	0
44	q	673	0	720	13	0
45	r	900	0	965	18	0
46	s	805	0	844	19	0
47	t	714	0	734	53	0
48	u	649	0	666	22	0
49	v	648	0	691	13	0
50	w	544	0	560	10	0
51	x	663	0	688	23	0
52	y	669	0	719	5	0
53	z	589	0	629	4	0
54	5	1627	0	832	22	0
55	A	2833	0	2729	76	0
56	6	32	0	28	1	0
57	1	2	0	0	0	0
57	2	1	0	0	0	0
57	3	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	i	1	0	0	0	0
58	a	1	0	0	0	0
58	f	1	0	0	0	0
All	All	146899	0	99407	1880	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 12.

All (1880) 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)
19:R:51:VAL:HG13	19:R:52:PRO:CD	1.51	1.40
19:R:51:VAL:CG1	19:R:52:PRO:HD3	1.55	1.36
1:1:402:A:C8	1:1:403:U:C6	2.18	1.30
6:C:151:THR:OG1	6:C:152:PRO:HD3	1.34	1.27
6:C:151:THR:HG23	6:C:152:PRO:CD	1.76	1.15
6:C:151:THR:CG2	6:C:152:PRO:HD2	1.81	1.10
19:R:52:PRO:HD2	19:R:53:PHE:H	1.13	1.07
1:1:402:A:N7	1:1:403:U:C6	2.25	1.02
1:1:403:U:H4'	1:1:406:G:O2'	1.61	1.00
6:C:151:THR:CG2	6:C:152:PRO:CD	2.40	0.99
1:1:402:A:C8	1:1:403:U:C5	2.51	0.98
19:R:52:PRO:CD	19:R:53:PHE:H	1.76	0.95
6:C:151:THR:OG1	6:C:152:PRO:CD	2.14	0.95
2:2:4:U:H3'	2:2:5:U:H5"	1.49	0.94
6:C:151:THR:HG23	6:C:152:PRO:HD2	0.93	0.93
47:t:57:LEU:HA	47:t:60:VAL:HB	1.49	0.93
6:C:151:THR:CB	6:C:152:PRO:CD	2.48	0.91
1:1:2875:C:HO2'	17:P:2:SER:N	1.70	0.88
1:1:139:U:H5'	1:1:140:C:O5'	1.73	0.88
1:1:2061:G:OP1	1:1:2503:2MA:CM2	2.21	0.88
2:2:357:G:H4'	2:2:368:U:H5"	1.55	0.87
1:1:402:A:H2'	1:1:403:U:O4'	1.74	0.87
1:1:402:A:N7	1:1:403:U:C5	2.44	0.84
6:C:151:THR:CB	6:C:152:PRO:HD3	2.06	0.84
1:1:402:A:C2	1:1:403:U:H1'	2.13	0.84
1:1:1065:U:O2'	1:1:1066:U:O4'	1.94	0.83
1:1:578:G:H21	1:1:1252:G:H22	1.25	0.83
47:t:56:LEU:O	47:t:60:VAL:HG23	1.79	0.83
1:1:402:A:C5	1:1:403:U:N1	2.47	0.82
19:R:52:PRO:HD2	19:R:53:PHE:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2061:G:OP1	1:1:2503:2MA:HM21	1.81	0.81
19:R:51:VAL:CB	19:R:52:PRO:HD3	2.10	0.81
1:1:402:A:C4	1:1:403:U:C1'	2.65	0.80
8:E:122:PHE:O	8:E:123:ASP:OD1	2.00	0.79
8:E:123:ASP:OD2	8:E:127:ASN:HB2	1.83	0.79
47:t:70:LEU:HA	47:t:73:LYS:HB2	1.64	0.78
19:R:52:PRO:CD	19:R:53:PHE:N	2.41	0.78
2:2:467:U:H3'	2:2:467:U:OP2	1.84	0.78
1:1:403:U:C4'	1:1:406:G:O2'	2.32	0.78
1:1:402:A:C5	1:1:403:U:C6	2.72	0.78
15:N:48:VAL:HA	15:N:51:LEU:HB2	1.67	0.77
2:2:136:C:H42	2:2:227:G:H1	1.31	0.77
19:R:51:VAL:HG13	19:R:52:PRO:HD3	0.78	0.77
1:1:402:A:C4	1:1:403:U:H1'	2.21	0.76
1:1:729:G:N3	1:1:729:G:H2'	1.99	0.76
2:2:667:G:H4'	47:t:51:HIS:HB2	1.68	0.75
47:t:53:ARG:O	47:t:57:LEU:HG	1.86	0.75
1:1:881:G:H1	1:1:895:U:H3	1.33	0.75
47:t:73:LYS:O	47:t:74:ASP:HB2	1.86	0.74
22:U:46:GLN:HB3	22:U:57:GLY:H	1.52	0.74
2:2:158:G:H1	2:2:163:C:H42	1.34	0.74
2:2:590:U:H3	2:2:649:A:H61	1.33	0.74
1:1:2402:U:O2'	1:1:2403:C:H5"	1.87	0.74
47:t:56:LEU:O	47:t:60:VAL:N	2.22	0.72
15:N:8:ARG:HD2	15:N:43:GLU:HB2	1.72	0.72
38:k:35:LYS:HB2	38:k:65:GLU:HB3	1.72	0.72
2:2:958:A:N3	2:2:985:C:O2'	2.22	0.71
34:g:87:CYS:O	34:g:88:ASP:OD1	2.07	0.71
47:t:57:LEU:CA	47:t:60:VAL:HB	2.21	0.71
1:1:228:C:N3	1:1:417:C:O2'	2.22	0.71
27:Z:31:ARG:HD2	27:Z:34:HIS:HB2	1.72	0.71
1:1:402:A:C6	1:1:403:U:H1'	2.26	0.71
1:1:2171:A:H5'	1:1:2174:C:H41	1.55	0.70
1:1:748:G:OP1	20:S:88:ARG:NE	2.25	0.70
1:1:2756:U:OP2	33:f:19:ARG:HG2	1.92	0.70
2:2:376:G:H1	2:2:387:U:H3	1.38	0.70
1:1:402:A:C8	1:1:403:U:H6	2.02	0.70
47:t:58:ARG:O	47:t:62:GLN:HB2	1.91	0.70
1:1:245:G:N7	32:e:8:ARG:NH2	2.40	0.69
1:1:369:U:O2'	1:1:404:A:N6	2.25	0.69
1:1:2709:G:OP1	15:N:18:GLN:NE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:667:G:O2'	47:t:52:SER:N	2.26	0.69
51:x:33:THR:HG22	51:x:35:SER:H	1.57	0.69
2:2:563:A:H3'	44:q:12:ARG:HH12	1.58	0.69
55:A:26:ASP:HB3	55:A:29:ALA:HB3	1.75	0.69
1:1:2358:A:H61	13:L:54:GLN:HE22	1.40	0.68
2:2:450:G:H1	2:2:483:C:H42	1.41	0.68
1:1:465:G:H5"	31:d:44:VAL:HG21	1.76	0.68
7:D:150:THR:HG22	7:D:152:GLU:H	1.57	0.68
2:2:452:A:N3	48:u:70:ARG:NH1	2.42	0.68
54:5:8:4SU:HN3	54:5:23:C:H41	1.40	0.68
35:h:58:GLU:HG2	35:h:60:PRO:HD3	1.75	0.68
24:W:50:ASN:HB2	24:W:82:ILE:HB	1.74	0.68
48:u:12:LYS:HG2	48:u:13:LYS:HG2	1.76	0.68
47:t:57:LEU:HA	47:t:60:VAL:CB	2.24	0.68
19:R:51:VAL:HG13	19:R:52:PRO:HD2	1.66	0.68
1:1:1915:3TD:H3'	1:1:1916:A:H8	1.58	0.67
9:F:155:GLU:HG2	9:F:157:TYR:H	1.60	0.67
1:1:402:A:C5	1:1:403:U:H1'	2.29	0.67
47:t:58:ARG:O	47:t:62:GLN:CB	2.42	0.67
1:1:402:A:C5	1:1:403:U:C1'	2.77	0.67
1:1:538:A:H5"	11:J:7:LYS:HE2	1.76	0.67
1:1:729:G:H2'	1:1:1775:U:H1'	1.75	0.67
2:2:668:G:OP1	47:t:50:HIS:CD2	2.49	0.66
1:1:1124:G:N3	33:f:37:GLN:NE2	2.44	0.66
1:1:468:G:N7	31:d:39:ARG:NH2	2.43	0.65
2:2:668:G:H1'	47:t:49:ASP:OD1	1.95	0.65
38:k:29:ILE:HG22	38:k:34:GLY:HA3	1.78	0.65
1:1:2880:C:O2'	15:N:90:ARG:NH2	2.30	0.65
2:2:201:G:H1	2:2:216:U:H3	1.44	0.65
2:2:451:A:H61	2:2:481:G:H5'	1.60	0.65
2:2:891:U:H2'	2:2:892:A:H8	1.60	0.65
12:K:78:ARG:HB2	17:P:71:GLU:HB2	1.77	0.65
2:2:401:C:OP2	36:i:70:ARG:NH1	2.29	0.65
35:h:88:ARG:HG2	35:h:99:ALA:HB3	1.78	0.65
1:1:2692:G:H1'	1:1:2847:U:H1'	1.79	0.65
2:2:107:G:OP1	2:2:325:A:N6	2.30	0.65
1:1:783:A:H2'	1:1:783:A:N3	2.11	0.65
35:h:156:ARG:HD3	35:h:193:TYR:HB3	1.78	0.65
25:X:33:LEU:HD23	25:X:50:ARG:HG2	1.79	0.64
2:2:390:U:H2'	2:2:391:G:C8	2.32	0.64
1:1:72:U:O4	26:Y:58:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2881:U:H5'	15:N:90:ARG:HH22	1.63	0.64
3:3:43:C:O2	8:E:92:ARG:NH2	2.30	0.64
2:2:668:G:OP1	47:t:50:HIS:HD2	1.81	0.64
2:2:1328:C:O2'	45:r:29:ARG:NH1	2.30	0.64
39:l:115:SER:H	39:l:118:LEU:HD12	1.61	0.64
2:2:4:U:C3'	2:2:5:U:H5"	2.26	0.63
19:R:74:ILE:HB	19:R:87:GLN:HB3	1.80	0.63
2:2:49:U:H3	2:2:362:G:H1'	1.62	0.63
36:i:172:GLU:HB3	36:i:181:THR:HB	1.80	0.63
2:2:376:G:H4'	48:u:5:ARG:HD3	1.80	0.63
2:2:1081:A:N7	37:j:52:LYS:NZ	2.46	0.63
1:1:1817:G:H3'	5:B:156:ARG:HH21	1.62	0.63
5:B:258:ARG:NH2	5:B:263:THR:OG1	2.32	0.63
47:t:58:ARG:O	47:t:62:GLN:N	2.30	0.63
16:O:29:HIS:HB3	16:O:36:TYR:HB2	1.79	0.63
33:f:16:ILE:HG12	33:f:25:VAL:HG22	1.81	0.63
2:2:1106:G:H5"	35:h:172:ARG:HB3	1.81	0.63
10:G:76:GLU:HG3	10:G:142:VAL:HA	1.81	0.63
41:n:6:TYR:HB2	41:n:21:ILE:HB	1.80	0.63
2:2:380:G:N2	2:2:383:A:OP2	2.32	0.62
29:b:9:THR:HG22	29:b:11:SER:H	1.64	0.62
47:t:36:ILE:HA	47:t:39:LEU:HB2	1.80	0.62
1:1:2029:G:N1	1:1:2033:A:OP2	2.30	0.62
2:2:979:C:O2	46:s:59:ARG:NH1	2.32	0.62
27:Z:9:GLN:HB2	27:Z:29:LEU:HD13	1.81	0.62
55:A:141:ALA:HA	55:A:144:TRP:HB3	1.80	0.62
1:1:1652:A:OP1	15:N:8:ARG:NH2	2.31	0.62
1:1:2425:A:H5"	1:1:2427:C:O4'	2.00	0.62
1:1:2200:C:H42	1:1:2223:G:H1	1.48	0.62
1:1:2788:C:O2'	1:1:2809:A:N3	2.33	0.62
13:L:74:THR:HG22	13:L:107:PHE:HB2	1.81	0.62
1:1:860:U:H2'	1:1:861:A:H8	1.65	0.62
20:S:7:HIS:HB3	20:S:103:ILE:HB	1.81	0.62
55:A:21:LEU:HD23	55:A:70:LEU:HD21	1.82	0.62
1:1:1754:A:O2'	17:P:103:ARG:NH2	2.32	0.62
1:1:698:C:O2'	1:1:734:A:N6	2.33	0.62
2:2:563:A:OP1	44:q:14:ARG:NH1	2.33	0.62
35:h:14:ILE:HG22	35:h:15:VAL:HG13	1.80	0.62
1:1:2134:A:N6	1:1:2157:G:O2'	2.32	0.62
6:C:151:THR:CG2	6:C:152:PRO:HD3	2.23	0.61
12:K:1:MET:SD	12:K:67:LYS:NZ	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:52:PRO:O	19:R:53:PHE:CG	2.52	0.61
22:U:86:ARG:NH2	22:U:102:THR:OG1	2.33	0.61
35:h:49:LYS:O	35:h:72:ARG:NH1	2.33	0.61
41:n:106:ARG:NH1	41:n:107:ASP:O	2.33	0.61
15:N:103:ARG:NH2	15:N:106:ASP:OD2	2.33	0.61
18:Q:44:GLN:HE21	19:R:77:PHE:HB3	1.65	0.61
19:R:51:VAL:CG1	19:R:52:PRO:CD	2.38	0.61
28:a:11:GLU:HA	28:a:25:ARG:HA	1.82	0.61
28:a:16:CYS:SG	28:a:17:SER:N	2.74	0.61
38:k:99:ALA:HB1	38:k:103:VAL:HG21	1.81	0.61
1:1:2117:A:N1	1:1:2165:C:N4	2.47	0.61
2:2:890:G:O2'	2:2:906:A:N6	2.34	0.61
16:O:32:PRO:HA	16:O:102:ARG:HH22	1.64	0.61
1:1:2579:C:O2'	6:C:136:ASN:ND2	2.32	0.61
2:2:1013:G:N2	2:2:1016:A:OP2	2.32	0.61
10:G:47:PHE:HA	10:G:51:ARG:HB2	1.82	0.61
43:p:113:VAL:HG12	50:w:73:ARG:HD2	1.81	0.61
2:2:59:A:H3'	2:2:331:G:H22	1.65	0.61
3:3:90:C:H5'	14:M:18:ARG:HB3	1.81	0.61
8:E:48:LYS:HA	8:E:51:ASP:HB3	1.83	0.61
1:1:65:U:O2'	1:1:456:C:N3	2.32	0.61
1:1:1263:U:OP1	29:b:13:ARG:NH1	2.34	0.61
38:k:1:MET:N	38:k:1:MET:SD	2.73	0.61
1:1:2010:G:H5"	20:S:42:LYS:HB2	1.81	0.61
9:F:98:VAL:HG22	9:F:103:ILE:HG12	1.82	0.61
22:U:52:LEU:HD23	22:U:52:LEU:O	2.01	0.61
2:2:4:U:H3'	2:2:5:U:C5'	2.27	0.60
6:C:111:GLY:HA2	6:C:201:LEU:HD22	1.83	0.60
38:k:2:ARG:HB3	38:k:91:ARG:HH12	1.66	0.60
1:1:885:C:H2'	1:1:886:A:H8	1.66	0.60
1:1:1305:C:N4	1:1:1607:C:OP1	2.34	0.60
2:2:2:A:N3	2:2:613:C:O2'	2.34	0.60
2:2:1031:C:O5'	2:2:1032:G:N2	2.34	0.60
18:Q:58:ARG:HE	18:Q:62:ILE:HD11	1.66	0.60
1:1:119:A:H4'	1:1:120:U:H5'	1.84	0.60
2:2:1033:G:H2'	2:2:1034:G:H8	1.66	0.60
35:h:11:ARG:NH2	35:h:177:THR:O	2.32	0.60
1:1:2188:U:H3'	1:1:2189:U:H5"	1.82	0.60
18:Q:76:TYR:OH	18:Q:92:ARG:NH1	2.34	0.60
25:X:17:ASN:OD1	25:X:27:ARG:NH1	2.35	0.60
1:1:402:A:N9	1:1:403:U:C6	2.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2279:G:N7	24:W:14:ARG:NH2	2.50	0.60
23:V:77:VAL:HG23	23:V:89:ILE:HG12	1.83	0.60
38:k:38:ARG:NH1	38:k:98:GLU:O	2.33	0.60
2:2:346:G:OP1	17:P:39:ARG:NH2	2.32	0.60
30:c:37:LYS:HA	30:c:48:ILE:HA	1.83	0.60
33:f:25:VAL:HB	33:f:35:GLN:HB2	1.83	0.60
1:1:819:A:OP2	1:1:1187:G:N2	2.34	0.60
1:1:1428:C:N4	1:1:1570:A:OP2	2.33	0.60
1:1:2061:G:N7	1:1:2501:C:O2'	2.35	0.60
6:C:179:ARG:HB3	6:C:188:LEU:HD12	1.84	0.60
1:1:2772:C:H5'	6:C:173:GLN:HE21	1.67	0.60
3:3:9:G:OP2	16:O:15:ARG:NH1	2.35	0.60
10:G:86:ASP:OD2	38:k:24:ARG:NH1	2.35	0.60
13:L:55:MET:O	13:L:60:ARG:NH2	2.35	0.60
1:1:340:A:O2'	7:D:162:ARG:NH1	2.35	0.59
3:3:36:C:N4	3:3:49:C:O2	2.35	0.59
23:V:36:ALA:O	23:V:93:ARG:NH2	2.35	0.59
2:2:933:G:O6	39:l:3:ARG:NH2	2.33	0.59
13:L:58:TYR:O	32:e:13:ARG:NH2	2.35	0.59
1:1:796:C:OP1	7:D:57:LYS:NZ	2.34	0.59
2:2:1071:C:OP1	37:j:54:ARG:NH2	2.35	0.59
38:k:6:ILE:HG12	38:k:89:VAL:HG22	1.84	0.59
55:A:140:GLU:OE2	55:A:203:ARG:NH2	2.36	0.59
1:1:226:A:N1	1:1:418:C:O2'	2.35	0.59
30:c:17:THR:HG22	30:c:19:HIS:H	1.67	0.59
1:1:1715:G:N2	1:1:1744:A:OP2	2.34	0.59
2:2:1368:A:OP1	42:o:64:GLN:NE2	2.35	0.59
2:2:1377:A:OP1	39:l:92:ARG:NH1	2.36	0.59
49:v:24:ALA:HA	49:v:43:LYS:HA	1.83	0.59
1:1:1693:U:O2	5:B:14:ARG:NH1	2.35	0.59
2:2:626:G:O3'	48:u:51:ARG:NH1	2.36	0.59
2:2:246:A:N1	2:2:278:G:O2'	2.35	0.59
2:2:1073:U:O2	34:g:103:ASN:ND2	2.35	0.59
9:F:35:ARG:NH1	9:F:75:MET:SD	2.75	0.59
1:1:1079:C:H41	1:1:1088:A:H5'	1.67	0.59
2:2:664:G:H22	2:2:741:G:H1	1.50	0.59
2:2:1318:A:N3	51:x:37:ARG:NH1	2.51	0.59
1:1:1266:G:OP1	29:b:16:ARG:NE	2.27	0.59
1:1:1417:C:N4	1:1:1581:G:O6	2.36	0.59
2:2:1033:G:O2'	2:2:1034:G:O5'	2.20	0.59
37:j:13:GLU:HG2	37:j:39:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1365:A:O2'	25:X:11:ARG:NH1	2.35	0.58
1:1:2293:G:H5"	16:O:94:ARG:HH22	1.68	0.58
1:1:2305:U:H5"	8:E:131:GLY:HA3	1.85	0.58
1:1:2885:G:N1	29:b:30:VAL:O	2.36	0.58
2:2:3:A:HO2'	2:2:612:C:HO2'	1.51	0.58
2:2:373:A:H61	2:2:391:G:H1'	1.68	0.58
2:2:811:C:H4'	2:2:901:A:H61	1.67	0.58
21:T:54:GLU:HB3	21:T:88:LYS:HD2	1.84	0.58
32:e:31:HIS:HD2	32:e:32:ILE:HG12	1.67	0.58
10:G:51:ARG:HA	10:G:54:LEU:HB3	1.85	0.58
49:v:76:VAL:HG23	49:v:77:ARG:HG2	1.85	0.58
55:A:124:ASP:OD1	55:A:193:ARG:NH1	2.36	0.58
1:1:2126:A:N3	1:1:2127:G:O2'	2.36	0.58
3:3:75:G:HO2'	23:V:88:HIS:HE2	1.51	0.58
20:S:83:LYS:HB3	20:S:97:LEU:HD13	1.85	0.58
35:h:34:ASP:HB2	46:s:65:ARG:HH21	1.69	0.58
1:1:517:C:OP2	29:b:10:ARG:NH2	2.36	0.58
2:2:45:G:H1	2:2:396:C:H42	1.49	0.58
2:2:229:U:O2'	48:u:25:ARG:NH2	2.37	0.58
2:2:1055:A:O2'	35:h:156:ARG:NH2	2.36	0.58
1:1:276:U:O2	1:1:278:A:N6	2.37	0.58
1:1:323:C:H5'	7:D:163:ASN:HD21	1.69	0.58
1:1:1287:A:H5'	15:N:103:ARG:HD2	1.85	0.58
1:1:2107:G:N1	1:1:2183:A:N1	2.51	0.58
1:1:2425:A:C5'	1:1:2427:C:O4'	2.51	0.58
1:1:2747:G:H1	1:1:2754:U:H2'	1.68	0.58
2:2:333:U:OP1	52:y:2:ALA:N	2.36	0.58
2:2:1136:C:H5'	2:2:1137:C:C6	2.39	0.58
55:A:11:ILE:HD11	55:A:84:LEU:HD12	1.86	0.58
12:K:21:CYS:HA	12:K:41:ILE:HG22	1.85	0.58
2:2:73:C:N3	2:2:74:A:N6	2.52	0.58
37:j:87:GLY:N	37:j:94:VAL:O	2.37	0.58
1:1:1266:G:O2'	1:1:2012:G:O6	2.21	0.58
1:1:2831:G:OP2	6:C:59:ARG:NH1	2.37	0.58
2:2:667:G:O3'	47:t:50:HIS:HB2	2.04	0.58
2:2:1101:A:OP2	34:g:95:ARG:NH1	2.37	0.58
2:2:1150:A:H4'	42:o:43:PRO:HG3	1.84	0.58
5:B:117:GLN:O	5:B:128:ASN:ND2	2.33	0.58
2:2:1048:G:N1	2:2:1210:C:N3	2.52	0.58
2:2:1414:U:H2'	2:2:1415:G:H8	1.68	0.58
54:5:7:U:O2'	54:5:21:A:N1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:402:A:N1	1:1:403:U:H1'	2.19	0.57
1:1:784:G:N7	1:1:792:A:C5	2.72	0.57
1:1:878:A:N6	1:1:899:A:O2'	2.35	0.57
1:1:2134:A:H1'	1:1:2159:G:H1'	1.85	0.57
1:1:2846:G:OP1	17:P:53:ARG:NH1	2.34	0.57
2:2:264:C:O3'	49:v:65:ARG:NH2	2.37	0.57
6:C:181:ASP:OD2	6:C:184:ARG:NH2	2.37	0.57
14:M:34:LYS:HA	14:M:101:VAL:HA	1.86	0.57
39:l:27:VAL:HG12	39:l:43:VAL:HG21	1.85	0.57
49:v:61:ILE:HA	49:v:75:LEU:HA	1.86	0.57
55:A:334:LYS:HG2	55:A:341:GLU:HG2	1.85	0.57
1:1:643:A:N1	1:1:2369:A:O2'	2.35	0.57
1:1:1935:G:H3'	1:1:1962:5MC:HN41	1.69	0.57
1:1:2061:G:N2	56:6:79:PHE:HB3	2.19	0.57
2:2:923:A:N6	2:2:1392:G:O6	2.37	0.57
5:B:71:LYS:NZ	5:B:100:GLU:OE1	2.35	0.57
1:1:601:C:O2'	7:D:99:LYS:NZ	2.37	0.57
15:N:44:LEU:O	15:N:48:VAL:N	2.36	0.57
17:P:30:VAL:HG12	17:P:81:VAL:HG12	1.86	0.57
37:j:133:PRO:HA	37:j:136:VAL:HG12	1.85	0.57
2:2:467:U:O2	2:2:467:U:H2'	2.04	0.57
51:x:3:ARG:HE	51:x:7:LYS:HB3	1.68	0.57
2:2:1297:G:O2'	39:l:114:LYS:NZ	2.35	0.57
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.37	0.57
1:1:1077:A:N1	1:1:1088:A:O2'	2.37	0.57
1:1:1871:A:N7	1:1:1872:A:N6	2.52	0.57
1:1:2114:A:N6	1:1:2167:U:O2'	2.38	0.57
1:1:2204:G:OP2	5:B:147:LYS:NZ	2.37	0.57
1:1:2419:U:OP1	32:e:41:LYS:NZ	2.36	0.57
2:2:626:G:OP1	48:u:35:ARG:NH2	2.38	0.57
6:C:6:GLY:N	6:C:201:LEU:O	2.31	0.57
45:r:11:ASP:HA	45:r:45:ILE:HB	1.86	0.57
1:1:799:G:H3'	1:1:800:A:H2'	1.86	0.57
36:i:85:ASN:HA	37:j:102:GLY:HA3	1.86	0.57
1:1:2163:A:H3'	1:1:2164:C:H4'	1.86	0.57
2:2:1033:G:H2'	2:2:1034:G:C8	2.39	0.57
13:L:23:ILE:HB	19:R:84:ARG:HH22	1.70	0.57
55:A:162:LYS:HB3	55:A:184:SER:HB3	1.87	0.57
1:1:477:A:N6	1:1:500:G:O3'	2.37	0.57
2:2:980:C:O2'	46:s:13:ARG:NH1	2.38	0.57
9:F:16:ASP:HB3	9:F:27:LYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:6:LEU:HD11	10:G:37:VAL:HG23	1.87	0.57
1:1:243:U:OP2	32:e:8:ARG:NH1	2.38	0.56
1:1:1170:C:H6	1:1:1170:C:H5"	1.70	0.56
2:2:1178:G:N2	2:2:1181:G:OP2	2.38	0.56
15:N:6:SER:OG	15:N:46:ARG:NE	2.34	0.56
17:P:60:THR:HG23	17:P:73:VAL:HG22	1.85	0.56
1:1:910:A:N3	1:1:2264:C:O2'	2.36	0.56
1:1:1901:A:OP2	5:B:253:LYS:NZ	2.39	0.56
2:2:86:G:O2'	2:2:87:C:O5'	2.23	0.56
2:2:405:U:O4	36:i:2:ALA:N	2.38	0.56
2:2:674:G:OP1	38:k:86:ARG:NH2	2.39	0.56
2:2:1072:G:O6	2:2:1102:A:N6	2.38	0.56
6:C:150:GLN:O	6:C:151:THR:O	2.23	0.56
1:1:918:A:OP2	1:1:2268:A:N6	2.38	0.56
1:1:2351:G:O6	32:e:42:ARG:NH1	2.39	0.56
5:B:142:HIS:ND1	5:B:193:GLY:O	2.34	0.56
5:B:258:ARG:NH1	5:B:264:ASP:OD1	2.38	0.56
7:D:6:LYS:O	7:D:9:GLN:NE2	2.38	0.56
10:G:72:ILE:HD11	10:G:108:VAL:HG23	1.86	0.56
10:G:127:GLU:HA	10:G:145:ASN:HA	1.86	0.56
22:U:46:GLN:NE2	22:U:54:GLN:OE1	2.39	0.56
39:l:72:THR:HA	39:l:96:ARG:HH12	1.71	0.56
55:A:126:ALA:HB1	55:A:225:GLU:HB3	1.86	0.56
1:1:563:A:OP2	19:R:79:ARG:NH2	2.37	0.56
2:2:151:A:OP2	2:2:169:C:N4	2.38	0.56
2:2:1451:U:OP2	2:2:1452:C:N4	2.39	0.56
3:3:66:A:O5'	3:3:108:A:N6	2.38	0.56
29:b:30:VAL:HG22	29:b:37:LYS:HG2	1.87	0.56
2:2:254:G:N2	49:v:18:GLU:OE2	2.32	0.56
2:2:728:A:H62	47:t:54:ARG:HD3	1.71	0.56
49:v:68:SER:HB3	49:v:71:LYS:HB3	1.88	0.56
1:1:574:A:N6	1:1:2034:U:OP1	2.39	0.56
1:1:1864:U:H3	1:1:1878:G:H1	1.53	0.56
8:E:122:PHE:HA	8:E:128:TYR:HA	1.88	0.56
1:1:668:A:H2'	1:1:670:A:H62	1.71	0.56
1:1:1779:U:OP2	1:1:1784:A:N6	2.39	0.56
1:1:1188:U:H2'	1:1:1189:A:H8	1.71	0.56
2:2:1086:U:H2'	2:2:1087:G:H8	1.71	0.56
10:G:129:GLU:HA	10:G:143:ILE:HA	1.88	0.56
23:V:58:SER:O	23:V:73:LYS:NZ	2.39	0.56
1:1:329:G:OP2	22:U:69:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:390:U:H2'	2:2:391:G:H8	1.68	0.56
1:1:2692:G:O2'	1:1:2847:U:O2	2.24	0.56
2:2:1376:U:O4	39:l:10:ARG:NH1	2.38	0.56
1:1:2119:A:N6	1:1:2167:U:O2'	2.39	0.55
5:B:2:ALA:N	5:B:20:VAL:O	2.39	0.55
8:E:29:PRO:HB2	8:E:169:LEU:HD22	1.88	0.55
13:L:29:LYS:HG3	13:L:30:THR:HG23	1.87	0.55
16:O:89:ASP:HA	16:O:116:GLN:HB3	1.88	0.55
2:2:1317:C:OP1	46:s:24:ARG:NH2	2.39	0.55
49:v:20:SER:OG	49:v:71:LYS:NZ	2.35	0.55
1:1:717:C:H3'	1:1:718:A:H8	1.71	0.55
1:1:1913:A:N7	2:2:1493:A:O2'	2.35	0.55
1:1:2530:A:O2'	1:1:2534:A:N6	2.40	0.55
2:2:376:G:O2'	48:u:5:ARG:NH1	2.39	0.55
2:2:1149:C:O2'	2:2:1280:A:N1	2.37	0.55
6:C:181:ASP:HB3	6:C:186:LEU:HB2	1.88	0.55
1:1:177:G:OP2	1:1:177:G:N2	2.38	0.55
1:1:2061:G:OP1	1:1:2503:2MA:HM23	2.06	0.55
2:2:795:C:H4'	43:p:128:ARG:HH21	1.71	0.55
3:3:48:U:OP1	16:O:30:ARG:NH2	2.38	0.55
39:l:118:LEU:O	39:l:122:ASN:ND2	2.39	0.55
1:1:1414:C:O2	1:1:1588:G:N2	2.39	0.55
1:1:2746:U:H5'	9:F:138:LYS:HG2	1.87	0.55
2:2:373:A:N1	2:2:391:G:O2'	2.38	0.55
8:E:131:GLY:HA2	8:E:153:ASP:HA	1.89	0.55
23:V:57:TYR:OH	23:V:79:ARG:NH2	2.40	0.55
29:b:31:ASP:OD2	29:b:34:SER:N	2.39	0.55
1:1:1040:A:OP1	23:V:46:LYS:NZ	2.39	0.55
1:1:1652:A:N6	15:N:11:ASN:OD1	2.39	0.55
2:2:110:C:H2'	2:2:111:G:O4'	2.06	0.55
2:2:374:A:N1	2:2:390:U:O2'	2.38	0.55
2:2:1425:U:H2'	2:2:1426:G:H8	1.71	0.55
19:R:6:GLN:HG2	19:R:11:GLN:HG2	1.88	0.55
47:t:59:MET:HA	47:t:62:GLN:HB3	1.87	0.55
1:1:673:C:OP1	7:D:49:ARG:NH2	2.38	0.55
1:1:1227:G:OP2	18:Q:16:LYS:NZ	2.38	0.55
1:1:1419:A:H5'	1:1:1579:A:H61	1.71	0.55
1:1:2507:C:OP1	55:A:256:ARG:NH1	2.40	0.55
19:R:52:PRO:O	19:R:53:PHE:CD2	2.59	0.55
34:g:3:THR:N	34:g:51:ASN:OD1	2.40	0.55
54:5:33:U:N3	54:5:36:A:OP2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:247:G:OP2	1:1:249:C:N4	2.34	0.55
1:1:1998:A:HO2'	1:1:2724:U:HO2'	1.53	0.55
2:2:222:C:H2'	2:2:223:A:H8	1.72	0.55
2:2:297:G:N2	2:2:300:A:OP2	2.36	0.55
2:2:362:G:N2	2:2:365:U:OP2	2.39	0.55
1:1:714:U:OP2	47:t:88:ARG:NH1	2.40	0.55
2:2:8:A:N6	36:i:202:GLU:O	2.39	0.55
2:2:405:U:OP2	36:i:3:ARG:NH1	2.40	0.55
2:2:429:U:H3'	36:i:9:LEU:HD12	1.89	0.55
2:2:1249:C:N4	2:2:1288:A:OP2	2.40	0.55
7:D:117:ARG:HH21	7:D:184:ASP:HA	1.72	0.55
25:X:5:CYS:HB2	25:X:33:LEU:HD11	1.88	0.55
25:X:36:HIS:ND1	25:X:37:ARG:O	2.38	0.55
1:1:2036:C:H2'	1:1:2037:A:H8	1.70	0.55
1:1:2308:G:H2'	1:1:2310:C:H41	1.72	0.55
2:2:373:A:O2'	2:2:451:A:N7	2.40	0.55
24:W:68:LYS:NZ	24:W:69:PHE:O	2.40	0.55
1:1:220:G:H22	1:1:427:U:H2'	1.72	0.54
1:1:861:A:N3	3:3:79:G:O2'	2.37	0.54
1:1:1363:C:O2'	1:1:1809:A:N3	2.39	0.54
2:2:216:U:O2'	2:2:468:A:N6	2.41	0.54
2:2:389:A:H2'	2:2:390:U:H5'	1.89	0.54
2:2:1304:G:H21	2:2:1333:A:H62	1.55	0.54
5:B:66:ASP:OD2	5:B:102:ARG:NH1	2.40	0.54
1:1:1789:A:OP2	5:B:221:ARG:NH1	2.39	0.54
2:2:309:A:O2'	2:2:607:A:N1	2.39	0.54
17:P:52:ASN:O	17:P:53:ARG:NH1	2.38	0.54
24:W:37:ILE:HG22	24:W:38:VAL:HG23	1.89	0.54
1:1:460:A:OP2	31:d:41:ARG:NH1	2.38	0.54
1:1:1528:A:N6	1:1:1543:G:O2'	2.39	0.54
14:M:47:GLU:OE2	14:M:50:ARG:NH1	2.41	0.54
1:1:402:A:H2'	1:1:403:U:H5'	1.90	0.54
2:2:542:G:O3'	36:i:14:ARG:NH2	2.38	0.54
12:K:102:PRO:HD2	17:P:68:GLU:HG3	1.90	0.54
15:N:87:PHE:HD1	15:N:90:ARG:HD3	1.71	0.54
47:t:57:LEU:O	47:t:60:VAL:HB	2.07	0.54
1:1:402:A:H2'	1:1:403:U:C5'	2.38	0.54
1:1:956:G:O6	14:M:14:LYS:NZ	2.41	0.54
1:1:2189:U:H4'	1:1:2189:U:OP1	2.07	0.54
2:2:120:A:O2'	2:2:122:G:N7	2.37	0.54
2:2:691:G:O6	43:p:53:ARG:NH2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1259:C:O2'	2:2:1283:U:O2	2.22	0.54
17:P:91:ALA:HB2	17:P:113:ARG:HA	1.90	0.54
50:w:11:CYS:SG	50:w:12:ARG:N	2.81	0.54
1:1:1250:G:N7	13:L:18:ARG:NH2	2.49	0.54
1:1:2532:G:O2'	1:1:2657:A:N1	2.40	0.54
2:2:376:G:H5'	48:u:5:ARG:HB2	1.88	0.54
2:2:841:C:H2'	2:2:843:U:H5"	1.89	0.54
2:2:865:A:N3	2:2:918:A:O2'	2.40	0.54
5:B:108:LYS:HA	5:B:196:GLY:HA2	1.88	0.54
36:i:139:PRO:HA	36:i:182:PHE:HD2	1.73	0.54
1:1:1807:G:N2	1:1:1810:A:OP2	2.35	0.54
2:2:71:A:H61	2:2:99:C:H1'	1.73	0.54
2:2:1015:G:N2	2:2:1218:C:O2	2.39	0.54
37:j:12:GLN:HE21	37:j:117:VAL:HA	1.73	0.54
45:r:68:ASP:OD1	45:r:71:ARG:NH1	2.38	0.54
2:2:197:A:N1	2:2:220:G:O2'	2.37	0.54
2:2:653:U:O4'	40:m:56:LYS:NZ	2.39	0.54
39:l:47:LEU:HD23	39:l:58:GLU:HB3	1.90	0.54
45:r:89:LEU:HA	45:r:92:ARG:HG2	1.89	0.54
1:1:2467:C:O2	14:M:123:LYS:NZ	2.41	0.54
2:2:510:A:HO2'	2:2:542:G:HO2'	1.55	0.54
35:h:131:ARG:NH1	35:h:166:GLU:OE2	2.41	0.54
1:1:2576:G:O2'	1:1:2579:C:OP2	2.24	0.54
1:1:2756:U:O4'	1:1:2757:A:C8	2.61	0.54
2:2:1071:C:H2'	2:2:1072:G:H8	1.72	0.54
1:1:2688:G:N1	1:1:2720:U:OP2	2.34	0.53
8:E:115:ARG:HA	28:a:47:LYS:HD2	1.90	0.53
20:S:77:ASP:HB2	20:S:102:HIS:HB2	1.89	0.53
1:1:2825:G:OP2	1:1:2825:G:N2	2.41	0.53
2:2:933:G:N7	39:l:3:ARG:NE	2.54	0.53
19:R:21:ARG:HD2	19:R:93:PHE:HB2	1.91	0.53
1:1:1068:G:O2'	1:1:1070:A:N6	2.40	0.53
1:1:2359:C:H2'	1:1:2360:G:C8	2.43	0.53
1:1:2451:A:N3	54:5:76:A:O2'	2.41	0.53
2:2:137:U:H2'	2:2:138:G:H8	1.73	0.53
8:E:34:ILE:HG12	8:E:156:ILE:HG12	1.90	0.53
10:G:117:LEU:HD21	10:G:130:VAL:HG22	1.89	0.53
30:c:8:LYS:HA	30:c:24:THR:HA	1.91	0.53
1:1:1418:G:N1	1:1:1579:A:OP2	2.41	0.53
1:1:2133:G:H1	1:1:2157:G:H2'	1.73	0.53
1:1:2484:G:OP1	14:M:44:ARG:NH1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:258:G:H1	2:2:268:U:H3	1.57	0.53
2:2:411:A:H4'	2:2:412:A:H5'	1.90	0.53
2:2:1060:U:OP1	46:s:85:ARG:NH1	2.41	0.53
14:M:66:ARG:NH1	14:M:104:GLU:OE2	2.41	0.53
43:p:28:ASN:O	43:p:57:LYS:NZ	2.34	0.53
55:A:274:CYS:SG	55:A:276:ASN:ND2	2.81	0.53
1:1:739:A:H1'	1:1:740:C:H5	1.74	0.53
1:1:1071:G:H1'	1:1:1089:A:H2'	1.90	0.53
1:1:2006:C:O2'	1:1:2823:A:N3	2.42	0.53
1:1:2449:U:O2'	1:1:2501:C:N4	2.42	0.53
2:2:1406:U:H5"	2:2:1407:5MC:HM52	1.90	0.53
43:p:88:GLY:H	43:p:114:THR:HG22	1.74	0.53
1:1:1365:A:OP2	25:X:2:SER:OG	2.27	0.53
22:U:40:ASN:ND2	22:U:64:ALA:O	2.42	0.53
36:i:73:ARG:HG3	36:i:77:LYS:HE2	1.91	0.53
41:n:36:GLU:OE1	41:n:45:ARG:NH1	2.41	0.53
6:C:46:ARG:NH1	6:C:85:ALA:O	2.38	0.53
55:A:117:ARG:NH1	55:A:358:GLU:O	2.42	0.53
1:1:265:A:O2'	1:1:428:A:N6	2.41	0.53
2:2:227:G:O2'	48:u:63:GLN:OE1	2.25	0.53
38:k:9:MET:HB2	38:k:86:ARG:H	1.73	0.53
1:1:807:U:OP2	13:L:41:ARG:NH1	2.40	0.53
1:1:973:A:OP2	19:R:81:LYS:NZ	2.35	0.53
1:1:2508:G:HO2'	1:1:2554:U:HO2'	1.54	0.53
21:T:22:THR:O	21:T:26:LYS:NZ	2.42	0.53
1:1:402:A:H2'	1:1:403:U:C4'	2.39	0.53
1:1:865:C:O2	1:1:867:C:N4	2.37	0.53
2:2:979:C:OP1	2:2:1223:C:N4	2.41	0.53
8:E:4:LEU:O	8:E:8:TYR:N	2.39	0.53
17:P:46:VAL:N	17:P:62:ARG:O	2.41	0.53
25:X:43:GLU:OE1	25:X:45:ARG:NH1	2.42	0.53
48:u:21:VAL:HG12	48:u:33:ILE:HB	1.91	0.53
1:1:2680:U:H5'	6:C:194:PRO:HA	1.91	0.52
2:2:338:A:H2	2:2:351:G:H22	1.56	0.52
12:K:43:ILE:HD12	12:K:56:ASP:HB2	1.91	0.52
51:x:36:ARG:NH2	51:x:72:GLY:O	2.43	0.52
52:y:4:ILE:HG22	52:y:6:SER:H	1.75	0.52
1:1:1364:G:N2	1:1:1367:A:OP2	2.34	0.52
1:1:2692:G:H2'	1:1:2693:G:H8	1.74	0.52
1:1:2901:C:H6	1:1:2901:C:H5"	1.74	0.52
2:2:299:G:N2	2:2:565:U:O2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:t:50:HIS:HA	47:t:53:ARG:HH11	1.73	0.52
1:1:402:A:C4	1:1:403:U:C6	2.97	0.52
1:1:1344:U:OP1	1:1:1345:C:N4	2.42	0.52
2:2:300:A:O2'	2:2:564:C:N3	2.35	0.52
2:2:579:A:H5'	2:2:728:A:H1'	1.89	0.52
2:2:728:A:N6	47:t:54:ARG:HD3	2.24	0.52
5:B:262:ARG:O	5:B:265:LYS:NZ	2.41	0.52
12:K:71:ARG:NE	12:K:106:GLU:OE2	2.42	0.52
15:N:47:VAL:O	15:N:51:LEU:N	2.42	0.52
40:m:49:PHE:HB2	40:m:59:LEU:HD11	1.91	0.52
40:m:74:SER:HB3	40:m:130:ALA:HB3	1.91	0.52
1:1:1682:G:OP2	1:1:1699:G:N2	2.42	0.52
1:1:1995:U:H3'	1:1:1996:C:H2'	1.91	0.52
2:2:265:G:H5'	49:v:65:ARG:HH22	1.73	0.52
2:2:1268:G:N3	2:2:1326:U:O2'	2.43	0.52
3:3:80:U:O4	23:V:14:LYS:NZ	2.39	0.52
11:J:68:LYS:HA	11:J:71:ASP:HB2	1.90	0.52
37:j:45:ARG:NH2	37:j:73:ASN:OD1	2.42	0.52
47:t:69:TYR:O	47:t:72:ARG:C	2.52	0.52
55:A:242:ASP:HB2	55:A:262:ARG:HB3	1.92	0.52
1:1:29:U:H2'	1:1:30:G:H8	1.74	0.52
1:1:279:A:OP2	1:1:361:G:N2	2.42	0.52
1:1:500:G:N1	1:1:503:A:OP2	2.34	0.52
1:1:2552:OMU:H2'	1:1:2554:U:OP2	2.09	0.52
2:2:202:G:H21	2:2:466:A:H61	1.56	0.52
6:C:111:GLY:N	6:C:170:VAL:O	2.42	0.52
1:1:307:G:N1	1:1:310:A:OP2	2.39	0.52
1:1:2584:U:H2'	1:1:2585:U:H2'	1.92	0.52
2:2:718:A:N6	50:w:70:TYR:O	2.41	0.52
2:2:1305:G:N2	2:2:1332:A:OP2	2.43	0.52
2:2:1441:A:H62	2:2:1461:G:H21	1.57	0.52
10:G:78:VAL:HG21	10:G:103:VAL:HG22	1.91	0.52
36:i:91:LEU:HD23	36:i:94:LEU:HD12	1.90	0.52
55:A:117:ARG:O	55:A:193:ARG:NH2	2.43	0.52
55:A:195:GLU:OE2	55:A:324:ARG:NH2	2.42	0.52
1:1:2689:U:OP2	1:1:2691:C:N4	2.42	0.52
2:2:826:C:O2	40:m:16:ASN:ND2	2.43	0.52
2:2:1227:A:OP1	51:x:80:TYR:OH	2.26	0.52
3:3:75:G:O2'	23:V:88:HIS:NE2	2.42	0.52
3:3:111:U:H2'	3:3:112:G:H8	1.75	0.52
20:S:4:ILE:HG12	20:S:106:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:t:50:HIS:HA	47:t:53:ARG:HD2	1.92	0.52
55:A:168:GLU:HA	55:A:179:VAL:HG12	1.92	0.52
1:1:287:G:O6	1:1:352:A:N6	2.43	0.52
1:1:781:A:OP1	5:B:217:ARG:NH2	2.43	0.52
2:2:1261:A:N6	2:2:1274:A:O2'	2.37	0.52
7:D:62:GLN:HG3	7:D:63:LYS:HG3	1.91	0.52
1:1:1817:G:OP1	5:B:87:ARG:NH2	2.39	0.52
1:1:1870:C:OP1	1:1:1871:A:N6	2.42	0.52
1:1:2753:A:O2'	33:f:15:LYS:NZ	2.42	0.52
2:2:1305:G:H21	2:2:1332:A:H2	1.57	0.52
3:3:39:A:H2	3:3:44:G:H5'	1.75	0.52
15:N:44:LEU:HA	15:N:47:VAL:HB	1.90	0.52
19:R:75:VAL:HG22	19:R:86:GLN:HE22	1.75	0.52
51:x:3:ARG:NH1	51:x:9:PRO:O	2.43	0.52
1:1:2112:G:OP1	1:1:2115:G:N2	2.42	0.52
2:2:1003:G:N2	2:2:1005:A:O5'	2.43	0.52
9:F:29:LYS:NZ	9:F:80:THR:O	2.40	0.52
9:F:95:ARG:HB2	9:F:128:GLN:HB3	1.92	0.52
15:N:98:LEU:HB2	15:N:112:TYR:HB2	1.90	0.52
19:R:8:GLY:O	19:R:10:LYS:NZ	2.41	0.52
27:Z:17:LEU:HB2	27:Z:20:HIS:HD2	1.74	0.52
37:j:12:GLN:HG3	37:j:117:VAL:HG12	1.91	0.52
1:1:402:A:C2'	1:1:403:U:H5'	2.40	0.51
1:1:442:G:N2	7:D:43:THR:O	2.43	0.51
1:1:2391:G:N1	1:1:2425:A:OP1	2.23	0.51
2:2:62:U:O2'	2:2:379:C:O2	2.27	0.51
7:D:46:GLN:HB3	7:D:83:VAL:HG21	1.92	0.51
12:K:88:ASN:HB3	12:K:92:GLU:H	1.74	0.51
1:1:335:C:O2	22:U:68:SER:OG	2.28	0.51
1:1:336:C:H6	1:1:336:C:H5"	1.75	0.51
1:1:482:A:N6	1:1:506:G:O2'	2.43	0.51
1:1:2045:C:O2	29:b:19:HIS:NE2	2.42	0.51
1:1:2590:A:O3'	5:B:238:ARG:NH1	2.43	0.51
2:2:34:C:H2'	2:2:35:G:H8	1.75	0.51
2:2:368:U:H2'	2:2:368:U:O2	2.09	0.51
10:G:76:GLU:HA	10:G:142:VAL:HG13	1.92	0.51
55:A:203:ARG:HD3	55:A:328:LEU:HD12	1.92	0.51
1:1:1941:C:H2'	1:1:1942:C:O4'	2.10	0.51
1:1:2134:A:OP1	1:1:2159:G:N2	2.43	0.51
1:1:2645:G:OP2	1:1:2645:G:N2	2.35	0.51
3:3:77:U:OP1	23:V:21:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:4:LEU:HA	8:E:7:TYR:HB3	1.92	0.51
10:G:51:ARG:HG3	10:G:54:LEU:HD23	1.92	0.51
39:l:139:GLU:O	39:l:143:ARG:N	2.42	0.51
54:5:18:G:OP2	54:5:60:U:O2'	2.28	0.51
1:1:1028:A:N6	1:1:1126:A:OP1	2.43	0.51
1:1:2131:U:H5'	1:1:2132:U:H5"	1.93	0.51
2:2:438:U:O2'	2:2:494:G:O6	2.24	0.51
3:3:28:C:H5"	16:O:31:THR:HG21	1.93	0.51
5:B:140:THR:HG22	5:B:163:GLN:HG2	1.92	0.51
36:i:75:TYR:OH	36:i:97:ARG:NH1	2.44	0.51
43:p:94:GLU:OE2	43:p:98:ARG:NH2	2.41	0.51
1:1:265:A:N1	1:1:427:U:O2'	2.42	0.51
1:1:298:G:O2'	1:1:322:A:N1	2.43	0.51
1:1:1020:A:N1	1:1:1141:U:O2'	2.44	0.51
2:2:217:C:H4'	2:2:217:C:OP1	2.10	0.51
19:R:38:VAL:HG13	19:R:54:VAL:HB	1.92	0.51
34:g:20:THR:HA	34:g:39:HIS:HE1	1.75	0.51
35:h:140:ASN:OD1	35:h:143:ARG:NH2	2.43	0.51
1:1:780:G:H5"	5:B:217:ARG:HH22	1.75	0.51
1:1:1326:U:O2'	1:1:2010:G:O2'	2.26	0.51
1:1:1798:U:OP2	5:B:271:ARG:NH2	2.41	0.51
1:1:2131:U:O5'	1:1:2158:A:N6	2.44	0.51
2:2:1209:C:O2'	2:2:1214:C:N4	2.39	0.51
22:U:72:ILE:HD12	22:U:83:VAL:HG21	1.93	0.51
1:1:1586:A:H3'	1:1:1587:G:H8	1.76	0.51
1:1:2684:U:O4'	12:K:70:ARG:NH1	2.42	0.51
2:2:1255:G:O2'	2:2:1258:G:N3	2.38	0.51
5:B:106:ALA:O	5:B:196:GLY:N	2.41	0.51
18:Q:47:TYR:OH	18:Q:51:ARG:NH2	2.34	0.51
23:V:72:VAL:HA	23:V:94:ALA:H	1.75	0.51
34:g:94:HIS:ND1	34:g:146:ASN:O	2.43	0.51
38:k:42:TRP:HB2	38:k:59:TYR:HB2	1.93	0.51
49:v:17:MET:HG3	49:v:20:SER:HB2	1.92	0.51
54:5:15:C:H5"	54:5:15:C:O2	2.10	0.51
1:1:994:C:O2'	1:1:996:A:OP1	2.28	0.51
1:1:1170:C:H5"	1:1:1170:C:C6	2.45	0.51
1:1:2061:G:H5'	1:1:2061:G:H8	1.76	0.51
1:1:2266:A:N6	1:1:2273:A:OP2	2.44	0.51
1:1:2521:C:H42	1:1:2544:G:H1	1.59	0.51
2:2:219:U:H2'	2:2:220:G:H8	1.75	0.51
2:2:868:C:H2'	2:2:869:G:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:66:A:O4'	3:3:108:A:N6	2.44	0.51
18:Q:12:ALA:HA	18:Q:15:LYS:HB2	1.92	0.51
1:1:1089:A:H2	1:1:1090:A:H62	1.58	0.51
1:1:1667:G:O2'	1:1:1991:U:O4	2.28	0.51
2:2:14:U:N3	2:2:17:U:OP2	2.43	0.51
2:2:80:A:OP2	2:2:83:C:N4	2.37	0.51
8:E:134:GLU:HG2	8:E:136:ILE:H	1.76	0.51
29:b:54:VAL:HG23	29:b:55:ILE:HG22	1.93	0.51
36:i:100:ASN:OD1	36:i:111:ARG:NH1	2.37	0.51
40:m:94:LYS:HG3	40:m:117:ARG:HH22	1.75	0.51
42:o:7:ARG:HB2	42:o:101:SER:HB2	1.92	0.51
3:3:76:G:OP1	23:V:9:ARG:NH2	2.35	0.51
6:C:97:SER:OG	6:C:98:VAL:N	2.44	0.51
8:E:47:LYS:HG2	8:E:51:ASP:HB2	1.93	0.51
15:N:37:THR:HA	15:N:110:MET:HA	1.92	0.51
39:l:111:ARG:NH1	39:l:126:ASP:OD2	2.43	0.51
1:1:514:A:N3	1:1:581:C:O2'	2.43	0.50
1:1:1340:U:OP1	21:T:19:LYS:NZ	2.44	0.50
2:2:427:U:OP1	36:i:13:ARG:NH1	2.44	0.50
1:1:447:A:OP1	18:Q:5:LYS:NZ	2.40	0.50
15:N:58:ASP:HB2	15:N:80:PHE:HB3	1.92	0.50
16:O:110:ALA:HB1	16:O:115:LEU:HD12	1.94	0.50
1:1:220:G:O2'	1:1:233:A:N3	2.36	0.50
1:1:336:C:H5"	1:1:336:C:C6	2.46	0.50
1:1:1490:A:O2'	5:B:98:ASP:OD2	2.28	0.50
7:D:117:ARG:NH2	7:D:183:PHE:O	2.45	0.50
10:G:47:PHE:O	10:G:52:ALA:N	2.45	0.50
21:T:22:THR:HG22	21:T:26:LYS:HZ1	1.76	0.50
35:h:36:ASP:OD1	35:h:59:ARG:NH2	2.45	0.50
35:h:60:PRO:HB3	42:o:94:ALA:HB2	1.93	0.50
47:t:48:LYS:C	47:t:50:HIS:H	2.19	0.50
1:1:61:C:OP1	26:Y:47:ARG:NH1	2.45	0.50
1:1:403:U:O2	1:1:403:U:H2'	2.10	0.50
1:1:572:A:OP2	19:R:79:ARG:NH1	2.45	0.50
1:1:1170:C:H3'	1:1:1171:G:H8	1.76	0.50
1:1:2164:C:H5"	1:1:2171:A:H62	1.76	0.50
2:2:562:U:H1'	44:q:12:ARG:HD2	1.92	0.50
6:C:4:LEU:HG	6:C:32:ASN:HD21	1.76	0.50
28:a:56:ARG:HH11	51:x:68:GLY:HA3	1.76	0.50
35:h:40:ARG:NH1	35:h:55:ILE:O	2.43	0.50
46:s:86:GLU:HB3	46:s:90:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A:80:VAL:HG13	55:A:99:ALA:HB1	1.94	0.50
1:1:458:G:O2'	1:1:469:G:O6	2.29	0.50
1:1:684:G:O2'	1:1:788:A:N7	2.42	0.50
1:1:1006:C:O2'	11:J:108:MET:O	2.27	0.50
2:2:178:C:H2'	2:2:179:A:H8	1.76	0.50
3:3:5:U:OP1	3:3:61:G:O2'	2.29	0.50
5:B:244:PRO:O	5:B:251:GLN:NE2	2.45	0.50
34:g:167:ASP:O	34:g:170:HIS:ND1	2.42	0.50
54:5:53:G:H3'	54:5:54:5MU:H73	1.94	0.50
55:A:150:ARG:HA	55:A:153:LEU:HB2	1.93	0.50
55:A:164:GLU:HB3	55:A:182:LYS:HB3	1.92	0.50
55:A:241:ILE:HG12	55:A:263:ILE:HG12	1.94	0.50
1:1:818:G:N1	1:1:1188:U:OP2	2.35	0.50
1:1:1712:U:H3'	1:1:1713:A:H2'	1.94	0.50
1:1:1822:C:H2'	1:1:1823:G:H8	1.77	0.50
1:1:2708:G:H2'	1:1:2709:G:H8	1.76	0.50
2:2:1136:C:H5'	2:2:1137:C:C5	2.47	0.50
17:P:60:THR:HA	17:P:73:VAL:HG13	1.92	0.50
18:Q:49:ASP:O	18:Q:53:ARG:N	2.42	0.50
25:X:5:CYS:O	25:X:9:GLY:N	2.37	0.50
46:s:49:GLN:NE2	51:x:11:ILE:O	2.34	0.50
1:1:404:A:H5'	1:1:406:G:H1'	1.93	0.50
1:1:545:U:O2'	1:1:547:A:OP1	2.27	0.50
1:1:672:C:OP2	13:L:42:SER:OG	2.29	0.50
1:1:824:U:O2'	1:1:2358:A:N7	2.42	0.50
1:1:1469:A:OP2	1:1:1522:A:N6	2.40	0.50
1:1:2756:U:O4'	1:1:2757:A:H8	1.95	0.50
2:2:816:A:OP1	2:2:1526:G:O2'	2.27	0.50
40:m:5:ASP:OD2	40:m:77:ARG:NH1	2.38	0.50
1:1:107:G:H2'	1:1:108:G:H8	1.77	0.50
1:1:2013:A:H4'	20:S:96:ILE:HG22	1.93	0.50
1:1:2138:G:N7	1:1:2139:U:O2'	2.43	0.50
1:1:2286:G:C8	1:1:2286:G:H5'	2.47	0.50
1:1:2790:U:OP2	1:1:2893:A:N6	2.45	0.50
2:2:404:G:H4'	2:2:439:U:H5	1.77	0.50
2:2:753:A:H4'	2:2:754:C:O4'	2.11	0.50
13:L:135:ILE:HG22	13:L:140:GLY:HA3	1.94	0.50
1:1:395:U:O2'	1:1:396:G:N7	2.41	0.50
1:1:581:C:OP2	18:Q:33:ARG:NH2	2.45	0.50
1:1:748:G:P	20:S:88:ARG:HE	2.34	0.50
2:2:126:G:OP1	2:2:605:U:O2'	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:490:C:H2'	2:2:491:G:H8	1.77	0.50
2:2:718:A:O2'	53:z:35:ARG:NH2	2.43	0.50
2:2:1218:C:H2'	2:2:1219:A:C8	2.47	0.50
10:G:124:THR:O	10:G:128:HIS:NE2	2.45	0.50
19:R:43:ASN:HB3	19:R:46:GLU:HB3	1.94	0.50
19:R:50:GLY:O	19:R:51:VAL:C	2.55	0.50
37:j:15:LEU:HA	37:j:37:THR:HG22	1.92	0.50
46:s:45:VAL:HG21	51:x:3:ARG:HH22	1.77	0.50
49:v:59:VAL:HG23	49:v:78:VAL:HG22	1.93	0.50
55:A:14:LEU:HB2	55:A:77:LEU:HD21	1.94	0.50
1:1:158:U:H2'	1:1:159:G:O4'	2.12	0.49
1:1:1416:G:O6	1:1:1583:A:N6	2.45	0.49
2:2:50:A:O2'	2:2:360:G:N2	2.45	0.49
2:2:721:G:H4'	2:2:722:G:O4'	2.12	0.49
6:C:122:VAL:HB	6:C:141:ARG:HH21	1.77	0.49
18:Q:83:LEU:HA	18:Q:86:ALA:HB3	1.92	0.49
21:T:11:LEU:HD11	21:T:47:VAL:HG22	1.94	0.49
22:U:36:VAL:HG11	22:U:39:ILE:HD12	1.94	0.49
1:1:138:U:H4'	1:1:139:U:C2	2.47	0.49
1:1:776:G:N7	1:1:793:A:O2'	2.43	0.49
1:1:1009:A:OP1	11:J:39:LYS:NZ	2.44	0.49
1:1:1324:G:O2'	1:1:1326:U:OP2	2.31	0.49
1:1:1936:A:N6	1:1:1963:U:O2	2.45	0.49
1:1:2519:U:O4'	1:1:2542:A:N6	2.45	0.49
2:2:254:G:O2'	49:v:18:GLU:O	2.30	0.49
5:B:37:ASN:HB2	5:B:62:TYR:HB2	1.93	0.49
18:Q:72:ASN:HD22	18:Q:110:VAL:HG21	1.77	0.49
36:i:202:GLU:OE1	37:j:112:ARG:NH1	2.45	0.49
55:A:87:ALA:O	55:A:92:ASP:N	2.40	0.49
1:1:138:U:O2'	1:1:139:U:O2	2.26	0.49
1:1:320:A:O2'	1:1:322:A:OP2	2.24	0.49
1:1:403:U:C5'	1:1:406:G:O2'	2.59	0.49
2:2:677:U:H3	2:2:713:G:H1	1.60	0.49
2:2:880:C:H2'	2:2:881:G:H8	1.77	0.49
2:2:1236:A:H4'	2:2:1304:G:H4'	1.95	0.49
3:3:43:C:H5"	28:a:1:MET:HG2	1.93	0.49
24:W:46:HIS:CD2	24:W:77:ARG:HB3	2.47	0.49
32:e:32:ILE:O	32:e:32:ILE:HG22	2.12	0.49
37:j:97:GLN:HB3	37:j:124:LEU:HB2	1.93	0.49
38:k:46:GLN:HE22	38:k:55:HIS:HB3	1.77	0.49
39:l:75:VAL:HA	39:l:88:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A:87:ALA:HA	55:A:92:ASP:HB3	1.92	0.49
1:1:48:G:N1	1:1:177:G:OP2	2.44	0.49
1:1:1418:G:H1'	1:1:1581:G:H22	1.76	0.49
1:1:1889:A:N3	1:1:2086:U:O2'	2.41	0.49
1:1:2704:C:H3'	1:1:2705:A:C8	2.48	0.49
2:2:108:G:H5'	2:2:109:A:H5"	1.93	0.49
2:2:792:A:O2'	2:2:794:A:N7	2.41	0.49
2:2:1060:U:O2'	42:o:58:ASN:OD1	2.28	0.49
2:2:1328:C:HO2'	45:r:29:ARG:HH11	1.56	0.49
23:V:1:MET:N	23:V:59:GLU:OE1	2.45	0.49
36:i:152:GLN:O	36:i:156:LYS:NZ	2.46	0.49
2:2:668:G:P	47:t:50:HIS:HB2	2.53	0.49
2:2:1422:G:O2'	12:K:49:ARG:NH2	2.46	0.49
6:C:4:LEU:O	6:C:203:VAL:N	2.43	0.49
16:O:52:SER:OG	16:O:53:THR:N	2.44	0.49
22:U:29:LEU:HD12	22:U:33:LYS:HB2	1.94	0.49
31:d:9:VAL:O	31:d:13:ASN:ND2	2.46	0.49
40:m:92:LEU:O	40:m:117:ARG:NH2	2.42	0.49
1:1:79:C:O2'	1:1:346:A:N3	2.42	0.49
1:1:495:G:H21	20:S:61:ASN:HD21	1.60	0.49
1:1:1231:U:H2'	1:1:1232:G:H8	1.77	0.49
1:1:2667:C:N3	9:F:110:SER:OG	2.43	0.49
23:V:64:VAL:HG22	23:V:69:GLU:HG3	1.94	0.49
55:A:27:TYR:HE1	55:A:67:VAL:HA	1.78	0.49
1:1:459:U:H2'	1:1:460:A:H8	1.77	0.49
1:1:662:G:H2'	1:1:663:G:H8	1.77	0.49
1:1:1028:A:OP2	1:1:1126:A:N6	2.36	0.49
1:1:1808:A:O2'	1:1:1809:A:O4'	2.30	0.49
1:1:2684:U:OP1	17:P:51:ARG:NH1	2.46	0.49
1:1:2815:C:O2'	29:b:41:HIS:ND1	2.42	0.49
2:2:1152:A:OP1	42:o:70:HIS:ND1	2.45	0.49
8:E:68:THR:N	8:E:86:GLY:O	2.46	0.49
8:E:129:SER:HA	8:E:155:THR:HA	1.93	0.49
22:U:8:ASP:O	22:U:24:LYS:NZ	2.40	0.49
1:1:371:A:H61	1:1:401:A:H3'	1.77	0.49
1:1:1133:A:N6	1:1:2025:C:O2'	2.46	0.49
2:2:411:A:OP1	36:i:26:ARG:NH1	2.46	0.49
10:G:48:GLU:HA	10:G:52:ALA:HB2	1.93	0.49
14:M:47:GLU:OE2	14:M:51:ARG:NE	2.45	0.49
19:R:78:ARG:HB2	19:R:83:TYR:HB3	1.95	0.49
21:T:65:GLY:N	21:T:79:ASP:OD1	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:180:ALA:HA	35:h:206:GLU:HA	1.93	0.49
47:t:39:LEU:HD23	47:t:43:PHE:HE2	1.77	0.49
1:1:402:A:N3	1:1:403:U:H1'	2.25	0.49
1:1:781:A:H2'	1:1:1777:U:H1'	1.94	0.49
2:2:494:G:H2'	2:2:496:A:H8	1.77	0.49
3:3:5:U:H2'	3:3:6:G:H8	1.77	0.49
7:D:1:MET:HB3	7:D:14:VAL:HG23	1.94	0.49
9:F:83:PHE:N	9:F:135:GLY:O	2.46	0.49
21:T:35:ALA:HB3	21:T:38:ALA:HB2	1.94	0.49
34:g:97:LEU:H	34:g:100:MET:HE3	1.77	0.49
37:j:55:GLU:HG3	37:j:57:PRO:HD2	1.94	0.49
40:m:64:LYS:HG2	40:m:71:VAL:HG21	1.94	0.49
48:u:77:GLU:HA	48:u:80:LYS:HB2	1.94	0.49
1:1:894:U:C6	1:1:895:U:H5	2.31	0.49
1:1:2668:G:H1'	9:F:110:SER:HB2	1.94	0.49
2:2:222:C:H2'	2:2:223:A:C8	2.48	0.49
2:2:1130:A:N6	2:2:1144:G:N3	2.56	0.49
40:m:78:VAL:HG12	40:m:85:ILE:HG13	1.95	0.49
1:1:1926:U:N3	1:1:1929:G:OP2	2.42	0.48
1:1:2756:U:H4'	1:1:2757:A:O5'	2.13	0.48
2:2:217:C:H6	2:2:217:C:H5"	1.78	0.48
3:3:43:C:OP1	28:a:6:HIS:NE2	2.37	0.48
29:b:39:LEU:HB2	29:b:42:HIS:HB2	1.95	0.48
47:t:57:LEU:HA	47:t:60:VAL:CG2	2.43	0.48
1:1:467:G:OP2	31:d:34:ARG:NH1	2.43	0.48
1:1:894:U:H1'	1:1:895:U:H5'	1.95	0.48
1:1:1297:C:O2'	1:1:1302:A:N1	2.41	0.48
1:1:1306:C:N4	1:1:1607:C:OP2	2.46	0.48
1:1:1310:G:O2'	1:1:1611:C:OP1	2.29	0.48
1:1:1919:A:O2'	2:2:1517:G:N3	2.42	0.48
1:1:2595:G:N2	1:1:2598:A:OP2	2.32	0.48
16:O:60:GLU:HG3	16:O:61:GLN:HE21	1.79	0.48
39:l:93:PRO:HA	39:l:96:ARG:HD3	1.95	0.48
41:n:21:ILE:HG23	41:n:61:LEU:HD13	1.96	0.48
1:1:139:U:C5'	1:1:140:C:O5'	2.53	0.48
1:1:1252:G:OP2	1:1:1252:G:H4'	2.13	0.48
1:1:2117:A:N1	1:1:2170:A:N6	2.60	0.48
2:2:780:A:N6	2:2:801:U:OP2	2.42	0.48
8:E:123:ASP:C	8:E:125:ARG:H	2.21	0.48
17:P:104:THR:HA	17:P:108:ALA:HB2	1.95	0.48
22:U:14:LEU:HD11	22:U:71:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:188:ARG:HH12	36:i:193:ALA:HA	1.78	0.48
45:r:2:ALA:O	45:r:9:ILE:N	2.45	0.48
47:t:57:LEU:C	47:t:60:VAL:HB	2.39	0.48
1:1:1688:U:O2'	1:1:1700:A:N7	2.37	0.48
1:1:2039:U:H2'	1:1:2040:G:H8	1.78	0.48
1:1:2039:U:H2'	1:1:2040:G:C8	2.48	0.48
1:1:2515:C:H2'	1:1:2516:A:H8	1.77	0.48
1:1:2582:G:H2'	1:1:2583:G:H8	1.79	0.48
2:2:22:G:O2'	2:2:913:A:N1	2.42	0.48
2:2:675:A:O2'	43:p:116:ILE:O	2.24	0.48
12:K:61:VAL:HB	12:K:87:LEU:HD11	1.95	0.48
36:i:202:GLU:OE2	37:j:105:ILE:N	2.46	0.48
55:A:19:ASP:HA	55:A:22:ARG:HH11	1.79	0.48
55:A:78:GLU:O	55:A:82:GLY:N	2.43	0.48
1:1:968:C:H2'	1:1:969:G:H8	1.78	0.48
1:1:1056:G:O2'	1:1:1103:A:N6	2.46	0.48
1:1:1482:G:O2'	1:1:1509:A:N1	2.41	0.48
1:1:2096:C:H2'	1:1:2097:A:C8	2.48	0.48
2:2:695:A:H61	2:2:797:C:H1'	1.79	0.48
2:2:1147:C:O2	41:n:18:ARG:NH2	2.47	0.48
3:3:7:G:O2'	16:O:38:GLN:NE2	2.46	0.48
5:B:69:ARG:NH2	5:B:127:GLY:O	2.39	0.48
9:F:84:THR:OG1	9:F:134:LYS:NZ	2.42	0.48
10:G:84:ALA:HA	10:G:91:PHE:H	1.77	0.48
10:G:132:PHE:HB2	10:G:140:ALA:HB3	1.96	0.48
17:P:88:ARG:NH2	17:P:110:ILE:O	2.46	0.48
21:T:4:GLU:HA	21:T:7:LEU:HD12	1.95	0.48
23:V:75:GLN:HB2	23:V:92:VAL:HG23	1.95	0.48
44:q:4:VAL:HA	44:q:7:LEU:HB2	1.96	0.48
47:t:73:LYS:HD2	47:t:73:LYS:HA	1.68	0.48
55:A:41:LEU:HD23	55:A:46:VAL:HG21	1.96	0.48
1:1:116:C:O2'	1:1:126:A:N3	2.40	0.48
5:B:84:ASP:OD1	5:B:86:ASN:ND2	2.46	0.48
20:S:34:ASP:OD2	29:b:37:LYS:NZ	2.36	0.48
38:k:59:TYR:HE2	50:w:67:LEU:HD21	1.78	0.48
40:m:39:VAL:O	40:m:43:GLU:N	2.46	0.48
55:A:141:ALA:O	55:A:145:ALA:N	2.43	0.48
1:1:282:A:H2'	1:1:283:G:H8	1.78	0.48
1:1:2130:U:H5"	1:1:2133:G:H4'	1.94	0.48
2:2:127:G:O2'	49:v:6:ARG:NH1	2.47	0.48
2:2:1256:A:O2'	2:2:1278:G:O6	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:51:ASN:HA	34:g:54:LEU:HD12	1.96	0.48
41:n:26:GLY:N	41:n:62:ASP:OD1	2.40	0.48
43:p:24:HIS:HB3	43:p:31:ILE:HB	1.95	0.48
47:t:69:TYR:CE2	47:t:73:LYS:HD3	2.49	0.48
55:A:26:ASP:O	55:A:30:LYS:N	2.43	0.48
1:1:532:A:N1	1:1:2035:G:N2	2.62	0.48
1:1:1189:A:OP1	19:R:82:HIS:CD2	2.67	0.48
6:C:125:TRP:NE1	6:C:161:MET:O	2.41	0.48
46:s:38:ASP:O	46:s:42:TRP:N	2.43	0.48
48:u:78:VAL:O	48:u:82:ALA:N	2.44	0.48
54:5:74:C:OP2	55:A:278:ARG:NH2	2.47	0.48
55:A:128:CYS:HB3	55:A:189:TYR:HB2	1.96	0.48
55:A:170:GLU:HA	55:A:176:ILE:HA	1.95	0.48
1:1:2559:C:H2'	1:1:2560:A:H8	1.79	0.48
2:2:66:A:H4'	2:2:173:U:C4	2.48	0.48
2:2:269:C:H2'	2:2:270:A:C8	2.49	0.48
2:2:666:G:H5'	2:2:726:C:H1'	1.94	0.48
2:2:1241:G:H2'	2:2:1242:G:H8	1.79	0.48
6:C:125:TRP:CG	6:C:160:LYS:HB3	2.49	0.48
36:i:62:ARG:NH1	36:i:69:GLU:OE1	2.46	0.48
1:1:1438:U:H2'	1:1:1439:A:H8	1.78	0.48
1:1:1568:G:OP2	5:B:63:ARG:NH1	2.42	0.48
1:1:1667:G:N1	1:1:1992:G:OP2	2.38	0.48
1:1:1721:G:H22	1:1:1738:G:H2'	1.79	0.48
2:2:413:G:O3'	2:2:428:G:N2	2.46	0.48
10:G:40:THR:HG22	10:G:42:LYS:H	1.79	0.48
36:i:27:ALA:O	36:i:30:THR:OG1	2.31	0.48
45:r:54:ASP:OD1	45:r:57:ARG:NH1	2.47	0.48
46:s:47:LYS:O	46:s:50:THR:OG1	2.29	0.48
1:1:182:A:N3	1:1:433:C:O2'	2.41	0.47
1:1:301:G:OP2	22:U:82:ARG:NH1	2.41	0.47
1:1:578:G:OP1	1:1:1255:U:O2'	2.29	0.47
1:1:894:U:C5	1:1:895:U:H5	2.32	0.47
1:1:1022:G:H4'	1:1:1023:U:H5'	1.96	0.47
1:1:1274:A:OP1	1:1:1646:C:N4	2.48	0.47
1:1:2796:U:O2'	1:1:2798:U:OP2	2.29	0.47
1:1:2881:U:O2'	15:N:95:THR:O	2.27	0.47
6:C:43:ASP:HB3	6:C:45:TYR:CE1	2.49	0.47
27:Z:37:GLU:O	27:Z:38:ARG:NH1	2.45	0.47
38:k:35:LYS:N	38:k:65:GLU:O	2.47	0.47
55:A:187:TYR:HD1	55:A:190:GLY:HA3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:859:G:O2'	1:1:916:G:O6	2.31	0.47
1:1:974:G:N2	1:1:989:G:O2'	2.47	0.47
1:1:2118:U:O2'	1:1:2172:U:O4	2.31	0.47
1:1:2692:G:H2'	1:1:2693:G:C8	2.49	0.47
2:2:217:C:H5"	2:2:217:C:C6	2.49	0.47
2:2:252:U:O4	2:2:253:A:N6	2.47	0.47
2:2:531:U:H2'	55:A:332:ARG:HH22	1.79	0.47
9:F:18:LYS:HE2	9:F:20:ASN:HB2	1.96	0.47
17:P:62:ARG:HD2	17:P:71:GLU:HG2	1.96	0.47
36:i:58:LYS:NZ	36:i:69:GLU:OE1	2.46	0.47
55:A:234:ILE:HD11	55:A:292:LYS:HB2	1.96	0.47
1:1:1849:G:H2'	1:1:1850:G:H8	1.80	0.47
1:1:1954:G:O2'	1:1:1956:U:O4	2.27	0.47
2:2:322:C:O2	2:2:332:G:N2	2.46	0.47
2:2:1314:C:N4	51:x:2:PRO:O	2.33	0.47
11:J:58:ASN:ND2	11:J:128:ASN:OD1	2.46	0.47
48:u:68:SER:OG	48:u:69:ASP:N	2.46	0.47
55:A:117:ARG:HH11	55:A:361:LEU:HB2	1.78	0.47
1:1:281:C:H2'	1:1:282:A:C8	2.50	0.47
1:1:1023:U:OP2	1:1:1025:G:O2'	2.33	0.47
1:1:2748:A:H5'	9:F:4:VAL:HG21	1.95	0.47
2:2:67:C:O2'	2:2:171:A:N3	2.46	0.47
2:2:362:G:H5"	44:q:58:THR:HG21	1.97	0.47
2:2:1238:A:H5'	2:2:1336:C:H41	1.80	0.47
10:G:78:VAL:HB	10:G:144:VAL:HG22	1.97	0.47
19:R:48:LYS:HE2	19:R:103:ALA:HB1	1.97	0.47
26:Y:21:LEU:HD12	26:Y:46:VAL:HG13	1.97	0.47
1:1:160:A:N3	1:1:2208:C:O2'	2.44	0.47
1:1:1386:C:H2'	1:1:1387:A:H8	1.80	0.47
1:1:1966:A:O2'	1:1:1967:C:OP2	2.24	0.47
1:1:2237:G:O2'	1:1:2239:G:N7	2.39	0.47
1:1:2681:C:O2	1:1:2683:C:N4	2.46	0.47
14:M:33:LEU:HD13	14:M:117:PHE:HB3	1.96	0.47
55:A:30:LYS:HZ2	55:A:63:LEU:HD23	1.79	0.47
1:1:75:G:N2	1:1:112:U:O2	2.43	0.47
1:1:1536:C:O2	1:1:1537:G:N2	2.47	0.47
1:1:1926:U:O2'	1:1:1928:A:N7	2.44	0.47
1:1:2060:A:N7	7:D:69:ARG:NH2	2.60	0.47
1:1:2704:C:H3'	1:1:2705:A:H8	1.79	0.47
25:X:68:LEU:HD23	25:X:71:LEU:HD12	1.96	0.47
1:1:373:U:H2'	1:1:374:A:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:690:G:O2'	1:1:780:G:OP1	2.33	0.47
1:1:729:G:N3	1:1:729:G:C2'	2.74	0.47
1:1:958:U:C2	3:3:89:U:H1'	2.49	0.47
1:1:1438:U:H2'	1:1:1439:A:C8	2.50	0.47
1:1:2241:A:H2'	1:1:2242:G:C8	2.50	0.47
1:1:2264:C:N4	24:W:15:ASP:OD2	2.47	0.47
1:1:2540:C:O2'	1:1:2740:A:N3	2.44	0.47
1:1:2572:A:O2'	1:1:2575:C:OP1	2.29	0.47
2:2:54:C:H2'	2:2:352:C:H41	1.80	0.47
2:2:429:U:H3	2:2:431:A:H62	1.61	0.47
2:2:618:C:H5'	2:2:619:U:H5"	1.96	0.47
2:2:671:G:O2'	38:k:79:ARG:NH1	2.44	0.47
5:B:63:ARG:H	5:B:86:ASN:HD21	1.61	0.47
8:E:140:GLU:OE2	28:a:26:SER:OG	2.31	0.47
8:E:158:THR:HG23	8:E:160:ALA:H	1.78	0.47
16:O:7:ARG:HH22	16:O:29:HIS:HE1	1.63	0.47
17:P:62:ARG:HB3	17:P:71:GLU:HA	1.96	0.47
20:S:10:ALA:HB3	20:S:101:SER:HB2	1.95	0.47
27:Z:49:ASN:HA	27:Z:52:SER:HB3	1.96	0.47
33:f:2:LYS:HB2	33:f:35:GLN:HG2	1.96	0.47
34:g:54:LEU:HD23	34:g:57:LEU:HD12	1.96	0.47
35:h:156:ARG:H	35:h:163:ALA:HA	1.80	0.47
36:i:147:GLU:O	36:i:151:LYS:NZ	2.43	0.47
45:r:34:LEU:HA	45:r:37:ALA:HB3	1.95	0.47
1:1:12:U:O4	1:1:13:A:N6	2.48	0.47
2:2:161:A:N6	2:2:347:G:O2'	2.45	0.47
2:2:1027:C:H2'	2:2:1034:G:H22	1.78	0.47
2:2:1222:G:H5"	51:x:78:ARG:HD2	1.97	0.47
2:2:1418:A:N6	2:2:1482:G:O2'	2.48	0.47
35:h:151:VAL:HG12	35:h:200:VAL:HG23	1.96	0.47
39:l:69:VAL:HG23	39:l:100:ALA:HB1	1.97	0.47
40:m:29:SER:HB3	40:m:57:PRO:HB2	1.97	0.47
40:m:112:THR:HG23	40:m:115:ALA:H	1.80	0.47
42:o:64:GLN:O	46:s:99:ALA:N	2.44	0.47
45:r:20:THR:HA	45:r:25:VAL:HG23	1.97	0.47
55:A:165:ILE:HA	55:A:181:ILE:HG13	1.97	0.47
1:1:2659:G:N2	1:1:2662:A:OP2	2.46	0.47
1:1:2861:U:H2'	1:1:2862:G:H8	1.80	0.47
2:2:1349:A:OP2	41:n:120:LYS:NZ	2.37	0.47
5:B:6:CYS:SG	5:B:13:ARG:NH2	2.88	0.47
6:C:110:THR:HA	6:C:171:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:98:LYS:HB3	7:D:102:ARG:HH22	1.79	0.47
10:G:128:HIS:O	10:G:144:VAL:N	2.41	0.47
1:1:370:G:O2'	1:1:424:G:OP1	2.26	0.47
1:1:658:U:O2'	7:D:97:ASN:OD1	2.29	0.47
1:1:958:U:N3	3:3:89:U:O2'	2.43	0.47
1:1:2193:G:O2'	1:1:2194:U:OP1	2.31	0.47
1:1:2296:U:OP2	16:O:9:ARG:NH2	2.47	0.47
2:2:401:C:N4	2:2:402:G:O6	2.48	0.47
2:2:974:A:H5'	46:s:71:HIS:HB3	1.97	0.47
2:2:1077:G:N2	2:2:1080:A:OP2	2.38	0.47
5:B:147:LYS:HD2	5:B:150:LYS:HD2	1.97	0.47
7:D:161:ALA:HA	7:D:164:LEU:HD12	1.97	0.47
26:Y:44:LYS:HG3	26:Y:47:ARG:HH11	1.80	0.47
30:c:35:GLU:HG2	30:c:50:LYS:HA	1.97	0.47
35:h:131:ARG:NH2	35:h:168:TYR:OH	2.47	0.47
39:l:12:ILE:HD13	39:l:28:ASN:HD21	1.79	0.47
1:1:910:A:N6	1:1:2277:G:O2'	2.36	0.46
1:1:1398:C:H2'	1:1:1399:C:H6	1.79	0.46
1:1:2278:A:OP2	24:W:12:ASN:ND2	2.39	0.46
2:2:521:G:H4'	44:q:70:GLU:HG2	1.96	0.46
2:2:921:U:O2'	37:j:24:THR:O	2.29	0.46
2:2:1183:U:O2'	2:2:1185:G:OP2	2.33	0.46
5:B:155:ALA:HB2	5:B:162:VAL:HG23	1.97	0.46
5:B:245:VAL:HG12	5:B:251:GLN:HA	1.96	0.46
6:C:116:LYS:HG3	15:N:1:MET:HE1	1.96	0.46
9:F:7:ALA:O	9:F:69:ARG:NE	2.47	0.46
10:G:3:VAL:HA	10:G:38:PRO:HA	1.97	0.46
37:j:84:PRO:HG3	37:j:97:GLN:HG3	1.97	0.46
41:n:130:ARG:HH12	54:5:32:4OC:H3'	1.79	0.46
1:1:26:G:H1'	1:1:515:A:H61	1.80	0.46
1:1:154:U:H2'	1:1:155:A:C8	2.50	0.46
1:1:183:C:O2'	1:1:432:A:N3	2.40	0.46
1:1:402:A:C5	1:1:403:U:C2	3.02	0.46
1:1:1062:G:O6	1:1:1075:C:N4	2.48	0.46
1:1:1463:C:H2'	1:1:1464:G:C8	2.50	0.46
2:2:510:A:O2'	2:2:542:G:O2'	2.30	0.46
2:2:776:G:N1	2:2:802:A:OP1	2.45	0.46
2:2:843:U:OP1	2:2:844:G:N2	2.47	0.46
2:2:1328:C:H5"	45:r:28:THR:HG21	1.96	0.46
37:j:111:MET:HA	37:j:114:VAL:HG12	1.97	0.46
38:k:100:SER:HB2	38:k:103:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:t:32:LEU:HA	47:t:35:GLN:HB3	1.97	0.46
55:A:40:GLU:HG3	55:A:43:GLN:HE21	1.81	0.46
1:1:411:G:OP2	1:1:2406:A:O2'	2.26	0.46
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.97	0.46
1:1:2286:G:H21	1:1:2287:A:H62	1.62	0.46
2:2:17:U:O2'	2:2:1079:G:N3	2.47	0.46
2:2:77:A:H2'	2:2:78:A:C8	2.50	0.46
2:2:563:A:O2'	2:2:566:G:O3'	2.33	0.46
2:2:1303:C:H2'	2:2:1304:G:O4'	2.15	0.46
25:X:33:LEU:HD12	25:X:52:SER:HB3	1.98	0.46
41:n:84:THR:HG21	41:n:103:PHE:HB3	1.97	0.46
44:q:54:ARG:HD2	44:q:62:GLU:HG3	1.97	0.46
47:t:50:HIS:CA	47:t:53:ARG:HD2	2.45	0.46
51:x:11:ILE:HG13	51:x:38:SER:HB3	1.97	0.46
1:1:143:C:H6	1:1:143:C:H5"	1.80	0.46
1:1:1155:A:O3'	18:Q:55:ARG:NH2	2.41	0.46
1:1:1530:G:N3	1:1:1530:G:H2'	2.31	0.46
1:1:1671:U:N3	1:1:1674:G:OP2	2.34	0.46
1:1:2096:C:H2'	1:1:2097:A:H8	1.80	0.46
1:1:2286:G:H3'	30:c:30:LYS:HE3	1.97	0.46
1:1:2717:C:H2'	1:1:2718:G:O4'	2.15	0.46
2:2:477:C:H2'	2:2:478:A:O4'	2.16	0.46
2:2:859:G:OP2	2:2:869:G:N1	2.38	0.46
6:C:68:PHE:O	6:C:72:GLY:N	2.48	0.46
27:Z:42:PRO:HA	27:Z:45:ARG:HB2	1.97	0.46
1:1:1019:U:H2'	1:1:1020:A:H8	1.81	0.46
1:1:1987:A:H2'	1:1:1988:G:H8	1.81	0.46
1:1:2226:C:H2'	1:1:2227:A:O4'	2.16	0.46
2:2:652:U:O4	2:2:752:G:O2'	2.27	0.46
2:2:739:C:O2'	47:t:42:HIS:ND1	2.47	0.46
2:2:790:A:OP1	54:5:38:A:O2'	2.32	0.46
5:B:63:ARG:H	5:B:86:ASN:ND2	2.13	0.46
7:D:121:VAL:HG21	7:D:124:PHE:HB2	1.97	0.46
23:V:18:ARG:O	23:V:22:ALA:N	2.48	0.46
36:i:61:VAL:HA	36:i:64:ILE:HD12	1.97	0.46
54:5:55:PSU:N3	54:5:58:A:OP2	2.40	0.46
55:A:242:ASP:N	55:A:262:ARG:O	2.37	0.46
1:1:1501:G:OP1	5:B:101:ARG:NH2	2.45	0.46
1:1:1722:A:N6	1:1:1738:G:O2'	2.48	0.46
1:1:1859:U:H2'	1:1:1860:G:C8	2.51	0.46
1:1:2832:U:H4'	1:1:2833:U:H2'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:740:U:OP1	47:t:38:HIS:NE2	2.42	0.46
2:2:937:A:N6	2:2:1345:U:O4	2.40	0.46
8:E:123:ASP:O	8:E:125:ARG:N	2.49	0.46
10:G:14:SER:OG	10:G:15:LEU:N	2.48	0.46
39:l:51:ALA:O	39:l:55:GLY:N	2.43	0.46
54:5:15:C:O2'	54:5:60:U:O2	2.32	0.46
1:1:1039:A:H2	1:1:1116:G:H22	1.64	0.46
1:1:1306:C:H2'	1:1:1307:A:C8	2.51	0.46
1:1:1788:C:H2'	1:1:1789:A:C8	2.50	0.46
1:1:1857:G:O2'	1:1:1884:G:N2	2.38	0.46
1:1:1967:C:H2'	1:1:1968:G:O4'	2.16	0.46
2:2:939:G:OP1	39:l:95:ARG:NH2	2.40	0.46
5:B:161:TYR:HB3	5:B:194:GLU:HG2	1.98	0.46
19:R:60:LYS:N	19:R:100:GLY:O	2.47	0.46
30:c:10:LYS:HA	30:c:22:THR:HA	1.97	0.46
40:m:48:ASP:O	40:m:62:THR:N	2.49	0.46
51:x:52:HIS:ND1	51:x:56:GLN:O	2.48	0.46
1:1:35:G:O6	1:1:446:G:N1	2.48	0.46
1:1:612:G:O2'	1:1:613:A:H5'	2.15	0.46
1:1:964:C:O2'	1:1:2273:A:N3	2.36	0.46
1:1:2655:G:N2	1:1:2656:U:O4	2.40	0.46
1:1:2806:C:H2'	1:1:2807:U:O4'	2.16	0.46
2:2:308:C:H2'	2:2:309:A:H8	1.80	0.46
2:2:1359:C:OP2	46:s:75:ARG:NE	2.49	0.46
12:K:70:ARG:HA	12:K:76:VAL:HA	1.97	0.46
34:g:65:GLY:O	34:g:225:ARG:NH1	2.48	0.46
35:h:56:VAL:HB	35:h:67:THR:HB	1.98	0.46
36:i:188:ARG:NH1	36:i:192:SER:O	2.49	0.46
47:t:33:THR:HA	47:t:63:ARG:HH11	1.81	0.46
1:1:581:C:H2'	1:1:582:A:H8	1.81	0.46
2:2:370:C:H2'	2:2:371:A:H8	1.80	0.46
2:2:509:A:H5'	36:i:51:TYR:HD2	1.80	0.46
18:Q:89:GLU:O	19:R:11:GLN:NE2	2.45	0.46
20:S:59:GLU:HB2	20:S:66:ILE:HD11	1.98	0.46
35:h:79:LYS:HB2	35:h:82:GLU:HB2	1.97	0.46
47:t:10:LYS:O	47:t:14:GLU:N	2.49	0.46
47:t:82:ILE:HG22	47:t:87:LEU:HD12	1.97	0.46
55:A:270:ILE:HB	55:A:291:MET:HE1	1.97	0.46
1:1:191:A:OP2	1:1:204:A:N6	2.42	0.46
1:1:282:A:H2'	1:1:283:G:C8	2.50	0.46
1:1:321:U:O3'	7:D:162:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:671:C:OP2	13:L:33:ARG:NH1	2.48	0.46
1:1:857:G:N2	1:1:921:C:O2	2.48	0.46
1:1:981:A:N1	1:1:2027:G:O2'	2.48	0.46
1:1:1364:G:OP1	25:X:50:ARG:NH1	2.42	0.46
1:1:1980:G:O2'	1:1:1982:U:OP2	2.32	0.46
1:1:2351:G:H2'	1:1:2365:G:H22	1.80	0.46
1:1:2642:G:H5'	11:J:80:HIS:CE1	2.51	0.46
2:2:1368:A:OP2	41:n:114:LYS:NZ	2.47	0.46
3:3:22:U:H2'	3:3:23:G:C8	2.51	0.46
3:3:116:G:H2'	3:3:117:G:C8	2.51	0.46
5:B:107:PRO:HD2	5:B:110:LEU:HD22	1.97	0.46
5:B:141:VAL:HG12	5:B:192:LEU:HA	1.97	0.46
6:C:150:GLN:O	6:C:151:THR:C	2.58	0.46
35:h:70:THR:O	35:h:106:VAL:N	2.41	0.46
1:1:205:G:H1'	1:1:206:U:H5	1.81	0.45
1:1:402:A:C6	1:1:403:U:C2	3.04	0.45
1:1:598:U:H2'	1:1:599:A:C8	2.52	0.45
1:1:1341:G:OP1	1:1:1397:U:N3	2.46	0.45
1:1:2529:G:H5'	9:F:175:LYS:HD3	1.98	0.45
2:2:437:U:O2'	36:i:120:HIS:ND1	2.44	0.45
2:2:1311:A:OP1	28:a:59:ARG:NH2	2.49	0.45
20:S:73:LYS:HB2	20:S:106:VAL:HB	1.98	0.45
36:i:26:ARG:HE	36:i:31:LYS:HG2	1.82	0.45
42:o:9:ARG:HB2	42:o:99:GLN:HB3	1.98	0.45
50:w:42:SER:OG	50:w:47:THR:O	2.25	0.45
55:A:56:LEU:HA	55:A:59:GLU:HB3	1.97	0.45
55:A:263:ILE:O	55:A:272:THR:N	2.49	0.45
1:1:581:C:H2'	1:1:582:A:C8	2.51	0.45
1:1:1528:A:OP2	1:1:1543:G:N2	2.40	0.45
1:1:1818:U:OP2	5:B:156:ARG:NE	2.37	0.45
1:1:1844:C:O3'	5:B:256:LYS:NZ	2.49	0.45
1:1:2056:G:O2'	29:b:5:GLN:NE2	2.43	0.45
1:1:2112:G:H5'	1:1:2115:G:H22	1.81	0.45
3:3:98:G:H1	23:V:14:LYS:HB2	1.81	0.45
8:E:111:ILE:HB	8:E:114:PHE:HB2	1.98	0.45
28:a:26:SER:OG	28:a:27:THR:N	2.49	0.45
51:x:15:LEU:HD13	51:x:33:THR:HG21	1.98	0.45
55:A:324:ARG:HG2	55:A:335:ASP:HA	1.99	0.45
1:1:154:U:H2'	1:1:155:A:H8	1.81	0.45
1:1:476:G:O2'	1:1:502:A:N6	2.45	0.45
1:1:2522:U:O2'	1:1:2647:U:OP1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:160:A:H61	2:2:347:G:H1'	1.81	0.45
21:T:24:MET:HE2	21:T:30:ILE:HA	1.98	0.45
26:Y:28:LEU:O	26:Y:32:ALA:N	2.39	0.45
38:k:11:HIS:HB3	38:k:14:GLN:HG2	1.97	0.45
42:o:45:ARG:HB3	42:o:69:THR:HB	1.98	0.45
45:r:25:VAL:HG12	45:r:29:ARG:HD2	1.99	0.45
47:t:56:LEU:C	47:t:60:VAL:HG23	2.41	0.45
1:1:201:C:OP1	25:X:18:ARG:NH1	2.48	0.45
1:1:1464:G:H2'	1:1:1465:G:C8	2.51	0.45
2:2:217:C:H2'	2:2:218:U:O4'	2.16	0.45
2:2:519:C:N4	2:2:529:G:O2'	2.50	0.45
2:2:673:A:H4'	38:k:86:ARG:HH12	1.81	0.45
2:2:1123:U:H4'	42:o:39:PRO:HD2	1.97	0.45
2:2:1222:G:OP2	2:2:1322:C:N4	2.42	0.45
8:E:41:GLY:HA2	8:E:85:ILE:HD11	1.99	0.45
12:K:24:VAL:HA	12:K:39:ILE:HG22	1.98	0.45
19:R:66:HIS:ND1	19:R:94:THR:OG1	2.38	0.45
35:h:81:GLY:HA2	35:h:84:VAL:HB	1.98	0.45
37:j:102:GLY:H	37:j:122:ASN:ND2	2.14	0.45
1:1:376:G:H2'	1:1:377:G:H8	1.82	0.45
1:1:1135:C:N4	1:1:1138:G:OP2	2.37	0.45
2:2:83:C:O2'	2:2:86:G:O6	2.30	0.45
2:2:1391:U:H2'	2:2:1392:G:C8	2.51	0.45
8:E:23:ASN:N	8:E:27:GLN:OE1	2.49	0.45
1:1:1078:U:O2'	1:1:1088:A:O5'	2.35	0.45
1:1:2353:G:N2	24:W:34:GLY:O	2.40	0.45
2:2:1309:G:OP2	45:r:98:ARG:NE	2.38	0.45
9:F:65:ALA:O	9:F:69:ARG:N	2.46	0.45
25:X:40:VAL:HG12	25:X:43:GLU:H	1.81	0.45
34:g:15:HIS:HB3	34:g:43:LEU:HD11	1.98	0.45
35:h:19:ASN:OD1	35:h:54:ARG:NH2	2.44	0.45
48:u:8:ARG:H	48:u:28:ARG:HD2	1.82	0.45
55:A:129:TYR:HE1	55:A:182:LYS:HE2	1.82	0.45
1:1:887:A:H4'	1:1:889:C:H5	1.82	0.45
1:1:1614:A:N6	20:S:88:ARG:O	2.49	0.45
1:1:2699:C:H2'	1:1:2700:A:C8	2.52	0.45
1:1:2785:C:O3'	6:C:70:LYS:NZ	2.46	0.45
2:2:1159:U:O4'	2:2:1182:G:N2	2.50	0.45
2:2:1356:G:H2'	2:2:1357:A:C8	2.52	0.45
5:B:132:MET:HE2	5:B:188:CYS:HB2	1.98	0.45
6:C:38:LYS:HD3	6:C:45:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:17:ASN:OD1	14:M:97:GLN:NE2	2.50	0.45
16:O:66:GLY:O	16:O:102:ARG:NH2	2.49	0.45
18:Q:69:ALA:HB1	18:Q:74:ILE:HG23	1.98	0.45
34:g:119:THR:O	34:g:124:GLY:N	2.45	0.45
38:k:40:GLU:OE1	38:k:100:SER:OG	2.32	0.45
1:1:414:C:H2'	1:1:415:A:C8	2.52	0.45
1:1:598:U:H2'	1:1:599:A:H8	1.81	0.45
1:1:828:U:H2'	1:1:829:A:C8	2.52	0.45
1:1:1992:G:N2	1:1:1996:C:O2'	2.49	0.45
1:1:2314:A:OP1	8:E:88:LYS:NZ	2.40	0.45
5:B:176:LEU:HD12	5:B:180:GLU:HB3	1.99	0.45
6:C:152:PRO:O	6:C:154:LYS:N	2.49	0.45
17:P:24:ASP:O	17:P:47:VAL:N	2.45	0.45
54:5:19:G:OP2	54:5:20:H2U:H51	2.16	0.45
54:5:51:C:H2'	54:5:52:G:H8	1.82	0.45
1:1:748:G:OP1	20:S:88:ARG:NH1	2.50	0.45
1:1:995:C:N3	11:J:3:THR:N	2.65	0.45
1:1:2368:C:H2'	1:1:2369:A:H8	1.80	0.45
1:1:2787:C:H1'	6:C:63:PRO:HG3	1.98	0.45
2:2:59:A:H2	2:2:330:C:H42	1.62	0.45
2:2:454:G:H2'	2:2:455:G:H8	1.81	0.45
2:2:1492:A:O2'	55:A:319:TRP:NE1	2.44	0.45
41:n:12:ARG:HA	41:n:12:ARG:HD2	1.70	0.45
46:s:41:ARG:NH2	51:x:6:LYS:O	2.50	0.45
1:1:151:C:H2'	1:1:152:A:C8	2.52	0.45
1:1:1267:U:H2'	1:1:1268:A:C8	2.52	0.45
1:1:1915:3TD:H3'	1:1:1916:A:C8	2.45	0.45
1:1:2128:G:N2	1:1:2174:C:O5'	2.50	0.45
2:2:452:A:O2'	48:u:70:ARG:NH2	2.44	0.45
2:2:531:U:OP2	55:A:213:ARG:NH2	2.50	0.45
2:2:957:U:H4'	51:x:79:THR:HG23	1.98	0.45
4:4:21:A:N6	55:A:215:THR:OG1	2.50	0.45
8:E:140:GLU:OE1	28:a:27:THR:OG1	2.28	0.45
10:G:83:LYS:HA	10:G:149:GLU:HB3	1.98	0.45
36:i:116:GLN:HE21	36:i:120:HIS:CE1	2.35	0.45
41:n:39:PHE:O	41:n:45:ARG:NH2	2.41	0.45
44:q:57:LEU:HD12	44:q:61:PHE:HB2	1.99	0.45
48:u:40:ASN:HB3	48:u:43:ALA:HB2	1.98	0.45
53:z:30:ALA:O	53:z:34:ARG:N	2.50	0.45
1:1:404:A:O5'	1:1:404:A:C8	2.70	0.44
1:1:711:G:H1	1:1:720:U:H3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1047:G:HO2'	1:1:1110:G:H1	1.63	0.44
1:1:1123:C:H2'	1:1:1124:G:C8	2.52	0.44
1:1:2271:G:H5'	24:W:20:ARG:HG2	1.99	0.44
1:1:2503:2MA:O2'	1:1:2505:G:OP2	2.35	0.44
2:2:157:U:H2'	2:2:158:G:H8	1.82	0.44
2:2:257:G:H2'	2:2:258:G:H8	1.81	0.44
3:3:112:G:N2	16:O:45:SER:O	2.42	0.44
6:C:45:TYR:HE2	6:C:81:GLU:OE2	2.00	0.44
47:t:36:ILE:HB	47:t:63:ARG:NH1	2.32	0.44
55:A:196:THR:HG22	55:A:222:VAL:H	1.82	0.44
1:1:894:U:C6	1:1:894:U:OP2	2.70	0.44
2:2:197:A:N3	2:2:198:G:H1'	2.32	0.44
5:B:145:GLU:HB2	5:B:188:CYS:HB3	1.98	0.44
8:E:58:ALA:HB2	8:E:65:PRO:HD3	1.99	0.44
11:J:45:THR:HB	11:J:48:VAL:HB	1.99	0.44
22:U:51:ALA:O	22:U:52:LEU:HB3	2.16	0.44
42:o:6:ILE:HB	42:o:76:ILE:HB	1.99	0.44
46:s:69:ARG:HD3	46:s:71:HIS:H	1.82	0.44
53:z:31:GLU:OE2	53:z:34:ARG:NH2	2.38	0.44
54:5:60:U:OP2	54:5:60:U:C6	2.71	0.44
1:1:558:U:H2'	1:1:559:G:H8	1.81	0.44
1:1:717:C:H3'	1:1:718:A:C8	2.51	0.44
1:1:1114:C:H2'	1:1:1115:G:C8	2.53	0.44
1:1:1419:A:O2'	1:1:1421:G:N7	2.43	0.44
1:1:2119:A:N7	1:1:2169:A:N6	2.64	0.44
1:1:2127:G:N1	1:1:2161:C:N3	2.65	0.44
1:1:296:U:H2'	1:1:297:G:C8	2.53	0.44
1:1:404:A:H5'	1:1:406:G:C1'	2.48	0.44
1:1:463:G:N2	1:1:466:A:OP2	2.38	0.44
1:1:1026:G:OP1	1:1:1134:A:O2'	2.30	0.44
1:1:1270:C:H5"	1:1:1271:G:H5"	1.99	0.44
1:1:1651:G:H4'	15:N:39:PRO:HG2	1.98	0.44
1:1:2216:G:H2'	1:1:2217:G:C8	2.52	0.44
1:1:2371:G:O2'	30:c:46:HIS:ND1	2.47	0.44
2:2:806:C:H2'	2:2:807:A:H8	1.83	0.44
26:Y:29:ARG:O	26:Y:33:ALA:N	2.50	0.44
35:h:65:ARG:HA	35:h:100:GLN:HB3	1.99	0.44
47:t:73:LYS:O	47:t:73:LYS:HD2	2.17	0.44
1:1:632:A:N3	1:1:2403:C:O2'	2.44	0.44
2:2:711:G:H2'	2:2:712:A:H8	1.82	0.44
10:G:125:THR:HG21	10:G:148:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:136:MET:HE3	23:V:57:TYR:HB3	2.00	0.44
20:S:20:VAL:HG21	20:S:43:ALA:HB3	2.00	0.44
53:z:7:ARG:HH22	53:z:18:ARG:HH12	1.65	0.44
54:5:18:G:N2	54:5:58:A:O5'	2.49	0.44
1:1:616:A:H3'	1:1:617:G:H8	1.83	0.44
1:1:1463:C:H2'	1:1:1464:G:H8	1.82	0.44
1:1:2314:A:H1'	8:E:155:THR:HG21	1.99	0.44
2:2:32:A:OP2	2:2:398:U:O2'	2.29	0.44
2:2:257:G:H2'	2:2:258:G:C8	2.53	0.44
2:2:769:G:H4'	2:2:1513:A:H4'	1.99	0.44
2:2:1158:C:O2	2:2:1158:C:H2'	2.17	0.44
2:2:1402:4OC:HM22	2:2:1403:C:H5'	2.00	0.44
39:l:141:VAL:O	39:l:145:ALA:N	2.43	0.44
47:t:2:SER:HA	47:t:35:GLN:HE22	1.82	0.44
48:u:44:SER:OG	48:u:45:GLU:N	2.49	0.44
1:1:402:A:H3'	1:1:403:U:H6	1.82	0.44
1:1:728:G:H4'	5:B:13:ARG:HD3	2.00	0.44
1:1:750:A:OP1	1:1:1615:C:N4	2.50	0.44
1:1:894:U:C4'	1:1:895:U:OP1	2.65	0.44
1:1:1076:C:H2'	1:1:1077:A:H8	1.83	0.44
1:1:1153:C:OP1	18:Q:76:TYR:OH	2.35	0.44
1:1:2098:U:H2'	1:1:2099:U:O4'	2.17	0.44
2:2:397:A:O2'	2:2:399:G:OP2	2.28	0.44
2:2:674:G:H2'	2:2:675:A:C8	2.53	0.44
35:h:148:GLY:HA2	35:h:171:GLY:HA3	2.00	0.44
36:i:152:GLN:HB2	36:i:155:VAL:HG23	1.99	0.44
41:n:49:ARG:O	41:n:53:GLU:N	2.50	0.44
44:q:4:VAL:O	44:q:8:VAL:N	2.49	0.44
47:t:57:LEU:C	47:t:60:VAL:H	2.25	0.44
55:A:41:LEU:HD11	55:A:56:LEU:HB3	1.99	0.44
1:1:1825:U:H2'	1:1:1826:G:C8	2.53	0.44
1:1:2200:C:OP2	25:X:37:ARG:NH1	2.50	0.44
1:1:2824:C:H3'	1:1:2825:G:H21	1.83	0.44
2:2:499:A:H4'	2:2:500:G:H5'	2.00	0.44
2:2:730:G:H1	47:t:51:HIS:HE1	1.64	0.44
2:2:1086:U:H3	2:2:1099:G:H22	1.66	0.44
2:2:1239:A:O2'	2:2:1298:U:O4	2.36	0.44
2:2:1297:G:N2	2:2:1298:U:O4	2.50	0.44
6:C:13:ARG:HG2	17:P:56:HIS:CE1	2.53	0.44
7:D:41:GLN:HG2	7:D:43:THR:HG23	1.99	0.44
21:T:15:HIS:HB3	21:T:31:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:38:ALA:O	21:T:81:LYS:NZ	2.38	0.44
34:g:76:ALA:HB1	34:g:210:VAL:HG11	1.99	0.44
51:x:50:ALA:HB1	51:x:57:HIS:HB3	1.99	0.44
55:A:325:SER:N	55:A:334:LYS:O	2.50	0.44
1:1:106:C:H2'	1:1:107:G:C8	2.53	0.44
1:1:729:G:C4	1:1:1775:U:C2	3.05	0.44
1:1:1589:U:O2'	1:1:1590:A:H5'	2.18	0.44
1:1:1854:A:N6	1:1:1888:G:O2'	2.50	0.44
1:1:2544:G:H2'	1:1:2545:G:H8	1.83	0.44
2:2:1078:U:O2	37:j:135:ASN:ND2	2.42	0.44
2:2:1162:C:H2'	2:2:1163:A:H8	1.82	0.44
3:3:5:U:H2'	3:3:6:G:C8	2.53	0.44
6:C:151:THR:HG1	6:C:152:PRO:HD3	1.66	0.44
54:5:63:G:H2'	54:5:64:G:C8	2.53	0.44
1:1:177:G:H3'	1:1:178:G:H8	1.82	0.43
1:1:558:U:H2'	1:1:559:G:C8	2.53	0.43
1:1:1044:C:O2'	1:1:1111:A:N1	2.47	0.43
1:1:1332:G:N7	1:1:1609:A:O2'	2.39	0.43
1:1:1443:U:H2'	1:1:1444:G:H8	1.83	0.43
1:1:1796:U:H2'	1:1:1797:G:C8	2.53	0.43
1:1:2002:G:H5"	15:N:9:GLN:HE21	1.82	0.43
2:2:1273:C:H2'	2:2:1274:A:O4'	2.17	0.43
2:2:1406:U:H3'	2:2:1407:5MC:H6	1.83	0.43
5:B:71:LYS:O	5:B:118:SER:OG	2.36	0.43
7:D:29:HIS:HD2	13:L:6:LEU:HB3	1.83	0.43
15:N:52:ILE:HD13	15:N:94:TYR:HB2	2.00	0.43
27:Z:45:ARG:HA	27:Z:48:ILE:HD12	1.99	0.43
31:d:17:GLY:HA2	31:d:45:SER:HB2	2.00	0.43
34:g:7:ARG:O	34:g:11:LYS:N	2.47	0.43
36:i:62:ARG:O	36:i:66:GLY:N	2.50	0.43
54:5:6:G:O2'	54:5:49:G:O4'	2.36	0.43
55:A:117:ARG:HH22	55:A:362:LYS:HE2	1.83	0.43
1:1:1273:U:O2	1:1:2002:G:O2'	2.32	0.43
1:1:1475:G:O2'	1:1:1514:G:O6	2.27	0.43
1:1:2461:A:N6	1:1:2488:G:O6	2.51	0.43
2:2:67:C:H2'	2:2:68:G:C8	2.53	0.43
2:2:199:A:H61	2:2:218:U:H3	1.66	0.43
2:2:366:A:O2'	2:2:394:G:N2	2.50	0.43
2:2:552:U:O2'	44:q:83:ARG:O	2.30	0.43
6:C:5:VAL:HG22	6:C:202:ILE:HG12	2.00	0.43
9:F:10:VAL:HA	9:F:49:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:9:ILE:O	30:c:22:THR:OG1	2.26	0.43
35:h:20:SER:HB3	35:h:22:TRP:HE1	1.83	0.43
43:p:46:THR:OG1	43:p:49:GLY:N	2.51	0.43
1:1:564:C:O4'	18:Q:37:GLN:NE2	2.51	0.43
1:1:593:U:H2'	1:1:594:U:C6	2.53	0.43
1:1:949:G:H2'	1:1:950:G:H8	1.81	0.43
1:1:1038:G:H2'	1:1:1039:A:C8	2.53	0.43
1:1:1358:G:N1	1:1:1372:U:OP2	2.32	0.43
1:1:1631:G:N2	1:1:1634:A:OP2	2.46	0.43
1:1:2291:U:OP1	1:1:2380:C:O2'	2.28	0.43
1:1:2549:G:H2'	1:1:2550:G:H8	1.82	0.43
2:2:1173:U:H2'	2:2:1174:G:H8	1.83	0.43
2:2:1297:G:H21	39:l:114:LYS:HB3	1.84	0.43
30:c:8:LYS:HD2	32:e:34:THR:HG21	1.98	0.43
35:h:59:ARG:HA	35:h:64:ILE:HA	2.00	0.43
36:i:103:TYR:O	36:i:165:ARG:NH2	2.51	0.43
42:o:8:ILE:HG12	42:o:100:ILE:HG22	1.99	0.43
51:x:52:HIS:CD2	51:x:54:GLY:H	2.36	0.43
55:A:242:ASP:O	55:A:262:ARG:N	2.52	0.43
55:A:271:VAL:O	55:A:294:LYS:NZ	2.50	0.43
1:1:402:A:C4	1:1:403:U:O4'	2.70	0.43
1:1:729:G:H4'	1:1:763:G:O5'	2.18	0.43
1:1:890:C:H2'	1:1:891:G:H4'	2.00	0.43
1:1:1030:C:OP2	14:M:127:LYS:NZ	2.49	0.43
1:1:1342:A:OP1	21:T:40:LYS:NZ	2.34	0.43
1:1:1791:A:N6	1:1:1828:G:O2'	2.48	0.43
1:1:1844:C:H2'	1:1:1845:G:H8	1.82	0.43
1:1:1859:U:H2'	1:1:1860:G:H8	1.83	0.43
1:1:2241:A:H2'	1:1:2242:G:H8	1.84	0.43
2:2:77:A:H2'	2:2:78:A:H8	1.83	0.43
2:2:376:G:H4'	48:u:5:ARG:HH11	1.82	0.43
2:2:1376:U:H2'	2:2:1377:A:C8	2.53	0.43
8:E:123:ASP:CG	8:E:127:ASN:HB2	2.42	0.43
22:U:8:ASP:HB2	22:U:24:LYS:HD3	1.99	0.43
31:d:23:ALA:O	31:d:28:ARG:NH1	2.51	0.43
34:g:32:PHE:N	34:g:40:ILE:O	2.48	0.43
36:i:34:ILE:HG23	36:i:35:GLU:HG2	1.99	0.43
45:r:101:ARG:HG3	45:r:104:THR:H	1.84	0.43
50:w:48:ARG:HD3	50:w:50:LYS:H	1.83	0.43
55:A:265:HIS:CD2	55:A:267:PRO:HD2	2.53	0.43
1:1:242:G:N2	1:1:255:A:OP2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1278:C:H2'	1:1:1279:G:H8	1.81	0.43
1:1:1464:G:H2'	1:1:1465:G:H8	1.84	0.43
2:2:111:G:H22	2:2:330:C:H41	1.65	0.43
2:2:137:U:H2'	2:2:138:G:C8	2.53	0.43
2:2:406:G:H21	36:i:116:GLN:HE22	1.67	0.43
2:2:1464:U:H2'	2:2:1465:A:H8	1.84	0.43
7:D:2:GLU:HB3	7:D:11:ALA:HB1	2.00	0.43
20:S:77:ASP:O	20:S:102:HIS:N	2.50	0.43
28:a:20:ASN:HB2	28:a:39:LYS:HD3	2.01	0.43
34:g:162:PHE:HA	34:g:184:PHE:HB2	1.99	0.43
37:j:97:GLN:N	37:j:124:LEU:O	2.51	0.43
1:1:7:G:H5"	11:J:123:LYS:HE2	2.01	0.43
1:1:784:G:C8	1:1:792:A:N7	2.87	0.43
1:1:968:C:H2'	1:1:969:G:C8	2.54	0.43
1:1:2128:G:H1'	1:1:2174:C:H1'	2.00	0.43
2:2:490:C:H2'	2:2:491:G:C8	2.54	0.43
2:2:496:A:H2'	2:2:496:A:N3	2.33	0.43
2:2:886:G:H1	2:2:911:U:H3	1.67	0.43
2:2:1412:C:H2'	2:2:1413:A:C8	2.53	0.43
7:D:181:ILE:HG23	13:L:1:MET:HG2	2.01	0.43
9:F:27:LYS:HG2	9:F:32:GLU:HB2	2.01	0.43
10:G:66:ASN:CG	10:G:135:HIS:HB3	2.44	0.43
29:b:31:ASP:HB3	29:b:36:GLU:H	1.83	0.43
34:g:19:GLN:HB2	34:g:22:TYR:HD2	1.83	0.43
37:j:114:VAL:HG13	37:j:115:LEU:HD22	2.00	0.43
39:l:26:PHE:HA	39:l:29:ILE:HD12	2.01	0.43
55:A:169:SER:HG	55:A:178:SER:HG	1.64	0.43
1:1:5:A:H2'	1:1:6:A:C8	2.53	0.43
1:1:458:G:N2	1:1:459:U:O4	2.50	0.43
1:1:1583:A:N3	1:1:1584:U:N3	2.66	0.43
1:1:2425:A:H5'	1:1:2427:C:O4'	2.19	0.43
1:1:2447:G:N2	1:1:2450:A:OP2	2.52	0.43
15:N:66:ALA:O	15:N:70:THR:OG1	2.27	0.43
25:X:69:ALA:O	25:X:73:ALA:N	2.43	0.43
26:Y:18:LEU:HB2	26:Y:53:VAL:HG11	2.00	0.43
37:j:84:PRO:HG3	37:j:98:PRO:HD2	2.01	0.43
38:k:78:PHE:HD1	38:k:84:VAL:HG11	1.83	0.43
52:y:35:VAL:HG11	52:y:79:LEU:HD13	2.01	0.43
52:y:67:ILE:HB	52:y:71:LYS:HD3	2.01	0.43
1:1:563:A:H2'	18:Q:37:GLN:HE21	1.82	0.43
1:1:974:G:O2'	1:1:989:G:N2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1065:U:O2	1:1:1073:A:N6	2.51	0.43
1:1:1820:U:N3	5:B:198:ALA:O	2.46	0.43
1:1:2087:G:H2'	1:1:2088:A:H8	1.83	0.43
1:1:2251:OMG:OP1	14:M:81:ARG:NH1	2.50	0.43
1:1:2392:A:OP1	32:e:31:HIS:NE2	2.52	0.43
1:1:2674:G:O2'	12:K:28:SER:O	2.31	0.43
2:2:1375:A:OP1	39:l:25:LYS:NZ	2.45	0.43
16:O:43:ASN:HD21	16:O:46:GLU:HG2	1.83	0.43
28:a:30:HIS:ND1	28:a:31:ASP:O	2.45	0.43
55:A:203:ARG:HH12	55:A:206:PRO:HD3	1.83	0.43
1:1:441:U:H2'	1:1:442:G:C8	2.53	0.43
1:1:1306:C:H2'	1:1:1307:A:H8	1.84	0.43
1:1:1820:U:O2'	5:B:157:SER:OG	2.34	0.43
1:1:1914:C:N3	1:1:1915:3TD:H1'	2.34	0.43
1:1:2572:A:OP1	1:1:2574:G:O2'	2.33	0.43
2:2:60:A:N1	2:2:107:G:O2'	2.49	0.43
2:2:750:C:O2'	47:t:21:ASP:O	2.27	0.43
2:2:940:C:H2'	2:2:941:G:C8	2.54	0.43
7:D:106:LYS:HG3	7:D:200:LEU:HD23	2.01	0.43
9:F:42:GLU:HA	9:F:55:ARG:NH2	2.34	0.43
10:G:103:VAL:HB	10:G:110:VAL:HG11	2.01	0.43
13:L:88:GLY:O	13:L:121:THR:N	2.45	0.43
41:n:97:GLU:O	41:n:101:ALA:N	2.46	0.43
51:x:39:THR:HA	51:x:70:LYS:HA	2.00	0.43
55:A:29:ALA:HA	55:A:32:GLU:HB3	1.99	0.43
1:1:1013:C:H2'	1:1:1014:A:C8	2.53	0.43
1:1:1128:G:N3	1:1:2516:A:O2'	2.43	0.43
1:1:1341:G:H1'	21:T:59:ASN:HB3	1.99	0.43
2:2:522:C:OP2	44:q:66:TYR:OH	2.25	0.43
2:2:1086:U:H3	2:2:1099:G:H1	1.67	0.43
2:2:1338:G:H21	54:5:41:C:H1'	1.84	0.43
3:3:23:G:H2'	3:3:24:G:C5	2.54	0.43
3:3:51:G:OP1	16:O:63:LYS:NZ	2.45	0.43
23:V:32:GLY:O	23:V:93:ARG:NH1	2.45	0.43
27:Z:8:THR:HB	27:Z:56:LYS:HB3	2.01	0.43
36:i:170:TRP:CD2	36:i:186:PRO:HB3	2.54	0.43
41:n:12:ARG:HG3	41:n:13:LYS:H	1.83	0.43
1:1:745:1MG:O2'	1:1:750:A:N6	2.52	0.42
1:1:1102:C:H2'	1:1:1103:A:C8	2.53	0.42
1:1:1602:U:OP2	21:T:64:LYS:NZ	2.52	0.42
1:1:2406:A:O4'	13:L:69:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:996:A:N1	2:2:1045:C:O2'	2.44	0.42
6:C:13:ARG:HH11	17:P:56:HIS:HA	1.84	0.42
35:h:107:ARG:HG3	35:h:108:LYS:HG3	2.01	0.42
37:j:38:VAL:HA	37:j:48:PHE:HA	2.00	0.42
41:n:34:SER:OG	41:n:35:LEU:N	2.52	0.42
50:w:51:TYR:O	50:w:55:LEU:N	2.50	0.42
1:1:45:G:H5"	1:1:46:G:H5'	2.01	0.42
1:1:935:C:H2'	1:1:936:A:C8	2.54	0.42
1:1:956:G:N2	1:1:960:A:OP2	2.37	0.42
1:1:1000:A:OP2	1:1:1154:G:N1	2.37	0.42
1:1:1222:U:H2'	1:1:1223:G:H8	1.84	0.42
1:1:2087:G:H2'	1:1:2088:A:C8	2.54	0.42
1:1:2368:C:H2'	1:1:2369:A:C8	2.54	0.42
2:2:269:C:H2'	2:2:270:A:H8	1.84	0.42
2:2:309:A:H5'	48:u:29:ASN:HB3	2.02	0.42
2:2:1095:U:OP1	2:2:1108:G:N1	2.46	0.42
6:C:48:ILE:HG23	6:C:84:LEU:HD11	2.01	0.42
20:S:73:LYS:HB3	20:S:75:PHE:HE2	1.83	0.42
34:g:120:GLN:HA	34:g:124:GLY:HA3	2.01	0.42
43:p:35:THR:OG1	43:p:36:ASP:N	2.51	0.42
46:s:63:ARG:HB3	46:s:68:GLY:HA2	2.01	0.42
1:1:577:G:O2'	1:1:1254:A:OP1	2.37	0.42
1:1:894:U:H4'	1:1:895:U:OP1	2.19	0.42
1:1:910:A:N6	14:M:11:LYS:O	2.52	0.42
1:1:1278:C:H2'	1:1:1279:G:C8	2.54	0.42
1:1:1700:A:H3'	1:1:1701:A:H8	1.84	0.42
1:1:1914:C:H2'	1:1:1915:3TD:O4'	2.20	0.42
1:1:2108:A:N6	1:1:2181:U:H3	2.17	0.42
2:2:504:C:H42	2:2:541:G:H1	1.67	0.42
2:2:711:G:H2'	2:2:712:A:C8	2.54	0.42
2:2:744:C:H2'	2:2:745:G:C8	2.53	0.42
5:B:199:GLU:HA	5:B:202:LEU:HD23	2.02	0.42
15:N:44:LEU:HG	15:N:48:VAL:HB	2.01	0.42
22:U:102:THR:HB	22:U:104:LYS:HE2	2.01	0.42
28:a:42:PRO:HB2	28:a:46:GLY:HA3	2.01	0.42
35:h:152:GLU:N	35:h:199:LYS:O	2.53	0.42
55:A:276:ASN:N	55:A:283:ASN:OD1	2.52	0.42
1:1:1287:A:N6	15:N:105:GLY:O	2.49	0.42
1:1:1948:G:O2'	2:2:1418:A:N1	2.48	0.42
1:1:2252:G:H2'	1:1:2253:G:H8	1.83	0.42
1:1:2880:C:HO2'	15:N:90:ARG:NH2	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:357:G:C4'	2:2:368:U:H5"	2.38	0.42
2:2:1134:G:H1	2:2:1140:C:H42	1.65	0.42
15:N:38:LEU:O	15:N:42:LYS:N	2.50	0.42
43:p:64:GLN:HB2	43:p:99:ALA:HB2	2.02	0.42
46:s:41:ARG:HH22	51:x:6:LYS:HB2	1.83	0.42
47:t:36:ILE:O	47:t:40:GLN:N	2.52	0.42
55:A:164:GLU:O	55:A:182:LYS:N	2.50	0.42
55:A:276:ASN:HD22	55:A:286:GLN:HG2	1.84	0.42
1:1:706:A:OP1	5:B:7:LYS:NZ	2.37	0.42
1:1:918:A:N3	3:3:80:U:O2'	2.50	0.42
1:1:1398:C:H2'	1:1:1399:C:C6	2.53	0.42
1:1:1954:G:N2	1:1:1956:U:O2	2.48	0.42
1:1:2233:U:H2'	1:1:2234:G:C8	2.54	0.42
2:2:335:C:H2'	2:2:336:A:H8	1.85	0.42
2:2:368:U:O2	2:2:368:U:C2'	2.68	0.42
2:2:404:G:O2'	2:2:498:A:N1	2.47	0.42
2:2:750:C:H2'	2:2:751:U:C6	2.55	0.42
2:2:950:U:H3'	45:r:101:ARG:HH22	1.84	0.42
2:2:1221:G:H5"	51:x:36:ARG:HH11	1.84	0.42
13:L:23:ILE:HG12	19:R:82:HIS:CE1	2.54	0.42
34:g:163:VAL:N	34:g:184:PHE:O	2.50	0.42
38:k:36:ILE:HD11	38:k:39:LEU:HB2	2.02	0.42
39:l:87:VAL:HA	39:l:88:PRO:HD3	1.94	0.42
1:1:69:C:O2	1:1:73:A:O2'	2.31	0.42
1:1:181:A:H2'	1:1:182:A:C8	2.54	0.42
1:1:347:A:H2'	1:1:348:A:C8	2.55	0.42
1:1:409:G:H2'	1:1:410:G:C8	2.54	0.42
1:1:851:C:O2'	27:Z:43:ALA:O	2.34	0.42
1:1:1059:G:H3'	1:1:1060:U:H3'	2.00	0.42
1:1:1067:A:OP1	55:A:54:GLN:NE2	2.52	0.42
1:1:1496:A:H2'	1:1:1498:C:C4	2.54	0.42
1:1:1580:A:H3'	1:1:1581:G:H8	1.83	0.42
1:1:2833:U:H3'	1:1:2834:G:C8	2.55	0.42
1:1:2861:U:H2'	1:1:2862:G:C8	2.55	0.42
6:C:101:PHE:HD1	6:C:104:VAL:HG21	1.85	0.42
12:K:16:ALA:HA	12:K:46:ALA:HA	2.02	0.42
22:U:51:ALA:O	22:U:52:LEU:CB	2.67	0.42
24:W:33:ALA:N	24:W:64:ASP:OD1	2.52	0.42
45:r:13:LYS:HD3	45:r:17:ILE:HG22	2.01	0.42
48:u:18:GLN:HE22	48:u:35:ARG:HH21	1.66	0.42
1:1:585:G:O6	1:1:1251:C:O2'	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:696:G:H2'	1:1:697:G:H8	1.83	0.42
1:1:1477:A:N6	1:1:1514:G:O2'	2.52	0.42
1:1:1583:A:H1'	1:1:1584:U:C2	2.54	0.42
1:1:2523:G:O2'	1:1:2764:A:O2'	2.34	0.42
1:1:2708:G:O2'	15:N:71:ARG:NH1	2.52	0.42
2:2:714:G:N2	2:2:777:A:N3	2.49	0.42
14:M:121:ALA:HA	14:M:124:LEU:HD12	2.01	0.42
35:h:32:ASN:OD1	35:h:59:ARG:NH1	2.51	0.42
39:l:78:ARG:HG2	39:l:80:VAL:HG13	2.01	0.42
51:x:3:ARG:HH11	51:x:10:PHE:HB2	1.83	0.42
1:1:219:A:N3	1:1:234:U:O2'	2.47	0.42
1:1:596:U:H2'	1:1:597:G:C8	2.55	0.42
1:1:1426:G:H3'	1:1:1427:A:H2'	2.02	0.42
1:1:1443:U:H2'	1:1:1444:G:C8	2.55	0.42
1:1:1934:C:H2'	1:1:1935:G:H8	1.84	0.42
1:1:2081:U:H2'	1:1:2082:A:H8	1.83	0.42
1:1:2251:OMG:HM23	1:1:2251:OMG:H1'	1.87	0.42
1:1:2821:A:H2'	1:1:2822:G:H8	1.84	0.42
2:2:21:G:H2'	2:2:22:G:C8	2.55	0.42
2:2:1060:U:H2'	2:2:1061:G:H8	1.85	0.42
7:D:58:LYS:HA	7:D:59:PRO:HD3	1.94	0.42
34:g:12:ALA:HB1	34:g:209:ALA:HA	2.02	0.42
38:k:8:PHE:HA	38:k:87:SER:HA	2.00	0.42
38:k:21:MET:HG2	38:k:24:ARG:HH21	1.84	0.42
40:m:28:PRO:HA	40:m:58:GLU:HA	2.02	0.42
52:y:28:MET:HE1	52:y:67:ILE:HG21	2.02	0.42
1:1:175:G:H2'	1:1:176:A:C8	2.54	0.42
1:1:1028:A:N3	1:1:2486:C:O2'	2.44	0.42
1:1:1295:C:H4'	15:N:22:ARG:HH21	1.85	0.42
1:1:2520:C:H2'	1:1:2521:C:H6	1.85	0.42
2:2:559:A:H4'	2:2:560:A:H3'	2.01	0.42
2:2:1386:G:H2'	2:2:1387:G:H8	1.85	0.42
3:3:86:G:H3'	3:3:88:C:H41	1.84	0.42
8:E:99:PHE:HA	8:E:102:ARG:HE	1.85	0.42
8:E:122:PHE:HE1	8:E:170:LEU:HD12	1.85	0.42
11:J:117:ALA:HA	11:J:120:ARG:HH21	1.85	0.42
12:K:23:LYS:HB3	12:K:40:LYS:HB3	2.02	0.42
16:O:30:ARG:HD3	16:O:102:ARG:NH1	2.35	0.42
26:Y:39:GLN:HB3	26:Y:41:HIS:CE1	2.55	0.42
47:t:49:ASP:O	47:t:52:SER:N	2.49	0.42
1:1:371:A:N6	1:1:402:A:OP2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:783:A:N3	1:1:783:A:C2'	2.81	0.42
1:1:1408:G:O6	1:1:1593:A:N6	2.52	0.42
1:1:2162:G:O2'	1:1:2163:A:N7	2.47	0.42
1:1:2193:G:HO2'	1:1:2194:U:P	2.43	0.42
1:1:2580:PSU:OP1	6:C:137:SER:OG	2.31	0.42
2:2:154:U:H2'	2:2:155:A:H8	1.84	0.42
2:2:375:U:O3'	48:u:6:LEU:HB2	2.20	0.42
9:F:127:THR:HB	9:F:130:GLU:HB3	2.01	0.42
42:o:42:LEU:HB2	42:o:71:LEU:HB3	2.01	0.42
55:A:208:ASP:OD2	55:A:211:GLY:N	2.53	0.42
1:1:82:U:H2'	1:1:83:A:C8	2.55	0.41
1:1:720:U:H2'	1:1:721:A:C8	2.55	0.41
1:1:741:U:H2'	1:1:742:A:H8	1.85	0.41
1:1:992:C:H2'	1:1:993:G:C8	2.54	0.41
1:1:1252:G:H5"	18:Q:32:TYR:HE2	1.85	0.41
1:1:2183:A:H2'	1:1:2184:A:C8	2.55	0.41
2:2:195:A:H2'	2:2:196:A:C8	2.55	0.41
2:2:231:U:H2'	2:2:232:G:H8	1.84	0.41
2:2:583:A:N6	2:2:758:C:O2'	2.53	0.41
2:2:770:C:H2'	2:2:771:G:H8	1.84	0.41
8:E:117:LEU:N	8:E:177:PHE:O	2.39	0.41
18:Q:31:VAL:HG12	18:Q:34:VAL:H	1.85	0.41
1:1:848:C:H2'	1:1:849:A:C8	2.55	0.41
1:1:2124:G:H1	1:1:2174:C:H42	1.68	0.41
1:1:2508:G:O2'	1:1:2554:U:O2'	2.25	0.41
2:2:34:C:H2'	2:2:35:G:C8	2.53	0.41
2:2:1241:G:H2'	2:2:1242:G:C8	2.55	0.41
6:C:46:ARG:NH2	6:C:88:GLU:O	2.36	0.41
14:M:36:VAL:H	14:M:128:THR:HA	1.85	0.41
19:R:51:VAL:CG2	19:R:52:PRO:HD3	2.50	0.41
25:X:33:LEU:HA	25:X:52:SER:HA	2.02	0.41
30:c:9:ILE:HA	30:c:54:ILE:HB	2.02	0.41
36:i:124:MET:HG3	36:i:146:ARG:HB3	2.02	0.41
41:n:65:ILE:HD13	41:n:79:ILE:HG23	2.01	0.41
55:A:198:VAL:HG22	55:A:219:SER:HB3	2.02	0.41
1:1:1653:G:C6	15:N:9:GLN:HB3	2.56	0.41
1:1:2175:C:H3'	1:1:2176:A:C8	2.55	0.41
2:2:1126:U:O4	42:o:9:ARG:NH1	2.51	0.41
2:2:1369:C:H2'	2:2:1370:G:C8	2.56	0.41
3:3:7:G:H5"	16:O:29:HIS:CE1	2.55	0.41
5:B:251:GLN:HB3	5:B:255:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:83:VAL:HB	7:D:86:ALA:HB2	2.02	0.41
9:F:123:ALA:HA	9:F:133:LEU:HA	2.02	0.41
15:N:28:LEU:HD13	15:N:34:ILE:HG12	2.02	0.41
17:P:89:ARG:NE	17:P:113:ARG:O	2.53	0.41
37:j:86:LYS:HA	37:j:95:PHE:HA	2.02	0.41
37:j:156:LYS:HG2	40:m:71:VAL:HG13	2.02	0.41
41:n:128:SER:OG	41:n:130:ARG:OXT	2.34	0.41
42:o:28:THR:O	42:o:32:THR:OG1	2.32	0.41
42:o:34:ALA:HB3	42:o:78:GLU:HB2	2.01	0.41
44:q:18:LYS:NZ	44:q:19:SER:O	2.48	0.41
47:t:51:HIS:HA	47:t:54:ARG:HB3	2.02	0.41
1:1:992:C:H2'	1:1:993:G:H8	1.85	0.41
1:1:1187:G:OP1	19:R:85:LYS:NZ	2.42	0.41
1:1:1269:A:H61	1:1:2011:U:H3	1.67	0.41
1:1:1864:U:O2	1:1:1878:G:N2	2.34	0.41
1:1:1870:C:O2'	1:1:1871:A:O4'	2.38	0.41
1:1:2002:G:H5'	15:N:13:ASN:HA	2.02	0.41
1:1:2216:G:H2'	1:1:2217:G:H8	1.85	0.41
1:1:2452:C:H5'	55:A:252:GLN:HB3	2.02	0.41
1:1:2838:G:O2'	15:N:49:GLU:OE1	2.23	0.41
2:2:452:A:H2'	2:2:453:G:O4'	2.21	0.41
2:2:493:A:H2'	2:2:494:G:C8	2.56	0.41
3:3:40:U:N3	3:3:44:G:OP2	2.39	0.41
15:N:77:ALA:O	15:N:81:ASN:ND2	2.47	0.41
18:Q:92:ARG:HA	18:Q:95:LEU:HB2	2.01	0.41
39:l:5:ARG:NH1	39:l:7:ILE:HA	2.34	0.41
41:n:25:ASN:H	41:n:62:ASP:CG	2.28	0.41
46:s:53:ARG:HD3	46:s:59:ARG:HH12	1.85	0.41
55:A:115:PHE:O	55:A:119:PHE:N	2.50	0.41
1:1:69:C:H2'	1:1:70:G:H8	1.85	0.41
1:1:1094:U:H2'	1:1:1095:A:H2'	2.01	0.41
1:1:1127:A:N7	1:1:2488:G:O2'	2.54	0.41
1:1:1691:C:H2'	1:1:1692:U:C6	2.55	0.41
1:1:2329:U:H2'	1:1:2330:G:C8	2.55	0.41
1:1:2428:G:H4'	1:1:2429:G:C4	2.55	0.41
2:2:672:U:H2'	2:2:673:A:C8	2.56	0.41
2:2:1071:C:H2'	2:2:1072:G:C8	2.52	0.41
13:L:57:LEU:HD13	13:L:60:ARG:HH11	1.86	0.41
17:P:63:LYS:HE2	17:P:65:SER:HB2	2.03	0.41
22:U:18:ASP:HB3	22:U:21:LYS:HD2	2.02	0.41
35:h:156:ARG:NH1	35:h:160:ALA:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:170:TRP:CE3	36:i:186:PRO:HB3	2.56	0.41
41:n:34:SER:H	41:n:37:GLN:HB2	1.85	0.41
49:v:25:ILE:N	49:v:42:THR:O	2.48	0.41
54:5:51:C:H2'	54:5:52:G:C8	2.55	0.41
1:1:6:A:H2'	1:1:7:G:C8	2.55	0.41
1:1:455:C:N3	1:1:473:G:H5'	2.36	0.41
1:1:544:C:H3'	1:1:545:U:O2	2.21	0.41
1:1:552:U:H2'	1:1:553:G:C8	2.56	0.41
1:1:1161:C:H2'	1:1:1162:G:C8	2.56	0.41
1:1:1837:C:O2'	1:1:1927:A:N3	2.46	0.41
1:1:2106:U:O5'	1:1:2178:C:N4	2.53	0.41
2:2:1162:C:H2'	2:2:1163:A:C8	2.55	0.41
8:E:158:THR:OG1	8:E:159:THR:N	2.53	0.41
14:M:42:THR:HA	14:M:93:VAL:HG12	2.01	0.41
34:g:138:THR:O	34:g:142:GLU:N	2.44	0.41
39:l:140:ASP:OD1	39:l:143:ARG:NH1	2.43	0.41
45:r:33:ILE:O	45:r:37:ALA:N	2.53	0.41
50:w:34:THR:HG23	50:w:37:GLY:H	1.85	0.41
1:1:321:U:H5"	7:D:131:THR:HG23	2.02	0.41
1:1:372:G:C8	25:X:61:LYS:HD2	2.56	0.41
1:1:948:C:H2'	1:1:949:G:C8	2.56	0.41
1:1:995:C:H42	11:J:3:THR:H	1.67	0.41
1:1:1388:G:O2'	1:1:1525:A:O2'	2.38	0.41
1:1:2064:C:H42	1:1:2446:G:H1	1.68	0.41
1:1:2291:U:H2'	1:1:2292:U:C6	2.56	0.41
1:1:2563:U:H4'	12:K:28:SER:HA	2.02	0.41
1:1:2796:U:H3	1:1:2799:A:H61	1.69	0.41
1:1:2840:C:H5"	15:N:56:LYS:HZ1	1.85	0.41
2:2:1116:U:H2'	2:2:1117:A:C8	2.55	0.41
6:C:33:ARG:NH1	6:C:53:GLY:O	2.38	0.41
7:D:181:ILE:HG12	13:L:1:MET:HE3	2.03	0.41
24:W:56:ASP:OD1	24:W:58:THR:OG1	2.34	0.41
31:d:18:PHE:HA	31:d:43:THR:HG21	2.02	0.41
34:g:46:THR:HG23	34:g:201:PRO:HD2	2.03	0.41
39:l:69:VAL:HG21	39:l:104:ILE:HD11	2.01	0.41
45:r:33:ILE:HD12	45:r:59:GLU:HB3	2.03	0.41
55:A:213:ARG:HH12	55:A:329:ASP:HB2	1.86	0.41
1:1:548:G:H3'	1:1:549:G:O4'	2.21	0.41
1:1:563:A:N3	18:Q:37:GLN:NE2	2.65	0.41
1:1:1223:G:OP1	19:R:68:ARG:NH2	2.53	0.41
1:1:1267:U:H2'	1:1:1268:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1529:G:C4	1:1:1530:G:C8	3.09	0.41
1:1:2818:U:OP2	15:N:45:ARG:NH2	2.50	0.41
2:2:309:A:H2'	2:2:310:G:H8	1.86	0.41
2:2:680:C:H2'	2:2:681:A:C8	2.55	0.41
2:2:1280:A:OP2	42:o:9:ARG:NH2	2.46	0.41
6:C:136:ASN:HD21	6:C:139:SER:HB2	1.86	0.41
47:t:43:PHE:CD1	47:t:56:LEU:HD22	2.56	0.41
55:A:310:MET:HA	55:A:313:ASN:HB2	2.01	0.41
55:A:310:MET:HA	55:A:313:ASN:HD22	1.85	0.41
1:1:693:A:O2'	1:1:1353:A:N3	2.48	0.41
1:1:922:C:H2'	1:1:923:G:H8	1.85	0.41
1:1:1170:C:N4	1:1:1171:G:O6	2.54	0.41
1:1:1426:G:O2'	1:1:1572:A:N6	2.54	0.41
1:1:2024:G:O3'	6:C:154:LYS:NZ	2.44	0.41
1:1:2489:U:O2'	1:1:2518:A:N6	2.53	0.41
2:2:105:G:H2'	2:2:106:C:C6	2.56	0.41
2:2:460:A:H2'	2:2:461:A:C8	2.56	0.41
2:2:719:C:O2'	50:w:39:ILE:O	2.37	0.41
2:2:720:C:O3'	50:w:52:GLN:NE2	2.53	0.41
2:2:842:U:O2'	2:2:845:A:OP2	2.32	0.41
2:2:1088:G:H21	2:2:1167:A:H61	1.69	0.41
2:2:1103:C:OP1	34:g:95:ARG:NH2	2.53	0.41
2:2:1304:G:N2	2:2:1333:A:H62	2.19	0.41
2:2:1385:G:H2'	2:2:1386:G:C8	2.55	0.41
6:C:184:ARG:HG3	6:C:186:LEU:HG	2.03	0.41
7:D:149:ILE:HG12	7:D:188:MET:HA	2.02	0.41
7:D:157:LEU:HG	7:D:169:VAL:HG21	2.03	0.41
7:D:176:ASP:N	7:D:176:ASP:OD1	2.53	0.41
8:E:8:TYR:HB2	8:E:173:PHE:HZ	1.86	0.41
9:F:124:GLU:N	9:F:132:VAL:O	2.54	0.41
10:G:126:GLY:O	10:G:146:VAL:N	2.52	0.41
11:J:18:VAL:HB	11:J:56:VAL:HA	2.02	0.41
12:K:78:ARG:N	17:P:71:GLU:O	2.38	0.41
19:R:6:GLN:HG3	19:R:39:LEU:HD11	2.02	0.41
24:W:46:HIS:N	24:W:78:LYS:O	2.44	0.41
34:g:72:THR:OG1	34:g:169:GLU:OE2	2.31	0.41
41:n:42:GLU:O	41:n:46:MET:N	2.54	0.41
47:t:29:VAL:HG22	47:t:67:LEU:HD22	2.02	0.41
48:u:76:LYS:O	48:u:80:LYS:N	2.51	0.41
55:A:83:LEU:O	55:A:87:ALA:N	2.53	0.41
55:A:141:ALA:HB2	55:A:216:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A:189:TYR:CG	55:A:224:PRO:HB3	2.56	0.41
55:A:316:ASP:OD1	55:A:316:ASP:N	2.53	0.41
1:1:242:G:C8	32:e:3:LYS:HE3	2.56	0.41
1:1:243:U:N3	1:1:255:A:N7	2.67	0.41
1:1:784:G:C5	1:1:792:A:C5	3.08	0.41
1:1:1857:G:N2	1:1:1884:G:O2'	2.42	0.41
1:1:1987:A:H2'	1:1:1988:G:C8	2.56	0.41
1:1:2167:U:O2'	1:1:2169:A:N7	2.42	0.41
1:1:2315:G:H2'	1:1:2316:G:H8	1.86	0.41
1:1:2594:C:H2'	1:1:2595:G:C8	2.56	0.41
1:1:2696:U:H2'	1:1:2697:G:C8	2.56	0.41
2:2:157:U:H2'	2:2:158:G:C8	2.56	0.41
5:B:67:PHE:CE1	5:B:156:ARG:HD2	2.56	0.41
10:G:15:LEU:HD22	10:G:56:ALA:HB2	2.03	0.41
13:L:79:LEU:HD11	13:L:112:LEU:HD12	2.02	0.41
24:W:25:ARG:HH12	24:W:35:SER:HB3	1.86	0.41
35:h:172:ARG:HE	35:h:174:PRO:HD3	1.86	0.41
38:k:19:PRO:HA	38:k:22:ILE:HD12	2.02	0.41
1:1:21:A:N6	1:1:518:G:O6	2.54	0.40
1:1:69:C:H2'	1:1:70:G:C8	2.56	0.40
1:1:1000:A:H62	1:1:1154:G:H2'	1.86	0.40
1:1:2394:C:H5"	13:L:63:LYS:HE2	2.03	0.40
1:1:2436:G:O2'	1:1:2598:A:N1	2.52	0.40
1:1:2602:A:C5	55:A:254:VAL:HG22	2.57	0.40
2:2:235:C:H2'	2:2:236:A:C8	2.56	0.40
2:2:537:G:H2'	2:2:538:G:H8	1.85	0.40
2:2:689:C:H2'	2:2:690:G:O4'	2.21	0.40
2:2:1135:U:O2'	2:2:1136:C:H5"	2.21	0.40
2:2:1152:A:H2'	2:2:1153:G:C8	2.56	0.40
12:K:53:LYS:N	12:K:56:ASP:OD2	2.54	0.40
16:O:67:ASN:OD1	16:O:70:ALA:N	2.52	0.40
26:Y:18:LEU:HD21	26:Y:50:VAL:HG13	2.02	0.40
34:g:56:GLU:HG2	34:g:198:PHE:HE2	1.86	0.40
35:h:157:LEU:HB2	35:h:164:ARG:CZ	2.51	0.40
44:q:56:ARG:NE	44:q:62:GLU:OE1	2.50	0.40
46:s:54:ASP:HA	46:s:59:ARG:HG2	2.03	0.40
51:x:52:HIS:HB2	51:x:57:HIS:CE1	2.57	0.40
1:1:329:G:H1	22:U:17:LYS:HD3	1.85	0.40
1:1:660:C:H2'	1:1:661:A:C8	2.56	0.40
1:1:704:G:N2	1:1:726:G:O2'	2.54	0.40
1:1:2552:OMU:HM22	1:1:2554:U:H5	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:47:LYS:O	8:E:51:ASP:N	2.42	0.40
12:K:121:GLU:OE1	17:P:65:SER:OG	2.32	0.40
43:p:81:ASN:OD1	43:p:106:ARG:NH1	2.54	0.40
45:r:89:LEU:HD23	45:r:92:ARG:HE	1.86	0.40
54:5:50:U:H3	54:5:64:G:H1	1.68	0.40
1:1:240:C:OP2	1:1:241:A:O2'	2.37	0.40
1:1:759:G:H2'	1:1:760:G:H8	1.87	0.40
1:1:2425:A:H4'	1:1:2426:A:O5'	2.21	0.40
2:2:114:U:H2'	2:2:115:G:C8	2.57	0.40
2:2:1339:A:O2'	54:5:40:C:O2'	2.35	0.40
2:2:1347:G:H1'	2:2:1348:U:H5	1.86	0.40
2:2:1425:U:H2'	2:2:1426:G:C8	2.54	0.40
6:C:4:LEU:HG	6:C:32:ASN:ND2	2.37	0.40
34:g:24:ASN:HD21	34:g:26:LYS:HD2	1.85	0.40
37:j:16:ILE:HD12	37:j:36:LEU:HG	2.03	0.40
1:1:196:A:N7	13:L:38:GLN:NE2	2.56	0.40
1:1:1094:U:H1'	1:1:1097:U:H5	1.87	0.40
1:1:1796:U:H2'	1:1:1797:G:H8	1.85	0.40
1:1:2113:U:O4	1:1:2114:A:N6	2.54	0.40
1:1:2374:C:N4	1:1:2375:G:O6	2.55	0.40
1:1:2591:C:H2'	1:1:2592:G:C8	2.57	0.40
2:2:166:U:H2'	2:2:167:A:C8	2.56	0.40
2:2:166:U:H2'	2:2:167:A:H8	1.85	0.40
2:2:458:U:H2'	2:2:459:A:C8	2.56	0.40
2:2:668:G:O2'	47:t:46:HIS:ND1	2.40	0.40
2:2:946:A:H2'	2:2:947:G:C8	2.56	0.40
2:2:1074:G:O2'	2:2:1101:A:N1	2.52	0.40
5:B:168:ASP:N	5:B:168:ASP:OD1	2.54	0.40
12:K:123:LEU:HA	17:P:41:GLN:HE22	1.86	0.40
16:O:56:LYS:HE2	16:O:56:LYS:HB2	1.93	0.40
18:Q:49:ASP:HA	18:Q:52:GLN:HB2	2.02	0.40
28:a:16:CYS:HA	28:a:34:LEU:HB2	2.03	0.40
37:j:99:ALA:HB2	37:j:124:LEU:HG	2.03	0.40
43:p:36:ASP:OD1	43:p:40:ASN:N	2.54	0.40
1:1:399:U:H2'	1:1:400:G:O4'	2.22	0.40
1:1:552:U:H2'	1:1:553:G:H8	1.86	0.40
1:1:2417:C:H2'	1:1:2418:A:H8	1.85	0.40
1:1:2789:C:H2'	1:1:2893:A:N7	2.36	0.40
2:2:129:A:H2	2:2:232:G:H22	1.69	0.40
2:2:1004:A:H5"	2:2:1025:U:C2	2.56	0.40
7:D:111:GLU:O	7:D:115:GLN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:72:LEU:HA	9:F:75:MET:HB2	2.03	0.40
25:X:70:GLU:O	25:X:74:ARG:N	2.52	0.40
35:h:20:SER:HB3	35:h:22:TRP:NE1	2.37	0.40
38:k:18:VAL:HA	38:k:21:MET:HE3	2.04	0.40
55:A:64:GLU:HA	55:A:67:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	269/271 (99%)	254 (94%)	15 (6%)	0	100	100
6	C	207/209 (99%)	198 (96%)	7 (3%)	2 (1%)	12	45
7	D	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
8	E	175/177 (99%)	160 (91%)	14 (8%)	1 (1%)	21	55
9	F	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
10	G	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
11	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
12	K	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
13	L	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
15	N	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
16	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
17	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
18	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
19	R	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	12	45
20	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
22	U	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
23	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
24	W	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
25	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
26	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
27	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
28	a	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
29	b	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
30	c	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
31	d	44/46 (96%)	44 (100%)	0	0	100	100
32	e	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	36
33	f	36/38 (95%)	36 (100%)	0	0	100	100
34	g	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
35	h	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
36	i	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
37	j	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
38	k	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	l	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
40	m	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
41	n	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
42	o	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
43	p	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
44	q	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
45	r	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
46	s	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
47	t	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	5	30
48	u	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
49	v	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
50	w	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
51	x	81/83 (98%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	y	84/86 (98%)	84 (100%)	0	0	100	100
53	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	A	355/357 (99%)	331 (93%)	24 (7%)	0	100	100
56	6	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5929/6031 (98%)	5627 (95%)	295 (5%)	7 (0%)	49	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	151	THR
47	t	50	HIS
47	t	74	ASP
19	R	52	PRO
32	e	32	ILE
8	E	124	GLY
6	C	153	GLY

5.3.2 Protein sidechains (i)

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	
5	B	216/216 (100%)	216 (100%)	0	100	100
6	C	164/164 (100%)	163 (99%)	1 (1%)	78	80
7	D	165/165 (100%)	165 (100%)	0	100	100
8	E	148/148 (100%)	147 (99%)	1 (1%)	76	78
9	F	136/136 (100%)	136 (100%)	0	100	100
10	G	114/114 (100%)	114 (100%)	0	100	100
11	J	116/116 (100%)	116 (100%)	0	100	100
12	K	104/104 (100%)	104 (100%)	0	100	100
13	L	103/103 (100%)	103 (100%)	0	100	100
14	M	109/109 (100%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	N	99/99 (100%)	97 (98%)	2 (2%)	48 65
16	O	86/86 (100%)	86 (100%)	0	100 100
17	P	99/99 (100%)	99 (100%)	0	100 100
18	Q	89/89 (100%)	89 (100%)	0	100 100
19	R	84/84 (100%)	83 (99%)	1 (1%)	63 72
20	S	93/93 (100%)	93 (100%)	0	100 100
21	T	81/81 (100%)	81 (100%)	0	100 100
22	U	84/84 (100%)	84 (100%)	0	100 100
23	V	78/78 (100%)	77 (99%)	1 (1%)	61 71
24	W	58/58 (100%)	58 (100%)	0	100 100
25	X	67/67 (100%)	67 (100%)	0	100 100
26	Y	54/54 (100%)	54 (100%)	0	100 100
27	Z	48/48 (100%)	48 (100%)	0	100 100
28	a	59/59 (100%)	59 (100%)	0	100 100
29	b	47/47 (100%)	47 (100%)	0	100 100
30	c	47/47 (100%)	47 (100%)	0	100 100
31	d	38/38 (100%)	38 (100%)	0	100 100
32	e	51/51 (100%)	51 (100%)	0	100 100
33	f	34/34 (100%)	34 (100%)	0	100 100
34	g	187/187 (100%)	186 (100%)	1 (0%)	81 82
35	h	171/171 (100%)	169 (99%)	2 (1%)	63 72
36	i	172/172 (100%)	172 (100%)	0	100 100
37	j	119/119 (100%)	119 (100%)	0	100 100
38	k	91/91 (100%)	91 (100%)	0	100 100
39	l	124/124 (100%)	124 (100%)	0	100 100
40	m	104/104 (100%)	104 (100%)	0	100 100
41	n	105/105 (100%)	105 (100%)	0	100 100
42	o	86/86 (100%)	86 (100%)	0	100 100
43	p	90/90 (100%)	90 (100%)	0	100 100
44	q	74/74 (100%)	74 (100%)	0	100 100
45	r	94/94 (100%)	94 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	s	83/83 (100%)	83 (100%)	0	100 100
47	t	76/76 (100%)	71 (93%)	5 (7%)	15 41
48	u	65/65 (100%)	65 (100%)	0	100 100
49	v	74/74 (100%)	74 (100%)	0	100 100
50	w	57/57 (100%)	57 (100%)	0	100 100
51	x	72/72 (100%)	72 (100%)	0	100 100
52	y	65/65 (100%)	65 (100%)	0	100 100
53	z	60/60 (100%)	60 (100%)	0	100 100
55	A	304/305 (100%)	304 (100%)	0	100 100
56	6	2/2 (100%)	2 (100%)	0	100 100
All	All	4946/4947 (100%)	4932 (100%)	14 (0%)	84 85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	151	THR
8	E	40	VAL
15	N	2	ARG
15	N	48	VAL
19	R	51	VAL
23	V	65	VAL
34	g	129	LEU
35	h	72	ARG
35	h	179	ARG
47	t	49	ASP
47	t	52	SER
47	t	53	ARG
47	t	60	VAL
47	t	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	53	HIS
5	B	86	ASN
5	B	197	ASN
5	B	260	ASN

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Mol	Chain	Res	Type
6	C	32	ASN
6	C	136	ASN
6	C	173	GLN
7	D	29	HIS
7	D	92	HIS
7	D	115	GLN
7	D	136	GLN
7	D	163	ASN
7	D	195	GLN
9	F	73	ASN
9	F	116	GLN
13	L	54	GLN
14	M	22	GLN
16	O	29	HIS
16	O	38	GLN
16	O	61	GLN
16	O	100	HIS
17	P	12	GLN
17	P	15	GLN
18	Q	37	GLN
18	Q	44	GLN
18	Q	72	ASN
19	R	12	HIS
20	S	7	HIS
20	S	40	ASN
20	S	61	ASN
21	T	70	HIS
22	U	46	GLN
22	U	54	GLN
23	V	75	GLN
25	X	34	HIS
26	Y	15	ASN
26	Y	20	ASN
26	Y	39	GLN
26	Y	45	GLN
27	Z	20	HIS
28	a	20	ASN
29	b	6	ASN
29	b	42	HIS
30	c	26	ASN
31	d	13	ASN
31	d	16	HIS

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Mol	Chain	Res	Type
32	e	26	HIS
33	f	37	GLN
34	g	39	HIS
34	g	51	ASN
34	g	177	ASN
35	h	8	ASN
35	h	41	GLN
36	i	59	GLN
36	i	116	GLN
36	i	198	HIS
37	j	12	GLN
37	j	121	HIS
38	k	46	GLN
38	k	63	ASN
38	k	68	GLN
39	l	28	ASN
39	l	130	ASN
43	p	40	ASN
43	p	119	ASN
44	q	5	ASN
45	r	8	ASN
47	t	20	ASN
47	t	40	GLN
47	t	50	HIS
47	t	51	HIS
48	u	26	ASN
50	w	52	GLN
51	x	52	HIS
51	x	57	HIS
52	y	48	GLN
52	y	52	ASN
55	A	43	GLN
55	A	199	HIS
55	A	255	ASN
55	A	276	ASN
55	A	281	HIS
55	A	313	ASN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	759 (26%)	16 (0%)
2	2	1532/1534 (99%)	415 (27%)	5 (0%)
3	3	119/120 (99%)	23 (19%)	0
4	4	8/9 (88%)	2 (25%)	0
54	5	75/76 (98%)	19 (25%)	0
All	All	4636/4642 (99%)	1218 (26%)	21 (0%)

All (1218) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	34	U
1	1	35	G
1	1	40	U
1	1	46	G
1	1	48	G
1	1	51	G
1	1	58	G
1	1	60	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	88	G
1	1	100	U
1	1	101	A
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U
1	1	126	A
1	1	132	G
1	1	136	G
1	1	137	U
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A

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Mol	Chain	Res	Type
1	1	146	A
1	1	158	U
1	1	163	C
1	1	171	U
1	1	184	C
1	1	196	A
1	1	199	A
1	1	206	U
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	226	A
1	1	228	C
1	1	230	G
1	1	233	A
1	1	248	G
1	1	255	A
1	1	266	G
1	1	267	C
1	1	270	A
1	1	271	G
1	1	273	G
1	1	275	C
1	1	276	U
1	1	277	G
1	1	278	A
1	1	284	U
1	1	285	G
1	1	295	G
1	1	311	A
1	1	317	G
1	1	318	C
1	1	322	A
1	1	329	G
1	1	330	A
1	1	346	A
1	1	353	C
1	1	361	G
1	1	367	G
1	1	371	A
1	1	372	G

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Mol	Chain	Res	Type
1	1	386	G
1	1	396	G
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	438	G
1	1	445	C
1	1	449	A
1	1	451	U
1	1	454	A
1	1	455	C
1	1	457	A
1	1	479	A
1	1	481	G
1	1	483	A
1	1	484	C
1	1	488	G
1	1	496	G
1	1	505	A
1	1	508	A
1	1	509	C
1	1	510	C
1	1	513	A
1	1	518	G
1	1	519	U
1	1	527	C
1	1	529	A
1	1	531	C
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	552	U
1	1	563	A
1	1	565	C

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Mol	Chain	Res	Type
1	1	568	U
1	1	573	U
1	1	575	A
1	1	581	C
1	1	582	A
1	1	586	A
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	627	A
1	1	637	A
1	1	645	C
1	1	646	U
1	1	651	G
1	1	654	A
1	1	655	A
1	1	656	G
1	1	664	G
1	1	670	A
1	1	681	G
1	1	686	U
1	1	714	U
1	1	717	C
1	1	726	G
1	1	727	A
1	1	730	A
1	1	740	C
1	1	744	U
1	1	747	5MU
1	1	748	G
1	1	752	A
1	1	757	G
1	1	762	U
1	1	763	G
1	1	764	A
1	1	765	C
1	1	770	G
1	1	775	G
1	1	776	G
1	1	781	A

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Mol	Chain	Res	Type
1	1	782	A
1	1	783	A
1	1	784	G
1	1	785	G
1	1	789	A
1	1	792	A
1	1	793	A
1	1	794	A
1	1	795	C
1	1	803	U
1	1	805	G
1	1	809	G
1	1	810	U
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	829	A
1	1	831	G
1	1	846	U
1	1	856	G
1	1	858	G
1	1	859	G
1	1	869	G
1	1	877	A
1	1	878	A
1	1	880	G
1	1	882	G
1	1	883	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	893	C
1	1	894	U
1	1	895	U
1	1	896	A
1	1	910	A
1	1	914	G
1	1	915	C
1	1	932	U

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Mol	Chain	Res	Type
1	1	941	A
1	1	945	A
1	1	946	C
1	1	947	A
1	1	948	C
1	1	958	U
1	1	959	A
1	1	961	C
1	1	965	C
1	1	973	A
1	1	974	G
1	1	980	A
1	1	981	A
1	1	983	A
1	1	989	G
1	1	990	A
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1014	A
1	1	1017	G
1	1	1020	A
1	1	1022	G
1	1	1023	U
1	1	1024	G
1	1	1026	G
1	1	1033	U
1	1	1041	G
1	1	1042	G
1	1	1044	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1058	U
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1064	C

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Mol	Chain	Res	Type
1	1	1066	U
1	1	1067	A
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1074	G
1	1	1075	C
1	1	1077	A
1	1	1078	U
1	1	1079	C
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1085	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1115	G
1	1	1119	U
1	1	1128	G
1	1	1129	A
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1141	U
1	1	1142	A
1	1	1151	A
1	1	1158	C
1	1	1161	C
1	1	1168	G
1	1	1169	A

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Mol	Chain	Res	Type
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1190	G
1	1	1206	G
1	1	1211	C
1	1	1212	G
1	1	1217	U
1	1	1218	G
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1248	G
1	1	1249	U
1	1	1251	C
1	1	1252	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1275	A
1	1	1287	A
1	1	1294	U
1	1	1300	G
1	1	1301	A
1	1	1306	C
1	1	1312	U
1	1	1324	G
1	1	1329	U
1	1	1332	G
1	1	1338	G
1	1	1341	G

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Mol	Chain	Res	Type
1	1	1345	C
1	1	1351	C
1	1	1355	G
1	1	1360	G
1	1	1361	G
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1385	A
1	1	1388	G
1	1	1394	U
1	1	1395	A
1	1	1396	U
1	1	1398	C
1	1	1403	A
1	1	1409	U
1	1	1410	G
1	1	1411	U
1	1	1412	U
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1425	G
1	1	1428	C
1	1	1437	C
1	1	1449	G
1	1	1455	G
1	1	1458	U
1	1	1461	C
1	1	1467	U
1	1	1476	U
1	1	1478	G
1	1	1479	G
1	1	1482	G
1	1	1484	U
1	1	1489	C
1	1	1490	A
1	1	1491	G

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Mol	Chain	Res	Type
1	1	1493	C
1	1	1494	A
1	1	1502	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1515	A
1	1	1516	G
1	1	1523	U
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1531	C
1	1	1532	A
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1550	C
1	1	1559	U
1	1	1560	G
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1586	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1607	C
1	1	1613	G
1	1	1616	A
1	1	1618	6MZ
1	1	1619	G
1	1	1626	A
1	1	1634	A
1	1	1639	C
1	1	1646	C

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Mol	Chain	Res	Type
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1657	U
1	1	1659	G
1	1	1660	G
1	1	1668	A
1	1	1669	A
1	1	1674	G
1	1	1693	U
1	1	1694	C
1	1	1695	G
1	1	1713	A
1	1	1715	G
1	1	1716	U
1	1	1722	A
1	1	1723	G
1	1	1724	G
1	1	1725	U
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1733	G
1	1	1738	G
1	1	1744	A
1	1	1751	U
1	1	1754	A
1	1	1756	G
1	1	1758	U
1	1	1759	A
1	1	1760	C
1	1	1764	C
1	1	1765	U
1	1	1773	A
1	1	1781	U
1	1	1784	A
1	1	1786	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1808	A

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Mol	Chain	Res	Type
1	1	1816	C
1	1	1820	U
1	1	1829	A
1	1	1830	C
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1858	A
1	1	1859	U
1	1	1862	G
1	1	1865	U
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1884	G
1	1	1889	A
1	1	1899	A
1	1	1900	A
1	1	1903	G
1	1	1906	G
1	1	1913	A
1	1	1914	C
1	1	1915	3TD
1	1	1916	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1941	C
1	1	1943	U
1	1	1955	U
1	1	1960	A
1	1	1962	5MC
1	1	1963	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G

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Mol	Chain	Res	Type
1	1	1982	U
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2010	G
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2032	G
1	1	2033	A
1	1	2034	U
1	1	2043	C
1	1	2047	C
1	1	2048	G
1	1	2049	G
1	1	2051	A
1	1	2052	A
1	1	2053	G
1	1	2055	C
1	1	2056	G
1	1	2057	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2094	A
1	1	2095	A
1	1	2102	G
1	1	2103	C
1	1	2105	U
1	1	2106	U
1	1	2108	A
1	1	2109	U
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A

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Mol	Chain	Res	Type
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2121	G
1	1	2122	U
1	1	2123	G
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2130	U
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2135	A
1	1	2136	G
1	1	2137	U
1	1	2138	G
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2153	C
1	1	2156	G
1	1	2158	A
1	1	2160	C
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2166	U
1	1	2167	U
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2174	C

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Mol	Chain	Res	Type
1	1	2175	C
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2214	C
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2266	A
1	1	2269	G
1	1	2278	A
1	1	2279	G
1	1	2283	C
1	1	2287	A
1	1	2305	U
1	1	2309	A
1	1	2315	G
1	1	2319	G
1	1	2320	U
1	1	2321	U
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2335	A
1	1	2336	A
1	1	2344	U
1	1	2347	C
1	1	2350	C

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Mol	Chain	Res	Type
1	1	2357	G
1	1	2361	G
1	1	2379	G
1	1	2383	G
1	1	2385	C
1	1	2388	A
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2410	G
1	1	2419	U
1	1	2422	C
1	1	2423	U
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2436	G
1	1	2439	A
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2484	G
1	1	2490	G
1	1	2491	U
1	1	2492	U
1	1	2494	G
1	1	2501	C
1	1	2502	G
1	1	2503	2MA
1	1	2504	PSU
1	1	2505	G
1	1	2507	C
1	1	2513	A

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Mol	Chain	Res	Type
1	1	2517	C
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2530	A
1	1	2531	A
1	1	2535	G
1	1	2547	A
1	1	2553	G
1	1	2554	U
1	1	2562	U
1	1	2564	A
1	1	2566	A
1	1	2567	G
1	1	2571	U
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2583	G
1	1	2585	U
1	1	2602	A
1	1	2604	U
1	1	2608	G
1	1	2609	U
1	1	2610	C
1	1	2613	U
1	1	2629	U
1	1	2630	G
1	1	2634	A
1	1	2636	C
1	1	2646	C
1	1	2654	A
1	1	2656	U
1	1	2673	G
1	1	2684	U
1	1	2689	U
1	1	2690	U
1	1	2707	U
1	1	2713	U
1	1	2716	C
1	1	2718	G
1	1	2719	G

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Mol	Chain	Res	Type
1	1	2725	A
1	1	2726	A
1	1	2729	G
1	1	2731	G
1	1	2732	G
1	1	2733	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2750	A
1	1	2751	G
1	1	2756	U
1	1	2757	A
1	1	2765	A
1	1	2766	A
1	1	2773	C
1	1	2778	A
1	1	2787	C
1	1	2789	C
1	1	2794	C
1	1	2796	U
1	1	2798	U
1	1	2802	G
1	1	2804	U
1	1	2805	C
1	1	2806	C
1	1	2810	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2832	U
1	1	2833	U
1	1	2834	G
1	1	2835	A
1	1	2837	A
1	1	2840	C
1	1	2841	C
1	1	2848	G
1	1	2849	U
1	1	2854	G
1	1	2861	U

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Mol	Chain	Res	Type
1	1	2865	U
1	1	2866	U
1	1	2867	G
1	1	2873	A
1	1	2875	C
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2886	A
1	1	2891	U
1	1	2893	A
1	1	2898	U
1	1	2901	C
2	2	4	U
2	2	5	U
2	2	6	G
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	29	U
2	2	32	A
2	2	39	G
2	2	41	G
2	2	42	G
2	2	43	C
2	2	44	A
2	2	47	C
2	2	48	C
2	2	49	U
2	2	50	A
2	2	51	A
2	2	54	C
2	2	61	G
2	2	64	G
2	2	65	A
2	2	66	A
2	2	68	G
2	2	70	U
2	2	71	A
2	2	72	A

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Mol	Chain	Res	Type
2	2	74	A
2	2	77	A
2	2	78	A
2	2	79	G
2	2	81	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	88	U
2	2	89	U
2	2	91	U
2	2	92	U
2	2	93	U
2	2	95	C
2	2	104	G
2	2	106	C
2	2	108	G
2	2	110	C
2	2	116	A
2	2	119	A
2	2	120	A
2	2	121	U
2	2	123	U
2	2	130	A
2	2	131	A
2	2	138	G
2	2	141	G
2	2	144	G
2	2	149	A
2	2	154	U
2	2	156	C
2	2	161	A
2	2	164	G
2	2	165	G
2	2	168	G
2	2	173	U
2	2	177	G
2	2	178	C
2	2	181	A

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Mol	Chain	Res	Type
2	2	182	A
2	2	183	C
2	2	184	G
2	2	188	C
2	2	191	G
2	2	195	A
2	2	197	A
2	2	201	G
2	2	202	G
2	2	204	G
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	215	C
2	2	217	C
2	2	222	C
2	2	225	C
2	2	234	C
2	2	240	G
2	2	243	A
2	2	245	U
2	2	247	G
2	2	251	G
2	2	253	A
2	2	266	G
2	2	267	C
2	2	279	A
2	2	281	G
2	2	289	G
2	2	293	G
2	2	306	A
2	2	308	C
2	2	310	G
2	2	319	G
2	2	321	A
2	2	328	C
2	2	330	C
2	2	332	G
2	2	345	C
2	2	347	G

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Mol	Chain	Res	Type
2	2	348	G
2	2	351	G
2	2	352	C
2	2	353	A
2	2	354	G
2	2	355	C
2	2	363	A
2	2	367	U
2	2	368	U
2	2	369	G
2	2	372	C
2	2	376	G
2	2	381	C
2	2	384	G
2	2	388	G
2	2	390	U
2	2	391	G
2	2	398	U
2	2	401	C
2	2	402	G
2	2	404	G
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	428	G
2	2	429	U
2	2	438	U
2	2	439	U
2	2	444	G
2	2	451	A
2	2	452	A
2	2	456	A
2	2	457	G
2	2	459	A
2	2	463	U
2	2	464	U
2	2	466	A

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Mol	Chain	Res	Type
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	482	A
2	2	486	U
2	2	488	C
2	2	490	C
2	2	495	A
2	2	496	A
2	2	497	G
2	2	505	G
2	2	511	C
2	2	515	G
2	2	517	G
2	2	518	C
2	2	521	G
2	2	524	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	545	C
2	2	547	A
2	2	554	A
2	2	562	U
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	578	C
2	2	581	G
2	2	587	G
2	2	588	G
2	2	596	A
2	2	603	U
2	2	615	G
2	2	618	C

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Mol	Chain	Res	Type
2	2	632	U
2	2	633	G
2	2	640	A
2	2	641	U
2	2	648	A
2	2	649	A
2	2	650	G
2	2	653	U
2	2	665	A
2	2	668	G
2	2	673	A
2	2	686	U
2	2	687	A
2	2	695	A
2	2	700	G
2	2	703	G
2	2	717	U
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	744	C
2	2	747	A
2	2	748	G
2	2	752	G
2	2	753	A
2	2	755	G
2	2	761	G
2	2	772	U
2	2	773	G
2	2	774	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	798	U
2	2	799	G
2	2	814	A
2	2	815	A
2	2	817	C
2	2	820	U

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Mol	Chain	Res	Type
2	2	821	G
2	2	823	C
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	849	G
2	2	851	G
2	2	864	A
2	2	876	C
2	2	877	G
2	2	878	A
2	2	884	U
2	2	885	G
2	2	893	C
2	2	902	G
2	2	913	A
2	2	914	A
2	2	926	G
2	2	930	C
2	2	934	C
2	2	935	A
2	2	942	G
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	969	A
2	2	971	G
2	2	975	A
2	2	976	G
2	2	977	A
2	2	987	G
2	2	989	U
2	2	992	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1003	G

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Mol	Chain	Res	Type
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1011	C
2	2	1017	U
2	2	1018	G
2	2	1019	A
2	2	1020	G
2	2	1023	U
2	2	1026	G
2	2	1028	C
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1035	A
2	2	1036	A
2	2	1037	C
2	2	1038	C
2	2	1043	G
2	2	1050	G
2	2	1053	G
2	2	1054	C
2	2	1056	U
2	2	1065	U
2	2	1067	A
2	2	1085	U
2	2	1086	U
2	2	1089	G
2	2	1092	A
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1102	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1126	U
2	2	1132	C
2	2	1133	G
2	2	1135	U

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Mol	Chain	Res	Type
2	2	1136	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1145	A
2	2	1151	A
2	2	1152	A
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1171	A
2	2	1176	A
2	2	1177	G
2	2	1184	G
2	2	1193	G
2	2	1196	A
2	2	1197	A
2	2	1200	C
2	2	1201	A
2	2	1206	G
2	2	1207	2MG
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1227	A
2	2	1228	C
2	2	1231	G
2	2	1238	A
2	2	1240	U
2	2	1241	G
2	2	1254	A
2	2	1256	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G

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Mol	Chain	Res	Type
2	2	1299	A
2	2	1301	U
2	2	1302	C
2	2	1305	G
2	2	1317	C
2	2	1320	C
2	2	1331	G
2	2	1336	C
2	2	1338	G
2	2	1340	A
2	2	1363	A
2	2	1368	A
2	2	1370	G
2	2	1379	G
2	2	1380	U
2	2	1384	C
2	2	1397	C
2	2	1398	A
2	2	1401	G
2	2	1402	4OC
2	2	1404	C
2	2	1419	G
2	2	1422	G
2	2	1429	A
2	2	1432	G
2	2	1441	A
2	2	1446	A
2	2	1451	U
2	2	1452	C
2	2	1453	G
2	2	1458	G
2	2	1475	G
2	2	1487	G
2	2	1489	G
2	2	1491	G
2	2	1492	A
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1507	A
2	2	1510	C
2	2	1511	G

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Mol	Chain	Res	Type
2	2	1512	U
2	2	1517	G
2	2	1519	MA6
2	2	1520	C
2	2	1529	G
2	2	1530	G
2	2	1531	A
2	2	1533	C
2	2	1534	A
3	3	9	G
3	3	13	G
3	3	15	A
3	3	24	G
3	3	31	C
3	3	32	U
3	3	35	C
3	3	36	C
3	3	40	U
3	3	41	G
3	3	42	C
3	3	44	G
3	3	45	A
3	3	56	G
3	3	58	A
3	3	66	A
3	3	68	C
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
3	3	119	A
4	4	20	A
4	4	21	A
54	5	8	4SU
54	5	12	C
54	5	13	A
54	5	16	C
54	5	17	U
54	5	19	G
54	5	20	H2U
54	5	43	A

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Mol	Chain	Res	Type
54	5	46	A
54	5	47	U
54	5	48	C
54	5	49	G
54	5	53	G
54	5	55	PSU
54	5	68	C
54	5	72	A
54	5	73	A
54	5	74	C
54	5	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	947	A
1	1	1170	C
1	1	1175	A
1	1	1252	G
1	1	1379	U
1	1	1530	G
1	1	2146	C
1	1	2189	U
1	1	2193	G
1	1	2286	G
1	1	2425	A
1	1	2756	U
2	2	83	C
2	2	210	C
2	2	496	A
2	2	516	PSU
2	2	1109	C

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

39 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	1MG	1	745	1	23,26,27	2.83	7 (30%)	33,39,42	2.07	9 (27%)
1	G7M	1	2069	1	23,26,27	2.58	8 (34%)	34,39,42	2.51	11 (32%)
54	5MU	5	54	54	19,22,23	4.81	7 (36%)	27,32,35	3.52	8 (29%)
1	5MU	1	1939	1	19,22,23	4.77	7 (36%)	27,32,35	3.82	10 (37%)
1	5MU	1	747	1	19,22,23	4.82	7 (36%)	27,32,35	3.92	9 (33%)
1	PSU	1	1911	1	18,21,22	1.13	2 (11%)	21,30,33	2.16	5 (23%)
2	5MC	2	1407	2	19,22,23	3.81	8 (42%)	26,32,35	1.12	3 (11%)
2	MA6	2	1519	2	23,26,27	1.53	4 (17%)	33,38,41	2.77	13 (39%)
54	4OC	5	32	54	20,23,24	3.00	8 (40%)	25,32,35	1.02	1 (4%)
1	6MZ	1	2030	1	22,25,26	2.89	6 (27%)	29,36,39	4.47	13 (44%)
2	G7M	2	527	2	23,26,27	3.59	12 (52%)	34,39,42	1.57	7 (20%)
1	3TD	1	1915	1	19,22,23	4.25	5 (26%)	23,32,35	2.02	4 (17%)
1	PSU	1	2580	1	18,21,22	1.10	2 (11%)	21,30,33	2.07	5 (23%)
1	PSU	1	2605	1	18,21,22	1.12	2 (11%)	21,30,33	2.10	5 (23%)
1	PSU	1	2504	1	18,21,22	1.22	2 (11%)	21,30,33	1.93	4 (19%)
2	2MG	2	1516	2	23,26,27	2.95	8 (34%)	33,38,41	2.14	10 (30%)
1	2MG	1	2445	1	23,26,27	2.94	6 (26%)	33,38,41	2.27	7 (21%)
54	4SU	5	8	54	18,21,22	3.69	7 (38%)	25,30,33	2.22	5 (20%)
2	5MC	2	967	2	19,22,23	3.83	8 (42%)	26,32,35	0.99	1 (3%)
1	6MZ	1	1618	1	22,25,26	2.85	6 (27%)	29,36,39	4.45	14 (48%)
1	2MA	1	2503	1	22,25,26	3.71	8 (36%)	32,37,40	2.44	7 (21%)
1	OMC	1	2498	1	19,22,23	2.91	7 (36%)	25,31,34	0.91	1 (4%)
2	4OC	2	1402	2	20,23,24	3.00	8 (40%)	25,32,35	1.25	4 (16%)
54	H2U	5	20	54	18,21,22	3.38	5 (27%)	19,30,33	1.55	4 (21%)
2	PSU	2	516	2	18,21,22	1.02	1 (5%)	21,30,33	1.95	5 (23%)
1	OMU	1	2552	1	19,22,23	2.88	8 (42%)	25,31,34	1.92	5 (20%)
56	FME	6	77	56	8,9,10	0.92	0	8,9,11	0.73	0
1	PSU	1	955	1	18,21,22	1.04	1 (5%)	21,30,33	1.80	3 (14%)
2	MA6	2	1518	2	23,26,27	1.56	5 (21%)	33,38,41	2.71	12 (36%)
1	PSU	1	2457	1	18,21,22	1.17	3 (16%)	21,30,33	2.02	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MG	1	1835	1	23,26,27	2.89	7 (30%)	33,38,41	2.20	10 (30%)
1	PSU	1	746	1	18,21,22	1.08	2 (11%)	21,30,33	1.81	4 (19%)
54	PSU	5	55	54	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
1	PSU	1	1917	1	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
2	2MG	2	966	2	23,26,27	2.99	7 (30%)	33,38,41	2.30	7 (21%)
1	OMG	1	2251	1,54	23,26,27	2.40	8 (34%)	32,38,41	1.95	8 (25%)
1	5MC	1	1962	1	19,22,23	3.79	8 (42%)	26,32,35	1.02	2 (7%)
2	2MG	2	1207	2	23,26,27	2.88	7 (30%)	33,38,41	2.34	9 (27%)
2	UR3	2	1498	2	19,22,23	2.53	7 (36%)	26,32,35	1.56	3 (11%)

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	1MG	1	745	1	-	0/7/25/26	0/3/3/3
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
54	5MU	5	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	1/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	3/11/29/30	0/3/3/3
54	4OC	5	32	54	-	0/9/29/30	0/2/2/2
1	6MZ	1	2030	1	-	3/9/27/28	0/3/3/3
2	G7M	2	527	2	-	2/7/25/26	0/3/3/3
1	3TD	1	1915	1	-	4/7/25/26	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
54	4SU	5	8	54	-	3/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/9/27/28	0/3/3/3
1	2MA	1	2503	1	-	5/7/25/26	0/3/3/3
1	OMC	1	2498	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
54	H2U	5	20	54	-	4/7/38/39	0/2/2/2
2	PSU	2	516	2	-	2/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	1/9/27/28	0/2/2/2
56	FME	6	77	56	-	3/7/9/11	-
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	PSU	1	746	1	-	2/7/25/26	0/2/2/2
54	PSU	5	55	54	-	1/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	0/9/27/28	0/3/3/3
1	OMG	1	2251	1,54	-	0/9/27/28	0/3/3/3
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	2/9/27/28	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	13.15	1.49	1.35
1	1	2503	2MA	C4-N3	11.48	1.49	1.34
1	1	2030	6MZ	C6-N6	11.32	1.47	1.34
1	1	747	5MU	C2-N1	11.29	1.56	1.38
54	5	20	H2U	C2-N1	11.13	1.51	1.35
1	1	1618	6MZ	C6-N6	11.01	1.46	1.34
54	5	54	5MU	C2-N1	10.95	1.55	1.38
1	1	1939	5MU	C2-N1	10.83	1.55	1.38
2	2	527	G7M	C8-N7	10.78	1.51	1.33
54	5	54	5MU	C6-N1	10.57	1.56	1.38
1	1	1939	5MU	C6-N1	10.20	1.55	1.38
1	1	747	5MU	C6-N1	10.03	1.55	1.38
1	1	747	5MU	C4-C5	9.79	1.60	1.44
1	1	1915	3TD	C2-N1	9.77	1.49	1.37
1	1	1939	5MU	C4-C5	9.76	1.60	1.44
54	5	54	5MU	C4-C5	9.74	1.60	1.44
1	1	1962	5MC	C6-C5	9.03	1.49	1.34
2	2	967	5MC	C6-C5	9.03	1.49	1.34
2	2	1407	5MC	C6-C5	8.97	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	747	5MU	C4-N3	-8.09	1.23	1.38
54	5	54	5MU	C4-N3	-8.06	1.23	1.38
54	5	8	4SU	C4-N3	8.02	1.45	1.37
1	1	1939	5MU	C4-N3	-7.98	1.23	1.38
54	5	8	4SU	C2-N1	7.71	1.50	1.38
2	2	966	2MG	C2-N3	7.56	1.46	1.32
1	1	2445	2MG	C2-N3	7.54	1.46	1.32
1	1	745	1MG	C2-N2	7.48	1.47	1.34
1	1	1835	2MG	C2-N3	7.24	1.45	1.32
2	2	1516	2MG	C2-N3	7.21	1.45	1.32
2	2	1207	2MG	C2-N3	7.18	1.45	1.32
2	2	967	5MC	C4-N3	7.10	1.45	1.34
1	1	2503	2MA	C2-N3	7.00	1.46	1.34
2	2	1402	4OC	C4-N3	6.94	1.44	1.32
1	1	1962	5MC	C4-N3	6.92	1.45	1.34
54	5	32	4OC	C4-N3	6.88	1.44	1.32
2	2	966	2MG	C4-N3	6.80	1.49	1.34
2	2	1407	5MC	C4-N3	6.65	1.44	1.34
1	1	2445	2MG	C4-N3	6.64	1.49	1.34
2	2	966	2MG	C2-N2	6.64	1.47	1.33
1	1	745	1MG	C2-N3	6.62	1.44	1.33
2	2	1516	2MG	C2-N2	6.62	1.47	1.33
54	5	20	H2U	C2-N3	6.60	1.49	1.38
1	1	2552	OMU	C2-N3	6.59	1.49	1.38
1	1	2069	G7M	C4-N3	6.56	1.49	1.34
1	1	745	1MG	C4-N3	6.56	1.49	1.34
2	2	1207	2MG	C4-N3	6.54	1.49	1.34
2	2	1516	2MG	C4-N3	6.49	1.49	1.34
1	1	2445	2MG	C2-N2	6.41	1.46	1.33
1	1	1835	2MG	C4-N3	6.41	1.48	1.34
1	1	2552	OMU	C2-N1	6.37	1.48	1.38
1	1	1835	2MG	C2-N2	6.31	1.46	1.33
2	2	1207	2MG	C2-N2	6.29	1.46	1.33
1	1	2498	OMC	C6-C5	6.28	1.49	1.35
2	2	1498	UR3	C2-N1	6.26	1.47	1.38
1	1	2251	OMG	C4-N3	6.23	1.48	1.34
2	2	967	5MC	C2-N3	6.20	1.48	1.36
1	1	1962	5MC	C5-C4	6.19	1.48	1.44
1	1	1962	5MC	C2-N3	6.09	1.48	1.36
1	1	2498	OMC	C2-N3	6.08	1.48	1.36
2	2	1407	5MC	C2-N3	6.08	1.48	1.36
2	2	1407	5MC	C5-C4	6.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	967	5MC	C5-C4	5.98	1.48	1.44
54	5	32	4OC	C6-C5	5.94	1.48	1.35
1	1	1939	5MU	C6-C5	5.90	1.44	1.34
54	5	8	4SU	C6-C5	5.86	1.48	1.35
2	2	1498	UR3	C6-C5	5.84	1.48	1.35
2	2	1402	4OC	C2-N3	5.82	1.47	1.36
54	5	32	4OC	C2-N3	5.77	1.47	1.36
54	5	8	4SU	C4-S4	-5.73	1.58	1.68
1	1	1915	3TD	C6-N1	5.73	1.45	1.36
2	2	1402	4OC	C6-C5	5.72	1.48	1.35
1	1	747	5MU	C6-C5	5.65	1.43	1.34
2	2	527	G7M	C2-N3	5.64	1.46	1.33
1	1	2503	2MA	C2-N1	5.64	1.43	1.34
54	5	54	5MU	C6-C5	5.63	1.43	1.34
1	1	2498	OMC	C4-N3	5.63	1.45	1.34
54	5	8	4SU	C2-N3	5.62	1.47	1.38
1	1	2503	2MA	C6-N1	5.58	1.42	1.35
2	2	527	G7M	C8-N9	5.49	1.50	1.35
2	2	527	G7M	C4-N3	5.43	1.46	1.34
1	1	2552	OMU	C6-C5	5.40	1.47	1.35
1	1	2069	G7M	C2-N3	5.26	1.45	1.33
1	1	2251	OMG	C2-N3	5.22	1.45	1.33
1	1	2069	G7M	C5-N7	-4.95	1.33	1.39
2	2	967	5MC	C4-N4	4.82	1.46	1.34
1	1	1962	5MC	C4-N4	4.80	1.46	1.34
2	2	1407	5MC	C4-N4	4.79	1.46	1.34
54	5	20	H2U	C4-N3	4.79	1.45	1.37
1	1	1915	3TD	C2-N3	4.76	1.48	1.38
2	2	527	G7M	C2-N2	4.75	1.45	1.34
1	1	2251	OMG	C2-N2	4.70	1.45	1.34
2	2	1402	4OC	C2-N1	4.54	1.49	1.40
2	2	1407	5MC	C6-N1	4.53	1.45	1.38
2	2	1498	UR3	C2-N3	4.49	1.47	1.39
2	2	1407	5MC	C2-N1	4.46	1.49	1.40
2	2	967	5MC	C6-N1	4.43	1.45	1.38
2	2	527	G7M	C5-N7	4.40	1.44	1.39
2	2	1516	2MG	C2-N1	4.26	1.43	1.36
1	1	2069	G7M	C2-N2	4.26	1.44	1.34
1	1	1962	5MC	C6-N1	4.22	1.45	1.38
1	1	2503	2MA	C5-C6	4.19	1.52	1.41
2	2	966	2MG	C2-N1	4.17	1.43	1.36
1	1	2504	PSU	C6-C5	4.13	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	967	5MC	C2-N1	4.08	1.48	1.40
1	1	1835	2MG	C2-N1	4.03	1.43	1.36
54	5	32	4OC	C4-N4	3.99	1.44	1.36
2	2	1207	2MG	C2-N1	3.98	1.43	1.36
54	5	32	4OC	C2-N1	3.96	1.48	1.40
1	1	2069	G7M	C5-C6	3.93	1.54	1.43
2	2	1402	4OC	C4-N4	3.93	1.44	1.36
1	1	2552	OMU	C4-N3	3.85	1.45	1.38
1	1	1962	5MC	C2-N1	3.79	1.48	1.40
1	1	2445	2MG	C2-N1	3.79	1.42	1.36
2	2	1519	MA6	C6-N6	3.74	1.47	1.36
1	1	2498	OMC	C2-N1	3.71	1.47	1.40
1	1	2498	OMC	C4-N4	3.69	1.42	1.33
1	1	2030	6MZ	C5-C4	-3.67	1.32	1.39
1	1	2445	2MG	C5-N7	-3.66	1.31	1.39
1	1	2503	2MA	C6-N6	-3.65	1.24	1.34
1	1	1618	6MZ	C5-C4	-3.62	1.32	1.39
54	5	55	PSU	C6-C5	3.61	1.39	1.35
1	1	2445	2MG	O6-C6	-3.61	1.16	1.23
1	1	2498	OMC	C6-N1	3.60	1.46	1.38
54	5	32	4OC	C5-C4	3.59	1.48	1.41
2	2	1518	MA6	C6-N6	3.56	1.46	1.36
2	2	966	2MG	C5-N7	-3.54	1.32	1.39
1	1	2030	6MZ	C8-N9	-3.53	1.31	1.37
1	1	1835	2MG	O6-C6	-3.52	1.16	1.23
2	2	966	2MG	O6-C6	-3.51	1.16	1.23
1	1	1835	2MG	C5-N7	-3.50	1.32	1.39
2	2	1516	2MG	C5-N7	-3.48	1.32	1.39
2	2	1207	2MG	C5-N7	-3.47	1.32	1.39
2	2	1516	2MG	O6-C6	-3.44	1.17	1.23
1	1	2457	PSU	C6-C5	3.43	1.39	1.35
1	1	2503	2MA	C5-N7	-3.42	1.32	1.39
1	1	2605	PSU	C6-C5	3.41	1.39	1.35
2	2	1207	2MG	O6-C6	-3.41	1.17	1.23
2	2	1518	MA6	C8-N9	-3.38	1.31	1.37
1	1	1618	6MZ	C8-N9	-3.37	1.31	1.37
2	2	527	G7M	C2-N1	3.37	1.45	1.37
1	1	745	1MG	C2-N1	3.37	1.43	1.37
1	1	1962	5MC	O2-C2	-3.35	1.17	1.23
1	1	1911	PSU	C6-C5	3.34	1.39	1.35
2	2	1402	4OC	C5-C4	3.34	1.48	1.41
2	2	1407	5MC	O2-C2	-3.32	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1917	PSU	C6-C5	3.32	1.39	1.35
54	5	8	4SU	C5-C4	3.31	1.46	1.42
1	1	1618	6MZ	C4-N9	-3.31	1.30	1.37
2	2	527	G7M	C5-C6	3.28	1.52	1.43
1	1	745	1MG	C5-N7	-3.21	1.32	1.39
2	2	967	5MC	O2-C2	-3.20	1.17	1.23
1	1	2251	OMG	C5-N7	-3.17	1.32	1.39
1	1	746	PSU	C6-C5	3.17	1.38	1.35
2	2	1518	MA6	C5-N7	-3.11	1.33	1.39
1	1	2552	OMU	O4-C4	-3.11	1.18	1.24
1	1	955	PSU	C6-C5	3.10	1.38	1.35
2	2	516	PSU	C6-C5	3.10	1.38	1.35
2	2	1519	MA6	C5-N7	-3.09	1.33	1.39
2	2	1518	MA6	C5-C4	-3.05	1.33	1.39
2	2	1519	MA6	C8-N9	-2.99	1.32	1.37
1	1	747	5MU	O4-C4	-2.98	1.17	1.23
1	1	1915	3TD	C4-N3	2.96	1.46	1.40
54	5	32	4OC	O2-C2	-2.94	1.18	1.23
1	1	1939	5MU	O4-C4	-2.93	1.18	1.23
1	1	2580	PSU	C6-C5	2.92	1.38	1.35
54	5	32	4OC	C6-N1	2.90	1.45	1.38
1	1	2498	OMC	O2-C2	-2.88	1.18	1.23
54	5	54	5MU	O4-C4	-2.88	1.18	1.23
1	1	747	5MU	O2-C2	-2.86	1.18	1.23
2	2	1402	4OC	C6-N1	2.85	1.44	1.38
1	1	2251	OMG	O6-C6	-2.83	1.18	1.23
2	2	1519	MA6	C5-C4	-2.81	1.34	1.39
1	1	2069	G7M	O6-C6	-2.80	1.18	1.23
1	1	2030	6MZ	C4-N9	-2.78	1.31	1.37
2	2	1402	4OC	O2-C2	-2.74	1.18	1.23
2	2	527	G7M	O6-C6	-2.72	1.18	1.23
1	1	2552	OMU	O2-C2	-2.71	1.18	1.23
54	5	8	4SU	O2-C2	-2.70	1.18	1.23
2	2	527	G7M	C6-N1	2.68	1.43	1.38
1	1	1939	5MU	O2-C2	-2.58	1.18	1.23
1	1	2251	OMG	C2-N1	2.54	1.43	1.37
2	2	1498	UR3	C6-N1	2.47	1.44	1.38
54	5	54	5MU	O2-C2	-2.46	1.18	1.23
1	1	2552	OMU	C6-N1	2.42	1.43	1.38
1	1	2069	G7M	C2-N1	2.41	1.43	1.37
1	1	1618	6MZ	C6-N1	-2.41	1.31	1.35
2	2	1498	UR3	O4-C4	-2.39	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2580	PSU	O4'-C1'	-2.39	1.40	1.43
2	2	1498	UR3	O2-C2	-2.38	1.18	1.22
1	1	2030	6MZ	C6-N1	-2.37	1.31	1.35
1	1	1618	6MZ	C5-C6	-2.36	1.36	1.41
54	5	20	H2U	O4-C4	-2.34	1.18	1.23
54	5	20	H2U	O2-C2	-2.33	1.18	1.23
2	2	1207	2MG	C5-C6	2.32	1.53	1.44
1	1	745	1MG	C5-C6	2.25	1.51	1.45
1	1	2069	G7M	C6-N1	2.25	1.43	1.38
1	1	2251	OMG	C4-N9	-2.23	1.32	1.38
1	1	2503	2MA	C4-N9	-2.22	1.33	1.37
1	1	2251	OMG	C5-C6	2.21	1.52	1.44
2	2	966	2MG	C5-C6	2.21	1.52	1.44
1	1	1835	2MG	C5-C6	2.18	1.52	1.44
1	1	2457	PSU	C4-C5	-2.17	1.38	1.44
1	1	2552	OMU	C5-C4	2.16	1.48	1.43
2	2	1516	2MG	C5-C6	2.14	1.52	1.44
1	1	745	1MG	C4-N9	-2.11	1.32	1.38
1	1	746	PSU	C4-C5	-2.10	1.38	1.44
1	1	1911	PSU	C4-C5	-2.10	1.38	1.44
2	2	1498	UR3	C5-C4	2.08	1.49	1.43
1	1	2030	6MZ	C5-C6	-2.07	1.36	1.41
2	2	1516	2MG	C4-N9	-2.06	1.32	1.38
2	2	527	G7M	C4-N9	2.05	1.43	1.38
2	2	527	G7M	C5-C4	2.03	1.43	1.38
1	1	2605	PSU	C4-C5	-2.03	1.38	1.44
1	1	2457	PSU	O4'-C1'	-2.02	1.41	1.43
1	1	2504	PSU	C4-C5	-2.02	1.38	1.44
2	2	1518	MA6	C5-C6	-2.00	1.36	1.41

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1618	6MZ	C4-N9-C8	14.23	120.68	105.74
1	1	2030	6MZ	C4-N9-C8	13.98	120.42	105.74
1	1	747	5MU	C5-C4-N3	12.88	126.52	115.32
1	1	1939	5MU	C5-C4-N3	12.51	126.19	115.32
54	5	54	5MU	C5-C4-N3	11.98	125.74	115.32
1	1	747	5MU	C5-C6-N1	-10.67	111.72	123.31
1	1	2030	6MZ	N9-C8-N7	-10.51	99.03	113.94
1	1	1618	6MZ	N9-C8-N7	-10.43	99.14	113.94
1	1	1939	5MU	C5-C6-N1	-10.42	112.00	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	5	54	5MU	C5-C6-N1	-9.21	113.31	123.31
1	1	2030	6MZ	C5-C6-N1	8.70	127.49	118.15
2	2	1519	MA6	N1-C6-N6	-8.58	106.41	116.86
1	1	1618	6MZ	C5-C6-N1	8.37	127.13	118.15
2	2	1518	MA6	N1-C6-N6	-8.24	106.81	116.86
1	1	2503	2MA	C5-C4-N3	-7.75	119.01	127.18
54	5	8	4SU	C4-N3-C2	-6.99	120.61	127.31
2	2	966	2MG	C2-N3-C4	6.83	120.54	112.00
2	2	1207	2MG	C2-N3-C4	6.76	120.46	112.00
1	1	2030	6MZ	N3-C4-N9	6.48	138.18	127.17
1	1	2445	2MG	C2-N3-C4	6.41	120.02	112.00
2	2	966	2MG	C5-C4-N3	-6.19	118.53	128.39
2	2	1519	MA6	N1-C2-N3	-6.19	119.21	128.58
2	2	1207	2MG	C5-C4-N3	-6.18	118.55	128.39
1	1	1835	2MG	C2-N3-C4	6.16	119.71	112.00
1	1	2503	2MA	N3-C4-N9	6.14	134.78	126.99
2	2	1516	2MG	C2-N3-C4	6.11	119.64	112.00
2	2	1518	MA6	N1-C2-N3	-6.09	119.37	128.58
1	1	2552	OMU	C4-N3-C2	-6.07	119.08	126.61
1	1	2445	2MG	C5-C4-N3	-6.06	118.74	128.39
1	1	2069	G7M	CN7-N7-C5	6.03	134.31	126.80
1	1	1618	6MZ	N3-C4-N9	5.77	136.98	127.17
1	1	1915	3TD	C1'-C5-C4	5.75	126.34	117.61
2	2	1519	MA6	C5-C6-N6	5.71	134.37	125.33
1	1	1939	5MU	O4-C4-C5	-5.68	118.42	124.92
1	1	747	5MU	C4-N3-C2	-5.60	120.00	127.34
1	1	2030	6MZ	N1-C2-N3	-5.57	120.15	128.58
1	1	1618	6MZ	C9-N6-C6	-5.55	117.70	122.85
1	1	747	5MU	O4-C4-C5	-5.55	118.57	124.92
1	1	1618	6MZ	N1-C2-N3	-5.54	120.20	128.58
1	1	1911	PSU	N1-C2-N3	5.53	121.00	115.17
1	1	2069	G7M	C2-N3-C4	5.51	121.79	112.30
1	1	1835	2MG	C5-C4-N3	-5.50	119.64	128.39
1	1	745	1MG	C1'-N9-C4	-5.41	110.49	126.49
1	1	1939	5MU	C4-N3-C2	-5.41	120.25	127.34
1	1	1911	PSU	C4-N3-C2	-5.40	118.94	126.37
1	1	2605	PSU	C4-N3-C2	-5.36	118.99	126.37
1	1	2251	OMG	C5-C4-N3	-5.34	119.89	128.39
1	1	2605	PSU	N1-C2-N3	5.32	120.78	115.17
2	2	1498	UR3	C4-N3-C2	-5.31	120.30	124.58
1	1	1618	6MZ	C5-C4-N9	-5.26	100.07	105.81
2	2	1516	2MG	C5-C4-N3	-5.24	120.05	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1915	3TD	N1-C2-N3	5.22	119.93	116.13
1	1	2503	2MA	N9-C8-N7	-5.19	106.57	113.94
2	2	1518	MA6	C5-C6-N6	5.19	133.54	125.33
1	1	2030	6MZ	C5-C4-N9	-5.18	100.16	105.81
1	1	2580	PSU	N1-C2-N3	5.16	120.61	115.17
1	1	2069	G7M	CN7-N7-C8	-5.11	117.05	124.79
54	5	8	4SU	C5-C4-N3	5.09	119.49	114.75
1	1	2457	PSU	N1-C2-N3	5.07	120.52	115.17
1	1	2069	G7M	C5-C4-N3	-5.06	118.58	128.15
54	5	54	5MU	O4-C4-C5	-4.97	119.23	124.92
1	1	955	PSU	C4-N3-C2	-4.94	119.56	126.37
54	5	55	PSU	N1-C2-N3	4.94	120.38	115.17
1	1	2457	PSU	C4-N3-C2	-4.92	119.60	126.37
1	1	2504	PSU	N1-C2-N3	4.86	120.30	115.17
2	2	516	PSU	N1-C2-N3	4.86	120.29	115.17
1	1	1917	PSU	C4-N3-C2	-4.85	119.69	126.37
2	2	1207	2MG	C2-N1-C6	-4.84	118.70	124.55
1	1	746	PSU	C4-N3-C2	-4.83	119.71	126.37
1	1	1917	PSU	N1-C2-N3	4.82	120.25	115.17
2	2	966	2MG	C2-N1-C6	-4.81	118.74	124.55
1	1	2504	PSU	C4-N3-C2	-4.79	119.78	126.37
1	1	2445	2MG	C2-N1-C6	-4.75	118.81	124.55
1	1	2580	PSU	C4-N3-C2	-4.74	119.85	126.37
1	1	1939	5MU	N3-C2-N1	4.69	121.00	114.89
1	1	745	1MG	C5-C4-N3	-4.68	120.94	128.39
2	2	516	PSU	C4-N3-C2	-4.68	119.93	126.37
54	5	55	PSU	C4-N3-C2	-4.64	119.97	126.37
1	1	1835	2MG	C2-N1-C6	-4.62	118.97	124.55
1	1	2251	OMG	C2-N3-C4	4.61	120.24	112.30
1	1	747	5MU	N3-C2-N1	4.59	120.87	114.89
1	1	2445	2MG	N9-C4-N3	4.50	134.95	125.95
1	1	745	1MG	C1'-N9-C8	4.49	139.48	126.73
2	2	1518	MA6	N9-C8-N7	-4.48	107.58	113.94
1	1	2069	G7M	C5-C6-N1	4.48	121.09	111.84
1	1	955	PSU	N1-C2-N3	4.47	119.88	115.17
1	1	2030	6MZ	C9-N6-C6	-4.39	118.78	122.85
1	1	746	PSU	N1-C2-N3	4.36	119.76	115.17
1	1	2030	6MZ	C5-N7-C8	4.34	110.27	103.45
1	1	2030	6MZ	C1'-N9-C8	-4.33	117.48	127.09
2	2	527	G7M	C2-N3-C4	4.32	119.73	112.30
2	2	1516	2MG	C2-N1-C6	-4.29	119.36	124.55
54	5	54	5MU	C4-N3-C2	-4.29	121.71	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	966	2MG	N9-C4-N3	4.27	134.49	125.95
2	2	1519	MA6	C5-C4-N3	-4.24	120.88	126.72
2	2	1519	MA6	N9-C8-N7	-4.21	107.97	113.94
2	2	1518	MA6	C5-C4-N3	-4.20	120.94	126.72
1	1	2503	2MA	C4-N9-C8	4.14	110.08	105.74
54	5	54	5MU	N3-C2-N1	4.11	120.25	114.89
2	2	1207	2MG	N9-C4-N3	4.10	134.15	125.95
1	1	2552	OMU	N3-C2-N1	3.94	120.02	114.89
54	5	54	5MU	C5M-C5-C4	3.91	122.95	118.78
1	1	1618	6MZ	C5-N7-C8	3.90	109.58	103.45
1	1	2069	G7M	N9-C4-N3	3.89	133.73	125.95
2	2	1519	MA6	C2-N1-C6	3.87	121.29	111.83
2	2	527	G7M	C5-C4-N3	-3.87	120.84	128.15
1	1	2552	OMU	C5-C4-N3	3.86	120.20	114.80
2	2	527	G7M	C5-C6-N1	3.79	119.68	111.84
1	1	1915	3TD	C4-N3-C2	-3.76	120.63	124.61
1	1	745	1MG	N9-C8-N7	-3.76	106.43	113.40
2	2	1498	UR3	C5-C4-N3	3.74	119.97	115.04
54	5	8	4SU	C5-C4-S4	-3.74	120.03	124.31
1	1	747	5MU	C5M-C5-C6	-3.74	117.79	122.85
2	2	1518	MA6	C2-N1-C6	3.73	120.95	111.83
1	1	2030	6MZ	C5-C4-N3	-3.68	121.64	126.72
1	1	1835	2MG	N9-C4-N3	3.67	133.29	125.95
1	1	2069	G7M	C2-N1-C6	-3.61	118.56	125.11
1	1	2069	G7M	C1'-N9-C4	-3.59	115.89	126.49
1	1	2580	PSU	O2-C2-N1	-3.58	119.09	122.79
54	5	20	H2U	C5-C6-N1	3.57	122.33	111.52
54	5	54	5MU	C5M-C5-C6	-3.57	118.03	122.85
1	1	1939	5MU	C5M-C5-C6	-3.48	118.15	122.85
1	1	1618	6MZ	C1'-N9-C8	-3.47	119.39	127.09
1	1	2030	6MZ	C2-N3-C4	3.46	120.28	111.83
1	1	2251	OMG	C2-N1-C6	-3.45	118.85	125.11
2	2	1516	2MG	N9-C4-N3	3.45	132.84	125.95
2	2	1519	MA6	C4-C5-C6	3.38	119.41	115.91
1	1	1962	5MC	C5-C6-N1	-3.38	119.64	123.31
1	1	2069	G7M	O6-C6-C5	-3.38	120.47	128.01
54	5	20	H2U	N3-C2-N1	3.37	120.04	116.65
1	1	2251	OMG	N9-C4-N3	3.36	132.68	125.95
54	5	8	4SU	N3-C2-N1	3.35	119.26	114.89
2	2	1519	MA6	C2-N3-C4	3.34	120.00	111.83
54	5	20	H2U	O2-C2-N3	-3.34	115.33	121.49
54	5	8	4SU	C1'-N1-C2	3.33	123.57	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	745	1MG	C2-N3-C4	3.33	119.46	111.98
2	2	1518	MA6	C4-C5-C6	3.28	119.31	115.91
1	1	745	1MG	N9-C4-N3	3.28	132.51	125.95
2	2	1518	MA6	C2-N3-C4	3.26	119.80	111.83
1	1	747	5MU	C5M-C5-C4	3.26	122.26	118.78
1	1	1911	PSU	O2-C2-N1	-3.24	119.44	122.79
2	2	1402	4OC	O2-C2-N3	-3.24	117.22	122.33
1	1	2251	OMG	N9-C8-N7	-3.21	107.45	113.40
1	1	2503	2MA	C5-N7-C8	3.20	108.48	103.45
2	2	967	5MC	C5-C6-N1	-3.19	119.84	123.31
1	1	1618	6MZ	C2-N3-C4	3.11	119.43	111.83
1	1	2580	PSU	C6-N1-C2	-3.10	119.82	122.69
1	1	1835	2MG	N9-C8-N7	-3.04	107.76	113.40
1	1	1939	5MU	C5M-C5-C4	3.04	122.03	118.78
1	1	2504	PSU	O2-C2-N1	-3.04	119.66	122.79
2	2	1518	MA6	C5-N7-C8	3.04	108.22	103.45
2	2	1519	MA6	C5-N7-C8	2.99	108.15	103.45
2	2	1207	2MG	N1-C2-N2	2.99	119.61	116.56
1	1	2552	OMU	O4-C4-C5	-2.99	120.01	125.16
1	1	2445	2MG	N9-C8-N7	-2.97	107.89	113.40
2	2	1516	2MG	N9-C8-N7	-2.91	108.00	113.40
2	2	966	2MG	C5-C6-N1	2.91	120.66	113.25
1	1	1618	6MZ	C4-N9-C1'	-2.89	119.88	126.63
1	1	1618	6MZ	C4-C5-C6	-2.88	114.38	116.78
1	1	2251	OMG	C5-C6-N1	2.87	120.56	113.25
1	1	2445	2MG	C5-C6-N1	2.87	120.56	113.25
1	1	2504	PSU	C6-N1-C2	-2.87	120.03	122.69
1	1	2503	2MA	N3-C2-N1	-2.86	120.72	125.77
2	2	1518	MA6	C4-N9-C8	2.85	108.73	105.74
54	5	55	PSU	O2-C2-N1	-2.83	119.87	122.79
2	2	516	PSU	C6-N1-C2	-2.82	120.07	122.69
1	1	1939	5MU	O2-C2-N1	-2.81	119.14	122.80
1	1	746	PSU	O2-C2-N1	-2.79	119.91	122.79
1	1	747	5MU	O4-C4-N3	-2.77	114.91	120.11
54	5	55	PSU	C6-N1-C2	-2.76	120.13	122.69
1	1	1917	PSU	O2-C2-N1	-2.75	119.95	122.79
1	1	1618	6MZ	C5-C4-N3	-2.75	122.94	126.72
1	1	2445	2MG	O6-C6-C5	-2.75	119.28	126.53
2	2	1207	2MG	C5-C6-N1	2.74	120.23	113.25
2	2	1407	5MC	C5-C6-N1	-2.74	120.34	123.31
1	1	1835	2MG	C5-C6-N1	2.73	120.19	113.25
1	1	2251	OMG	O6-C6-C5	-2.72	119.35	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1516	2MG	C1'-N9-C4	-2.71	118.49	126.49
54	5	54	5MU	O4-C4-N3	-2.71	115.03	120.11
1	1	2069	G7M	C1'-N9-C8	2.70	135.84	126.74
2	2	966	2MG	O6-C6-C5	-2.69	119.43	126.53
2	2	1519	MA6	C4-C5-N7	-2.67	107.53	110.58
1	1	2457	PSU	C6-C5-C4	2.67	119.97	118.17
2	2	1516	2MG	O6-C6-C5	-2.66	119.50	126.53
2	2	1516	2MG	C5-C6-N1	2.65	119.99	113.25
1	1	1911	PSU	C6-N1-C2	-2.65	120.23	122.69
2	2	527	G7M	C2-N1-C6	-2.64	120.32	125.11
2	2	1407	5MC	O2-C2-N3	-2.63	118.18	122.33
2	2	966	2MG	N9-C8-N7	-2.62	108.54	113.40
1	1	1917	PSU	C6-N1-C2	-2.60	120.28	122.69
2	2	1207	2MG	N9-C8-N7	-2.58	108.61	113.40
1	1	2503	2MA	C6-C5-C4	2.58	120.70	117.18
54	5	32	4OC	C6-C5-C4	2.57	120.10	117.00
2	2	1207	2MG	CM2-N2-C2	-2.56	118.14	123.65
2	2	527	G7M	N9-C8-N7	-2.56	106.27	112.48
1	1	2457	PSU	C6-N1-C2	-2.53	120.34	122.69
1	1	745	1MG	C5-C6-N1	2.52	119.68	115.02
1	1	2605	PSU	O2-C2-N1	-2.52	120.18	122.79
2	2	1518	MA6	N3-C4-N9	2.52	131.45	127.17
1	1	2552	OMU	O2-C2-N1	-2.52	119.52	122.80
1	1	1939	5MU	O4-C4-N3	-2.51	115.39	120.11
1	1	1835	2MG	N1-C2-N2	2.49	119.10	116.56
1	1	1835	2MG	O6-C6-C5	-2.47	120.02	126.53
1	1	1618	6MZ	C6-C5-N7	2.46	135.11	132.43
2	2	516	PSU	O2-C2-N1	-2.45	120.27	122.79
2	2	527	G7M	C5-C4-N9	2.44	111.09	105.88
2	2	1207	2MG	O6-C6-C5	-2.39	120.23	126.53
2	2	1518	MA6	C4-C5-N7	-2.39	107.86	110.58
1	1	2580	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	1	1835	2MG	CM2-N2-C2	-2.36	118.57	123.65
2	2	527	G7M	O6-C6-C5	-2.36	122.75	128.01
1	1	1835	2MG	C1'-N9-C4	-2.34	119.56	126.49
1	1	2605	PSU	C6-N1-C2	-2.34	120.52	122.69
1	1	747	5MU	C6-C5-C4	2.34	119.95	118.02
2	2	516	PSU	O3'-C3'-C4'	2.33	117.78	111.08
1	1	745	1MG	C8-N7-C5	2.31	108.38	104.26
2	2	1519	MA6	C5-C4-N9	2.31	108.33	105.81
1	1	2457	PSU	O2-C2-N1	-2.30	120.42	122.79
1	1	2030	6MZ	C6-C5-N7	2.30	134.94	132.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	5	20	H2U	C5-C4-N3	2.30	119.13	116.69
2	2	1402	4OC	C1'-N1-C2	2.28	123.47	118.44
1	1	2605	PSU	C6-C5-C4	2.24	119.69	118.17
1	1	2498	OMC	O2-C2-N3	-2.24	118.80	122.33
1	1	1911	PSU	C6-C5-C4	2.23	119.68	118.17
1	1	1915	3TD	O4-C4-N3	-2.20	116.33	120.36
2	2	1498	UR3	C1'-N1-C2	2.20	120.64	117.04
1	1	2030	6MZ	C4-C5-C6	-2.19	114.95	116.78
1	1	1939	5MU	C6-C5-C4	2.19	119.83	118.02
2	2	1519	MA6	C4-N9-C8	2.18	108.03	105.74
2	2	1516	2MG	C1'-N9-C8	2.18	132.91	126.73
2	2	1402	4OC	C6-C5-C4	2.16	119.60	117.00
2	2	1516	2MG	N1-C2-N2	2.14	118.74	116.56
2	2	1519	MA6	N3-C4-N9	2.13	130.79	127.17
1	1	745	1MG	C8-N9-C4	2.12	110.00	106.03
1	1	2251	OMG	C8-N7-C5	2.11	108.01	104.26
1	1	955	PSU	O2-C2-N1	-2.10	120.62	122.79
1	1	2069	G7M	N2-C2-N1	2.09	121.17	116.76
1	1	2457	PSU	O4'-C1'-C2'	2.05	107.98	105.15
1	1	746	PSU	C6-N1-C2	-2.02	120.82	122.69
2	2	1402	4OC	O2-C2-N1	2.02	122.85	118.90
1	1	1962	5MC	CM5-C5-C6	-2.01	120.13	122.85
2	2	1407	5MC	C5-C4-N3	-2.01	119.70	121.75

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	2552	OMU	C1'-C2'-O2'-CM2
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	1207	2MG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
54	5	20	H2U	O4'-C1'-N1-C2
54	5	20	H2U	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
56	6	77	FME	O1-CN-N-CA
56	6	77	FME	N-CA-CB-CG
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	1207	2MG	C3'-C4'-C5'-O5'
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
54	5	20	H2U	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
54	5	20	H2U	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C1'-N9-C4
54	5	8	4SU	O4'-C1'-N1-C6
54	5	8	4SU	O4'-C1'-N1-C2
1	1	2503	2MA	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C1'-N9-C8
56	6	77	FME	C-CA-CB-CG
1	1	2030	6MZ	C4'-C5'-O5'-P
1	1	2503	2MA	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	747	5MU	C4'-C5'-O5'-P
54	5	8	4SU	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C6
1	1	1962	5MC	C2'-C1'-N1-C6
1	1	746	PSU	C2'-C1'-C5-C6
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	5	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

17 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	745	1MG	1	0
54	5	54	5MU	1	0
2	2	1407	5MC	2	0
2	2	1519	MA6	1	0
54	5	32	4OC	1	0
1	1	2030	6MZ	1	0
1	1	1915	3TD	4	0
1	1	2580	PSU	1	0
2	2	1516	2MG	1	0
54	5	8	4SU	1	0
1	1	2503	2MA	4	0
2	2	1402	4OC	1	0
54	5	20	H2U	1	0
1	1	2552	OMU	2	0
54	5	55	PSU	1	0
1	1	2251	OMG	2	0
1	1	1962	5MC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 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.

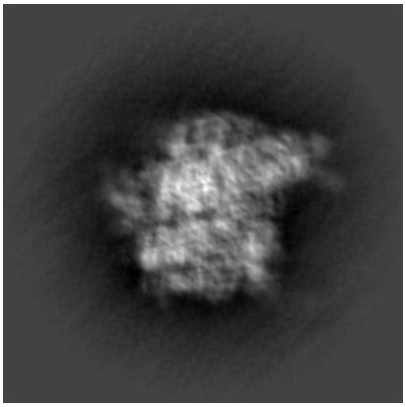
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20193. These allow visual inspection of the internal detail of the map and identification of artifacts.

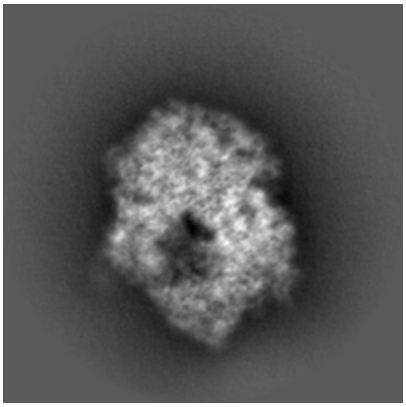
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

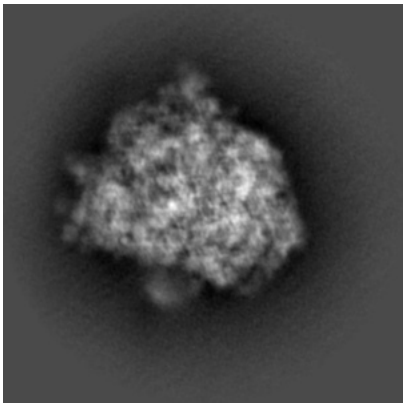
6.1.1 Primary map



X



Y

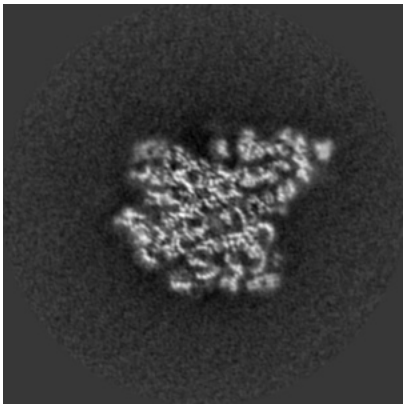


Z

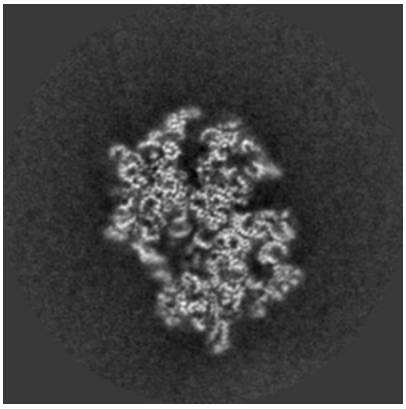
The images above show the map projected in three orthogonal directions.

6.2 Central slices

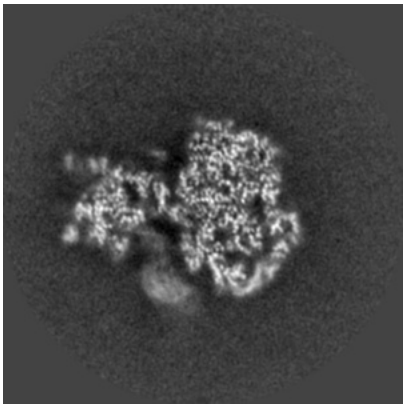
6.2.1 Primary map



X Index: 128



Y Index: 128

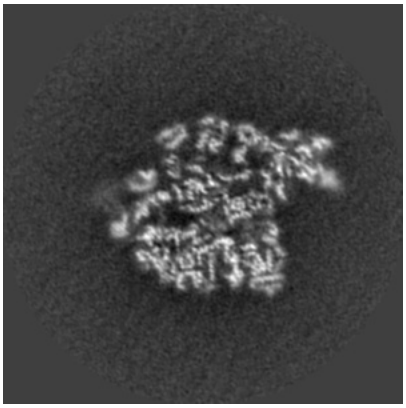


Z Index: 128

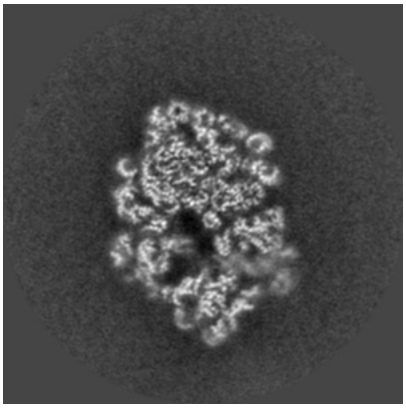
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

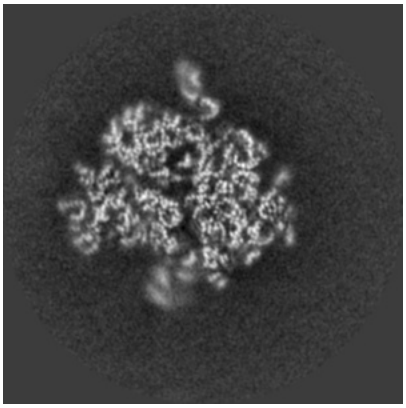
6.3.1 Primary map



X Index: 122



Y Index: 114

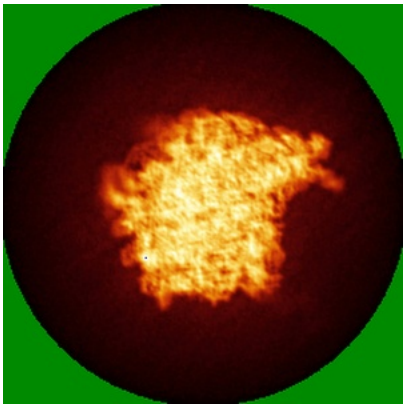


Z Index: 143

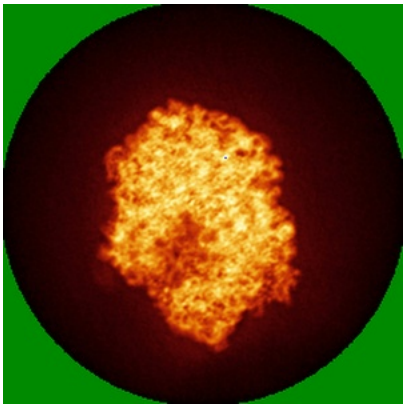
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

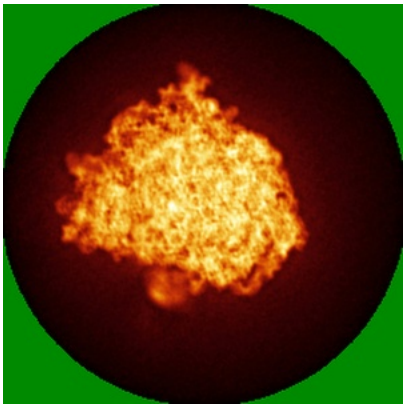
6.4.1 Primary map



X



Y

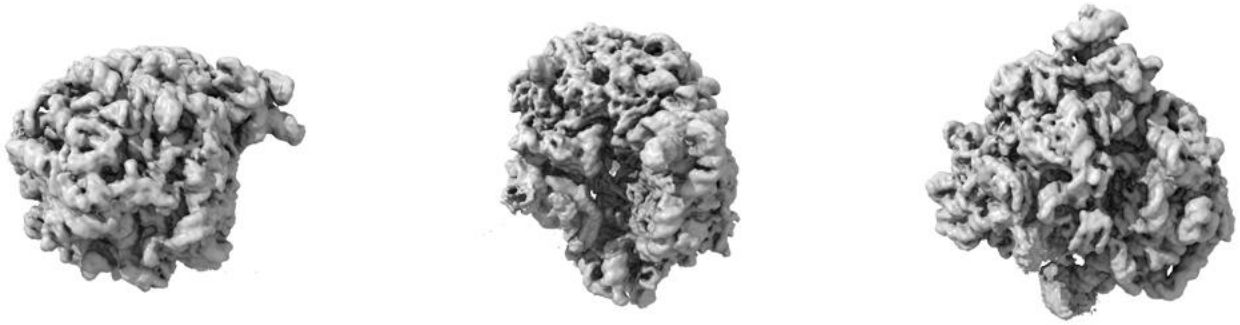


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

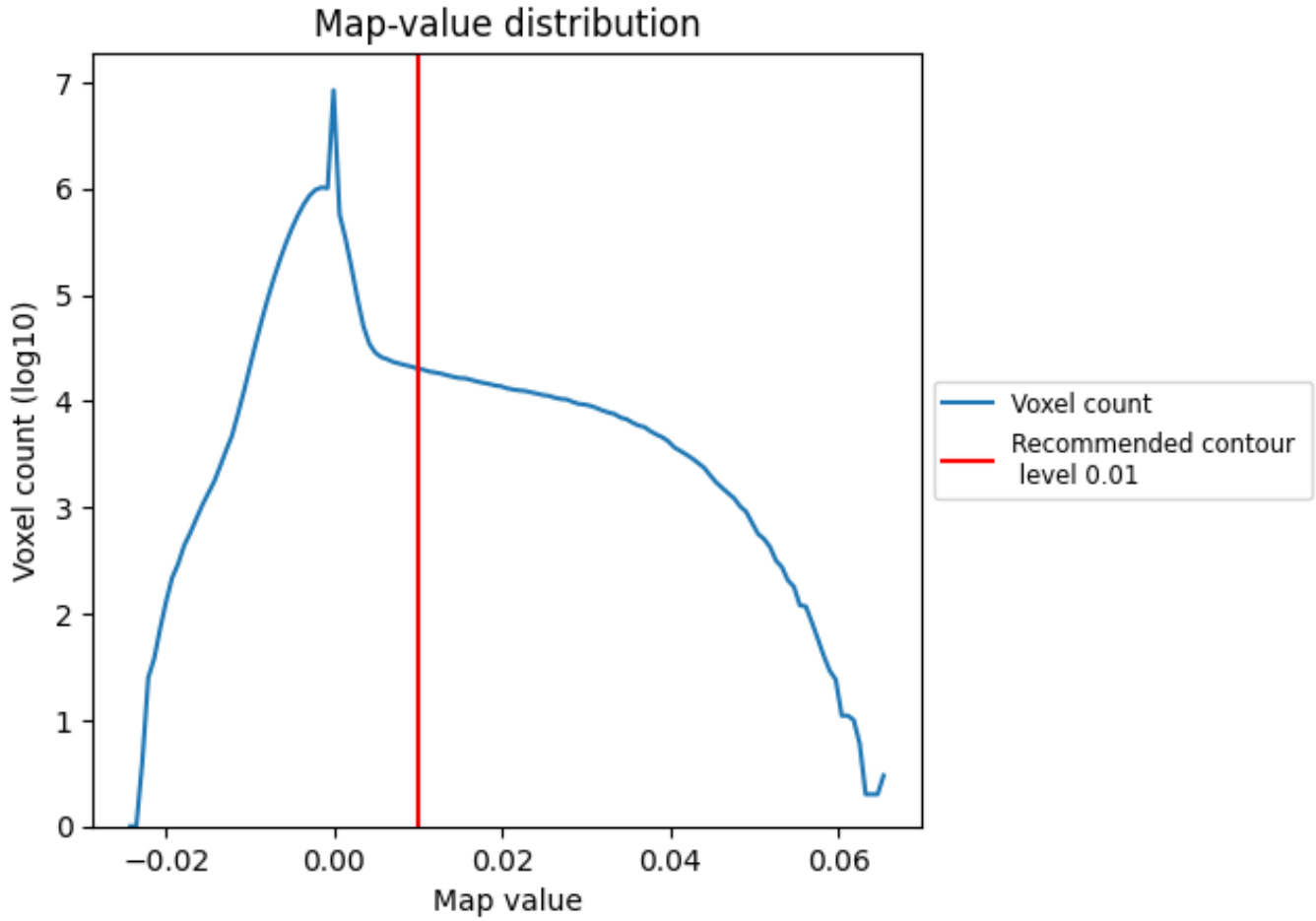
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

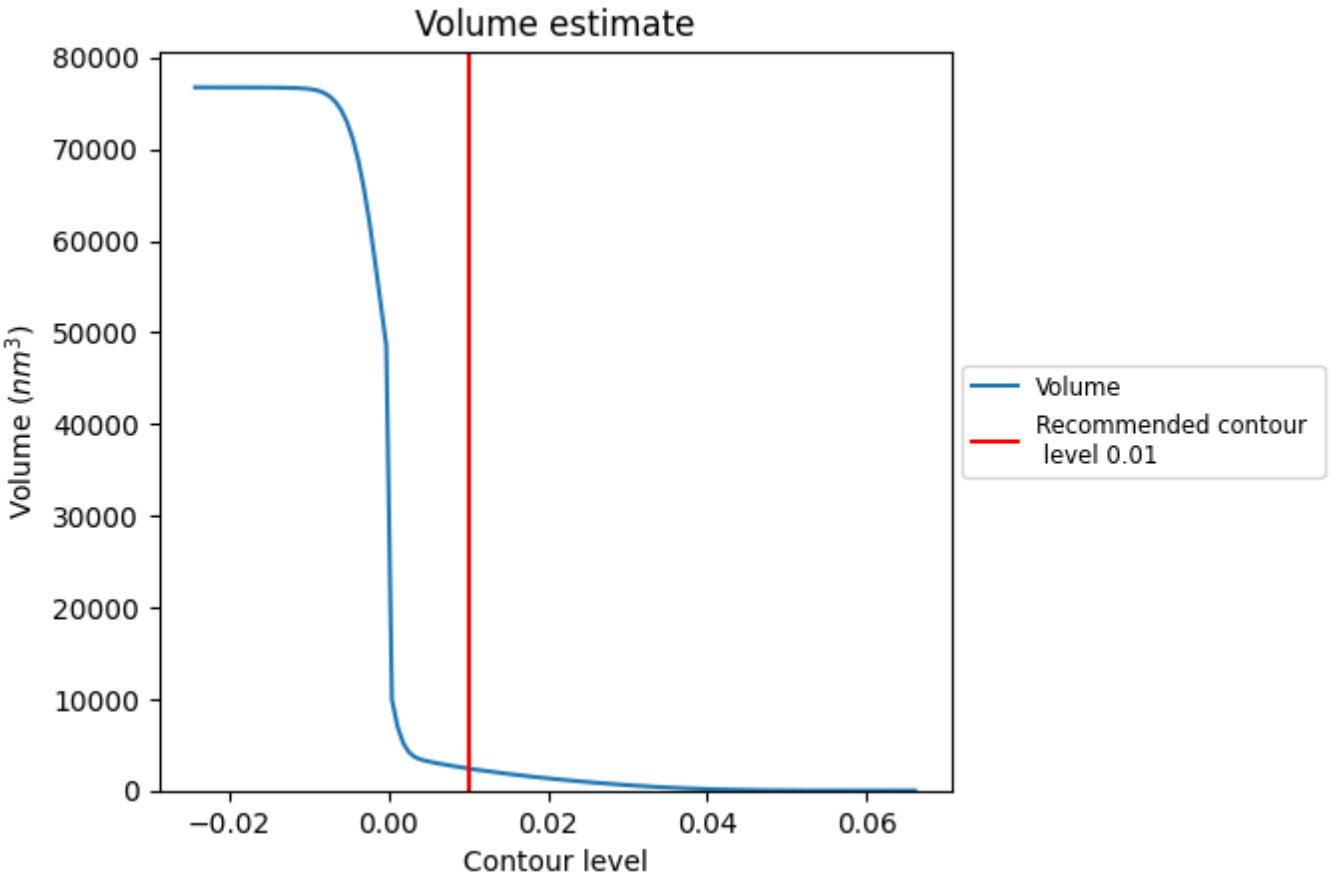
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

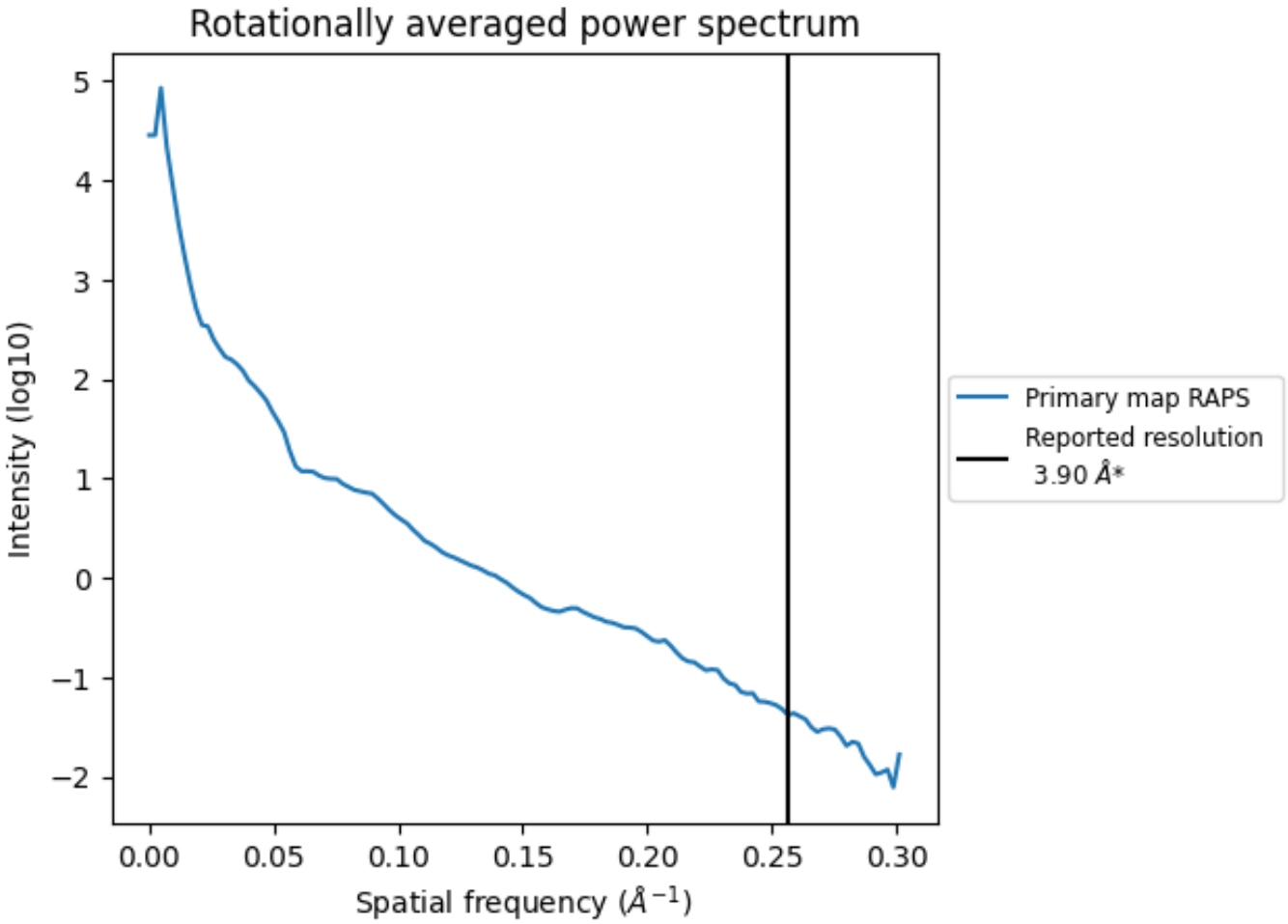
7.2 Volume estimate



The volume at the recommended contour level is 2414 nm^3; this corresponds to an approximate mass of 2180 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

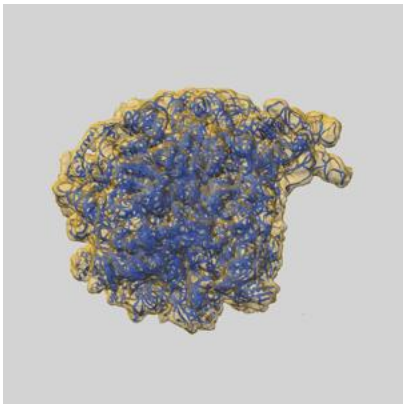
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

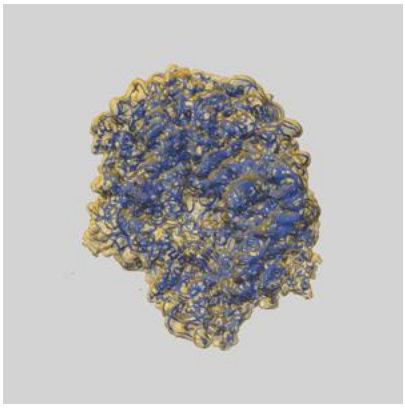
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20193 and PDB model 6OT3. Per-residue inclusion information can be found in section 3 on page 15.

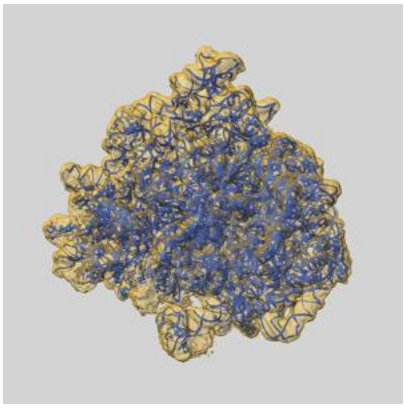
9.1 Map-model overlay



X



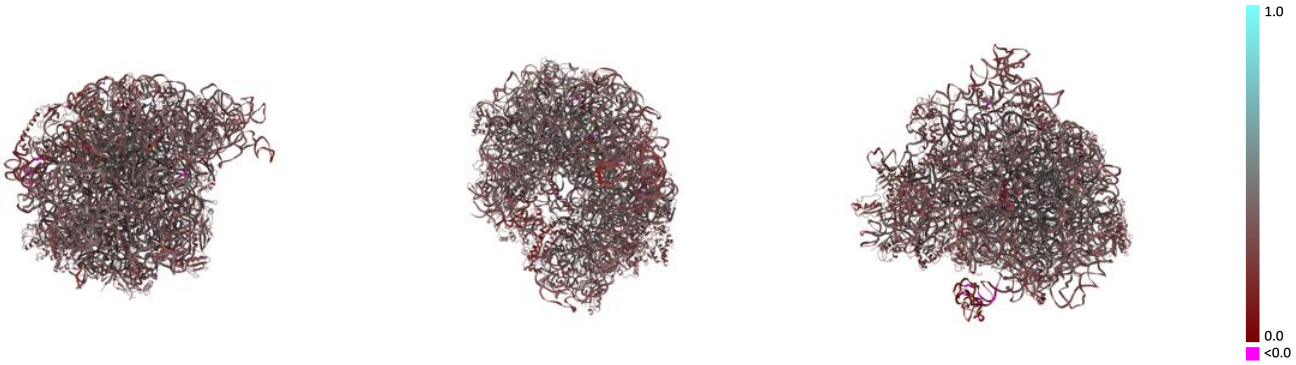
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

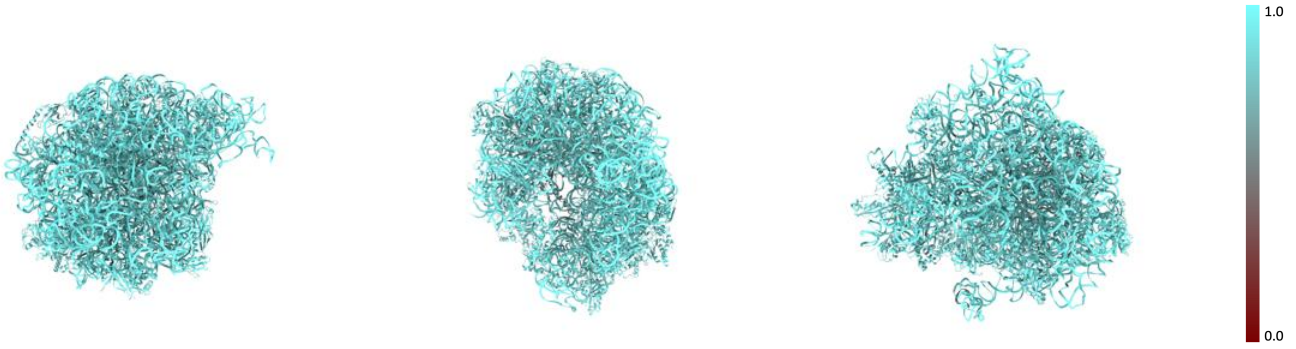
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

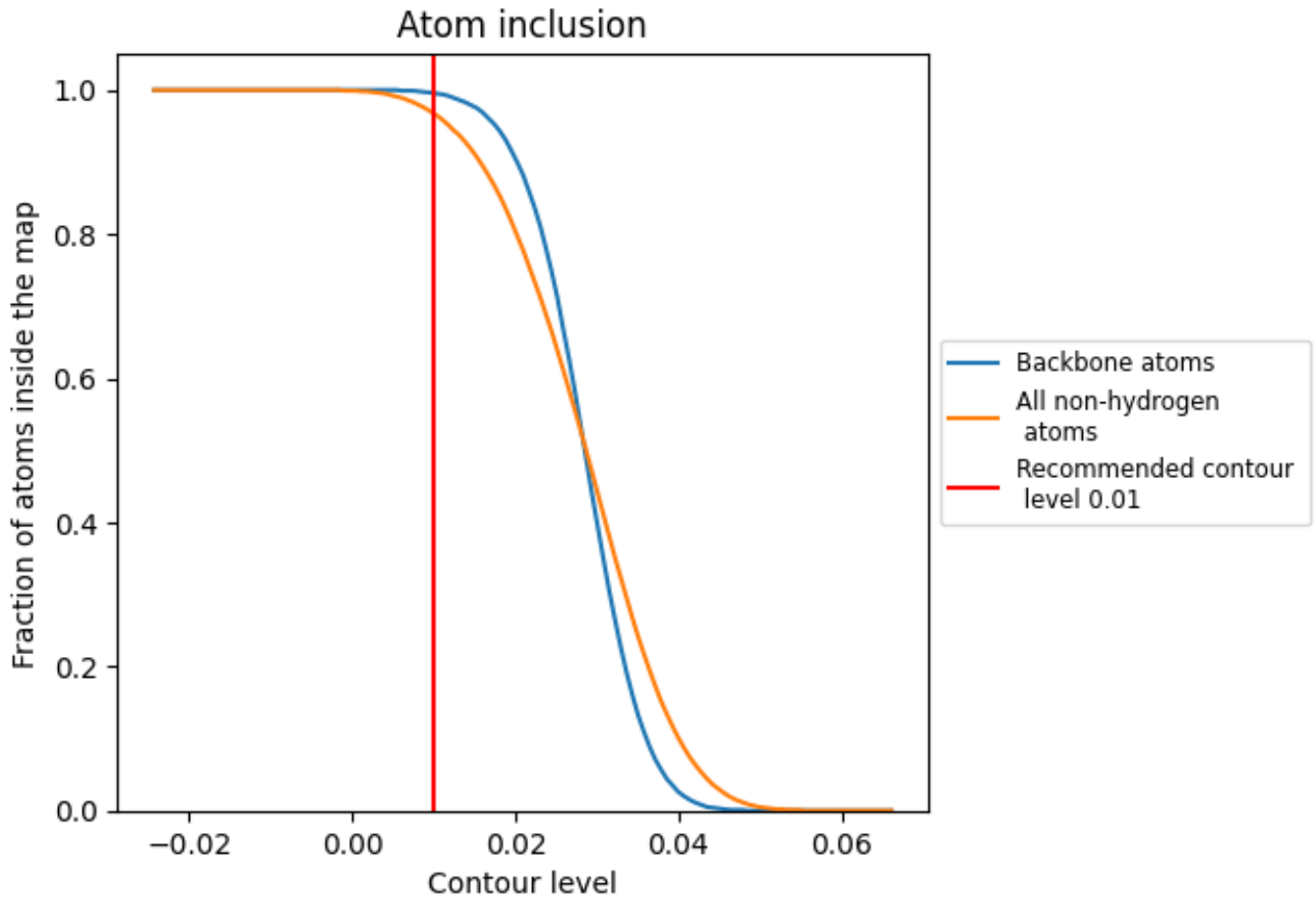
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.3480
1	0.9960	0.3640
2	0.9980	0.3560
3	0.9990	0.3490
4	0.9950	0.3690
5	0.9740	0.3360
6	0.7190	0.2220
A	0.8140	0.2480
B	0.8930	0.3790
C	0.9180	0.3550
D	0.9160	0.3480
E	0.9160	0.2980
F	0.9440	0.3200
G	0.8460	0.2660
J	0.9140	0.3540
K	0.8350	0.3410
L	0.9240	0.3660
M	0.8970	0.3630
N	0.9070	0.2820
O	0.9590	0.3270
P	0.8960	0.3220
Q	0.9220	0.3150
R	0.9280	0.3610
S	0.8740	0.3610
T	0.8990	0.3340
U	0.9500	0.3290
V	0.9550	0.3380
W	0.9130	0.3650
X	0.9000	0.3440
Y	0.9490	0.2730
Z	0.9130	0.3570
a	0.8980	0.2840
b	0.9250	0.3540
c	0.9280	0.3520
d	0.8930	0.3530



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Chain	Atom inclusion	Q-score
e	0.8840	0.3580
f	0.9250	0.3470
g	0.9020	0.2960
h	0.8910	0.3320
i	0.9350	0.3090
j	0.9200	0.3470
k	0.8980	0.3010
l	0.9080	0.2950
m	0.9270	0.3470
n	0.9350	0.3150
o	0.9050	0.3120
p	0.9070	0.3450
q	0.8620	0.3460
r	0.9170	0.2960
s	0.9330	0.3170
t	0.8970	0.2190
u	0.9520	0.3230
v	0.9290	0.3360
w	0.8720	0.3110
x	0.9300	0.3120
y	0.9250	0.2880
z	0.8300	0.2790