



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 03:21 PM GMT

PDB ID : 4K0Q
Title : Crystal structure of Thermus thermophilus 70S containing tRNAs and mRNA stop codon with pseudouridine
Authors : Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.
Deposited on : 2013-04-04
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

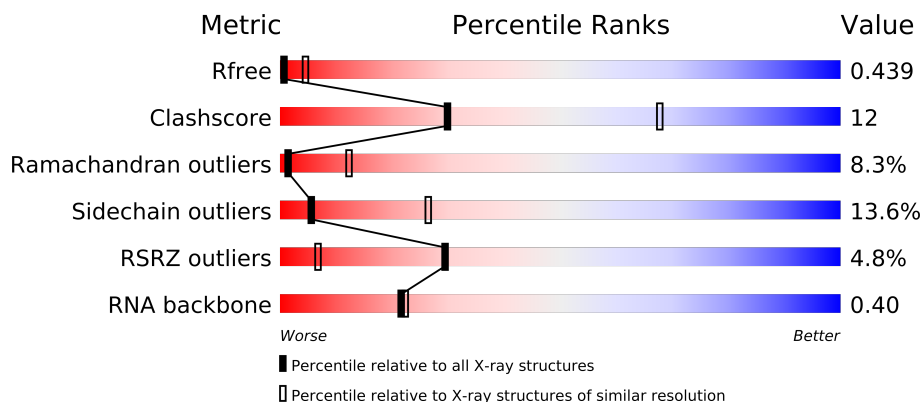
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	119	
3	C	196	
4	D	271	
5	E	204	
6	F	207	
7	G	181	
8	H	159	
9	I	145	
10	J	130	
11	N	138	
12	O	122	

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Mol	Chain	Length	Quality of chain
13	P	146	
14	Q	141	
15	R	117	
16	S	98	
17	T	137	
18	U	117	
19	V	101	
20	W	113	
21	X	92	
22	Y	100	
23	Z	176	
24	0	84	
25	1	93	
26	2	71	
27	3	59	
28	4	30	
29	5	59	
30	6	44	
31	7	48	
32	8	63	
33	9	36	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 91380 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1151	A	G	CONFLICT	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 3 is a protein called 50S Ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	0	0	0
			1157	706	220	231			

- Molecule 4 is a protein called 50S Ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 5 is a protein called 50S Ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 6 is a protein called 50S Ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			

- Molecule 7 is a protein called 50S Ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 8 is a protein called 50S Ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 9 is a protein called 50S Ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			

- Molecule 10 is a protein called 50S Ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	130	Total	C	N	O	S	0	0	0
			651	390	130	131				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	R	117	Total	C	N	O		0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	S	98	Total	C	N	O		0	0	0
			771	486	154	131				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	T	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	ALA	PHE	CONFLICT	UNP P60491

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	113	ALA	LYS	CONFLICT	UNP Q5SHP3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	X	92	Total	C	N	O	S	0	0	0
			726	471	131	124				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	81	ARG	LYS	CONFLICT	UNP P60494

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

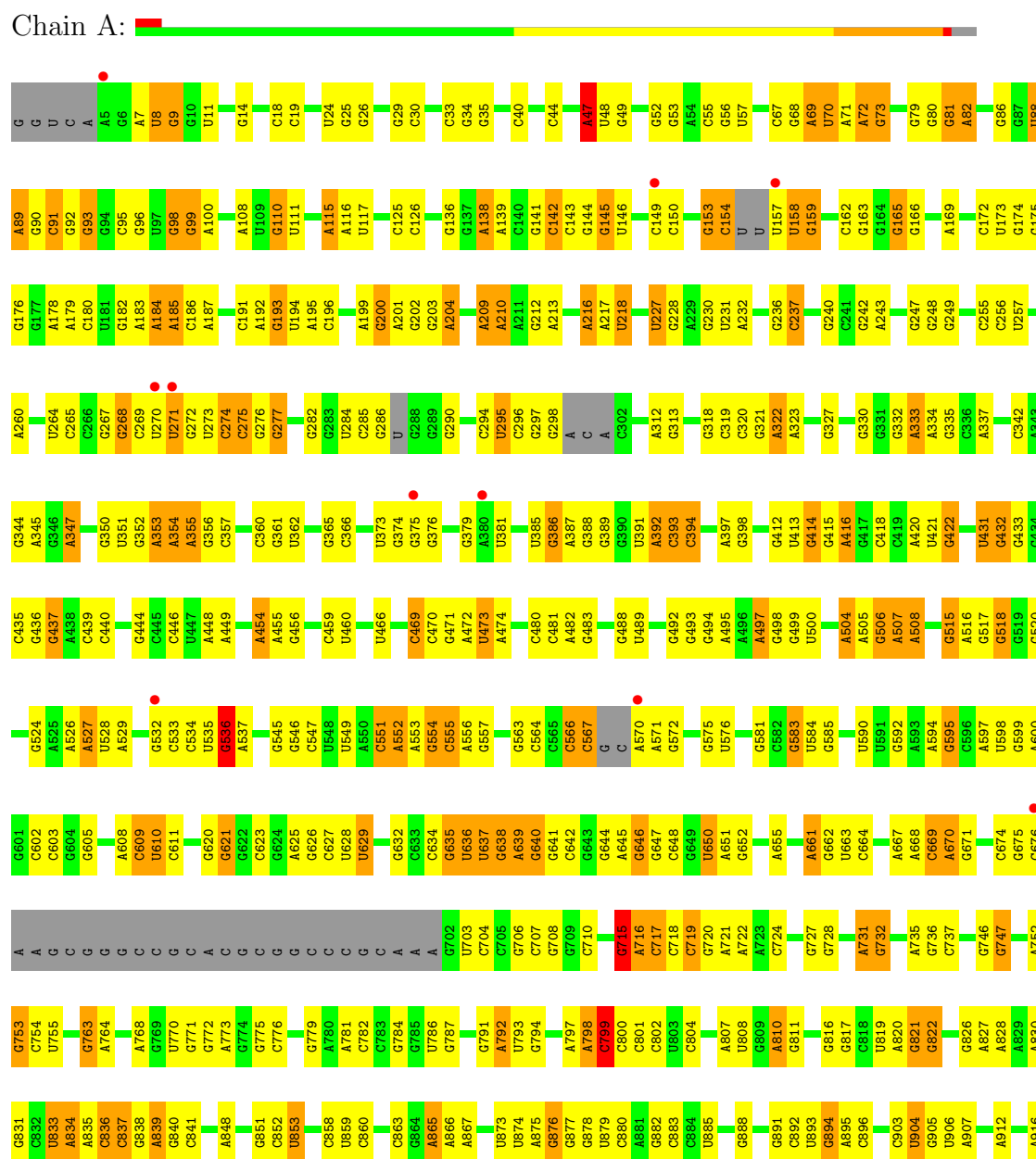
- Molecule 33 is a protein called 50S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

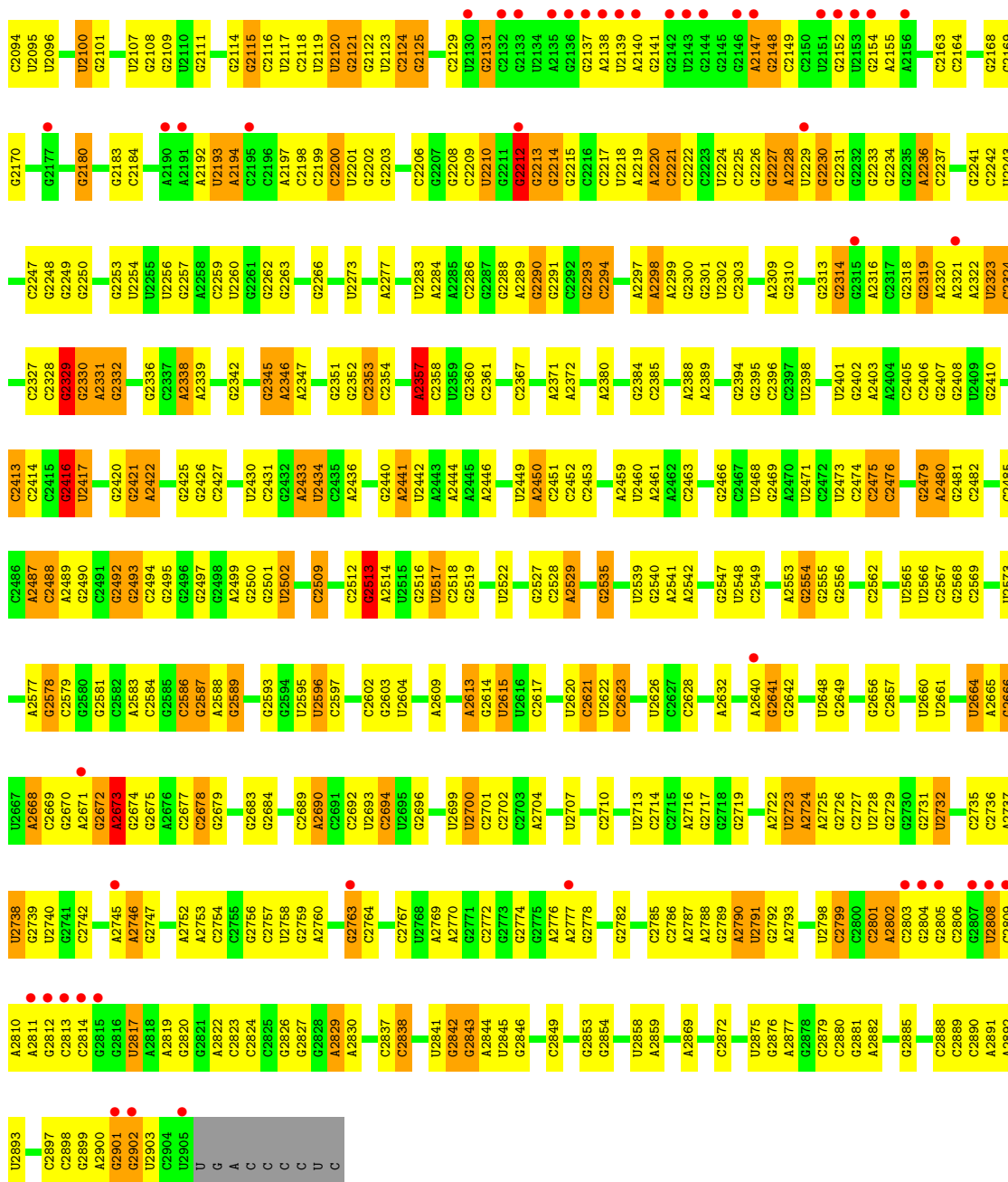
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA

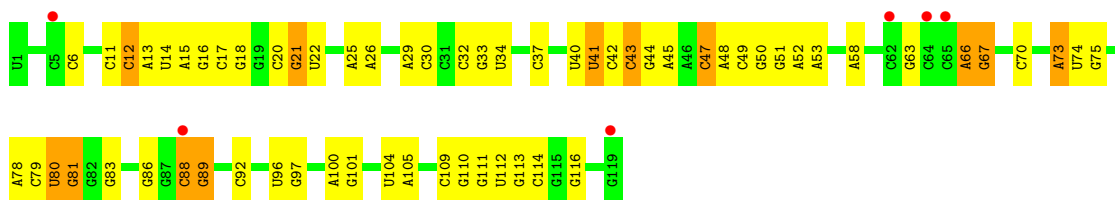


G2018	G2019	G2020	G2021	G2027	G2028	G2029	G2030	G2031	G2032	G2033	A2034	A2035	A2036	U2037	A2041	A2042	U2043	G2044	G2047	A2052	G2053	A2054	U2055	G2056	G2057	G2058	G2059	G2060	G2061	A2063	G2064	G2071	A2072	G2076	G2077	A2078	A2080	A2081	G2082	A2083	G2084	G2085	G2086	G2087	G2088	U2089	G2090	G2091				
G1854	A1855	G1856	G1857	G1858	A1859	U1863	U1864	G1865	G1868	G1869	C1873	G1874	G1875	G1876	U1877	A1878	G1879	A1883	G1887	G1888	A1889	U1894	A1895	G1896	G1897	A1898	G1899	C1900	C1901	G1902	C1903	G1904	A1905	A1906	C1907	C1908	C1909	A1910	U1914	C1915	C1916	G1917	G1920	A1921	A1922	C1923	G1927	U1930				
A1933	A1934	U1935	A1936	A1937	G1943	U1944	C1945	G1946	U1947	A1948	A1949	G1950	G1951	C1955	G1956	A1957	A1958	U1959	U1960	U1961	U1967	C1968	A1973	A1974	U1975	U1976	C1983	U1984	G1985	C1986	A1987	C1988	G1989	A1990	A1991	A1992	A1993	G1994	C1995	G2001	A2002	C2003	C2004	G2005	G2008	C2009	G2010	U2012	U2089	G2090	G2091	
G1775	G1776	G1777	G1778	G1779	G1780	G1783	G1786	G1787	G1788	A1789	C1792	C1793	G1794	C1797	U1798	G1802	A1803	G1806	U1807	U1808	U1809	A1810	C1811	C1812	A1813	A1814	A1815	A1816	A1817	C1818	A1819	C1820	A1821	U1824	C1825	U1826	C1827	U1828	G1829	C1830	G1831	A1832	A1833	C1834	U1835	G1846	A1849	U1850	A1851			
G1689	C1690	G1691	G1692	G1693	G1694	G1695	A1698	G1699	A1612	A1613	G1614	A1615	A1616	C1621	U1622	C1623	U1624	A1625	C1628	A1629	C1630	A1631	C1632	C1633	G1636	G1637	G1638	G1639	C1643	U1647	A1648	C1652	A1653	A1654	A1655	C1656	A1659	C1660	A1661	A1662	A1663	G1667	C1670	G1671	U1685	C1686	U1687	C1688	C1774			
G1536	G1537	C1538	A1539	A1540	A1541	U1542	C1543	C1544	G1545	G1546	C1547	A1548	C1549	C1550	A1553	C1554	A1555	A1556	C1557	U1558	U1559	U1560	U1561	G1562	C1563	U1564	U1565	U1566	G1567	G1570	A1574	G1575	C1576	C1577	C1578	C1579	A	C	C	C	U	C1589	A1590	A1591	C1592	C1593	C1594	C1595	C1596	C1597	U1598	A1599
G1461	C1462	G1463	C1464	U1465	G1466	G1467	G1470	G1471	A1472	C1473	G1474	C1475	U1476	U1477	U1478	A1479	C1482	G1488	G1489	A1490	C1491	G1413	C1414	C1415	A1495	G1496	C1497	C1498	A1499	U1500	C1504	G1505	A1506	G1507	C1513	G1516	A1517	G1521	C1522	A1523	G1524	G1526	U1527	C1528	C1529	C1530	A1531	G1532	G1533	U1534	A1535	
C1375	A1376	C1377	C1378	G1379	U1380	A1381	G1382	G1383	G1392	G1393	A1394	A1399	G1400	G1401	U1402	G1403	A1404	A1405	G1409	A1410	G1413	G1414	C1415	C1420	C1421	G1422	C1423	A1424	G1425	A1429	G1430	C1431	U1436	U1439	A1440	U1441	C1442	C1443	C1447	C1448	C1449	U1450	A1451	C1452	C1453	C1454	G1455	C1456	A1457	G1458		
G1295	C1296	C1297	A1298	G1301	C1302	G1309	A1310	G1311	U1312	A1313	A1314	C1315	G1316	A1317	U1318	A1323	G1324	C1325	U1326	U1327	G1328	A1329	C1330	A1331	A1332	U1333	C1334	C1335	C1336	U1337	C1338	U1345	A1346	A1347	G1348	C1351	A1352	A1353	G1354	G1355	U1358	C1359	G1364	C1365	A1366	A1367	G1370	U1371	C1372	G1373	U1374	
G1205	C1206	G1207	G1208	G1209	U1210	C1211	U1212	G1213	G1216	G1217	A1218	U1219	G1220	A1221	C1222	C1223	A1226	G1227	U1232	A1233	G1239	C1244	U1249	C1252	G1253	U1255	U1256	A1257	U1258	G1259	C1260	C1261	G1262	G1263	A1264	C1265	C1269	G1272	A1286	A1287	G1288	G1289	G1290	A1291	A1292	G1293	U1294					
A	G	A	G	U	U	G	A	A	U	A	G	C	U	U	C	A	A1151	G1152	G1155	A1156	G1157	U1158	G1160	C1161	G1162	C1163	G1167	C1168	A1173	A1174	U1175	G1176	C1179	G1180	G1181	G1182	G1183	U1185	U1186	A1187	A1188	G1189	G1194	C1195	C1198	G1199	A1200	A1201				
G1067	U1068	G1069	G1070	U1071	A1072	G1075	G1076	A1077	U1078	C1083	G1084	C1085	C1086	G1087	C1088	G1089	A1090	A1091	G1092	A1093	C1094	A1095	G1096	C1097	A	G	G	A	G	U	G	C	U	A	A	G	C	A	G	C	A	U	C	U	U	U	A	A				
G992	G996	U1002	A1003	A1004	C1005	G1006	U1007	C1008	C1009	G1010	U1013	C1014	G1015	A1017	G1018	C1021	G1022	A1025	A1026	C1027	A1028	G1032	C1036	G1037	C1038	G1039	A1040	A1041	G1042	C1043	U1044	A1045	A1046	G1047	C1048	C1049	C1050	C1051	A1054	A1055	G1056	U1057	C1058	U1059	C1060	G1061	G1062	C1063	A1064	A1066		
G920	A924	G929	C930	C931	C932	C933	C934	C935	A936	G937	C938	C939	U940	A941	C942	C943	A944	A945	C948	C949	U952	C953	A954	A955	C959	C960	G961	A962	A963	G964	G965	G966	U967	C968	G972	G973	U974	G975	G976	A977	G978	U981	G982	A985	G986	U987	G988	A989	G990	G991		



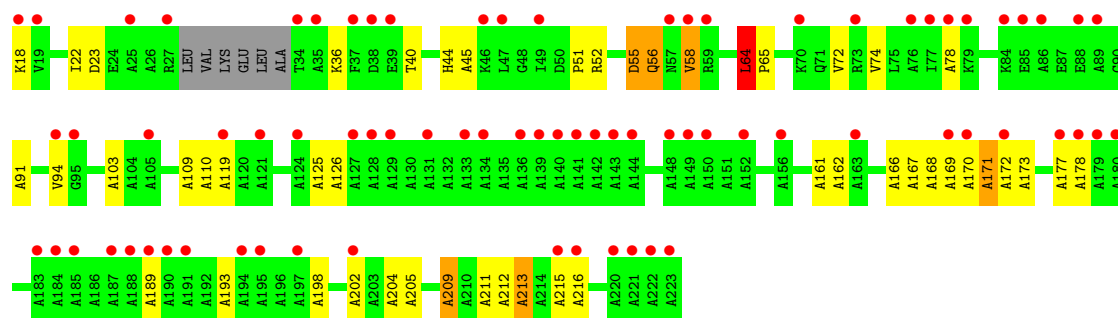
• Molecule 2: 5S rRNA

Chain B:



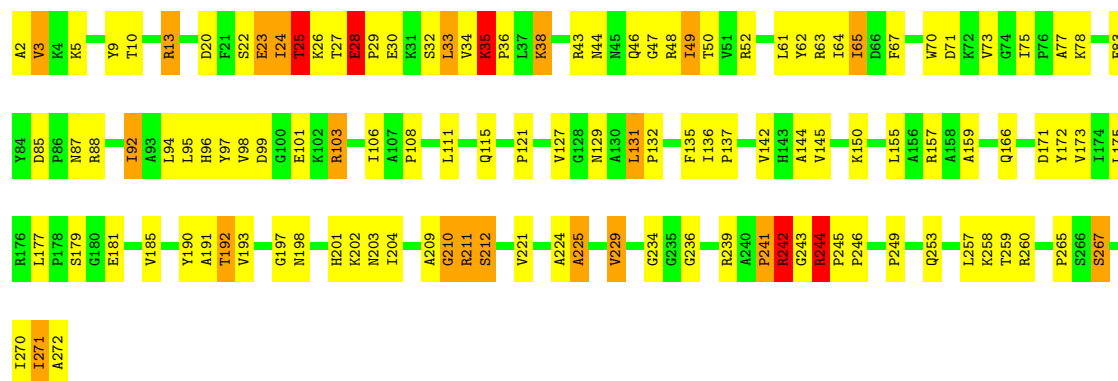
• Molecule 3: 50S Ribosomal protein L1

Chain C:



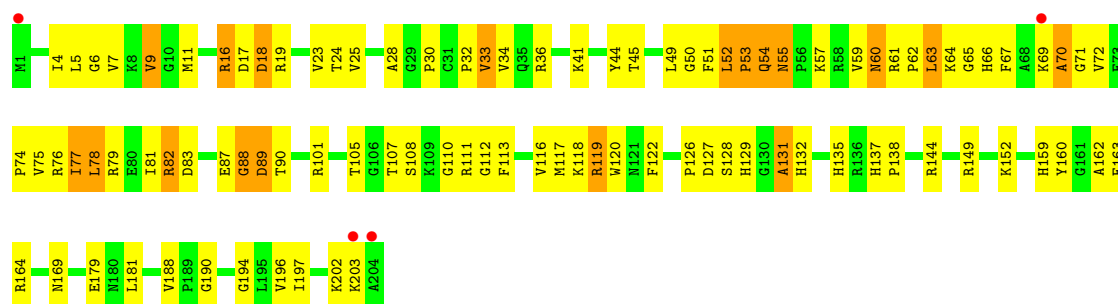
• Molecule 4: 50S Ribosomal protein L2

Chain D:



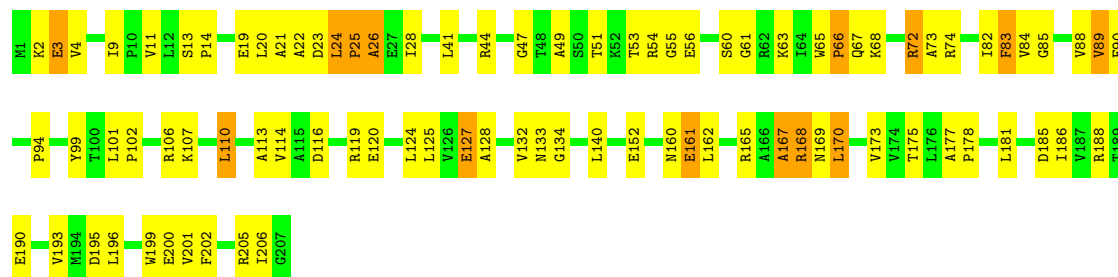
• Molecule 5: 50S Ribosomal protein L3

Chain E:



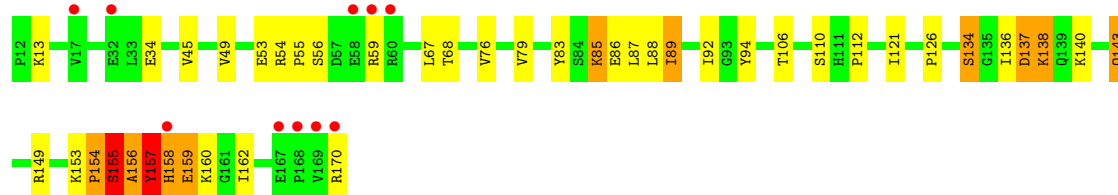
• Molecule 6: 50S Ribosomal protein L4

Chain F:

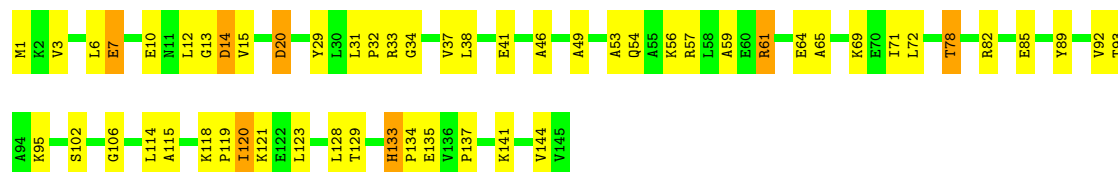


• Molecule 7: 50S Ribosomal protein L5

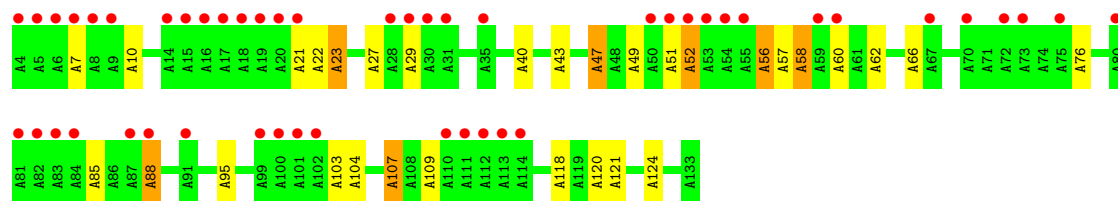
- Molecule 8: 50S Ribosomal protein L6



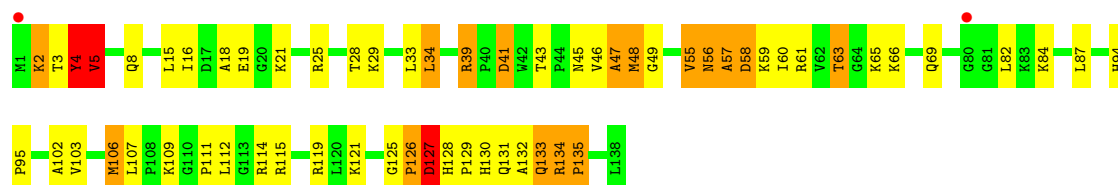
- Molecule 9: 50S Ribosomal protein L9



- Molecule 10: 50S Ribosomal protein L10

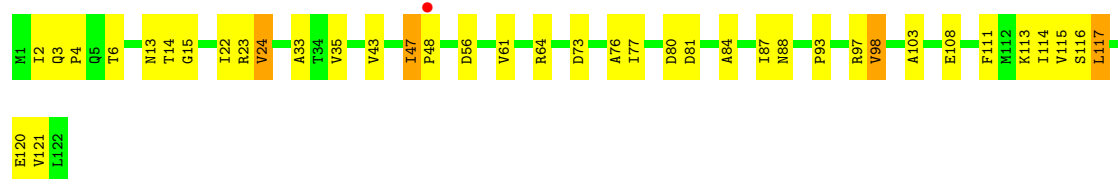


- Molecule 11: 50S Ribosomal protein L13



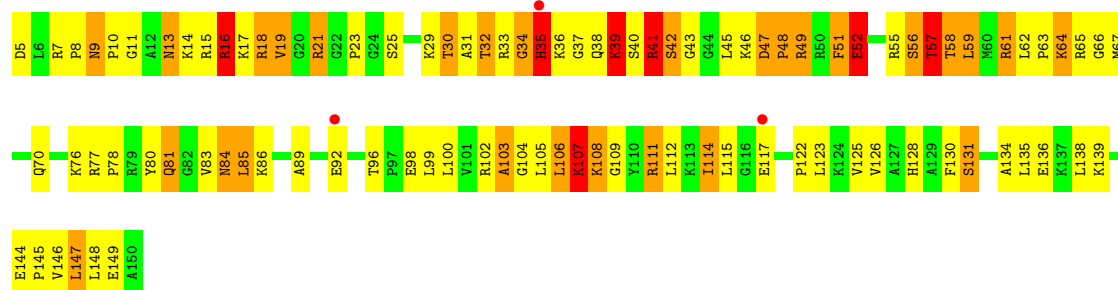
- Molecule 12: 50S Ribosomal protein L14

Chain O: 



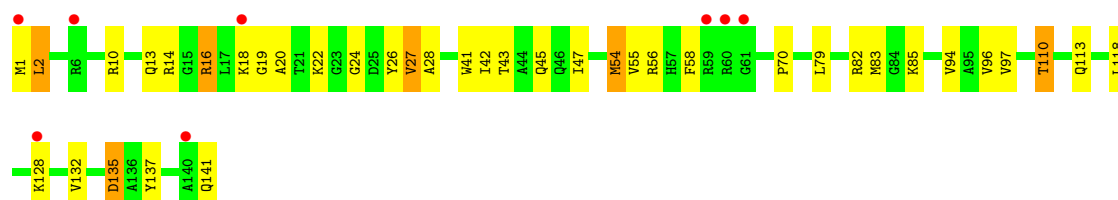
- Molecule 13: 50S Ribosomal protein L15

Chain P: 



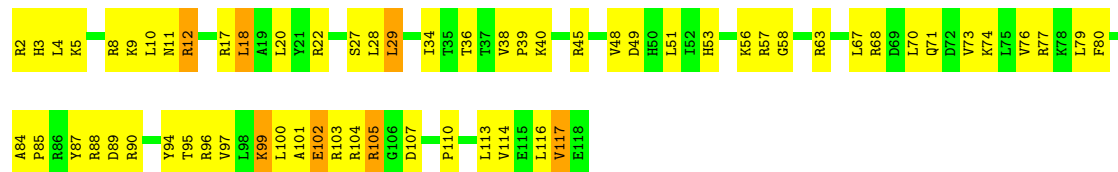
- Molecule 14: 50S Ribosomal protein L16

Chain Q: 



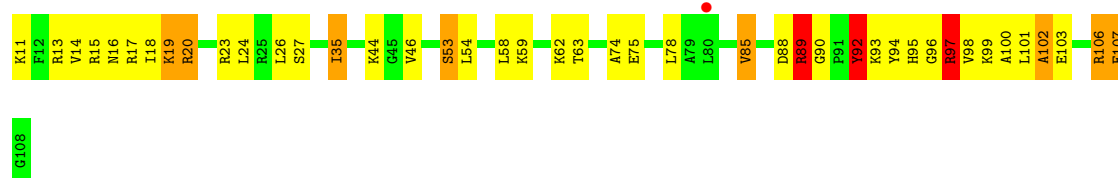
- Molecule 15: 50S Ribosomal protein L17

Chain R: 



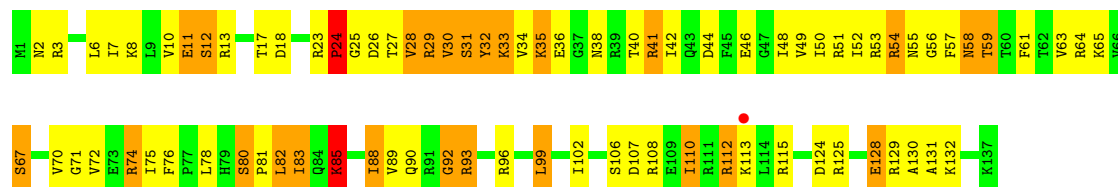
- Molecule 16: 50S Ribosomal protein L18

Chain S: 



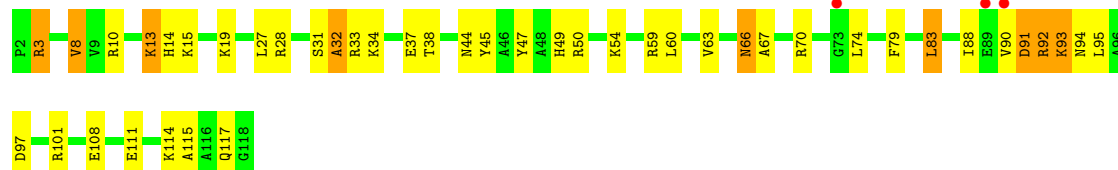
- Molecule 17: 50S Ribosomal protein L19

Chain T:



- Molecule 18: 50S Ribosomal protein L20

Chain U:



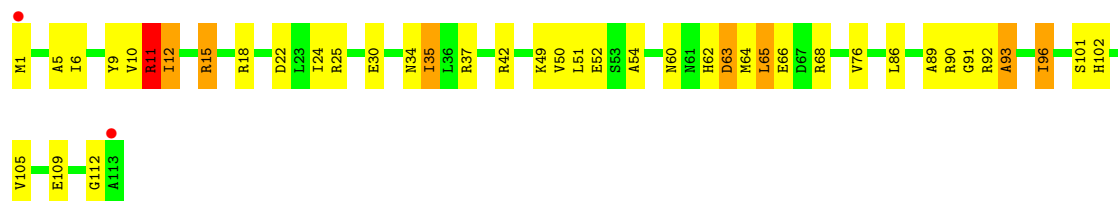
- Molecule 19: 50S Ribosomal protein L21

Chain V:



- Molecule 20: 50S Ribosomal protein L22

Chain W:



- Molecule 21: 50S Ribosomal protein L23

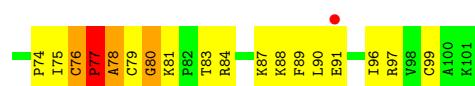
Chain X:



- Molecule 22: 50S Ribosomal protein L24

Chain Y:





- Molecule 23: 50S Ribosomal protein L25

Chain Z:



- Molecule 24: 50S Ribosomal protein L27

Chain 0:



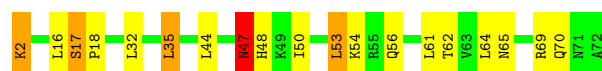
- Molecule 25: 50S Ribosomal protein L28

Chain 1:



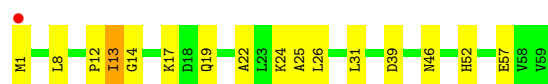
- Molecule 26: 50S Ribosomal protein L29

Chain 2:



- Molecule 27: 50S Ribosomal protein L30

Chain 3:



- Molecule 28: 50S Ribosomal protein L31

Chain 4:



- Molecule 29: 50S Ribosomal protein L32

Chain 5:



- Molecule 30: 50S Ribosomal protein L33

Chain 6: 



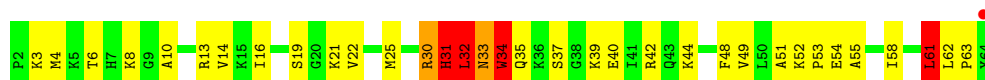
- Molecule 31: 50S Ribosomal protein L34

Chain 7: 



- Molecule 32: 50S Ribosomal protein L35

Chain 8: 



- Molecule 33: 50S Ribosomal protein L36

Chain 9: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.92Å 449.90Å 624.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 3.30 39.57 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.57-3.30) 95.6 (39.57-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
R, R_{free}	0.225 , 0.279 0.436 , 0.439	Depositor DCC
R_{free} test set	41955 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 839115 reflections	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	91380	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	5/67709 (0.0%)	0.80	93/105690 (0.1%)
2	B	0.35	0/2853	0.72	0/4451
3	C	0.48	0/1160	0.55	0/1584
4	D	0.60	0/2155	0.85	0/2905
5	E	0.56	1/1597 (0.1%)	0.83	2/2153 (0.1%)
6	F	0.52	0/1659	0.75	0/2244
7	G	0.44	0/1499	0.67	0/2016
8	H	0.47	0/1246	0.67	1/1682 (0.1%)
9	I	0.47	0/1147	0.72	0/1551
10	J	0.44	0/650	0.53	0/907
11	N	0.49	0/1132	0.77	0/1525
12	O	0.53	0/943	0.78	0/1269
13	P	0.57	0/1131	0.98	2/1504 (0.1%)
14	Q	0.46	0/1143	0.68	0/1527
15	R	0.54	0/974	0.87	0/1302
16	S	0.48	0/779	0.79	0/1036
17	T	0.58	0/1156	0.95	0/1542
18	U	0.50	0/975	0.75	0/1297
19	V	0.47	0/790	0.76	0/1057
20	W	0.52	0/907	0.77	0/1216
21	X	0.52	0/740	0.74	0/993
22	Y	0.53	0/789	0.83	0/1051
23	Z	0.44	0/1436	0.66	0/1949
24	0	0.51	0/671	0.76	0/892
25	1	0.53	0/741	0.84	1/984 (0.1%)
26	2	0.48	0/600	0.79	0/793
27	3	0.44	0/473	0.70	0/634
28	4	0.49	0/229	0.75	0/309
29	5	0.57	0/473	0.88	0/639
30	6	0.83	0/388	1.06	2/518 (0.4%)
31	7	0.58	0/427	0.85	0/561
32	8	0.54	0/516	0.88	1/679 (0.1%)
33	9	0.45	0/302	0.73	0/397
All	All	0.47	6/99390 (0.0%)	0.79	102/148857 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	20	0
4	D	0	2
5	E	0	1
13	P	0	4
15	R	0	1
30	6	0	1
All	All	20	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1851	A	O3'-P	-6.02	1.53	1.61
1	A	1987	A	O3'-P	-5.96	1.54	1.61
1	A	2234	G	O3'-P	-5.77	1.54	1.61
1	A	839	A	O3'-P	-5.63	1.54	1.61
5	E	127	ASP	CB-CG	5.59	1.63	1.51
1	A	2838	C	O3'-P	-5.09	1.55	1.61

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1345	U	C2'-C3'-O3'	11.83	135.53	109.50
1	A	989	A	N9-C1'-C2'	11.32	128.72	114.00
1	A	2013	G	C2'-C3'-O3'	11.20	134.14	109.50
1	A	2297	A	N9-C1'-C2'	11.08	128.41	114.00
1	A	1955	C	C2'-C3'-O3'	10.95	133.58	109.50
1	A	715	G	C2'-C3'-O3'	10.78	133.21	109.50
1	A	1590	A	N9-C1'-C2'	10.42	127.55	114.00
1	A	98	G	N9-C1'-C2'	10.24	127.31	114.00
1	A	1983	C	N1-C1'-C2'	9.91	126.88	114.00
1	A	839	A	O5'-P-OP2	-9.70	96.97	105.70
1	A	2587	G	O5'-P-OP2	-9.67	97.00	105.70
1	A	1345	U	N1-C1'-C2'	9.43	126.26	114.00
1	A	497	A	C2'-C3'-O3'	8.81	128.89	109.50
1	A	1662	C	O5'-P-OP1	-8.65	97.91	105.70
1	A	1740	C	C4'-C3'-O3'	8.65	130.29	113.00
1	A	2623	C	O5'-P-OP2	-8.54	98.02	105.70
1	A	2673	A	N9-C1'-C2'	8.49	125.04	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	715	G	N9-C1'-C2'	8.39	124.91	114.00
1	A	536	G	O5'-P-OP1	-8.35	98.19	105.70
1	A	2212	G	C2'-C3'-O3'	8.32	127.81	109.50
30	6	10	LEU	CA-CB-CG	8.23	134.23	115.30
1	A	715	G	C5'-C4'-O4'	8.16	118.89	109.10
1	A	1740	C	C2'-C3'-O3'	8.10	127.33	109.50
1	A	2236	A	C2'-C3'-O3'	8.10	127.32	109.50
1	A	534	C	O5'-P-OP2	-8.04	98.47	105.70
1	A	2212	G	C4'-C3'-O3'	7.66	128.32	113.00
1	A	1829	G	C2'-C3'-O3'	7.56	126.13	109.50
1	A	1424	A	N9-C1'-C2'	7.46	123.69	114.00
1	A	1699	G	C2'-C3'-O3'	7.31	125.58	109.50
1	A	833	U	O5'-P-OP1	7.20	119.34	110.70
1	A	2609	A	O5'-P-OP2	-7.19	99.23	105.70
30	6	46	HIS	N-CA-C	7.15	130.30	111.00
1	A	497	A	C4'-C3'-O3'	7.14	127.28	113.00
1	A	2517	U	C2'-C3'-O3'	7.01	124.92	109.50
1	A	1700	A	O5'-P-OP1	-6.96	99.43	105.70
1	A	2623	C	O5'-P-OP1	6.91	118.99	110.70
1	A	1983	C	C2'-C3'-O3'	6.86	124.68	113.70
1	A	536	G	O5'-P-OP2	6.81	118.88	110.70
1	A	2449	U	O5'-P-OP2	-6.72	99.65	105.70
1	A	1802	G	N9-C1'-C2'	-6.47	104.88	112.00
5	E	127	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	799	C	O5'-P-OP2	-6.36	99.98	105.70
1	A	787	G	O5'-P-OP2	-6.32	100.01	105.70
1	A	2100	U	O5'-P-OP1	-6.31	100.02	105.70
1	A	715	G	C5'-C4'-C3'	6.28	126.04	116.00
1	A	2115	G	C2'-C3'-O3'	6.27	123.73	113.70
1	A	1983	C	C5'-C4'-O4'	6.22	116.56	109.10
1	A	191	C	C2'-C3'-O3'	6.15	123.54	113.70
1	A	1810	A	O5'-P-OP1	6.11	118.03	110.70
1	A	1955	C	C4'-C3'-O3'	6.08	125.15	113.00
1	A	549	U	C2'-C3'-O3'	6.07	123.42	113.70
1	A	1410	A	C5'-C4'-O4'	6.04	116.35	109.10
25	1	46	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	98	G	O4'-C1'-N9	6.00	113.00	108.20
1	A	1744	A	C4'-C3'-O3'	-5.93	96.94	109.40
1	A	1044	U	O5'-P-OP1	-5.88	100.41	105.70
1	A	833	U	O5'-P-OP2	-5.82	100.46	105.70
1	A	2621	C	C4'-C3'-O3'	-5.79	97.24	109.40
1	A	1740	C	C5'-C4'-C3'	5.78	125.24	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1820	C	O5'-P-OP2	5.70	117.54	110.70
1	A	2329	G	C2'-C3'-O3'	5.68	122.79	113.70
1	A	1740	C	C5'-C4'-O4'	5.67	115.90	109.10
1	A	1693	G	O5'-P-OP1	-5.61	100.65	105.70
1	A	2028	C	O5'-P-OP2	-5.61	100.65	105.70
1	A	2259	C	O5'-P-OP2	5.59	117.40	110.70
1	A	2513	G	O5'-P-OP1	-5.58	100.67	105.70
1	A	1810	A	O5'-P-OP2	-5.58	100.68	105.70
1	A	1345	U	C5'-C4'-O4'	5.56	115.77	109.10
1	A	1726	U	C2'-C3'-O3'	5.55	122.58	113.70
1	A	1544	C	C2'-C3'-O3'	5.54	122.56	113.70
1	A	1661	A	O4'-C1'-C2'	-5.53	100.27	105.80
1	A	1325	G	C2'-C3'-O3'	5.45	122.42	113.70
1	A	1698	A	C4'-C3'-O3'	5.43	123.86	113.00
1	A	1816	A	O4'-C1'-C2'	-5.43	100.37	105.80
1	A	598	U	O5'-P-OP2	-5.39	100.84	105.70
1	A	2416	G	C2'-C3'-O3'	5.36	122.27	113.70
1	A	1709	C	C2'-C3'-O3'	5.35	122.26	113.70
1	A	1643	C	C2'-C3'-O3'	5.34	122.25	113.70
13	P	16	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	1392	G	C2'-C3'-O3'	5.33	122.22	113.70
1	A	2829	A	N9-C1'-C2'	5.31	120.91	114.00
1	A	47	A	C2'-C3'-O3'	5.31	122.19	113.70
1	A	534	C	O5'-P-OP1	5.26	117.02	110.70
1	A	715	G	C4'-C3'-O3'	5.26	123.52	113.00
32	8	32	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	1991	A	C1'-O4'-C4'	-5.24	105.71	109.90
1	A	2259	C	O5'-P-OP1	-5.24	100.98	105.70
1	A	2357	A	C1'-O4'-C4'	-5.24	105.71	109.90
1	A	1345	U	C5'-C4'-C3'	5.21	124.34	116.00
1	A	2587	G	O5'-P-OP1	5.21	116.96	110.70
1	A	839	A	O5'-P-OP1	5.20	116.94	110.70
1	A	2449	U	O5'-P-OP1	5.19	116.93	110.70
5	E	44	TYR	N-CA-C	5.17	124.95	111.00
1	A	1539	A	C2'-C3'-O3'	5.15	121.94	113.70
1	A	1174	A	C5'-C4'-O4'	5.15	115.28	109.10
13	P	41	ARG	N-CA-C	-5.10	97.22	111.00
1	A	2425	G	C2'-C3'-O3'	5.10	121.86	113.70
1	A	1811	C	C4'-C3'-O3'	-5.09	98.72	109.40
1	A	2586	C	O5'-P-OP2	5.08	116.80	110.70
1	A	2596	U	C4'-C3'-O3'	-5.06	98.77	109.40
8	H	155	SER	N-CA-C	5.05	124.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2609	A	O5'-P-OP1	5.00	116.70	110.70

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	98	G	C1'
1	A	497	A	C3'
1	A	715	G	C4',C1',C3'
1	A	989	A	C1'
1	A	1345	U	C4',C1',C3'
1	A	1424	A	C1'
1	A	1590	A	C1'
1	A	1740	C	C4',C3'
1	A	1955	C	C3'
1	A	1983	C	C4',C1'
1	A	2212	G	C3'
1	A	2297	A	C1'
1	A	2673	A	C1'
1	A	2808	U	C1'

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	6	45	LYS	Peptide
4	D	197	GLY	Peptide
4	D	244	ARG	Peptide
5	E	131	ALA	Peptide
13	P	41	ARG	Peptide
13	P	51	PHE	Peptide
13	P	52	GLU	Peptide
13	P	57	THR	Peptide
15	R	4	LEU	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60459	0	30488	990	0
2	B	2551	0	1295	35	0
3	C	1157	0	1160	22	0
4	D	2105	0	2182	89	0
5	E	1564	0	1629	66	0
6	F	1624	0	1677	63	0
7	G	1474	0	1535	48	0
8	H	1223	0	1282	22	0
9	I	1132	0	1218	29	0
10	J	651	0	649	14	0
11	N	1105	0	1180	42	0
12	O	933	0	996	27	0
13	P	1114	0	1187	82	0
14	Q	1122	0	1179	28	0
15	R	960	0	1021	46	0
16	S	771	0	832	33	0
17	T	1142	0	1202	67	0
18	U	958	0	1018	52	0
19	V	779	0	852	39	0
20	W	896	0	956	23	0
21	X	726	0	778	20	0
22	Y	776	0	870	45	0
23	Z	1404	0	1432	30	0
24	0	662	0	688	19	0
25	1	734	0	808	21	0
26	2	598	0	653	13	0
27	3	468	0	523	12	0
28	4	226	0	229	4	0
29	5	459	0	478	21	0
30	6	381	0	391	30	0
31	7	419	0	467	15	0
32	8	508	0	576	33	0
33	9	299	0	324	7	0
All	All	91380	0	61755	1840	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (1840) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1331:A:O2'	1:A:1333:U:OP2	1.62	1.13
1:A:1377:G:N2	1:A:1654:A:O2'	1.90	1.02
33:9:11:CYS:HB3	33:9:14:CYS:SG	1.99	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1424:A:O2'	1:A:1425:G:OP1	1.78	1.00
1:A:2492:G:O2'	1:A:2493:G:OP2	1.79	0.99
1:A:2273:U:OP2	24:0:16:SER:OG	1.80	0.97
1:A:26:G:N2	1:A:536:G:O2'	1.99	0.95
1:A:893:U:OP2	1:A:973:G:O6	1.85	0.94
1:A:2001:G:O2'	1:A:2003:C:OP2	1.85	0.94
12:O:35:VAL:HG11	12:O:103:ALA:HB3	1.50	0.94
1:A:1067:G:O2'	1:A:1068:U:OP2	1.87	0.91
16:S:89:ARG:HG2	16:S:92:TYR:HA	1.50	0.90
1:A:1704:C:OP1	5:E:132:HIS:O	1.91	0.89
18:U:90:VAL:HG21	19:V:47:VAL:HG21	1.54	0.88
1:A:2043:U:OP2	29:5:15:ARG:NH2	2.06	0.88
2:B:66:A:O2'	2:B:67:G:OP2	1.91	0.88
15:R:10:LEU:HB3	15:R:17:ARG:NE	1.89	0.88
29:5:46:CYS:SG	29:5:48:GLU:HG2	2.14	0.88
13:P:59:LEU:HA	13:P:61:ARG:NH1	1.90	0.87
1:A:996:G:P	14:Q:16:ARG:HH22	1.98	0.87
1:A:518:G:O2'	20:W:5:ALA:O	1.92	0.86
1:A:1875:G:C2'	1:A:1876:G:H5'	2.06	0.86
1:A:2416:G:O2'	1:A:2422:A:N6	2.08	0.85
1:A:138:A:C8	1:A:1453:C:O2'	2.27	0.85
1:A:1875:G:H2'	1:A:1876:G:H5'	1.57	0.84
1:A:552:A:O2'	1:A:553:A:H5'	1.75	0.84
1:A:1724:G:N2	1:A:2010:G:H22	1.75	0.83
1:A:1777:G:H2'	1:A:1778:G:H5'	1.59	0.83
1:A:2819:A:O2'	5:E:61:ARG:NH1	2.11	0.83
1:A:2694:C:OP1	17:T:53:ARG:NH2	2.12	0.83
1:A:138:A:H8	1:A:1453:C:O2'	1.58	0.83
17:T:27:THR:O	17:T:28:VAL:HG23	1.79	0.83
5:E:111:ARG:HG3	15:R:2:ARG:HE	1.43	0.82
1:A:1704:C:OP1	5:E:132:HIS:ND1	2.13	0.82
11:N:57:ALA:O	11:N:58:ASP:O	1.96	0.82
1:A:1346:A:O2'	1:A:1347:A:H2'	1.79	0.82
1:A:1464:A:O2'	1:A:1466:G:N7	2.11	0.82
1:A:2131:G:O2'	1:A:2141:G:OP2	1.99	0.81
1:A:144:G:H2'	1:A:145:G:H5'	1.62	0.81
1:A:2723:U:H5'	1:A:2723:U:O2	1.81	0.81
1:A:1185:U:OP2	11:N:63:THR:OG1	1.98	0.80
1:A:2475:C:O2'	1:A:2476:C:O5'	1.99	0.80
1:A:2487:A:N3	1:A:2488:C:H5''	1.96	0.80
1:A:708:G:OP1	13:P:18:ARG:HD2	1.82	0.80
1:A:1290:G:OP1	13:P:16:ARG:NE	2.14	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:U:114:LYS:HA	18:U:117:GLN:HB2	1.63	0.79
1:A:836:C:O2'	1:A:837:C:OP1	1.98	0.79
17:T:50:ILE:HD11	17:T:102:ILE:HD11	1.65	0.79
1:A:1833:A:O3'	4:D:259:THR:HG21	1.81	0.79
30:6:47:THR:OG1	30:6:48:VAL:N	2.15	0.79
4:D:44:ASN:HB3	4:D:49:ILE:HA	1.64	0.79
30:6:15:GLU:OE1	30:6:43:CYS:SG	2.41	0.78
22:Y:2:ARG:O	22:Y:4:LYS:N	2.17	0.78
30:6:16:CYS:SG	30:6:48:VAL:HG22	2.23	0.78
1:A:1903:C:H5'	1:A:1904:G:OP2	1.84	0.78
1:A:2548:U:H2'	1:A:2549:C:C6	2.17	0.78
4:D:77:ALA:HB2	4:D:97:TYR:CD2	2.19	0.77
24:O:12:ASN:O	24:O:14:ARG:N	2.17	0.77
4:D:35:LYS:HE2	4:D:36:PRO:HB3	1.65	0.77
1:A:1160:G:H2'	1:A:1161:C:C6	2.20	0.77
7:G:77:ILE:HG22	7:G:80:PHE:H	1.49	0.76
1:A:508:A:H4'	22:Y:49:VAL:HG22	1.67	0.76
25:1:5:CYS:SG	25:1:62:VAL:HG23	2.25	0.76
1:A:144:G:C2'	1:A:145:G:H5'	2.15	0.76
1:A:718:C:C2'	1:A:719:C:H5'	2.16	0.75
1:A:1527:U:H5'	1:A:1528:G:OP2	1.86	0.75
15:R:38:VAL:HB	15:R:39:PRO:HD3	1.68	0.75
6:F:101:LEU:O	6:F:106:ARG:NH1	2.20	0.75
20:W:18:ARG:NH1	20:W:76:VAL:O	2.18	0.75
5:E:11:MET:HB2	5:E:23:VAL:O	1.86	0.75
1:A:2323:U:H2'	1:A:2324:C:H5'	1.69	0.75
1:A:1821:A:N6	1:A:1858:G:O2'	2.19	0.74
30:6:43:CYS:O	30:6:43:CYS:SG	2.45	0.74
2:B:41:U:N3	7:G:70:VAL:O	2.20	0.73
22:Y:79:CYS:SG	22:Y:80:GLY:N	2.62	0.73
21:X:12:VAL:HG13	21:X:27:THR:O	1.87	0.73
1:A:798:A:O2'	1:A:799:C:OP2	2.04	0.73
1:A:2492:G:O2'	1:A:2493:G:P	2.46	0.73
1:A:82:A:N1	1:A:96:G:O2'	2.21	0.73
13:P:83:VAL:HG11	13:P:112:LEU:HD21	1.71	0.73
7:G:28:VAL:O	7:G:31:VAL:HG12	1.89	0.73
25:1:29:GLY:O	25:1:30:VAL:HG22	1.89	0.72
1:A:715:G:H4'	1:A:716:A:OP2	1.89	0.72
1:A:879:U:O2	13:P:55:ARG:NH1	2.23	0.72
1:A:987:U:OP2	13:P:38:GLN:CD	2.27	0.72
13:P:64:LYS:O	13:P:66:GLY:N	2.21	0.72
17:T:55:ASN:HD22	17:T:58:ASN:HD21	1.38	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1002:U:OP2	14:Q:14:ARG:NH1	2.23	0.72
1:A:1448:C:H5''	1:A:1517:A:H1'	1.72	0.72
16:S:74:ALA:HB1	16:S:103:GLU:HB2	1.72	0.71
15:R:11:ASN:OD1	15:R:12:ARG:N	2.22	0.71
16:S:96:GLY:O	16:S:98:VAL:N	2.23	0.71
17:T:30:VAL:HA	17:T:44:ASP:HA	1.72	0.71
22:Y:2:ARG:C	22:Y:4:LYS:H	1.93	0.71
1:A:1054:A:H5''	18:U:63:VAL:HG21	1.73	0.71
13:P:58:THR:O	13:P:61:ARG:NE	2.24	0.70
5:E:4:ILE:HD13	5:E:28:ALA:HB1	1.71	0.70
1:A:609:C:C5	13:P:33:ARG:HD3	2.26	0.70
1:A:1549:C:O2'	1:A:1550:C:O5'	2.08	0.70
12:O:80:ASP:OD1	17:T:64:ARG:NH2	2.23	0.70
17:T:23:ARG:O	17:T:25:GLY:N	2.24	0.70
30:6:40:CYS:HA	30:6:46:HIS:CB	2.21	0.70
13:P:61:ARG:NH1	32:8:13:ARG:HD2	2.06	0.70
1:A:230:G:H5''	32:8:62:LEU:HD13	1.73	0.70
1:A:1450:U:H2'	1:A:1451:U:C6	2.27	0.70
17:T:13:ARG:CZ	17:T:13:ARG:HA	2.22	0.70
1:A:355:A:O2'	1:A:357:C:OP2	2.08	0.69
1:A:2672:G:H3'	1:A:2673:A:O4'	1.92	0.69
16:S:20:ARG:NE	16:S:20:ARG:HA	2.06	0.69
1:A:2405:C:OP1	13:P:63:PRO:HD2	1.92	0.69
1:A:865:A:C4	1:A:1233:A:C2	2.81	0.69
30:6:40:CYS:HA	30:6:46:HIS:HB3	1.74	0.69
16:S:89:ARG:CG	16:S:92:TYR:HA	2.23	0.69
5:E:111:ARG:HG3	15:R:2:ARG:NE	2.08	0.69
1:A:1346:A:H4'	1:A:1347:A:OP1	1.92	0.69
1:A:718:C:O2'	1:A:719:C:H5'	1.92	0.69
13:P:107:LYS:O	13:P:109:GLY:N	2.25	0.69
13:P:23:PRO:HB2	13:P:33:ARG:CD	2.23	0.69
1:A:775:G:OP2	4:D:13:ARG:NH1	2.26	0.69
32:8:54:GLU:O	32:8:58:ILE:HG12	1.93	0.69
1:A:852:C:OP2	13:P:39:LYS:HD3	1.93	0.69
13:P:58:THR:O	13:P:61:ARG:CZ	2.41	0.68
1:A:139:A:C8	1:A:1453:C:H1'	2.28	0.68
4:D:44:ASN:CB	4:D:49:ILE:HA	2.23	0.68
7:G:20:ILE:O	7:G:24:GLY:HA2	1.93	0.68
1:A:634:C:H2'	1:A:635:G:H5''	1.73	0.68
1:A:1712:G:HO2'	12:O:6:THR:HG1	1.40	0.68
3:C:78:ALA:HB3	3:C:94:VAL:HG13	1.75	0.68
1:A:95:C:H5''	26:2:2:LYS:HB2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2672:G:H2'	1:A:2673:A:N3	2.08	0.68
1:A:276:G:O2'	1:A:277:G:H8	1.76	0.68
1:A:2147:A:H4'	1:A:2148:G:O5'	1.94	0.68
6:F:53:THR:HG22	6:F:56:GLU:OE2	1.93	0.68
1:A:2030:G:H1'	15:R:107:ASP:O	1.93	0.68
1:A:276:G:HO2'	1:A:277:G:H8	1.42	0.68
1:A:1232:U:O2'	1:A:1233:A:H5'	1.94	0.68
12:O:114:ILE:H	12:O:114:ILE:HD12	1.57	0.68
1:A:260:A:N1	1:A:290:G:O2'	2.23	0.68
1:A:1888:G:O2'	1:A:1905:A:N6	2.26	0.67
17:T:7:ILE:O	17:T:10:VAL:HB	1.94	0.67
1:A:1185:U:OP1	11:N:25:ARG:NH1	2.27	0.67
1:A:1628:C:O2'	1:A:1631:A:C8	2.47	0.67
29:5:33:CYS:HB2	29:5:40:LYS:HE3	1.75	0.67
17:T:88:ILE:HG22	17:T:89:VAL:HG23	1.76	0.67
18:U:31:SER:O	18:U:33:ARG:N	2.27	0.67
1:A:1441:U:H2'	1:A:1441:U:O2	1.94	0.67
1:A:1851:A:OP1	4:D:201:HIS:NE2	2.26	0.67
8:H:106:THR:HG22	8:H:112:PRO:HB3	1.76	0.67
5:E:119:ARG:HD2	5:E:120:TRP:NE1	2.10	0.67
4:D:24:ILE:O	4:D:25:THR:O	2.12	0.67
1:A:1354:G:HO2'	1:A:1656:C:HO2'	1.43	0.67
30:6:18:ARG:HD2	30:6:43:CYS:SG	2.34	0.67
6:F:165:ARG:HA	6:F:168:ARG:HD3	1.77	0.67
1:A:2420:G:H2'	1:A:2421:G:O4'	1.95	0.66
9:I:133:HIS:HB2	9:I:134:PRO:CD	2.25	0.66
6:F:185:ASP:OD1	6:F:188:ARG:NH1	2.27	0.66
1:A:209:A:H4'	1:A:210:A:O5'	1.94	0.66
1:A:47:A:H5'	1:A:49:G:O4'	1.94	0.66
1:A:202:G:H1'	1:A:204:A:O2'	1.95	0.66
2:B:21:G:O2'	2:B:22:U:O5'	2.14	0.66
1:A:1850:U:H4'	1:A:1851:A:OP2	1.95	0.66
1:A:985:A:H4'	13:P:35:HIS:CE1	2.30	0.66
1:A:2220:A:H3'	1:A:2221:C:H6	1.61	0.66
1:A:2221:C:H5'	1:A:2222:C:OP2	1.95	0.66
1:A:524:G:N1	1:A:527:A:OP2	2.27	0.66
5:E:112:GLY:O	5:E:159:HIS:HA	1.96	0.66
1:A:2885:G:H4'	17:T:3:ARG:HE	1.60	0.66
1:A:108:A:O3'	26:2:69:ARG:NH2	2.28	0.66
1:A:91:C:H5'	1:A:92:G:OP2	1.95	0.65
6:F:24:LEU:O	6:F:26:ALA:N	2.30	0.65
24:0:51:VAL:HG21	24:0:79:VAL:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:6:35:GLU:OE1	30:6:36:LEU:N	2.30	0.65
1:A:1724:G:H22	1:A:2010:G:H22	1.45	0.65
2:B:21:G:O2'	2:B:22:U:O4'	2.13	0.65
1:A:92:G:N3	26:2:47:ASN:ND2	2.44	0.65
1:A:1920:G:N2	1:A:1923:C:H41	1.93	0.65
5:E:30:PRO:O	5:E:32:PRO:HD3	1.96	0.65
22:Y:75:ILE:HA	22:Y:79:CYS:O	1.97	0.65
1:A:1210:U:H2'	1:A:1211:C:C6	2.32	0.65
29:5:33:CYS:O	29:5:36:CYS:O	2.15	0.65
1:A:852:C:OP2	13:P:39:LYS:HB3	1.96	0.64
6:F:110:LEU:HD21	6:F:181:LEU:HG	1.78	0.64
1:A:948:C:C2'	1:A:949:C:H5'	2.27	0.64
5:E:81:ILE:O	5:E:81:ILE:HG22	1.97	0.64
1:A:2656:G:H3'	1:A:2657:C:H5'	1.79	0.64
13:P:126:VAL:HG12	13:P:148:LEU:HD11	1.78	0.64
1:A:2475:C:O2'	1:A:2476:C:P	2.55	0.64
1:A:2354:C:HO2'	1:A:2384:G:HO2'	1.36	0.64
7:G:120:LEU:N	7:G:179:PRO:O	2.30	0.64
13:P:23:PRO:HB2	13:P:33:ARG:HD2	1.79	0.64
29:5:41:PRO:O	29:5:44:THR:OG1	2.11	0.64
22:Y:17:SER:HB2	22:Y:71:LYS:HE2	1.79	0.64
9:I:118:LYS:HG2	9:I:119:PRO:HD2	1.79	0.64
20:W:86:LEU:HD22	20:W:96:ILE:HD12	1.79	0.64
1:A:1540:A:H2'	1:A:1540:A:N3	2.11	0.64
1:A:1041:A:C2	1:A:1042:G:C8	2.85	0.64
2:B:104:U:H5''	14:Q:141:GLN:OE1	1.97	0.64
1:A:158:U:H4'	1:A:159:G:C8	2.33	0.64
1:A:1013:U:OP1	27:3:17:LYS:HG2	1.97	0.64
1:A:88:U:H2'	1:A:88:U:O2	1.98	0.64
1:A:718:C:H2'	1:A:719:C:H5'	1.79	0.64
1:A:2469:G:O2'	1:A:2471:U:O4	2.14	0.64
17:T:102:ILE:HB	17:T:110:ILE:HD13	1.78	0.64
18:U:97:ASP:OD2	18:U:101:ARG:NH1	2.31	0.63
21:X:12:VAL:CG1	21:X:17:ALA:HB1	2.27	0.63
1:A:2120:U:H2'	1:A:2120:U:O2	1.97	0.63
1:A:566:C:H2'	1:A:567:C:OP1	1.98	0.63
18:U:83:LEU:HD12	18:U:88:ILE:HD11	1.80	0.63
1:A:1041:A:OP2	18:U:92:ARG:NH2	2.32	0.63
1:A:1286:A:C2'	1:A:1287:A:O5'	2.46	0.63
11:N:58:ASP:O	11:N:60:ILE:N	2.31	0.63
4:D:30:GLU:HB3	4:D:35:LYS:HG3	1.79	0.63
19:V:55:ALA:HA	19:V:101:GLY:HA2	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1777:G:C2'	1:A:1778:G:H5'	2.28	0.63
1:A:1309:G:H3'	1:A:1310:A:H5''	1.81	0.63
1:A:663:U:H2'	1:A:664:C:C6	2.33	0.63
1:A:1182:G:N2	11:N:106:MET:SD	2.69	0.63
1:A:139:A:H8	1:A:1453:C:H1'	1.63	0.63
1:A:552:A:O2'	1:A:553:A:C5'	2.44	0.63
1:A:230:G:C5'	32:8:62:LEU:HD13	2.29	0.63
3:C:56:GLN:NE2	3:C:168:ALA:HB2	2.13	0.63
1:A:422:G:O2'	25:1:43:TYR:O	2.14	0.63
1:A:2666:G:O2'	1:A:2675:G:N1	2.31	0.63
19:V:62:LEU:HD21	19:V:95:LEU:HB2	1.81	0.63
1:A:1897:A:H2'	1:A:1898:A:C8	2.34	0.63
1:A:1269:C:HO2'	19:V:85:LYS:HA	1.64	0.63
1:A:1475:C:H2'	1:A:1476:U:C6	2.34	0.63
11:N:57:ALA:O	11:N:58:ASP:C	2.37	0.62
1:A:1820:C:H5''	1:A:1821:A:OP1	1.99	0.62
13:P:83:VAL:CG1	13:P:112:LEU:HD21	2.29	0.62
1:A:644:G:H5''	1:A:644:G:N3	2.13	0.62
1:A:505:A:O4'	22:Y:44:ILE:HG21	1.98	0.62
19:V:2:PHE:O	19:V:14:VAL:O	2.18	0.62
1:A:1920:G:H22	1:A:1923:C:N4	1.97	0.62
1:A:2209:C:H2'	1:A:2210:U:C1'	2.30	0.62
17:T:27:THR:OG1	17:T:28:VAL:N	2.29	0.62
1:A:906:U:H5	1:A:962:A:N7	1.97	0.62
5:E:87:GLU:O	5:E:87:GLU:HG3	1.99	0.62
1:A:25:G:C6	1:A:26:G:N1	2.68	0.62
1:A:952:U:OP1	14:Q:24:GLY:N	2.31	0.62
5:E:16:ARG:O	5:E:18:ASP:N	2.32	0.62
15:R:10:LEU:HD22	15:R:17:ARG:HD2	1.82	0.62
6:F:101:LEU:HD12	6:F:102:PRO:HD2	1.79	0.62
1:A:1541:A:C8	1:A:1623:C:O2'	2.53	0.62
1:A:473:U:O4	1:A:605:G:H1'	1.99	0.62
1:A:2535:G:H8	1:A:2535:G:H5''	1.65	0.62
1:A:1269:C:O2'	19:V:85:LYS:HA	2.00	0.62
25:1:67:ILE:N	25:1:68:PRO:HD2	2.15	0.62
4:D:210:GLY:O	4:D:211:ARG:HB3	2.00	0.62
3:C:55:ASP:HB2	3:C:56:GLN:HE21	1.65	0.62
7:G:46:ALA:HB2	7:G:88:ILE:HG12	1.82	0.62
13:P:107:LYS:C	13:P:109:GLY:H	2.03	0.61
21:X:63:LYS:HA	21:X:72:LYS:HA	1.82	0.61
1:A:2054:A:O2'	1:A:2056:G:OP2	2.12	0.61
1:A:2529:A:C8	1:A:2529:A:H5'	2.35	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:A:H2	1:A:1254:A:H2'	1.64	0.61
1:A:820:A:O2'	1:A:821:G:OP2	2.16	0.61
17:T:24:PRO:HA	17:T:49:VAL:HG13	1.81	0.61
1:A:493:G:N7	31:7:39:ARG:NH2	2.47	0.61
30:6:16:CYS:SG	30:6:47:THR:OG1	2.57	0.61
1:A:1920:G:H22	1:A:1923:C:H41	1.49	0.61
1:A:1092:G:OP1	1:A:1092:G:H4'	2.00	0.61
7:G:51:ARG:HA	7:G:51:ARG:HE	1.64	0.61
17:T:58:ASN:HD22	17:T:58:ASN:C	2.04	0.61
1:A:1765:G:C2	1:A:1767:U:OP2	2.53	0.61
1:A:1069:G:H3'	1:A:1070:G:H5''	1.81	0.61
1:A:987:U:OP2	13:P:38:GLN:OE1	2.19	0.61
1:A:1051:C:C2	1:A:1182:G:N2	2.69	0.61
17:T:90:GLN:NE2	17:T:124:ASP:OD2	2.34	0.61
1:A:819:U:H4'	4:D:47:GLY:HA2	1.82	0.61
4:D:65:ILE:H	4:D:65:ILE:HD13	1.64	0.61
1:A:1740:C:O2'	1:A:1741:G:C4	2.54	0.61
17:T:29:ARG:HB3	17:T:85:LYS:HA	1.82	0.61
1:A:2228:A:H1'	1:A:2230:G:C5	2.36	0.61
1:A:2672:G:H2'	1:A:2673:A:C4	2.35	0.61
1:A:1064:U:HO2'	1:A:1066:A:H2	1.44	0.61
23:Z:53:ILE:HG21	23:Z:71:VAL:O	2.01	0.61
1:A:670:A:H2'	1:A:671:G:O4'	2.01	0.61
1:A:1091:A:H1'	10:J:10:ALA:HB3	1.83	0.60
7:G:96:ARG:O	7:G:98:ARG:N	2.34	0.60
1:A:2488:C:O2	1:A:2492:G:O6	2.19	0.60
1:A:605:G:OP2	18:U:10:ARG:HD2	2.01	0.60
13:P:8:PRO:C	13:P:10:PRO:HD2	2.22	0.60
32:8:51:ALA:C	32:8:53:PRO:HD2	2.22	0.60
1:A:2077:G:N3	1:A:2077:G:H2'	2.16	0.60
18:U:31:SER:C	18:U:33:ARG:H	2.03	0.60
2:B:50:G:OP1	16:S:63:THR:HG23	2.00	0.60
1:A:1403:G:O2'	1:A:1404:A:H5''	2.00	0.60
1:A:2402:G:OP1	32:8:32:LEU:HD13	2.02	0.60
13:P:85:LEU:HD23	13:P:85:LEU:H	1.65	0.60
1:A:655:A:OP1	13:P:64:LYS:HE2	2.02	0.60
30:6:22:ALA:O	30:6:23:THR:OG1	2.16	0.60
17:T:82:LEU:HD12	17:T:82:LEU:H	1.67	0.60
30:6:37:ARG:O	30:6:48:VAL:O	2.19	0.60
5:E:111:ARG:HB2	5:E:160:TYR:O	2.02	0.60
8:H:156:ALA:O	8:H:157:TYR:C	2.40	0.60
17:T:28:VAL:O	17:T:29:ARG:HD3	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2735:C:OP1	15:R:2:ARG:NH1	2.35	0.59
1:A:1346:A:O2'	1:A:1347:A:C2'	2.48	0.59
17:T:23:ARG:HA	17:T:52:ILE:HD11	1.84	0.59
3:C:78:ALA:HB3	3:C:94:VAL:CG1	2.32	0.59
9:I:133:HIS:O	9:I:135:GLU:HG3	2.01	0.59
1:A:142:C:H4'	21:X:38:GLU:OE2	2.01	0.59
29:5:16:ARG:NH1	29:5:17:ASP:OD1	2.35	0.59
1:A:391:U:H5'	1:A:392:A:OP2	2.02	0.59
19:V:28:GLU:HB3	19:V:29:PRO:HD2	1.84	0.59
3:C:51:PRO:HB3	3:C:204:ALA:HB2	1.83	0.59
14:Q:2:LEU:O	14:Q:70:PRO:HG2	2.02	0.59
1:A:2036:A:O2'	29:5:2:ALA:HA	2.01	0.59
5:E:132:HIS:HA	5:E:135:HIS:CE1	2.38	0.59
12:O:111:PHE:HB3	12:O:114:ILE:HD13	1.84	0.59
1:A:1920:G:O2'	1:A:1921:A:OP2	2.20	0.59
1:A:1207:G:H4'	19:V:24:LYS:HB2	1.84	0.59
1:A:595:G:N1	1:A:2052:A:OP2	2.28	0.59
1:A:2889:C:O3'	15:R:90:ARG:NH1	2.35	0.59
13:P:64:LYS:HD2	32:8:25:MET:SD	2.43	0.59
7:G:95:ARG:O	7:G:96:ARG:HG2	2.02	0.59
1:A:2095:U:H2'	1:A:2096:U:C6	2.37	0.59
30:6:33:LYS:HA	30:6:33:LYS:HE2	1.84	0.59
13:P:59:LEU:HA	13:P:61:ARG:CZ	2.32	0.59
1:A:1833:A:O3'	4:D:259:THR:CG2	2.50	0.59
1:A:948:C:H2'	1:A:949:C:H5'	1.85	0.59
1:A:906:U:O4'	1:A:906:U:O2	2.20	0.59
1:A:154:C:O4'	1:A:154:C:O2	2.18	0.59
1:A:1685:U:O2'	1:A:1686:C:H5''	2.02	0.59
1:A:590:U:O2'	1:A:592:G:N7	2.28	0.59
32:8:33:ASN:O	32:8:34:TRP:HB3	2.02	0.59
1:A:1450:U:H2'	1:A:1451:U:H6	1.68	0.59
4:D:108:PRO:HD2	4:D:111:LEU:HG	1.85	0.59
1:A:2893:U:O2	29:5:52:TYR:OH	2.21	0.59
1:A:1690:C:O2	1:A:1690:C:H2'	2.01	0.59
19:V:64:HIS:ND1	19:V:92:THR:HG22	2.17	0.59
22:Y:90:LEU:HG	22:Y:91:GLU:HG2	1.84	0.59
13:P:21:ARG:HD3	13:P:29:LYS:HE3	1.85	0.59
1:A:2885:G:H4'	17:T:3:ARG:NE	2.18	0.59
12:O:87:ILE:HG22	12:O:88:ASN:O	2.01	0.59
1:A:1075:G:OP2	14:Q:128:LYS:NZ	2.27	0.59
7:G:29:TRP:O	7:G:33:ARG:NH1	2.36	0.59
6:F:178:PRO:HB2	6:F:201:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:R:10:LEU:HD22	15:R:17:ARG:CD	2.33	0.58
1:A:483:G:O2'	31:7:39:ARG:HD3	2.03	0.58
1:A:594:A:OP2	19:V:78:LYS:NZ	2.35	0.58
1:A:2433:A:H4'	1:A:2434:U:OP1	2.02	0.58
1:A:2107:U:H2'	1:A:2108:G:C8	2.37	0.58
11:N:2:LYS:O	11:N:4:TYR:CZ	2.56	0.58
1:A:415:G:O5'	1:A:415:G:H8	1.86	0.58
4:D:44:ASN:HB2	4:D:48:ARG:O	2.03	0.58
1:A:628:U:H4'	1:A:704:C:H4'	1.85	0.58
5:E:59:VAL:HG13	5:E:63:LEU:HG	1.84	0.58
1:A:72:A:H4'	1:A:73:G:O5'	2.03	0.58
1:A:232:A:C2	1:A:243:A:C4	2.90	0.58
19:V:98:GLU:OE1	19:V:100:ARG:HB3	2.04	0.58
1:A:1039:C:OP2	18:U:54:LYS:NZ	2.31	0.58
32:8:52:LYS:N	32:8:53:PRO:HD2	2.18	0.58
13:P:84:ASN:HA	13:P:115:LEU:O	2.04	0.58
13:P:56:SER:O	13:P:58:THR:N	2.31	0.58
1:A:180:C:O2'	1:A:848:A:N3	2.35	0.58
5:E:7:VAL:HA	5:E:194:GLY:O	2.04	0.58
1:A:1050:C:O2'	11:N:28:THR:OG1	2.22	0.58
13:P:32:THR:HG21	13:P:37:GLY:HA2	1.85	0.58
16:S:20:ARG:HE	16:S:20:ARG:HA	1.66	0.58
1:A:489:U:H4'	31:7:5:TRP:CZ3	2.38	0.58
15:R:2:ARG:HD2	15:R:5:LYS:HE2	1.86	0.58
29:5:40:LYS:NZ	29:5:49:CYS:SG	2.75	0.58
1:A:859:U:H2'	1:A:860:C:C6	2.39	0.58
1:A:1770:G:N7	1:A:1771:C:C4	2.72	0.58
22:Y:66:PRO:O	22:Y:67:LEU:HB3	2.03	0.58
1:A:1087:G:H2'	1:A:1087:G:N3	2.19	0.58
1:A:2479:G:N2	1:A:2492:G:O2'	2.36	0.58
30:6:13:CYS:O	30:6:21:TYR:HA	2.04	0.58
1:A:1698:A:H3'	1:A:1699:G:C8	2.37	0.58
1:A:149:C:H2'	1:A:150:C:C6	2.39	0.58
25:1:51:VAL:O	25:1:57:GLU:O	2.22	0.58
1:A:2817:U:H5'	1:A:2899:G:O6	2.03	0.58
1:A:955:A:C8	14:Q:13:GLN:HG3	2.39	0.58
6:F:65:TRP:CZ3	6:F:72:ARG:HB2	2.39	0.58
1:A:267:G:O2'	1:A:268:G:OP2	2.21	0.57
1:A:2263:G:O6	24:0:4:LYS:HD3	2.05	0.57
32:8:21:LYS:HD3	32:8:48:PHE:CZ	2.39	0.57
19:V:19:LYS:HG3	19:V:20:LEU:N	2.19	0.57
1:A:2499:A:O2'	1:A:2500:G:H5'	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:T:10:VAL:O	17:T:13:ARG:HG2	2.05	0.57
1:A:620:G:H2'	1:A:621:G:O4'	2.04	0.57
1:A:1735:A:H62	1:A:1744:A:H2	1.51	0.57
13:P:49:ARG:HA	32:8:55:ALA:HB1	1.85	0.57
1:A:2121:G:C6	1:A:2122:G:C6	2.93	0.57
1:A:138:A:H8	1:A:1453:C:HO2'	0.76	0.57
1:A:2799:C:O2	5:E:61:ARG:NH1	2.38	0.57
5:E:4:ILE:HG12	5:E:5:LEU:O	2.04	0.57
11:N:125:GLY:HA3	11:N:126:PRO:O	2.03	0.57
2:B:29:A:O2'	2:B:58:A:N1	2.38	0.57
13:P:57:THR:OG1	13:P:59:LEU:HB2	2.05	0.57
17:T:28:VAL:HG22	17:T:46:GLU:HA	1.85	0.57
1:A:2613:A:H4'	1:A:2614:G:C5'	2.34	0.57
26:2:65:ASN:HB3	26:2:69:ARG:NH2	2.19	0.57
1:A:1973:A:C6	1:A:1974:A:N1	2.73	0.57
32:8:61:LEU:HD12	32:8:62:LEU:H	1.69	0.57
6:F:113:ALA:HB1	6:F:186:ILE:HG21	1.87	0.57
1:A:2227:G:H3'	1:A:2227:G:N3	2.20	0.57
5:E:61:ARG:HB3	5:E:62:PRO:HD3	1.87	0.57
1:A:2566:U:C5	1:A:2567:C:C2	2.93	0.57
1:A:2845:U:H2'	1:A:2846:G:C8	2.40	0.57
10:J:21:ALA:HB3	10:J:88:ALA:O	2.05	0.57
6:F:65:TRP:HB3	6:F:66:PRO:HD2	1.86	0.56
1:A:2032:U:OP1	20:W:42:ARG:NH1	2.37	0.56
1:A:2648:U:OP1	5:E:82:ARG:NE	2.37	0.56
6:F:89:VAL:HG12	6:F:90:PHE:N	2.19	0.56
15:R:9:LYS:O	15:R:10:LEU:HD23	2.05	0.56
17:T:28:VAL:HG13	17:T:46:GLU:HA	1.87	0.56
1:A:2656:G:H3'	1:A:2657:C:C5'	2.35	0.56
1:A:2802:A:H2'	1:A:2802:A:N3	2.20	0.56
23:Z:150:LEU:HG	23:Z:171:ILE:HD11	1.86	0.56
9:I:129:THR:HA	9:I:137:PRO:HA	1.85	0.56
25:1:90:ILE:O	25:1:94:LEU:HB2	2.04	0.56
1:A:2200:C:N4	1:A:2203:G:O6	2.38	0.56
30:6:26:ASN:O	30:6:27:LYS:HD3	2.06	0.56
1:A:1553:A:N3	1:A:1553:A:H2'	2.20	0.56
16:S:88:ASP:OD2	16:S:89:ARG:N	2.38	0.56
6:F:24:LEU:HB3	6:F:25:PRO:HD2	1.87	0.56
1:A:1543:C:O4'	1:A:1623:C:H4'	2.04	0.56
11:N:102:ALA:O	11:N:106:MET:HG3	2.05	0.56
17:T:42:ILE:HD13	17:T:83:ILE:HD11	1.86	0.56
4:D:129:ASN:O	4:D:193:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:149:ARG:HA	8:H:162:ILE:HD11	1.87	0.56
1:A:2213:G:H2'	1:A:2214:G:H5'	1.88	0.56
1:A:1424:A:O2'	1:A:1425:G:P	2.63	0.56
1:A:1539:A:H2'	1:A:1540:A:H5''	1.87	0.56
1:A:1098:C:O3'	1:A:1151:A:P	2.64	0.56
1:A:2826:G:OP1	15:R:99:LYS:NZ	2.39	0.56
1:A:639:A:N3	1:A:640:G:H1'	2.21	0.56
2:B:66:A:C2'	2:B:67:G:OP2	2.54	0.56
10:J:62:ALA:O	10:J:66:ALA:HB3	2.06	0.56
1:A:2193:U:H1'	1:A:2194:A:OP1	2.06	0.56
1:A:770:U:H2'	1:A:771:G:O4'	2.05	0.56
2:B:14:U:OP2	2:B:70:C:O2'	2.20	0.56
6:F:107:LYS:HD2	6:F:205:ARG:O	2.06	0.56
1:A:1727:G:H8	1:A:1727:G:OP2	1.88	0.56
4:D:71:ASP:OD2	4:D:103:ARG:NH2	2.37	0.56
11:N:18:ALA:HB1	11:N:21:LYS:HB2	1.88	0.56
1:A:1824:U:H1'	1:A:1921:A:N3	2.21	0.56
6:F:9:ILE:HA	6:F:13:SER:O	2.04	0.56
1:A:276:G:O2'	1:A:277:G:P	2.64	0.56
1:A:2221:C:C5'	1:A:2222:C:OP2	2.54	0.56
22:Y:46:LYS:H	22:Y:62:GLU:HG2	1.71	0.56
1:A:2214:G:C4	1:A:2215:G:C8	2.93	0.56
23:Z:24:LEU:HD21	23:Z:86:VAL:HG23	1.88	0.56
32:8:14:VAL:HG21	32:8:22:VAL:HG13	1.86	0.56
1:A:2492:G:HO2'	1:A:2493:G:P	2.17	0.55
1:A:1685:U:C2'	1:A:1686:C:H5''	2.37	0.55
1:A:1863:U:O2'	1:A:1990:A:N1	2.35	0.55
30:6:17:LYS:O	30:6:18:ARG:HB3	2.06	0.55
9:I:6:LEU:O	9:I:7:GLU:C	2.43	0.55
2:B:74:U:H2'	2:B:75:G:O4'	2.06	0.55
14:Q:41:TRP:CD1	14:Q:96:VAL:HG22	2.42	0.55
1:A:1393:G:H2'	1:A:1394:A:H5'	1.88	0.55
11:N:58:ASP:C	11:N:60:ILE:H	2.10	0.55
1:A:2212:G:H2'	1:A:2212:G:N3	2.21	0.55
1:A:344:G:O4'	6:F:165:ARG:NH1	2.39	0.55
1:A:2262:G:OP1	14:Q:82:ARG:NH1	2.36	0.55
1:A:853:U:O2'	1:A:2081:A:N1	2.37	0.55
1:A:141:G:H4'	21:X:35:THR:HG21	1.89	0.55
1:A:2502:U:H4'	1:A:2581:G:OP1	2.06	0.55
9:I:13:GLY:O	9:I:14:ASP:C	2.44	0.55
7:G:51:ARG:HA	7:G:51:ARG:NE	2.21	0.55
31:7:5:TRP:CD1	31:7:7:PRO:HD3	2.42	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:T:102:ILE:HB	17:T:110:ILE:CD1	2.37	0.55
1:A:154:C:O3'	1:A:157:U:P	2.65	0.55
1:A:1314:A:O2'	1:A:1370:G:O6	2.25	0.55
1:A:967:U:H2'	1:A:968:C:C6	2.42	0.55
30:6:51:GLU:O	30:6:52:VAL:HG23	2.05	0.55
1:A:454:A:H3'	1:A:455:A:H8	1.70	0.55
5:E:117:MET:HA	5:E:122:PHE:N	2.21	0.55
6:F:185:ASP:HA	6:F:188:ARG:HD3	1.88	0.55
1:A:1920:G:C2'	1:A:1921:A:OP2	2.55	0.55
1:A:1286:A:H2'	1:A:1287:A:O5'	2.06	0.55
1:A:644:G:H4'	1:A:645:A:OP1	2.06	0.55
4:D:65:ILE:HG13	4:D:67:PHE:CZ	2.41	0.55
4:D:65:ILE:HD11	4:D:67:PHE:CE1	2.42	0.55
13:P:96:THR:O	13:P:99:LEU:HB3	2.06	0.55
4:D:121:PRO:HB3	4:D:135:PHE:CE1	2.42	0.55
22:Y:76:CYS:SG	22:Y:77:PRO:HD2	2.46	0.55
1:A:231:U:OP1	32:8:6:THR:CG2	2.55	0.55
22:Y:87:LYS:O	22:Y:88:LYS:HB2	2.07	0.55
15:R:29:LEU:HD23	15:R:70:LEU:HD11	1.88	0.55
27:3:1:MET:HE2	27:3:39:ASP:HB3	1.89	0.55
3:C:169:ALA:O	3:C:171:ALA:N	2.39	0.55
1:A:274:C:O2'	1:A:275:C:C6	2.57	0.55
7:G:32:PRO:HB2	7:G:172:LEU:HD13	1.88	0.55
1:A:1541:A:H8	1:A:1623:C:O2'	1.90	0.54
1:A:610:U:H1'	6:F:90:PHE:CG	2.42	0.54
4:D:85:ASP:HB2	4:D:92:ILE:HD12	1.89	0.54
1:A:1067:G:N2	1:A:1187:A:C2	2.72	0.54
15:R:2:ARG:CD	15:R:5:LYS:HE2	2.37	0.54
9:I:53:ALA:O	9:I:57:ARG:HB2	2.06	0.54
1:A:1184:C:OP2	11:N:66:LYS:NZ	2.38	0.54
15:R:103:ARG:NH1	15:R:110:PRO:HD3	2.23	0.54
1:A:2413:C:C2'	1:A:2414:C:H5'	2.37	0.54
1:A:1579:G:O3'	1:A:1589:C:P	2.65	0.54
1:A:1636:G:H8	1:A:1636:G:H5''	1.71	0.54
1:A:2487:A:N1	1:A:2488:C:C5	2.75	0.54
16:S:24:LEU:HB3	16:S:85:VAL:HG12	1.88	0.54
16:S:27:SER:HA	16:S:88:ASP:HB3	1.88	0.54
1:A:237:C:OP2	1:A:2405:C:O2'	2.25	0.54
4:D:34:VAL:O	4:D:35:LYS:C	2.44	0.54
1:A:275:C:O2'	1:A:276:G:H5'	2.06	0.54
1:A:1824:U:H1'	1:A:1921:A:C2	2.43	0.54
1:A:1254:A:H5''	1:A:1256:G:O4'	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:8:51:ALA:N	32:8:53:PRO:HD2	2.22	0.54
5:E:36:ARG:HH21	5:E:88:GLY:HA2	1.72	0.54
1:A:975:G:O3'	27:3:24:LYS:NZ	2.40	0.54
1:A:2293:G:H5''	1:A:2294:C:O4'	2.07	0.54
1:A:1083:C:H3'	1:A:1084:G:H5''	1.89	0.54
1:A:2475:C:HO2'	1:A:2476:C:P	2.30	0.54
21:X:26:TYR:OH	21:X:88:LYS:HB2	2.08	0.54
1:A:896:C:O2'	27:3:46:ASN:ND2	2.41	0.54
1:A:2197:A:HO2'	3:C:44:HIS:CE1	2.25	0.54
13:P:8:PRO:O	13:P:9:ASN:CB	2.55	0.54
1:A:1443:C:OP1	21:X:53:LYS:NZ	2.41	0.54
7:G:61:ALA:HB2	7:G:68:PRO:HD3	1.90	0.54
1:A:583:G:O2'	18:U:45:TYR:OH	2.04	0.54
1:A:1441:U:C2'	1:A:1441:U:O2	2.54	0.54
1:A:1090:A:O2'	10:J:60:ALA:HB1	2.08	0.54
6:F:124:LEU:O	6:F:193:VAL:HA	2.08	0.54
1:A:439:C:H4'	1:A:1901:C:O2'	2.07	0.54
1:A:2302:U:H2'	1:A:2303:C:C6	2.43	0.54
1:A:185:A:H8	1:A:185:A:H5'	1.72	0.54
4:D:201:HIS:O	4:D:203:ASN:N	2.41	0.54
1:A:2084:C:O2	1:A:2461:A:N1	2.41	0.54
1:A:1935:C:O4'	1:A:1935:C:O2	2.26	0.54
22:Y:17:SER:OG	22:Y:18:GLY:N	2.35	0.54
1:A:1538:C:O2	1:A:1538:C:C2'	2.54	0.54
1:A:1008:C:O2'	1:A:2284:A:N3	2.26	0.54
1:A:2323:U:C2'	1:A:2324:C:H5'	2.36	0.53
1:A:1920:G:O2'	1:A:1921:A:P	2.65	0.53
4:D:85:ASP:OD2	4:D:88:ARG:NH1	2.41	0.53
1:A:863:C:O2'	1:A:885:U:H5''	2.08	0.53
1:A:2728:U:O2'	1:A:2729:G:H5'	2.07	0.53
1:A:2849:C:H5''	15:R:53:HIS:CD2	2.44	0.53
1:A:2058:G:H2'	1:A:2059:G:C8	2.43	0.53
17:T:28:VAL:O	17:T:29:ARG:HB2	2.08	0.53
11:N:57:ALA:C	11:N:58:ASP:O	2.45	0.53
1:A:708:G:P	13:P:18:ARG:HD2	2.47	0.53
27:3:52:HIS:CD2	27:3:52:HIS:H	2.24	0.53
1:A:2854:G:OP1	17:T:56:GLY:N	2.37	0.53
1:A:1947:U:O2	1:A:1949:A:C8	2.61	0.53
1:A:1540:A:P	1:A:1540:A:O4'	2.66	0.53
1:A:2228:A:H1'	1:A:2230:G:C4	2.43	0.53
1:A:650:U:O2	13:P:105:LEU:HG	2.07	0.53
32:8:61:LEU:CD1	32:8:62:LEU:HD12	2.38	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:20:C:H2'	2:B:21:G:H5'	1.89	0.53
7:G:124:SER:HB2	7:G:131:TYR:CE1	2.43	0.53
1:A:69:A:C8	1:A:69:A:H5'	2.43	0.53
8:H:76:VAL:O	8:H:79:VAL:HG22	2.09	0.53
13:P:81:GLN:HG2	13:P:106:LEU:HA	1.90	0.53
1:A:2014:U:H2'	1:A:2015:C:O4'	2.09	0.53
4:D:145:VAL:HG13	4:D:191:ALA:HB2	1.90	0.53
1:A:1346:A:O2'	1:A:1347:A:H3'	2.09	0.53
18:U:111:GLU:O	18:U:115:ALA:N	2.42	0.53
1:A:1824:U:O4'	1:A:1921:A:C2	2.62	0.53
13:P:115:LEU:HA	13:P:134:ALA:HB2	1.90	0.53
12:O:120:GLU:OE1	17:T:67:SER:OG	2.25	0.53
1:A:216:A:H2'	1:A:218:U:O4'	2.08	0.53
1:A:1902:C:H5''	1:A:1902:C:C6	2.44	0.53
4:D:30:GLU:HG3	4:D:63:ARG:CZ	2.38	0.53
1:A:1819:A:H2'	1:A:1820:C:O4'	2.09	0.53
1:A:2220:A:H3'	1:A:2221:C:C6	2.41	0.53
19:V:38:LEU:C	19:V:39:LEU:HD13	2.29	0.53
24:O:53:MET:HG3	24:O:59:LEU:HD23	1.90	0.53
1:A:2573:U:O2'	12:O:23:ARG:HD3	2.07	0.53
17:T:46:GLU:O	17:T:65:LYS:HD2	2.09	0.53
21:X:12:VAL:HB	21:X:17:ALA:HB1	1.91	0.53
5:E:4:ILE:CD1	5:E:28:ALA:HB1	2.38	0.53
1:A:566:C:C2'	1:A:567:C:OP1	2.56	0.53
19:V:2:PHE:O	19:V:3:ALA:HB3	2.09	0.53
1:A:493:G:H2'	1:A:494:G:O4'	2.08	0.53
1:A:69:A:OP2	1:A:69:A:H3'	2.08	0.53
1:A:515:G:O6	20:W:49:LYS:HD3	2.09	0.53
5:E:101:ARG:HD2	5:E:169:ASN:ND2	2.24	0.53
5:E:87:GLU:O	5:E:89:ASP:N	2.41	0.53
9:I:92:VAL:HG13	9:I:120:ILE:HB	1.91	0.53
30:6:40:CYS:HA	30:6:46:HIS:HB2	1.90	0.53
1:A:1895:G:H5'	1:A:1896:C:P	2.49	0.53
1:A:1920:G:N2	1:A:1923:C:N4	2.55	0.52
1:A:1254:A:H8	1:A:1254:A:H5'	1.74	0.52
1:A:1765:G:N1	1:A:1767:U:OP2	2.42	0.52
1:A:1038:G:N3	19:V:89:GLN:NE2	2.57	0.52
1:A:610:U:H1'	6:F:90:PHE:CD1	2.44	0.52
4:D:83:GLU:HG3	4:D:92:ILE:HD11	1.91	0.52
1:A:1025:A:N3	1:A:2058:G:O2'	2.36	0.52
3:C:103:ALA:HB1	3:C:110:ALA:HB2	1.91	0.52
17:T:32:TYR:CD2	17:T:81:PRO:HB2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2089:U:N3	1:A:2441:A:H2	2.07	0.52
10:J:57:ALA:O	10:J:58:ALA:HB2	2.10	0.52
1:A:935:C:O4'	1:A:935:C:O2	2.25	0.52
1:A:894:G:H2'	1:A:895:A:C8	2.44	0.52
11:N:134:ARG:O	11:N:135:PRO:C	2.46	0.52
1:A:172:C:H2'	1:A:173:U:C6	2.44	0.52
24:O:26:TYR:O	24:O:29:GLN:HB2	2.09	0.52
1:A:1381:A:O2'	1:A:1382:G:H5'	2.09	0.52
19:V:5:VAL:HG22	19:V:6:LYS:N	2.24	0.52
1:A:545:G:H2'	1:A:546:G:C8	2.45	0.52
1:A:2799:C:O2	1:A:2799:C:H2'	2.10	0.52
13:P:16:ARG:HD3	13:P:18:ARG:H	1.73	0.52
8:H:137:ASP:O	8:H:138:LYS:HB2	2.10	0.52
4:D:70:TRP:CH2	4:D:150:LYS:HA	2.45	0.52
1:A:1021:C:H5'	1:A:1201:A:N6	2.24	0.52
1:A:2487:A:C2	1:A:2488:C:C6	2.97	0.52
4:D:35:LYS:HG2	4:D:63:ARG:HG3	1.90	0.52
1:A:92:G:H2'	1:A:93:G:O4'	2.10	0.52
6:F:51:THR:HB	6:F:88:VAL:CG1	2.39	0.52
4:D:159:ALA:HB1	4:D:198:ASN:O	2.10	0.52
1:A:1345:U:O2'	1:A:1671:G:C2	2.61	0.52
5:E:111:ARG:HD2	5:E:160:TYR:CD1	2.45	0.52
1:A:836:C:O2'	1:A:837:C:P	2.67	0.52
1:A:1064:U:O2'	1:A:1066:A:C2	2.57	0.52
11:N:28:THR:HG23	11:N:29:LYS:N	2.25	0.52
1:A:1326:G:H8	1:A:1326:G:C5'	2.23	0.52
11:N:65:LYS:O	11:N:69:GLN:HG3	2.08	0.52
1:A:1815:A:O2'	1:A:1816:A:H2'	2.09	0.52
1:A:563:G:H2'	1:A:564:C:C6	2.44	0.52
15:R:87:TYR:O	15:R:89:ASP:N	2.41	0.52
1:A:1770:G:N7	1:A:1771:C:N3	2.58	0.52
13:P:102:ARG:O	13:P:103:ALA:HB2	2.09	0.52
1:A:2288:G:OP2	24:O:10:THR:HG21	2.09	0.52
1:A:1218:A:OP1	1:A:1220:G:N7	2.43	0.52
1:A:2578:G:H2'	1:A:2579:C:C6	2.45	0.52
1:A:2450:A:C8	1:A:2450:A:H5'	2.44	0.52
33:9:14:CYS:HA	33:9:27:CYS:HA	1.92	0.52
6:F:178:PRO:CB	6:F:201:VAL:HG11	2.40	0.52
1:A:2086:C:H2'	1:A:2087:C:C6	2.45	0.52
6:F:65:TRP:CZ3	6:F:73:ALA:O	2.62	0.52
1:A:69:A:H5''	1:A:71:A:C8	2.44	0.52
1:A:2345:G:N3	16:S:18:ILE:HD11	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:40:THR:HG23	3:C:215:ALA:HB3	1.92	0.52
14:Q:110:THR:HG23	14:Q:113:GLN:HB2	1.92	0.52
7:G:36:LYS:HD2	7:G:160:VAL:HG21	1.91	0.52
1:A:552:A:C2	1:A:2064:C:H4'	2.45	0.52
1:A:1039:C:H3'	18:U:54:LYS:HE3	1.92	0.52
1:A:1040:C:OP2	18:U:54:LYS:HE3	2.09	0.52
9:I:78:THR:HA	9:I:141:LYS:O	2.09	0.52
24:O:43:THR:HG23	24:O:43:THR:O	2.10	0.52
1:A:1824:U:C1'	1:A:1921:A:C2	2.93	0.51
1:A:1326:G:C8	1:A:1326:G:C5'	2.92	0.51
13:P:136:GLU:O	13:P:139:LYS:HB2	2.10	0.51
11:N:34:LEU:O	11:N:49:GLY:HA3	2.11	0.51
28:4:42:CYS:SG	28:4:62:CYS:HB3	2.49	0.51
16:S:17:ARG:HA	16:S:20:ARG:NH1	2.25	0.51
1:A:1355:G:OP2	31:7:9:ARG:NE	2.36	0.51
1:A:1489:G:H2'	1:A:1491:C:C5	2.45	0.51
1:A:2694:C:N3	1:A:2739:G:O2'	2.37	0.51
7:G:20:ILE:O	7:G:24:GLY:CA	2.58	0.51
7:G:46:ALA:HB3	7:G:82:LEU:HD11	1.91	0.51
1:A:1200:A:OP1	18:U:59:ARG:NH2	2.43	0.51
5:E:9:VAL:HG13	5:E:25:VAL:O	2.10	0.51
1:A:736:G:H2'	1:A:737:C:C6	2.45	0.51
1:A:195:A:H2'	1:A:196:C:O4'	2.11	0.51
1:A:2319:G:O6	1:A:2321:A:H2'	2.10	0.51
1:A:2225:C:O2	1:A:2231:G:C2	2.63	0.51
4:D:65:ILE:H	4:D:65:ILE:CD1	2.23	0.51
4:D:108:PRO:HG2	4:D:111:LEU:HB2	1.92	0.51
1:A:2786:C:H2'	1:A:2787:A:O4'	2.11	0.51
1:A:669:C:O2	1:A:669:C:O4'	2.26	0.51
1:A:1039:C:O2'	1:A:1041:A:OP1	2.28	0.51
24:O:53:MET:HA	24:O:58:THR:O	2.10	0.51
1:A:345:A:H3'	6:F:169:ASN:HD21	1.76	0.51
16:S:99:LYS:O	16:S:101:LEU:N	2.43	0.51
4:D:265:PRO:O	4:D:267:SER:O	2.29	0.51
1:A:2020:C:H2'	1:A:2021:G:O4'	2.11	0.51
1:A:2649:G:OP2	5:E:82:ARG:NH2	2.43	0.51
1:A:2089:U:H3	1:A:2441:A:H2	1.57	0.51
15:R:87:TYR:OH	15:R:117:VAL:O	2.27	0.51
1:A:1614:G:OP1	4:D:63:ARG:NH1	2.41	0.51
1:A:966:G:C6	1:A:967:U:C4	2.99	0.51
1:A:2767:C:C4	33:9:19:ARG:NH1	2.79	0.51
1:A:1068:U:OP2	1:A:1069:G:N7	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:N:56:ASN:O	11:N:57:ALA:O	2.28	0.51
2:B:37:C:O2	16:S:95:HIS:NE2	2.39	0.51
1:A:634:C:C2'	1:A:635:G:H5''	2.40	0.51
1:A:1856:G:H4'	4:D:242:ARG:HH21	1.74	0.51
1:A:2535:G:H8	1:A:2535:G:C5'	2.23	0.51
1:A:820:A:O2'	1:A:821:G:P	2.68	0.51
25:1:3:LYS:HG3	25:1:4:VAL:HG12	1.93	0.51
1:A:1906:A:H3'	1:A:1907:C:C6	2.45	0.51
1:A:1548:U:C4	1:A:1549:C:N4	2.79	0.51
16:S:13:ARG:O	16:S:15:ARG:HG3	2.10	0.51
8:H:85:LYS:CE	8:H:87:LEU:HG	2.41	0.51
1:A:2338:A:H2'	1:A:2339:A:C8	2.46	0.51
1:A:1261:C:OP2	18:U:15:LYS:NZ	2.23	0.51
1:A:1574:A:N7	1:A:1575:G:C8	2.79	0.51
1:A:1346:A:HO2'	1:A:1347:A:P	2.33	0.51
1:A:1346:A:O2'	1:A:1347:A:C3'	2.59	0.51
16:S:97:ARG:NH2	16:S:98:VAL:HA	2.25	0.51
1:A:231:U:OP1	32:8:6:THR:HG21	2.11	0.51
5:E:36:ARG:HH21	5:E:88:GLY:CA	2.24	0.51
1:A:347:A:N6	1:A:362:U:O4'	2.44	0.51
1:A:2876:G:O2'	1:A:2877:A:OP2	2.29	0.51
30:6:14:THR:O	30:6:49:HIS:HA	2.10	0.51
1:A:933:A:H1'	1:A:935:C:N3	2.27	0.50
1:A:545:G:H2'	1:A:546:G:H8	1.75	0.50
1:A:79:G:HO2'	1:A:318:G:HO2'	1.57	0.50
9:I:46:ALA:O	9:I:49:ALA:HB3	2.12	0.50
1:A:1557:G:H2'	1:A:1558:C:C6	2.45	0.50
5:E:132:HIS:CD2	5:E:135:HIS:CE1	3.00	0.50
1:A:2044:G:H5'	1:A:2628:C:H4'	1.93	0.50
30:6:39:TYR:O	30:6:46:HIS:HB2	2.11	0.50
1:A:2817:U:O2	1:A:2900:A:N6	2.45	0.50
1:A:2613:A:N3	1:A:2613:A:H2'	2.27	0.50
1:A:2613:A:H4'	1:A:2614:G:H5''	1.93	0.50
28:4:44:CYS:SG	28:4:65:CYS:SG	3.09	0.50
1:A:1659:A:H62	20:W:93:ALA:HB2	1.75	0.50
1:A:1565:U:H2'	1:A:1566:G:O4'	2.12	0.50
1:A:2529:A:H8	1:A:2529:A:H5'	1.76	0.50
16:S:15:ARG:O	16:S:18:ILE:HB	2.12	0.50
1:A:1806:G:C2	1:A:1807:U:C6	2.99	0.50
1:A:183:A:H5''	1:A:184:A:OP2	2.10	0.50
1:A:1780:G:O2'	1:A:2869:A:N1	2.40	0.50
8:H:155:SER:O	8:H:157:TYR:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:876:G:H4'	1:A:877:G:OP2	2.11	0.50
1:A:2752:A:H2'	1:A:2753:A:C8	2.47	0.50
1:A:720:G:H1'	6:F:74:ARG:HD3	1.93	0.50
1:A:2689:C:H2'	1:A:2690:A:O4'	2.11	0.50
1:A:1875:G:O2'	1:A:1876:G:H5'	2.12	0.50
4:D:30:GLU:HB2	4:D:35:LYS:HE3	1.93	0.50
1:A:2197:A:HO2'	3:C:44:HIS:CG	2.30	0.50
1:A:602:C:H2'	1:A:603:C:C6	2.47	0.50
1:A:1809:U:H5	1:A:1814:A:N7	2.09	0.50
1:A:459:C:C4	1:A:460:U:O4	2.65	0.50
6:F:83:PHE:O	6:F:85:GLY:N	2.43	0.50
4:D:35:LYS:HD3	4:D:63:ARG:HD2	1.92	0.50
6:F:53:THR:HG23	6:F:55:GLY:H	1.77	0.50
1:A:489:U:C4'	31:7:5:TRP:CZ3	2.95	0.50
32:8:19:SER:HB2	32:8:21:LYS:HD2	1.93	0.50
6:F:167:ALA:O	6:F:169:ASN:N	2.44	0.50
1:A:2756:G:N2	8:H:143:GLN:OE1	2.38	0.50
1:A:920:G:H5''	23:Z:175:VAL:HG11	1.94	0.50
12:O:2:ILE:HB	12:O:33:ALA:HB3	1.93	0.50
6:F:132:VAL:HG22	6:F:133:ASN:H	1.76	0.50
1:A:2699:U:O2	1:A:2699:U:O5'	2.29	0.50
1:A:2819:A:O2'	5:E:61:ARG:CZ	2.60	0.50
17:T:29:ARG:CB	17:T:85:LYS:HA	2.40	0.50
16:S:97:ARG:HH21	16:S:98:VAL:HA	1.76	0.50
1:A:1041:A:N6	1:A:1205:G:C6	2.80	0.50
6:F:65:TRP:HZ3	6:F:73:ALA:O	1.95	0.50
1:A:2309:A:H2'	1:A:2310:G:O4'	2.12	0.50
1:A:609:C:C5	1:A:717:C:H1'	2.46	0.50
23:Z:70:LEU:O	23:Z:88:PHE:HA	2.11	0.50
6:F:167:ALA:HB1	6:F:173:VAL:HG11	1.92	0.50
1:A:1878:A:C2'	1:A:1879:G:O5'	2.60	0.50
1:A:1313:A:OP1	1:A:2027:C:OP1	2.30	0.50
18:U:92:ARG:O	18:U:95:LEU:N	2.38	0.49
1:A:2089:U:N3	1:A:2441:A:C2	2.77	0.49
13:P:86:LYS:HB2	13:P:117:GLU:O	2.12	0.49
3:C:45:ALA:HA	3:C:209:ALA:O	2.12	0.49
1:A:2808:U:O4'	1:A:2808:U:O2	2.28	0.49
9:I:133:HIS:HB2	9:I:134:PRO:HD2	1.93	0.49
6:F:66:PRO:O	6:F:67:GLN:HB3	2.13	0.49
16:S:85:VAL:HG22	16:S:106:ARG:HB2	1.94	0.49
1:A:2753:A:H2'	1:A:2754:C:O4'	2.11	0.49
1:A:312:A:H2'	1:A:313:G:O4'	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2004:C:H4'	1:A:2617:C:O3'	2.12	0.49
1:A:2589:G:OP2	1:A:2589:G:H4'	2.11	0.49
7:G:114:ILE:O	7:G:115:ARG:C	2.50	0.49
1:A:1724:G:N2	1:A:2010:G:N2	2.52	0.49
17:T:11:GLU:O	17:T:13:ARG:N	2.45	0.49
17:T:56:GLY:O	17:T:59:THR:CG2	2.60	0.49
1:A:2155:A:C2	1:A:2180:G:H1'	2.46	0.49
1:A:1533:G:H5'	1:A:1534:U:OP2	2.13	0.49
7:G:38:VAL:HG22	7:G:93:THR:HG23	1.93	0.49
21:X:65:ARG:HD3	21:X:70:LEU:HD12	1.94	0.49
2:B:44:G:C2	2:B:48:A:C2	3.00	0.49
17:T:106:SER:HA	17:T:110:ILE:CG1	2.43	0.49
1:A:1549:C:O2'	1:A:1550:C:P	2.70	0.49
19:V:64:HIS:CE1	19:V:92:THR:HG22	2.47	0.49
30:6:30:THR:O	30:6:31:PRO:C	2.51	0.49
1:A:2277:A:C2	1:A:2283:U:C5	3.01	0.49
5:E:107:THR:O	5:E:190:GLY:HA2	2.12	0.49
7:G:56:ALA:HB1	7:G:153:ARG:CZ	2.42	0.49
7:G:107:LEU:HD11	7:G:178:PHE:CE1	2.48	0.49
29:5:55:ARG:NE	29:5:55:ARG:HA	2.28	0.49
15:R:10:LEU:HB3	15:R:17:ARG:CD	2.42	0.49
20:W:5:ALA:HB2	20:W:54:ALA:HB2	1.95	0.49
17:T:8:LYS:O	17:T:11:GLU:N	2.45	0.49
5:E:119:ARG:HD2	5:E:120:TRP:CE2	2.47	0.49
11:N:47:ALA:HB2	11:N:112:LEU:HD11	1.94	0.49
17:T:58:ASN:O	17:T:58:ASN:ND2	2.45	0.49
1:A:1297:G:C2	1:A:1298:A:C2	3.00	0.49
1:A:2301:G:C2	1:A:2354:C:O2	2.65	0.49
13:P:115:LEU:HA	13:P:134:ALA:CB	2.42	0.49
7:G:56:ALA:HB1	7:G:153:ARG:NH1	2.27	0.49
13:P:77:ARG:HB2	13:P:78:PRO:HD2	1.93	0.49
19:V:22:VAL:O	19:V:23:GLU:CB	2.60	0.49
18:U:83:LEU:CD1	18:U:88:ILE:HD11	2.43	0.49
1:A:1740:C:C2'	1:A:1740:C:O2	2.58	0.49
1:A:1685:U:H4'	1:A:2710:C:H4'	1.94	0.49
1:A:2293:G:O2'	1:A:2401:U:O4	2.29	0.49
25:1:4:VAL:HB	25:1:11:ARG:HB3	1.93	0.49
11:N:46:VAL:O	11:N:47:ALA:HB3	2.13	0.49
2:B:17:C:H2'	2:B:18:G:O4'	2.13	0.49
6:F:114:VAL:HG21	6:F:202:PHE:CZ	2.47	0.49
1:A:2331:A:H2'	1:A:2331:A:N3	2.27	0.49
8:H:88:LEU:N	8:H:88:LEU:HD22	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2214:G:C5	1:A:2215:G:N7	2.81	0.49
1:A:661:A:H2'	13:P:117:GLU:OE2	2.13	0.49
1:A:2111:G:H21	25:1:45:ASN:HD21	1.59	0.49
3:C:74:VAL:HB	3:C:91:ALA:HB2	1.94	0.49
1:A:797:A:H5'	20:W:90:ARG:HA	1.95	0.49
23:Z:38:TYR:O	23:Z:38:TYR:HD1	1.96	0.49
1:A:257:U:O2	1:A:257:U:H2'	2.13	0.49
17:T:36:GLU:O	17:T:36:GLU:HG2	2.12	0.49
1:A:2487:A:C2	1:A:2488:C:H5''	2.48	0.49
13:P:63:PRO:HB3	32:8:13:ARG:HB3	1.95	0.49
13:P:33:ARG:O	13:P:34:GLY:C	2.52	0.49
12:O:93:PRO:HD3	12:O:114:ILE:HD11	1.94	0.49
18:U:92:ARG:HB2	19:V:11:GLN:OE1	2.13	0.49
1:A:1336:C:H2'	1:A:1337:U:C6	2.48	0.49
1:A:7:A:H2'	1:A:8:U:C6	2.48	0.49
13:P:25:SER:O	13:P:30:THR:HG23	2.13	0.49
1:A:1069:G:C3'	1:A:1070:G:H5''	2.42	0.48
1:A:1574:A:H3'	1:A:1575:G:H5''	1.95	0.48
1:A:2660:U:H2'	1:A:2661:U:C6	2.48	0.48
1:A:722:A:H8	1:A:2090:G:H21	1.59	0.48
6:F:152:GLU:HA	6:F:190:GLU:OE2	2.13	0.48
21:X:10:ALA:HB1	21:X:11:PRO:CD	2.43	0.48
1:A:1056:G:OP2	18:U:66:ASN:OD1	2.31	0.48
1:A:29:G:H2'	1:A:30:C:C6	2.47	0.48
1:A:1835:U:O2	4:D:50:THR:HB	2.13	0.48
19:V:21:ARG:HG2	19:V:91:TYR:CD2	2.48	0.48
1:A:88:U:C2'	1:A:88:U:O2	2.60	0.48
13:P:9:ASN:O	13:P:10:PRO:C	2.48	0.48
22:Y:76:CYS:HB3	22:Y:96:ILE:HD11	1.95	0.48
17:T:80:SER:HB3	17:T:81:PRO:HD3	1.95	0.48
6:F:51:THR:HB	6:F:88:VAL:HG11	1.95	0.48
1:A:2298:A:C2	1:A:2357:A:N1	2.81	0.48
1:A:179:A:HO2'	1:A:724:C:HO2'	1.60	0.48
1:A:274:C:O2'	1:A:275:C:H6	1.95	0.48
1:A:2535:G:C8	1:A:2535:G:C5'	2.96	0.48
1:A:1217:G:H3'	1:A:1218:A:C5'	2.43	0.48
23:Z:97:GLU:CG	23:Z:125:LEU:HD11	2.43	0.48
1:A:2716:A:H2'	1:A:2717:G:O4'	2.13	0.48
4:D:22:SER:O	4:D:23:GLU:C	2.51	0.48
1:A:2020:C:H4'	1:A:2735:C:O2	2.13	0.48
1:A:2131:G:O2'	1:A:2141:G:H5'	2.14	0.48
22:Y:60:PHE:HA	22:Y:62:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:70:TRP:C	4:D:70:TRP:CD1	2.87	0.48
2:B:81:G:O6	2:B:96:U:O2	2.31	0.48
20:W:64:MET:O	20:W:65:LEU:HB3	2.13	0.48
4:D:175:LEU:HD12	4:D:185:VAL:HG21	1.94	0.48
1:A:1889:A:C2	1:A:1905:A:H1'	2.49	0.48
1:A:570:A:H2'	1:A:570:A:N3	2.28	0.48
1:A:2052:A:C6	1:A:2509:C:H1'	2.48	0.48
1:A:1615:A:H2'	1:A:1616:A:C8	2.48	0.48
1:A:1826:U:H2'	1:A:1827:C:C6	2.49	0.48
1:A:2791:U:H1'	1:A:2793:A:C6	2.48	0.48
1:A:996:G:C6	1:A:1010:G:C6	3.02	0.48
1:A:2122:G:H2'	1:A:2123:U:O4'	2.14	0.48
23:Z:24:LEU:HB2	23:Z:41:LEU:HD23	1.96	0.48
17:T:125:ARG:O	17:T:128:GLU:HG3	2.13	0.48
4:D:132:PRO:HG3	4:D:190:TYR:CE1	2.48	0.48
1:A:2678:C:H2'	1:A:2679:G:O4'	2.14	0.48
18:U:28:ARG:NH1	18:U:38:THR:OG1	2.41	0.48
1:A:2602:C:H2'	1:A:2603:G:C8	2.49	0.48
1:A:636:U:O4'	1:A:636:U:O2	2.28	0.48
32:8:62:LEU:N	32:8:63:PRO:HD2	2.28	0.48
12:O:114:ILE:H	12:O:114:ILE:CD1	2.27	0.48
1:A:1973:A:C5	12:O:22:ILE:HD12	2.48	0.48
1:A:1393:G:H2'	1:A:1394:A:C5'	2.44	0.48
1:A:1659:A:N1	20:W:91:GLY:HA2	2.29	0.48
10:J:103:ALA:O	10:J:109:ALA:HA	2.13	0.48
1:A:2480:A:O2'	14:Q:56:ARG:CZ	2.62	0.48
17:T:34:VAL:HG12	17:T:35:LYS:N	2.29	0.48
1:A:721:A:OP1	6:F:63:LYS:HE2	2.14	0.48
7:G:6:ALA:HB3	7:G:104:GLU:OE2	2.14	0.48
1:A:393:C:H2'	1:A:394:C:H5'	1.94	0.48
5:E:196:VAL:HG23	5:E:196:VAL:O	2.13	0.48
1:A:2732:U:O2	1:A:2732:U:H2'	2.14	0.48
33:9:27:CYS:HB2	33:9:32:HIS:HB2	1.96	0.48
1:A:1070:G:C4	1:A:1179:C:H1'	2.49	0.48
1:A:1538:C:H2'	1:A:1538:C:O2	2.13	0.48
4:D:172:TYR:HD1	4:D:185:VAL:C	2.16	0.48
9:I:3:VAL:HB	9:I:37:VAL:O	2.14	0.48
1:A:2121:G:H2'	1:A:2122:G:O4'	2.13	0.48
1:A:2083:A:HO2'	1:A:2084:C:C5'	2.27	0.48
10:J:47:ALA:HB1	10:J:95:ALA:HB2	1.95	0.48
20:W:34:ASN:O	20:W:35:ILE:C	2.52	0.48
11:N:94:HIS:N	11:N:95:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:Y:42:VAL:CG1	22:Y:65:ALA:HB3	2.44	0.48
1:A:1943:G:H2'	1:A:1944:U:O4'	2.14	0.48
18:U:31:SER:C	18:U:33:ARG:N	2.67	0.47
9:I:102:SER:O	9:I:106:GLY:N	2.47	0.47
6:F:47:GLY:O	6:F:94:PRO:HA	2.14	0.47
13:P:80:TYR:CE1	13:P:111:ARG:HB3	2.48	0.47
1:A:2842:G:H3'	1:A:2843:G:H5'	1.96	0.47
1:A:2890:C:H2'	1:A:2891:A:O4'	2.13	0.47
1:A:2668:A:O2'	8:H:160:LYS:NZ	2.38	0.47
1:A:1821:A:H61	1:A:1858:G:HO2'	1.59	0.47
1:A:504:A:H4'	1:A:505:A:OP1	2.14	0.47
4:D:65:ILE:HD11	4:D:67:PHE:CD1	2.49	0.47
1:A:267:G:O2'	1:A:268:G:H8	1.97	0.47
1:A:1217:G:H3'	1:A:1218:A:H5'	1.96	0.47
22:Y:74:PRO:O	22:Y:80:GLY:HA2	2.15	0.47
32:8:54:GLU:O	32:8:58:ILE:CG1	2.62	0.47
1:A:2108:G:C2'	1:A:2109:G:H5'	2.44	0.47
25:1:84:GLY:O	25:1:86:SER:N	2.47	0.47
1:A:1421:C:C2'	1:A:1422:G:O5'	2.63	0.47
1:A:1301:G:C6	1:A:1302:C:C4	3.01	0.47
12:O:116:SER:OG	12:O:117:LEU:N	2.46	0.47
1:A:641:G:H2'	1:A:642:C:O4'	2.15	0.47
1:A:373:U:H2'	1:A:374:G:O4'	2.13	0.47
1:A:1367:A:N1	1:A:1378:C:O2'	2.39	0.47
5:E:137:HIS:HB3	5:E:138:PRO:HD2	1.96	0.47
11:N:3:THR:O	11:N:5:VAL:N	2.47	0.47
1:A:2700:U:P	1:A:2731:G:H22	2.37	0.47
1:A:2595:U:O2	1:A:2595:U:O5'	2.33	0.47
15:R:10:LEU:HB3	15:R:17:ARG:CZ	2.43	0.47
18:U:92:ARG:O	18:U:94:ASN:N	2.47	0.47
1:A:1906:A:H3'	1:A:1907:C:H6	1.79	0.47
17:T:128:GLU:O	17:T:130:ALA:N	2.47	0.47
1:A:227:U:H2'	1:A:228:G:O4'	2.14	0.47
1:A:2430:U:O4	32:8:30:ARG:CZ	2.62	0.47
4:D:2:ALA:O	4:D:3:VAL:HB	2.15	0.47
1:A:1700:A:P	15:R:3:HIS:HB2	2.54	0.47
4:D:245:PRO:O	4:D:246:PRO:C	2.52	0.47
13:P:17:LYS:O	13:P:19:VAL:N	2.47	0.47
1:A:575:G:C5	1:A:576:U:C5	3.02	0.47
18:U:90:VAL:HG21	19:V:47:VAL:CG2	2.36	0.47
17:T:28:VAL:HG22	17:T:46:GLU:HG3	1.96	0.47
4:D:34:VAL:HG23	4:D:35:LYS:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1543:C:O4'	1:A:1623:C:C4'	2.63	0.47
7:G:94:LEU:HD22	7:G:98:ARG:HB2	1.96	0.47
4:D:177:LEU:HD12	4:D:181:GLU:HB3	1.96	0.47
1:A:2823:C:C5	1:A:2824:C:C5	3.02	0.47
30:6:15:GLU:CD	30:6:43:CYS:SG	2.93	0.47
1:A:276:G:O2'	1:A:277:G:OP2	2.33	0.47
1:A:1935:C:H2'	1:A:1936:U:O4'	2.14	0.47
1:A:1152:G:OP1	10:J:56:ALA:O	2.32	0.47
9:I:71:ILE:HG13	9:I:72:LEU:HG	1.96	0.47
1:A:2746:A:H5''	1:A:2747:G:OP2	2.13	0.47
4:D:78:LYS:N	4:D:96:HIS:O	2.36	0.47
1:A:200:G:C2'	1:A:201:A:H5'	2.44	0.47
18:U:90:VAL:O	18:U:91:ASP:C	2.53	0.47
13:P:61:ARG:HH11	32:8:13:ARG:HD2	1.78	0.47
18:U:115:ALA:C	18:U:117:GLN:H	2.17	0.47
22:Y:2:ARG:C	22:Y:4:LYS:N	2.62	0.47
4:D:24:ILE:HG12	4:D:25:THR:N	2.30	0.47
1:A:2885:G:O5'	17:T:2:ASN:O	2.33	0.47
6:F:22:ALA:HB1	6:F:26:ALA:HB2	1.96	0.47
4:D:209:ALA:C	4:D:210:GLY:O	2.53	0.47
23:Z:52:SER:OG	23:Z:53:ILE:N	2.47	0.47
22:Y:38:ILE:HG13	22:Y:64:GLU:HB3	1.96	0.47
1:A:454:A:H3'	1:A:455:A:C8	2.48	0.47
1:A:1409:G:OP2	25:1:3:LYS:HD3	2.14	0.47
1:A:183:A:H61	1:A:186:C:H3'	1.80	0.47
1:A:186:C:O5'	1:A:186:C:H6	1.98	0.47
1:A:2163:C:H2'	1:A:2164:C:C6	2.49	0.47
1:A:1606:G:OP1	1:A:1607:G:OP2	2.32	0.47
12:O:64:ARG:NH1	12:O:81:ASP:OD1	2.47	0.47
7:G:57:ALA:O	7:G:60:LEU:HB3	2.15	0.47
1:A:667:A:N1	1:A:2380:A:O2'	2.46	0.47
15:R:97:VAL:HG22	15:R:114:VAL:HG22	1.95	0.47
7:G:149:VAL:HG13	7:G:149:VAL:O	2.15	0.47
8:H:121:ILE:HA	8:H:134:SER:O	2.14	0.47
12:O:15:GLY:O	12:O:47:ILE:HB	2.15	0.47
1:A:581:G:H22	18:U:49:HIS:CD2	2.32	0.47
29:5:36:CYS:SG	29:5:49:CYS:SG	3.11	0.47
14:Q:141:GLN:O	23:Z:72:ARG:HD3	2.14	0.47
18:U:97:ASP:OD1	18:U:97:ASP:C	2.53	0.47
1:A:819:U:H4'	4:D:47:GLY:CA	2.44	0.47
1:A:1064:U:O2'	1:A:1066:A:H2	1.95	0.47
1:A:72:A:OP1	26:2:54:LYS:NZ	2.38	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:8:10:ALA:O	32:8:14:VAL:HG12	2.14	0.47
2:B:83:G:H4'	27:3:52:HIS:CG	2.50	0.47
2:B:73:A:C4	2:B:105:A:C2	3.03	0.47
6:F:60:SER:OG	6:F:61:GLY:N	2.48	0.47
1:A:437:G:OP2	1:A:2417:U:O2'	2.31	0.47
30:6:40:CYS:SG	30:6:45:LYS:HD3	2.55	0.47
1:A:1541:A:H8	1:A:1623:C:HO2'	1.51	0.47
29:5:51:TYR:CD2	29:5:52:TYR:CZ	3.03	0.47
1:A:2214:G:C6	1:A:2215:G:C5	3.03	0.47
1:A:720:G:H1'	6:F:74:ARG:CD	2.45	0.47
1:A:1960:U:OP1	1:A:2615:U:O2'	2.23	0.47
1:A:2351:G:O2'	1:A:2352:G:H5'	2.14	0.47
3:C:212:ALA:O	3:C:213:ALA:CB	2.63	0.47
1:A:1908:C:H2'	1:A:1909:G:C5'	2.45	0.47
13:P:13:ASN:HD22	13:P:13:ASN:C	2.18	0.47
1:A:1703:C:H2'	1:A:1704:C:C6	2.50	0.47
1:A:810:A:C6	1:A:827:A:C2	3.03	0.47
1:A:1326:G:H8	1:A:1326:G:H5''	1.79	0.47
7:G:130:ASN:HB3	7:G:160:VAL:HA	1.97	0.47
9:I:1:MET:O	9:I:20:ASP:HA	2.15	0.47
7:G:91:ARG:HD2	7:G:92:VAL:N	2.30	0.47
1:A:1500:U:OP1	15:R:77:ARG:HD3	2.15	0.47
1:A:888:G:N2	1:A:981:U:C2	2.83	0.47
5:E:126:PRO:HB2	5:E:128:SER:O	2.14	0.47
1:A:1194:G:H2'	1:A:1195:C:C6	2.50	0.47
1:A:295:U:OP2	1:A:295:U:C6	2.68	0.47
1:A:879:U:H2'	1:A:880:C:C6	2.50	0.46
17:T:57:PHE:CG	17:T:58:ASN:N	2.83	0.46
1:A:1378:C:H2'	1:A:1379:G:H8	1.80	0.46
19:V:49:THR:HB	19:V:50:PRO:HD2	1.96	0.46
2:B:92:C:O3'	23:Z:79:ARG:NH2	2.48	0.46
5:E:55:ASN:O	5:E:57:LYS:N	2.46	0.46
1:A:623:C:O2	1:A:627:C:H4'	2.15	0.46
1:A:474:A:OP1	6:F:84:VAL:O	2.33	0.46
1:A:1333:U:H4'	1:A:1334:C:OP2	2.15	0.46
32:8:61:LEU:HD13	32:8:62:LEU:HD12	1.97	0.46
5:E:63:LEU:O	5:E:64:LYS:C	2.54	0.46
13:P:115:LEU:HB2	13:P:131:SER:HB3	1.96	0.46
1:A:7:A:H2'	1:A:8:U:C5	2.50	0.46
13:P:51:PHE:O	13:P:52:GLU:HB2	2.15	0.46
1:A:992:G:C2	1:A:1014:C:O2	2.69	0.46
1:A:1495:A:H5'	1:A:1496:G:OP2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:P:34:GLY:O	13:P:35:HIS:CG	2.68	0.46
1:A:230:G:N2	1:A:242:G:H2'	2.30	0.46
1:A:1740:C:O2'	1:A:1741:G:N3	2.48	0.46
19:V:24:LYS:HA	19:V:92:THR:HG23	1.97	0.46
1:A:2124:C:C3'	1:A:2125:G:H5''	2.46	0.46
1:A:2124:C:H3'	1:A:2125:G:H5''	1.97	0.46
4:D:267:SER:HA	4:D:270:ILE:HG13	1.98	0.46
1:A:1797:C:H2'	1:A:1798:U:O4'	2.15	0.46
5:E:54:GLN:O	5:E:75:VAL:HG23	2.16	0.46
21:X:41:ASN:N	21:X:41:ASN:HD22	2.13	0.46
8:H:13:LYS:HA	8:H:13:LYS:CE	2.45	0.46
17:T:28:VAL:HG22	17:T:46:GLU:CA	2.45	0.46
1:A:1297:G:N2	18:U:37:GLU:OE2	2.35	0.46
1:A:1476:U:O2'	1:A:1477:C:H5'	2.15	0.46
1:A:563:G:H2'	1:A:564:C:H6	1.80	0.46
1:A:2298:A:N1	1:A:2357:A:C2	2.83	0.46
1:A:1401:G:H2'	1:A:1402:U:O4'	2.14	0.46
17:T:61:PHE:CE2	17:T:76:PHE:HB2	2.51	0.46
3:C:64:LEU:HD22	3:C:65:PRO:HD2	1.96	0.46
11:N:132:ALA:O	11:N:133:GLN:CB	2.62	0.46
7:G:73:ALA:N	7:G:87:PRO:HG3	2.31	0.46
1:A:473:U:C4	1:A:605:G:H1'	2.50	0.46
1:A:2802:A:O2'	1:A:2901:G:N2	2.48	0.46
9:I:56:LYS:O	9:I:59:ALA:N	2.48	0.46
1:A:330:G:N1	1:A:333:A:OP2	2.48	0.46
1:A:2371:A:H2'	1:A:2372:A:O4'	2.15	0.46
29:5:46:CYS:SG	29:5:47:PRO:HD2	2.55	0.46
1:A:2421:G:C2	1:A:2422:A:H1'	2.50	0.46
17:T:42:ILE:HG13	17:T:42:ILE:O	2.16	0.46
23:Z:96:VAL:HG22	23:Z:97:GLU:H	1.81	0.46
15:R:18:LEU:HD22	15:R:22:ARG:HG3	1.98	0.46
1:A:2539:U:H2'	1:A:2541:A:O5'	2.16	0.46
8:H:158:HIS:O	8:H:159:GLU:HB3	2.16	0.46
13:P:144:GLU:N	13:P:145:PRO:CD	2.79	0.46
1:A:731:A:C4	1:A:735:A:N6	2.84	0.46
1:A:794:G:C8	20:W:89:ALA:HB1	2.51	0.46
1:A:1479:A:H61	1:A:1604:A:H62	1.64	0.46
33:9:14:CYS:SG	33:9:32:HIS:ND1	2.89	0.46
1:A:332:G:O3'	22:Y:18:GLY:HA2	2.16	0.46
1:A:906:U:O2'	1:A:907:A:H5'	2.15	0.46
1:A:2289:A:C2'	1:A:2290:G:O5'	2.63	0.46
1:A:1914:C:C5	1:A:1915:C:C5	3.04	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1067:G:H22	1:A:1187:A:H2	1.56	0.46
1:A:554:G:N1	1:A:2043:U:OP1	2.49	0.46
1:A:718:C:O2'	1:A:719:C:C5'	2.61	0.46
1:A:799:C:O5'	1:A:799:C:H6	1.97	0.46
1:A:1540:A:OP1	1:A:1540:A:O4'	2.33	0.46
18:U:92:ARG:HD3	18:U:94:ASN:HB3	1.97	0.46
23:Z:53:ILE:HG22	23:Z:70:LEU:HD22	1.98	0.46
1:A:610:U:H2'	1:A:611:C:C6	2.50	0.46
1:A:771:G:C6	1:A:772:G:N1	2.84	0.46
1:A:2849:C:H4'	15:R:53:HIS:CD2	2.50	0.46
23:Z:8:TYR:HB2	23:Z:38:TYR:CE1	2.51	0.46
1:A:8:U:C5	1:A:2640:A:N6	2.84	0.46
1:A:2398:U:H4'	24:O:41:ARG:NH2	2.31	0.46
15:R:94:TYR:O	15:R:116:LEU:O	2.34	0.46
1:A:551:C:O2	1:A:551:C:O4'	2.33	0.46
2:B:66:A:O2'	2:B:67:G:P	2.74	0.46
1:A:1612:A:OP1	4:D:211:ARG:NH1	2.48	0.46
9:I:92:VAL:CG1	9:I:120:ILE:HB	2.46	0.46
1:A:2822:A:C6	1:A:2823:C:C4	3.03	0.46
3:C:58:VAL:HG21	3:C:166:ALA:N	2.30	0.46
1:A:1198:C:H2'	1:A:1199:G:O4'	2.16	0.46
1:A:2820:G:OP1	5:E:60:ASN:HB2	2.16	0.46
6:F:4:VAL:HA	6:F:19:GLU:HB3	1.98	0.46
31:7:31:LEU:HD23	31:7:42:LEU:HB3	1.98	0.46
1:A:552:A:N1	1:A:2064:C:O5'	2.49	0.46
1:A:552:A:C2	1:A:2063:A:H2'	2.51	0.46
17:T:28:VAL:O	17:T:29:ARG:CB	2.62	0.46
1:A:2426:G:H4'	13:P:67:MET:N	2.31	0.46
17:T:55:ASN:HD22	17:T:58:ASN:ND2	2.09	0.46
5:E:117:MET:HA	5:E:122:PHE:H	1.81	0.46
16:S:24:LEU:O	16:S:85:VAL:HB	2.16	0.46
18:U:44:ASN:HD21	19:V:75:PHE:HB3	1.80	0.46
2:B:11:C:H3'	2:B:12:C:C6	2.51	0.46
1:A:2788:A:H4'	1:A:2789:G:H5''	1.98	0.46
11:N:103:VAL:O	11:N:107:LEU:HG	2.16	0.46
1:A:81:G:H5'	22:Y:5:MET:SD	2.55	0.46
1:A:2416:G:O2'	1:A:2417:U:P	2.73	0.45
27:3:19:GLN:HE22	27:3:52:HIS:CE1	2.34	0.45
1:A:323:A:OP1	22:Y:84:ARG:NH2	2.49	0.45
26:2:35:LEU:HD22	26:2:50:ILE:HG13	1.97	0.45
20:W:9:TYR:H	20:W:102:HIS:HD2	1.64	0.45
10:J:27:ALA:HB3	10:J:85:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:241:PRO:O	4:D:243:GLY:N	2.48	0.45
1:A:143:C:H2'	1:A:144:G:H8	1.81	0.45
1:A:2723:U:O2'	1:A:2724:A:OP2	2.30	0.45
6:F:25:PRO:HB3	6:F:119:ARG:HD3	1.98	0.45
19:V:11:GLN:O	19:V:12:TYR:CG	2.69	0.45
19:V:25:LEU:H	19:V:92:THR:HG21	1.81	0.45
6:F:177:ALA:HB1	6:F:178:PRO:HD2	1.96	0.45
1:A:2107:U:H2'	1:A:2108:G:H8	1.82	0.45
1:A:955:A:C4	14:Q:13:GLN:NE2	2.84	0.45
1:A:1045:A:N6	1:A:1200:A:C8	2.84	0.45
28:4:61:VAL:HG13	28:4:65:CYS:SG	2.57	0.45
23:Z:38:TYR:O	23:Z:38:TYR:CD1	2.69	0.45
23:Z:97:GLU:HG2	23:Z:125:LEU:HD11	1.98	0.45
1:A:2791:U:H1'	1:A:2793:A:C5	2.51	0.45
13:P:144:GLU:N	13:P:145:PRO:HD3	2.31	0.45
5:E:24:THR:HG21	5:E:188:VAL:HG12	1.98	0.45
9:I:65:ALA:O	9:I:69:LYS:CB	2.64	0.45
22:Y:26:LYS:O	22:Y:27:VAL:C	2.54	0.45
1:A:1624:U:H2'	1:A:1625:A:H5'	1.98	0.45
5:E:65:GLY:HA2	5:E:70:ALA:CB	2.46	0.45
5:E:50:GLY:HA3	5:E:74:PRO:HG2	1.98	0.45
1:A:752:A:H2'	1:A:753:G:O5'	2.15	0.45
1:A:2388:A:H2'	1:A:2389:A:C8	2.50	0.45
1:A:176:G:H1'	1:A:1410:A:N1	2.31	0.45
1:A:992:G:OP1	1:A:1006:G:OP1	2.33	0.45
1:A:1048:G:N2	1:A:1198:C:C2	2.84	0.45
13:P:47:ASP:HB3	13:P:48:PRO:CA	2.46	0.45
2:B:88:C:N4	2:B:89:G:C6	2.85	0.45
12:O:76:ALA:HB3	17:T:75:ILE:HD12	1.97	0.45
1:A:2094:C:H5'	4:D:229:VAL:HG13	1.99	0.45
1:A:779:G:O6	1:A:807:A:C8	2.69	0.45
1:A:1755:U:H2'	1:A:1756:C:C6	2.52	0.45
1:A:1260:G:OP1	18:U:8:VAL:CG2	2.65	0.45
1:A:1652:C:N4	1:A:1667:G:OP2	2.43	0.45
1:A:247:G:H21	1:A:645:A:H8	1.64	0.45
1:A:1403:G:O2'	1:A:1404:A:C5'	2.65	0.45
22:Y:38:ILE:HD12	22:Y:66:PRO:HA	1.97	0.45
1:A:2567:C:H2'	1:A:2568:G:O4'	2.16	0.45
1:A:1325:G:H3'	1:A:1326:G:H5''	1.98	0.45
1:A:1615:A:O2'	4:D:38:LYS:HG3	2.16	0.45
1:A:1328:G:N2	1:A:1330:G:H3'	2.32	0.45
5:E:6:GLY:HA2	5:E:51:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:X:3:THR:O	21:X:4:ALA:HB3	2.16	0.45
1:A:1621:C:O2	1:A:1621:C:H2'	2.16	0.45
30:6:24:GLU:HA	30:6:24:GLU:OE1	2.16	0.45
1:A:2043:U:O2'	1:A:2628:C:H5'	2.17	0.45
1:A:1066:A:C8	1:A:1066:A:H3'	2.52	0.45
1:A:1066:A:H8	1:A:1066:A:H3'	1.80	0.45
30:6:13:CYS:HB2	30:6:22:ALA:HB3	1.99	0.45
1:A:2500:G:C6	1:A:2501:G:N1	2.85	0.45
5:E:137:HIS:HB3	5:E:138:PRO:CD	2.47	0.45
1:A:1694:C:H2'	1:A:1695:G:O5'	2.16	0.45
1:A:2810:A:N3	1:A:2810:A:H2'	2.31	0.45
1:A:1976:U:H5'	1:A:2562:C:O2'	2.16	0.45
30:6:19:ARG:HG3	30:6:20:ASN:N	2.32	0.45
1:A:2587:G:OP1	1:A:2588:A:OP1	2.34	0.45
4:D:144:ALA:HB3	4:D:192:THR:HG23	1.98	0.45
1:A:1311:G:O2'	1:A:2033:G:O6	2.28	0.45
1:A:1855:A:OP1	4:D:249:PRO:HD3	2.16	0.45
30:6:15:GLU:OE2	30:6:43:CYS:SG	2.72	0.45
4:D:35:LYS:HB3	4:D:36:PRO:HD3	1.98	0.45
1:A:1740:C:O2	1:A:1740:C:H2'	2.17	0.45
1:A:29:G:H2'	1:A:30:C:O4'	2.17	0.45
11:N:3:THR:HG22	11:N:5:VAL:HB	1.99	0.45
4:D:181:GLU:HA	4:D:272:ALA:HB3	1.99	0.45
10:J:40:ALA:HA	10:J:43:ALA:HB3	1.99	0.45
1:A:2229:U:O2'	25:1:52:ARG:NH1	2.50	0.45
1:A:1916:C:C2	1:A:1917:G:C8	3.05	0.45
1:A:2479:G:H2'	1:A:2487:A:C8	2.51	0.45
1:A:552:A:N1	1:A:2063:A:H2'	2.32	0.45
22:Y:75:ILE:HD12	22:Y:79:CYS:SG	2.57	0.45
1:A:1286:A:O2'	1:A:1287:A:O5'	2.34	0.45
22:Y:77:PRO:O	22:Y:99:CYS:SG	2.75	0.45
1:A:2388:A:H4'	16:S:107:GLU:HG3	1.98	0.45
1:A:200:G:O2'	1:A:201:A:H5'	2.17	0.45
1:A:420:A:C6	1:A:421:U:C4	3.05	0.45
18:U:14:HIS:CD2	18:U:32:ALA:HB1	2.52	0.45
22:Y:52:SER:O	22:Y:54:LYS:N	2.49	0.45
1:A:746:G:H2'	1:A:747:G:O4'	2.17	0.45
16:S:26:LEU:O	16:S:88:ASP:HB3	2.17	0.45
11:N:55:VAL:O	11:N:56:ASN:C	2.54	0.45
16:S:78:LEU:HD11	16:S:103:GLU:HB3	1.99	0.45
19:V:13:ARG:CG	19:V:13:ARG:HH11	2.29	0.45
4:D:210:GLY:O	4:D:211:ARG:CB	2.64	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1337:U:H2'	1:A:1338:C:C6	2.51	0.45
5:E:128:SER:OG	5:E:129:HIS:N	2.45	0.45
20:W:10:VAL:O	20:W:11:ARG:CB	2.64	0.45
10:J:51:ALA:O	10:J:52:ALA:HB2	2.17	0.45
14:Q:42:ILE:HD12	14:Q:42:ILE:N	2.31	0.45
29:5:4:HIS:HB3	29:5:5:PRO:HD3	1.99	0.45
26:2:64:LEU:HD23	26:2:64:LEU:O	2.17	0.45
11:N:15:LEU:HD13	11:N:16:ILE:N	2.32	0.45
1:A:2342:G:H4'	24:0:43:THR:H	1.82	0.45
5:E:196:VAL:O	5:E:196:VAL:CG2	2.65	0.45
1:A:1463:G:N1	1:A:1625:A:OP2	2.43	0.45
1:A:1694:C:C2'	1:A:1695:G:O5'	2.65	0.45
24:0:50:ASN:HB3	24:0:63:VAL:HG22	1.99	0.45
1:A:791:G:O6	1:A:792:A:C6	2.70	0.45
15:R:48:VAL:O	15:R:49:ASP:C	2.53	0.45
26:2:16:LEU:O	26:2:17:SER:HB3	2.16	0.45
1:A:1424:A:HO2'	1:A:1425:G:P	2.34	0.45
4:D:77:ALA:HA	4:D:97:TYR:HA	1.99	0.45
1:A:2672:G:H2'	1:A:2673:A:C2	2.52	0.45
1:A:108:A:H4'	26:2:69:ARG:NH2	2.32	0.45
26:2:47:ASN:O	26:2:48:HIS:C	2.55	0.45
1:A:29:G:O2'	1:A:1258:A:N3	2.49	0.45
1:A:2139:U:H5	1:A:2169:G:HO2'	1.64	0.45
1:A:319:C:H2'	1:A:320:C:O5'	2.17	0.45
1:A:2242:C:H2'	1:A:2243:U:O4'	2.17	0.45
1:A:469:C:H4'	6:F:49:ALA:HB2	1.99	0.45
4:D:62:TYR:HA	4:D:87:ASN:HD21	1.82	0.45
1:A:2037:U:H1'	29:5:6:VAL:HG13	1.98	0.45
9:I:31:LEU:N	9:I:32:PRO:CD	2.80	0.45
8:H:136:ILE:HD12	8:H:136:ILE:N	2.32	0.45
1:A:2416:G:O2'	1:A:2417:U:OP2	2.32	0.44
1:A:1090:A:H4'	1:A:1092:G:C1'	2.47	0.44
1:A:1767:U:O2	1:A:1767:U:H5''	2.17	0.44
14:Q:1:MET:O	14:Q:2:LEU:HB2	2.16	0.44
1:A:628:U:H4'	1:A:704:C:C4'	2.46	0.44
14:Q:137:TYR:CE2	23:Z:81:ARG:NH1	2.86	0.44
23:Z:137:ILE:HG21	23:Z:155:LEU:HD12	1.98	0.44
11:N:82:LEU:HD21	11:N:84:LYS:HE3	1.98	0.44
1:A:2247:C:H2'	1:A:2248:G:O4'	2.17	0.44
7:G:125:PHE:CB	7:G:166:ASP:HB2	2.47	0.44
1:A:351:U:H4'	22:Y:68:HIS:CD2	2.52	0.44
24:0:24:LYS:N	24:0:37:LEU:O	2.27	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:63:G:H2'	2:B:63:G:N3	2.32	0.44
7:G:133:LEU:HD12	7:G:133:LEU:C	2.38	0.44
1:A:620:G:H5'	13:P:15:ARG:HB2	1.98	0.44
3:C:74:VAL:HB	3:C:91:ALA:CB	2.48	0.44
1:A:1916:C:H2'	1:A:1917:G:O4'	2.17	0.44
6:F:116:ASP:O	6:F:120:GLU:HG2	2.18	0.44
14:Q:43:THR:HA	14:Q:94:VAL:HG12	1.99	0.44
1:A:2266:G:N2	24:O:9:SER:HB3	2.32	0.44
23:Z:28:MET:SD	23:Z:28:MET:C	2.96	0.44
13:P:96:THR:O	13:P:100:LEU:HD23	2.17	0.44
1:A:178:A:C4	1:A:195:A:C2	3.05	0.44
1:A:2875:U:C6	1:A:2877:A:H1'	2.52	0.44
1:A:602:C:H2'	1:A:603:C:H6	1.82	0.44
13:P:125:VAL:CG1	13:P:138:LEU:HD21	2.48	0.44
2:B:114:C:H4'	16:S:46:VAL:HG22	1.99	0.44
1:A:2785:C:OP1	5:E:164:ARG:NE	2.48	0.44
17:T:106:SER:HA	17:T:110:ILE:HG12	1.99	0.44
16:S:95:HIS:CG	16:S:96:GLY:N	2.85	0.44
1:A:276:G:O2'	1:A:277:G:C8	2.54	0.44
18:U:92:ARG:O	18:U:93:LYS:C	2.55	0.44
1:A:2119:U:H2'	1:A:2120:U:O4'	2.18	0.44
1:A:1057:U:O4	11:N:28:THR:HG21	2.17	0.44
32:8:14:VAL:HG21	32:8:22:VAL:CG1	2.47	0.44
9:I:53:ALA:O	9:I:57:ARG:CB	2.66	0.44
1:A:1887:G:O2'	1:A:1906:A:N6	2.45	0.44
11:N:3:THR:C	11:N:5:VAL:N	2.70	0.44
1:A:752:A:C2	1:A:753:G:H1'	2.52	0.44
29:5:4:HIS:CB	29:5:5:PRO:HD3	2.47	0.44
12:O:61:VAL:O	12:O:84:ALA:HB1	2.17	0.44
1:A:2554:G:H2'	1:A:2555:G:C8	2.52	0.44
1:A:1085:C:O2'	1:A:1086:C:P	2.75	0.44
1:A:2769:A:N1	8:H:67:LEU:HD22	2.33	0.44
17:T:70:VAL:HG12	17:T:71:GLY:O	2.17	0.44
1:A:115:A:N3	1:A:166:G:H1'	2.32	0.44
1:A:25:G:N1	1:A:26:G:N2	2.66	0.44
6:F:165:ARG:HA	6:F:168:ARG:CD	2.44	0.44
1:A:2221:C:H5'	1:A:2222:C:P	2.57	0.44
8:H:154:PRO:O	8:H:156:ALA:N	2.38	0.44
30:6:27:LYS:HB2	30:6:30:THR:HB	2.00	0.44
1:A:1946:C:O2'	1:A:1947:U:H5'	2.17	0.44
25:1:45:ASN:HD21	25:1:47:GLN:HE21	1.65	0.44
1:A:1421:C:H2'	1:A:1422:G:O5'	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:U:44:ASN:ND2	19:V:75:PHE:HB3	2.32	0.44
2:B:111:G:C6	2:B:112:U:C4	3.05	0.44
1:A:2517:U:H4'	1:A:2518:C:OP1	2.16	0.44
21:X:24:GLY:O	21:X:82:GLN:HA	2.17	0.44
1:A:2183:G:H2'	1:A:2184:C:O4'	2.18	0.44
1:A:431:U:H3'	1:A:432:G:C5'	2.48	0.44
7:G:15:VAL:HG21	7:G:176:LEU:HD23	1.99	0.44
13:P:146:VAL:HG13	13:P:147:LEU:N	2.32	0.44
1:A:2407:G:O2'	1:A:2408:G:H5'	2.18	0.44
24:O:40:GLN:HG3	24:O:42:GLY:O	2.18	0.44
1:A:763:G:H2'	1:A:764:A:O4'	2.17	0.44
20:W:22:ASP:HA	20:W:25:ARG:NH1	2.33	0.44
17:T:31:SER:OG	17:T:32:TYR:N	2.46	0.44
1:A:1326:G:H5'	1:A:1326:G:C8	2.53	0.44
1:A:2342:G:H4'	24:O:43:THR:N	2.33	0.44
13:P:13:ASN:ND2	13:P:13:ASN:C	2.71	0.44
25:1:52:ARG:HA	25:1:52:ARG:HD3	1.90	0.44
1:A:2072:A:H8	1:A:2072:A:OP2	2.00	0.44
1:A:1046:A:H2'	1:A:1047:G:O4'	2.18	0.44
1:A:2837:C:O2'	1:A:2838:C:H5'	2.18	0.44
1:A:1457:A:C6	1:A:1458:G:C5	3.06	0.44
9:I:29:TYR:CE1	9:I:33:ARG:NE	2.86	0.44
1:A:2547:G:C6	1:A:2548:U:C4	3.05	0.44
17:T:64:ARG:HA	17:T:72:VAL:O	2.18	0.44
1:A:732:G:N2	1:A:834:A:H61	2.16	0.44
1:A:1325:G:N2	1:A:1336:C:C2	2.85	0.44
2:B:47:C:O2'	16:S:93:LYS:HG2	2.18	0.44
27:3:12:PRO:O	27:3:13:ILE:C	2.55	0.44
7:G:27:ASN:HB2	7:G:30:GLU:HB2	2.00	0.44
3:C:18:LYS:CG	3:C:22:ILE:HD11	2.47	0.44
1:A:2431:C:OP1	32:8:33:ASN:O	2.35	0.44
12:O:98:VAL:CG1	12:O:117:LEU:HB3	2.48	0.44
1:A:2789:G:H5''	1:A:2790:A:H5'	1.99	0.44
1:A:1311:G:O4'	20:W:15:ARG:NH2	2.42	0.44
12:O:115:VAL:HG13	12:O:121:VAL:HG21	1.99	0.44
1:A:418:C:H5''	1:A:435:C:H5''	2.00	0.44
1:A:916:A:C2	1:A:953:C:C2	3.05	0.44
1:A:2664:U:O2'	8:H:110:SER:HB2	2.18	0.44
1:A:727:G:H2'	1:A:728:G:O4'	2.17	0.44
31:7:12:ARG:HD3	31:7:46:VAL:CG2	2.48	0.44
1:A:1763:G:O2'	1:A:1764:U:H5'	2.17	0.44
1:A:1789:A:C8	1:A:2707:U:H1'	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:53:LEU:HD22	7:G:53:LEU:N	2.32	0.44
1:A:535:U:C5	1:A:536:G:C5	3.06	0.44
1:A:2799:C:H1'	5:E:61:ARG:CD	2.48	0.44
1:A:1889:A:N6	1:A:1904:G:O2'	2.51	0.44
1:A:1765:G:N3	1:A:1765:G:H5''	2.33	0.44
1:A:267:G:O2'	1:A:268:G:P	2.76	0.44
1:A:2568:G:H2'	1:A:2569:C:C6	2.53	0.44
19:V:45:THR:O	19:V:46:VAL:HG12	2.18	0.44
1:A:55:C:H2'	1:A:56:G:O4'	2.17	0.44
1:A:2492:G:C2'	1:A:2493:G:OP2	2.64	0.43
13:P:32:THR:HG21	13:P:37:GLY:CA	2.47	0.43
1:A:2752:A:C6	1:A:2753:A:C6	3.06	0.43
1:A:735:A:O2'	1:A:826:G:H5'	2.18	0.43
10:J:22:ALA:O	10:J:23:ALA:HB2	2.18	0.43
1:A:1783:G:N1	1:A:1786:G:C2	2.86	0.43
1:A:1461:G:C4	1:A:1462:C:C5	3.05	0.43
1:A:1288:G:H2'	1:A:1289:G:O4'	2.17	0.43
18:U:83:LEU:CG	18:U:88:ILE:HD11	2.48	0.43
18:U:33:ARG:O	18:U:37:GLU:HG3	2.18	0.43
1:A:2666:G:N3	1:A:2666:G:H2'	2.33	0.43
1:A:353:A:HO2'	1:A:354:A:H8	1.59	0.43
1:A:1973:A:C6	1:A:1974:A:C6	3.07	0.43
1:A:934:C:H2'	1:A:935:C:H5'	1.98	0.43
1:A:1220:G:O2'	1:A:1221:A:H5'	2.19	0.43
2:B:43:C:H5''	2:B:44:G:OP2	2.17	0.43
14:Q:42:ILE:HD13	14:Q:97:VAL:CG2	2.47	0.43
14:Q:27:VAL:O	14:Q:28:ALA:HB3	2.18	0.43
1:A:89:A:H2'	1:A:90:G:O4'	2.18	0.43
17:T:112:ARG:HA	17:T:115:ARG:HE	1.83	0.43
5:E:49:LEU:O	5:E:78:LEU:CB	2.66	0.43
1:A:1470:G:H2'	1:A:1471:G:C8	2.53	0.43
1:A:942:C:H2'	1:A:943:C:C6	2.53	0.43
1:A:1216:G:H2'	1:A:1216:G:N3	2.33	0.43
1:A:25:G:C2	1:A:26:G:N2	2.87	0.43
1:A:505:A:O3'	22:Y:46:LYS:HA	2.18	0.43
1:A:1910:A:N3	1:A:2107:U:O2'	2.51	0.43
6:F:167:ALA:HA	6:F:170:LEU:CD2	2.48	0.43
18:U:66:ASN:ND2	18:U:70:ARG:HE	2.16	0.43
4:D:244:ARG:HA	4:D:245:PRO:HA	1.85	0.43
1:A:1908:C:H2'	1:A:1909:G:H5''	1.99	0.43
9:I:65:ALA:O	9:I:69:LYS:HB3	2.18	0.43
30:6:11:LEU:HD22	30:6:12:GLU:H	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2693:U:O4	1:A:2740:U:H1'	2.19	0.43
13:P:112:LEU:H	13:P:128:HIS:CD2	2.36	0.43
13:P:23:PRO:HB2	13:P:33:ARG:NE	2.33	0.43
9:I:119:PRO:O	9:I:121:LYS:N	2.52	0.43
22:Y:44:ILE:HG22	22:Y:45:VAL:N	2.33	0.43
1:A:2209:C:H2'	1:A:2210:U:O4'	2.17	0.43
1:A:72:A:H5'	1:A:73:G:O4'	2.19	0.43
22:Y:37:VAL:HG22	22:Y:67:LEU:O	2.19	0.43
27:3:26:LEU:HD21	27:3:46:ASN:HB2	2.00	0.43
12:O:113:LYS:HG3	12:O:117:LEU:HD12	2.01	0.43
31:7:12:ARG:CG	31:7:46:VAL:HG21	2.48	0.43
11:N:128:HIS:HD2	11:N:130:HIS:O	2.01	0.43
1:A:516:A:H2'	1:A:517:G:O4'	2.19	0.43
1:A:212:G:N7	1:A:446:C:H4'	2.34	0.43
1:A:1088:C:HO2'	1:A:1089:G:H8	1.62	0.43
22:Y:8:LYS:HB2	22:Y:28:LYS:NZ	2.33	0.43
30:6:15:GLU:O	30:6:18:ARG:HG2	2.18	0.43
1:A:1054:A:H5''	18:U:63:VAL:CG2	2.45	0.43
1:A:865:A:N3	1:A:1233:A:C2	2.86	0.43
18:U:31:SER:HB3	18:U:34:LYS:HB2	2.01	0.43
1:A:567:C:C5	1:A:570:A:N7	2.87	0.43
1:A:1254:A:C8	1:A:1254:A:H5'	2.53	0.43
23:Z:51:ALA:O	23:Z:52:SER:HB3	2.18	0.43
17:T:54:ARG:HA	17:T:59:THR:HB	2.00	0.43
1:A:69:A:O2'	1:A:70:U:OP2	2.30	0.43
13:P:30:THR:HG22	13:P:31:ALA:N	2.34	0.43
25:1:53:VAL:HG22	25:1:74:VAL:HG13	2.01	0.43
26:2:53:LEU:O	26:2:56:GLN:HB2	2.18	0.43
1:A:1721:C:H2'	1:A:1722:A:H5'	2.00	0.43
21:X:12:VAL:CB	21:X:17:ALA:HB1	2.48	0.43
17:T:11:GLU:OE2	17:T:11:GLU:N	2.51	0.43
1:A:1538:C:H4'	1:A:1539:A:OP1	2.18	0.43
1:A:506:G:O2'	1:A:507:A:OP2	2.36	0.43
1:A:2431:C:H6	1:A:2431:C:O5'	2.02	0.43
1:A:2031:G:H5''	20:W:42:ARG:HB2	2.01	0.43
12:O:23:ARG:HG3	12:O:24:VAL:N	2.33	0.43
1:A:1575:G:H2'	1:A:1575:G:N3	2.34	0.43
1:A:735:A:HO2'	1:A:826:G:H5'	1.83	0.43
1:A:2785:C:P	5:E:164:ARG:HE	2.41	0.43
33:9:17:ILE:HG13	33:9:26:ILE:HD11	1.99	0.43
1:A:2442:U:O2'	1:A:2444:A:N7	2.45	0.43
1:A:1526:G:C2	1:A:1559:U:O2	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2217:C:O2'	1:A:2218:U:H5'	2.18	0.43
1:A:822:G:C8	1:A:839:A:C2	3.07	0.43
29:5:50:GLY:HA3	29:5:56:LYS:HB3	2.00	0.43
23:Z:57:ILE:HG22	23:Z:58:VAL:N	2.34	0.43
1:A:1467:G:H4'	1:A:1538:C:OP1	2.19	0.43
1:A:594:A:H2'	1:A:595:G:O4'	2.18	0.43
6:F:66:PRO:O	6:F:68:LYS:N	2.51	0.43
19:V:20:LEU:HD12	19:V:20:LEU:N	2.34	0.43
2:B:83:G:H5''	27:3:52:HIS:CE1	2.54	0.43
1:A:2406:C:C2	1:A:2407:G:C8	3.07	0.43
1:A:1967:U:C2	1:A:1968:C:C5	3.06	0.43
1:A:2367:C:O3'	24:0:20:ARG:HD3	2.19	0.43
6:F:41:LEU:O	6:F:44:ARG:HG2	2.19	0.43
15:R:101:ALA:O	15:R:102:GLU:HB2	2.18	0.43
1:A:1766:A:H2	1:A:1768:G:H2'	1.84	0.43
1:A:11:U:H2'	1:A:11:U:O2	2.18	0.43
5:E:110:GLY:O	15:R:2:ARG:HD3	2.17	0.43
1:A:1562:G:C2	1:A:1563:C:C2	3.06	0.43
1:A:722:A:H2	1:A:848:A:H61	1.65	0.43
9:I:61:ARG:HA	9:I:64:GLU:HB2	2.01	0.43
1:A:555:C:OP1	1:A:583:G:N1	2.51	0.43
16:S:101:LEU:HD12	16:S:102:ALA:O	2.18	0.43
1:A:1574:A:N7	1:A:1575:G:H8	2.16	0.43
14:Q:132:VAL:HG11	23:Z:81:ARG:HE	1.82	0.43
1:A:1984:U:H4'	1:A:1985:G:OP1	2.18	0.43
16:S:35:ILE:H	16:S:53:SER:HB2	1.83	0.43
1:A:1383:G:N7	21:X:62:LYS:NZ	2.52	0.43
1:A:2313:G:C6	1:A:2314:G:C5	3.07	0.43
12:O:77:ILE:HD13	17:T:74:ARG:HD3	2.01	0.43
4:D:46:GLN:OE1	4:D:46:GLN:N	2.52	0.43
15:R:2:ARG:HD3	15:R:5:LYS:CE	2.49	0.43
1:A:717:C:H41	13:P:42:SER:HA	1.84	0.43
1:A:1540:A:N3	1:A:1541:A:C2	2.87	0.43
2:B:80:U:H2'	2:B:81:G:H21	1.84	0.43
1:A:1311:G:OP2	29:5:19:ARG:NH1	2.52	0.43
1:A:1213:G:C2	1:A:1226:A:C2	3.07	0.43
1:A:2360:G:OP2	32:8:42:ARG:NE	2.45	0.43
1:A:801:C:H2'	1:A:802:C:C6	2.54	0.43
23:Z:15:PRO:O	23:Z:19:ARG:HG2	2.19	0.43
1:A:271:U:H4'	1:A:272:G:C6	2.54	0.43
7:G:9:ARG:C	7:G:11:TYR:H	2.22	0.43
19:V:18:LEU:CD1	19:V:18:LEU:N	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1423:A:O2'	1:A:1424:A:H5''	2.19	0.43
1:A:1346:A:C2'	1:A:1347:A:H3'	2.49	0.43
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.43
1:A:546:G:H2'	1:A:547:C:C6	2.54	0.43
1:A:435:C:O2'	1:A:436:G:H5'	2.17	0.43
1:A:706:G:C6	1:A:707:C:C4	3.07	0.43
31:7:27:GLY:O	31:7:30:VAL:HB	2.19	0.43
5:E:108:SER:O	5:E:162:ALA:HA	2.19	0.43
22:Y:29:GLU:OE1	22:Y:29:GLU:N	2.51	0.43
18:U:83:LEU:HG	18:U:88:ILE:HD11	2.01	0.42
11:N:55:VAL:HG13	11:N:56:ASN:N	2.34	0.42
17:T:50:ILE:HA	17:T:99:LEU:CD1	2.49	0.42
13:P:64:LYS:C	13:P:66:GLY:N	2.72	0.42
18:U:34:LYS:HA	18:U:34:LYS:CE	2.49	0.42
21:X:35:THR:O	21:X:36:LYS:C	2.57	0.42
7:G:56:ALA:O	7:G:59:GLU:OE1	2.37	0.42
1:A:2759:G:O2'	8:H:67:LEU:HD13	2.19	0.42
14:Q:19:GLY:O	14:Q:20:ALA:HB3	2.18	0.42
1:A:773:A:H2	4:D:9:TYR:CD2	2.36	0.42
1:A:2692:C:H5	1:A:2737:A:H62	1.66	0.42
1:A:1439:U:H2'	1:A:1440:A:O4'	2.19	0.42
1:A:1173:A:N3	1:A:2527:G:O2'	2.42	0.42
1:A:110:G:H5''	1:A:111:U:OP1	2.19	0.42
1:A:2799:C:O2'	5:E:61:ARG:HD3	2.19	0.42
1:A:143:C:C2	1:A:144:G:C8	3.08	0.42
16:S:20:ARG:NE	16:S:20:ARG:CA	2.80	0.42
1:A:1628:C:O2'	1:A:1631:A:H8	2.00	0.42
1:A:524:G:N2	1:A:526:A:H3'	2.33	0.42
14:Q:2:LEU:HD22	14:Q:47:ILE:HG21	2.01	0.42
32:8:33:ASN:H	32:8:33:ASN:ND2	2.18	0.42
1:A:1050:C:C2	1:A:1188:A:C5	3.08	0.42
9:I:6:LEU:HD12	9:I:34:GLY:O	2.18	0.42
21:X:21:PHE:CE2	21:X:26:TYR:CD2	3.06	0.42
20:W:64:MET:O	20:W:65:LEU:CB	2.67	0.42
2:B:78:A:H2'	2:B:79:C:O4'	2.19	0.42
1:A:414:G:C6	1:A:416:A:C2	3.08	0.42
1:A:903:C:C4	1:A:904:U:O4	2.71	0.42
21:X:83:VAL:HG12	21:X:87:GLN:HB2	2.01	0.42
1:A:1022:G:C6	1:A:1032:G:C6	3.07	0.42
12:O:3:GLN:HB2	12:O:4:PRO:HD2	2.01	0.42
23:Z:65:GLN:HB3	23:Z:67:LEU:HD11	2.00	0.42
1:A:2476:C:O2	1:A:2497:G:C2	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:1:5:CYS:SG	25:1:62:VAL:CG2	3.04	0.42
1:A:1309:G:H2'	1:A:2035:A:N6	2.34	0.42
1:A:504:A:HO2'	1:A:506:G:H8	1.66	0.42
1:A:667:A:O2'	1:A:668:A:H5'	2.19	0.42
1:A:781:A:C8	1:A:782:C:C5	3.07	0.42
1:A:174:G:O2'	1:A:175:G:H5'	2.19	0.42
1:A:866:A:H2'	1:A:867:A:O4'	2.20	0.42
1:A:1829:G:N7	4:D:179:SER:OG	2.43	0.42
23:Z:77:ASP:O	23:Z:78:LYS:HB2	2.19	0.42
1:A:931:C:C2	1:A:932:C:N4	2.87	0.42
1:A:1873:C:H5'	4:D:253:GLN:OE1	2.19	0.42
1:A:1723:A:H2'	1:A:1724:G:C8	2.55	0.42
1:A:2798:U:C4	1:A:2799:C:C5	3.08	0.42
1:A:1517:A:OP2	1:A:1566:G:N1	2.42	0.42
1:A:1209:G:C5	1:A:1210:U:C4	3.08	0.42
1:A:1902:C:O2	1:A:1902:C:H2'	2.20	0.42
7:G:129:GLY:O	7:G:130:ASN:CB	2.67	0.42
14:Q:26:TYR:HA	23:Z:81:ARG:HH22	1.84	0.42
1:A:2079:A:H5''	1:A:2080:A:OP2	2.20	0.42
1:A:646:G:O2'	1:A:647:G:H5'	2.19	0.42
23:Z:29:TYR:HA	23:Z:33:LEU:O	2.20	0.42
1:A:800:C:O4'	1:A:1663:A:H2	2.02	0.42
4:D:95:LEU:HD12	4:D:95:LEU:O	2.20	0.42
1:A:24:U:H2'	1:A:25:G:C8	2.55	0.42
1:A:1698:A:O3'	1:A:1699:G:C8	2.72	0.42
19:V:22:VAL:O	19:V:23:GLU:CG	2.67	0.42
1:A:752:A:C2'	1:A:753:G:O5'	2.67	0.42
1:A:2810:A:O2'	1:A:2903:U:H5'	2.19	0.42
27:3:12:PRO:O	27:3:14:GLY:N	2.52	0.42
1:A:1956:G:H1'	1:A:1985:G:N2	2.34	0.42
1:A:2314:G:O2'	7:G:132:ASN:HB2	2.19	0.42
1:A:882:G:C5	1:A:883:C:C4	3.07	0.42
1:A:2696:G:O2'	1:A:2738:U:H5	2.03	0.42
10:J:118:ALA:HB3	10:J:121:ALA:HB3	2.01	0.42
20:W:62:HIS:O	20:W:63:ASP:C	2.57	0.42
20:W:68:ARG:O	20:W:109:GLU:HA	2.20	0.42
1:A:1358:U:H3'	1:A:1359:C:H5'	2.01	0.42
1:A:1454:C:H2'	1:A:1455:G:O4'	2.19	0.42
1:A:193:G:O2'	1:A:194:U:OP2	2.37	0.42
2:B:33:G:C6	2:B:34:U:N3	2.87	0.42
1:A:1702:C:C2	1:A:1703:C:C5	3.08	0.42
18:U:88:ILE:HG22	19:V:47:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:T:57:PHE:O	17:T:58:ASN:C	2.58	0.42
6:F:181:LEU:O	6:F:205:ARG:NH2	2.51	0.42
1:A:2213:G:C2'	1:A:2214:G:H5'	2.48	0.42
4:D:270:ILE:O	4:D:270:ILE:HD12	2.18	0.42
1:A:2111:G:H21	25:1:45:ASN:ND2	2.17	0.42
1:A:393:C:C2'	1:A:394:C:H5'	2.50	0.42
12:O:98:VAL:HG12	12:O:117:LEU:HB3	2.02	0.42
1:A:2595:U:O4'	1:A:2595:U:O2	2.38	0.42
1:A:472:A:H4'	1:A:474:A:N7	2.33	0.42
1:A:351:U:H4'	22:Y:68:HIS:CG	2.54	0.42
11:N:39:ARG:C	18:U:67:ALA:HB1	2.40	0.42
16:S:16:ASN:O	16:S:19:LYS:N	2.40	0.42
1:A:716:A:H5'	13:P:43:GLY:O	2.19	0.42
7:G:20:ILE:O	7:G:24:GLY:N	2.52	0.42
1:A:1209:G:C6	1:A:1210:U:C4	3.08	0.42
1:A:1041:A:N3	1:A:1042:G:C8	2.87	0.42
1:A:158:U:H4'	1:A:159:G:N9	2.34	0.42
22:Y:88:LYS:HB3	22:Y:90:LEU:HD23	2.02	0.42
3:C:74:VAL:HA	3:C:119:ALA:HB3	2.01	0.42
19:V:21:ARG:HG2	19:V:91:TYR:CG	2.55	0.42
14:Q:42:ILE:HD13	14:Q:97:VAL:HB	2.00	0.42
14:Q:54:MET:SD	14:Q:118:LEU:HD23	2.59	0.42
1:A:365:G:H2'	1:A:366:C:O5'	2.19	0.42
30:6:9:LEU:HD22	30:6:10:LEU:N	2.34	0.42
1:A:840:G:H2'	1:A:841:C:C6	2.55	0.42
14:Q:83:MET:SD	14:Q:83:MET:N	2.92	0.42
18:U:79:PHE:CE2	18:U:83:LEU:HD11	2.55	0.42
22:Y:31:LEU:HB2	22:Y:32:PRO:HA	2.01	0.42
1:A:1613:A:O2'	4:D:63:ARG:NH2	2.53	0.42
1:A:732:G:N7	31:7:5:TRP:CH2	2.88	0.42
1:A:1670:C:H2'	1:A:1671:G:O4'	2.20	0.42
5:E:9:VAL:HG22	5:E:25:VAL:HB	2.01	0.42
19:V:21:ARG:HG3	19:V:93:GLU:CG	2.49	0.42
1:A:1829:G:H5'	1:A:1849:A:N6	2.35	0.42
1:A:1608:A:H2'	1:A:1609:G:O4'	2.19	0.42
1:A:1176:G:O6	1:A:2061:C:H1'	2.20	0.42
1:A:1597:C:C5	1:A:1598:G:N7	2.88	0.42
1:A:1293:G:C5	18:U:3:ARG:HB2	2.54	0.42
1:A:386:G:N7	1:A:387:A:N7	2.68	0.42
1:A:2879:C:H2'	1:A:2880:C:O4'	2.20	0.42
1:A:554:G:C5	1:A:2043:U:H5''	2.55	0.42
1:A:1207:G:N3	19:V:89:GLN:NE2	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:29:A:H2'	2:B:30:C:O4'	2.20	0.42
1:A:2566:U:C4	1:A:2567:C:C2	3.08	0.42
1:A:2194:A:N3	1:A:2194:A:H2'	2.35	0.42
4:D:101:GLU:OE1	4:D:103:ARG:NH1	2.47	0.42
5:E:65:GLY:HA2	5:E:70:ALA:HB3	2.00	0.42
1:A:2518:C:H2'	1:A:2519:G:O4'	2.18	0.42
1:A:1332:A:OP1	15:R:105:ARG:O	2.37	0.42
22:Y:20:TYR:O	22:Y:23:ARG:HG2	2.20	0.42
1:A:18:C:H2'	1:A:19:C:H6	1.84	0.42
6:F:2:LYS:O	6:F:3:GLU:HB3	2.19	0.42
15:R:56:LYS:HE3	15:R:88:ARG:HA	2.02	0.42
1:A:488:G:N1	1:A:492:G:C6	2.88	0.42
1:A:924:A:N6	1:A:944:A:O2'	2.53	0.42
7:G:113:ARG:HE	7:G:113:ARG:HA	1.85	0.42
32:8:6:THR:CG2	32:8:63:PRO:HD3	2.50	0.42
29:5:33:CYS:CB	29:5:40:LYS:HE3	2.46	0.42
1:A:1538:C:C4	1:A:2226:G:O2'	2.71	0.42
1:A:1475:C:H2'	1:A:1476:U:H6	1.80	0.42
1:A:644:G:C4'	1:A:645:A:OP1	2.68	0.42
1:A:1973:A:C4	12:O:22:ILE:HD12	2.55	0.42
1:A:731:A:OP1	31:7:11:LYS:NZ	2.39	0.42
1:A:68:G:H2'	1:A:110:G:O2'	2.20	0.42
1:A:2253:G:H2'	1:A:2254:U:O4'	2.20	0.42
1:A:2100:U:H2'	1:A:2101:G:O4'	2.20	0.42
11:N:111:PRO:HA	11:N:114:ARG:CZ	2.50	0.42
3:C:189:ALA:O	3:C:193:ALA:HB3	2.19	0.42
1:A:1854:G:OP1	4:D:52:ARG:NH1	2.53	0.42
1:A:1563:C:O2'	1:A:1564:G:H5'	2.20	0.41
11:N:15:LEU:HB2	11:N:134:ARG:HB2	2.01	0.41
1:A:1381:A:H2'	1:A:1382:G:C8	2.55	0.41
1:A:1494:G:O2'	1:A:1574:A:N1	2.31	0.41
31:7:31:LEU:HD22	31:7:42:LEU:HD13	2.02	0.41
13:P:47:ASP:HB3	13:P:48:PRO:HA	2.01	0.41
1:A:1763:G:C6	1:A:1764:U:C4	3.08	0.41
1:A:1994:G:H2'	1:A:1995:C:C6	2.55	0.41
1:A:1175:U:O2	5:E:149:ARG:NH2	2.40	0.41
4:D:136:ILE:HA	4:D:137:PRO:HD3	1.92	0.41
1:A:2719:G:OP1	15:R:68:ARG:HD3	2.20	0.41
1:A:1026:A:N1	1:A:2048:G:O2'	2.42	0.41
1:A:2020:C:OP1	1:A:2735:C:O2'	2.37	0.41
1:A:810:A:N1	1:A:1819:A:O2'	2.51	0.41
32:8:4:MET:HB3	32:8:61:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:P:107:LYS:C	13:P:109:GLY:N	2.71	0.41
1:A:422:G:O3'	25:1:44:PRO:HA	2.20	0.41
1:A:391:U:H3'	1:A:392:A:O4'	2.19	0.41
11:N:125:GLY:CA	11:N:126:PRO:O	2.69	0.41
1:A:1578:C:O2'	1:A:1579:G:C2	2.74	0.41
1:A:1381:A:H2'	1:A:1382:G:H8	1.84	0.41
1:A:1045:A:C6	1:A:1200:A:C8	3.08	0.41
1:A:8:U:O2'	1:A:9:G:P	2.78	0.41
11:N:128:HIS:CD2	11:N:130:HIS:O	2.73	0.41
1:A:2353:C:O2'	1:A:2385:C:H5''	2.20	0.41
1:A:2332:G:N3	1:A:2332:G:H2'	2.35	0.41
1:A:1333:U:C2	1:A:1372:C:O2	2.73	0.41
1:A:996:G:P	14:Q:16:ARG:NH2	2.80	0.41
1:A:2723:U:O2	1:A:2723:U:C5'	2.60	0.41
22:Y:4:LYS:HB2	22:Y:32:PRO:HG2	2.02	0.41
6:F:161:GLU:O	6:F:165:ARG:HG3	2.21	0.41
7:G:111:LEU:N	7:G:112:PRO:CD	2.83	0.41
22:Y:17:SER:HA	22:Y:71:LYS:HB3	2.01	0.41
3:C:56:GLN:NE2	3:C:168:ALA:CB	2.82	0.41
1:A:2433:A:O2'	1:A:2434:U:O5'	2.34	0.41
1:A:2603:G:C6	1:A:2604:U:N3	2.88	0.41
1:A:2891:A:OP1	15:R:96:ARG:NE	2.50	0.41
8:H:13:LYS:HE2	8:H:13:LYS:HA	2.02	0.41
4:D:62:TYR:HA	4:D:87:ASN:ND2	2.34	0.41
1:A:637:U:H4'	1:A:638:G:H5''	2.02	0.41
17:T:92:GLY:O	17:T:93:ARG:C	2.58	0.41
3:C:72:VAL:HG21	3:C:161:ALA:HB1	2.02	0.41
1:A:1167:G:C2	1:A:1168:C:C6	3.08	0.41
26:2:61:LEU:O	26:2:62:THR:C	2.57	0.41
9:I:93:THR:HG23	9:I:95:LYS:HB2	2.02	0.41
1:A:1647:U:H3'	1:A:1648:A:H5'	2.03	0.41
7:G:64:THR:HG23	7:G:66:GLN:H	1.85	0.41
1:A:895:A:N6	1:A:973:G:O2'	2.49	0.41
15:R:2:ARG:CD	15:R:5:LYS:CE	2.98	0.41
1:A:1564:G:C6	1:A:1565:U:C4	3.07	0.41
1:A:1309:G:H8	1:A:1309:G:O5'	2.03	0.41
1:A:819:U:C4'	4:D:47:GLY:HA2	2.48	0.41
1:A:1883:A:N1	1:A:2108:G:H1'	2.35	0.41
6:F:65:TRP:CZ3	6:F:72:ARG:CB	3.03	0.41
1:A:2728:U:HO2'	1:A:2729:G:H5'	1.84	0.41
1:A:257:U:O2	1:A:257:U:C2'	2.66	0.41
19:V:21:ARG:HG3	19:V:93:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:53:PRO:O	5:E:54:GLN:C	2.58	0.41
15:R:18:LEU:HD11	15:R:22:ARG:CZ	2.50	0.41
6:F:116:ASP:OD2	13:P:5:ASP:N	2.53	0.41
4:D:73:VAL:C	4:D:75:ILE:H	2.24	0.41
1:A:2199:C:H4'	3:C:172:ALA:HB2	2.03	0.41
6:F:127:GLU:OE1	6:F:127:GLU:HA	2.21	0.41
1:A:145:G:H2'	1:A:146:U:O4'	2.20	0.41
15:R:38:VAL:HB	15:R:39:PRO:CD	2.47	0.41
1:A:662:G:C6	1:A:663:U:C4	3.09	0.41
1:A:494:G:C6	31:7:39:ARG:NH1	2.88	0.41
25:1:86:SER:O	25:1:90:ILE:HG12	2.21	0.41
1:A:455:A:H2'	1:A:456:G:C8	2.55	0.41
9:I:57:ARG:O	9:I:61:ARG:NH1	2.54	0.41
1:A:1816:A:N9	1:A:1959:A:N6	2.69	0.41
1:A:79:G:O2'	1:A:318:G:O2'	2.31	0.41
1:A:2843:G:N2	1:A:2891:A:N6	2.68	0.41
5:E:51:PHE:O	5:E:52:LEU:C	2.58	0.41
4:D:142:VAL:HG23	4:D:192:THR:C	2.41	0.41
1:A:1244:C:C2	1:A:1291:A:C2	3.08	0.41
1:A:2641:G:C6	1:A:2642:G:C6	3.09	0.41
1:A:264:U:H2'	1:A:265:C:C6	2.55	0.41
29:5:46:CYS:SG	29:5:47:PRO:N	2.93	0.41
1:A:99:G:OP1	1:A:99:G:H4'	2.19	0.41
1:A:2220:A:C5'	1:A:2221:C:OP2	2.68	0.41
22:Y:46:LYS:N	22:Y:62:GLU:HG2	2.34	0.41
1:A:819:U:C5'	4:D:47:GLY:HA2	2.49	0.41
1:A:2052:A:O2'	1:A:2466:G:O2'	2.34	0.41
1:A:1806:G:N3	1:A:1806:G:H2'	2.36	0.41
1:A:920:G:O2'	23:Z:170:THR:HG21	2.21	0.41
18:U:66:ASN:HD21	18:U:70:ARG:NE	2.18	0.41
1:A:2603:G:C6	1:A:2604:U:C4	3.09	0.41
6:F:134:GLY:HA2	6:F:162:LEU:O	2.21	0.41
27:3:22:ALA:O	27:3:25:ALA:HB3	2.21	0.41
1:A:2902:G:N3	1:A:2902:G:H2'	2.34	0.41
21:X:47:PHE:O	21:X:48:LYS:C	2.59	0.41
6:F:195:ASP:OD1	6:F:196:LEU:N	2.54	0.41
14:Q:85:LYS:CG	24:0:8:GLY:O	2.69	0.41
12:O:13:ASN:ND2	12:O:97:ARG:HB2	2.36	0.41
2:B:51:G:N7	16:S:62:LYS:NZ	2.68	0.41
24:0:34:GLY:O	24:0:35:ASN:C	2.57	0.41
15:R:84:ALA:N	15:R:85:PRO:CD	2.82	0.41
1:A:1704:C:H2'	1:A:1705:U:C6	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:629:U:OP1	6:F:102:PRO:HA	2.20	0.41
17:T:12:SER:O	17:T:13:ARG:NE	2.53	0.41
1:A:2466:G:C2	1:A:2509:C:N4	2.89	0.41
7:G:68:PRO:HB2	7:G:90:LEU:HD11	2.02	0.41
2:B:48:A:H2'	2:B:49:C:C6	2.55	0.41
17:T:34:VAL:O	17:T:35:LYS:HB3	2.21	0.41
7:G:125:PHE:HB2	7:G:166:ASP:HB2	2.03	0.41
1:A:165:G:H3'	1:A:166:G:H8	1.86	0.41
1:A:1059:U:C2'	1:A:1060:G:H5'	2.51	0.41
1:A:2473:U:H2'	1:A:2474:C:O4'	2.21	0.41
1:A:448:A:C2	1:A:449:A:C4	3.08	0.41
28:4:57:ILE:HG22	28:4:59:VAL:HG23	2.02	0.41
1:A:470:C:H2'	1:A:471:G:O4'	2.21	0.41
17:T:33:LYS:O	17:T:40:THR:O	2.39	0.41
1:A:599:G:C6	1:A:600:A:C6	3.09	0.41
18:U:47:TYR:HA	18:U:50:ARG:NH2	2.36	0.41
1:A:1865:G:H2'	1:A:1865:G:N3	2.36	0.41
1:A:1377:G:N2	1:A:1654:A:HO2'	2.12	0.41
22:Y:31:LEU:CB	22:Y:32:PRO:HA	2.51	0.41
1:A:1092:G:C8	1:A:1155:G:C6	3.09	0.41
13:P:7:ARG:O	13:P:10:PRO:HG2	2.21	0.41
1:A:2319:G:N7	1:A:2321:A:O5'	2.54	0.41
32:8:30:ARG:O	32:8:31:HIS:HB3	2.21	0.41
8:H:158:HIS:NE2	8:H:170:ARG:O	2.54	0.41
2:B:6:C:C2	2:B:116:G:N2	2.89	0.41
1:A:963:A:C5	1:A:964:G:H1'	2.56	0.41
1:A:327:G:C2	1:A:337:A:C2	3.09	0.41
15:R:34:ILE:HG22	15:R:36:THR:HG23	2.03	0.41
1:A:2522:U:O4	1:A:2586:C:N3	2.54	0.41
1:A:1423:A:C8	1:A:1425:G:C6	3.09	0.41
1:A:972:G:H3'	1:A:973:G:H8	1.86	0.41
1:A:655:A:O2'	13:P:67:MET:HB3	2.21	0.41
1:A:2427:C:OP1	13:P:64:LYS:O	2.39	0.41
1:A:1530:G:H1'	1:A:1550:C:N4	2.36	0.41
4:D:203:ASN:O	4:D:204:ILE:C	2.58	0.41
1:A:209:A:C4'	1:A:210:A:O5'	2.65	0.41
18:U:101:ARG:HD3	19:V:13:ARG:HH21	1.85	0.41
1:A:2054:A:H4'	1:A:2055:U:OP1	2.21	0.41
7:G:94:LEU:HD22	7:G:98:ARG:CB	2.51	0.41
1:A:153:G:C6	1:A:154:C:C4	3.08	0.41
22:Y:38:ILE:CG2	22:Y:39:VAL:N	2.83	0.41
6:F:66:PRO:C	6:F:68:LYS:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1727:G:O2'	1:A:1792:A:C2'	2.69	0.41
5:E:116:VAL:HG22	5:E:122:PHE:CG	2.56	0.41
1:A:2876:G:O2'	1:A:2877:A:P	2.77	0.41
1:A:2163:C:O5'	1:A:2163:C:H6	2.03	0.41
1:A:81:G:N2	1:A:100:A:OP2	2.43	0.41
5:E:108:SER:O	5:E:162:ALA:N	2.54	0.41
8:H:89:ILE:HD13	8:H:94:TYR:HB3	2.03	0.41
1:A:1728:G:H2'	1:A:1729:C:C6	2.55	0.41
1:A:1593:C:O2'	1:A:1594:C:H5'	2.21	0.41
23:Z:17:ALA:HA	23:Z:20:ARG:CD	2.51	0.41
5:E:69:LYS:O	5:E:71:GLY:N	2.54	0.41
1:A:2757:C:H2'	1:A:2758:U:O4'	2.21	0.41
21:X:55:ASN:O	21:X:79:ALA:HA	2.20	0.41
7:G:111:LEU:HB2	7:G:112:PRO:HD3	2.02	0.41
1:A:2468:U:C4	1:A:2469:G:C6	3.09	0.41
4:D:210:GLY:O	4:D:212:SER:N	2.53	0.41
1:A:2121:G:C6	1:A:2122:G:C5	3.09	0.41
1:A:2200:C:C2	1:A:2202:G:O6	2.74	0.41
1:A:2214:G:C5	1:A:2215:G:C8	3.08	0.41
22:Y:77:PRO:O	22:Y:78:ALA:HB2	2.20	0.41
6:F:170:LEU:HB2	6:F:173:VAL:HB	2.03	0.41
7:G:138:GLN:OE1	7:G:153:ARG:HG2	2.20	0.41
1:A:1827:C:H5''	4:D:258:LYS:HA	2.03	0.41
1:A:1721:C:C2'	1:A:1722:A:H5'	2.50	0.41
1:A:706:G:H5'	6:F:99:TYR:CD2	2.56	0.41
20:W:12:ILE:O	20:W:101:SER:OG	2.32	0.41
15:R:73:VAL:O	15:R:76:VAL:HG12	2.21	0.41
1:A:535:U:O4	1:A:536:G:C2	2.74	0.40
1:A:1824:U:H2'	1:A:1825:C:C6	2.56	0.40
1:A:2413:C:C3'	1:A:2414:C:H5'	2.51	0.40
1:A:1816:A:N3	1:A:1816:A:C2'	2.84	0.40
1:A:1410:A:O3'	25:1:11:ARG:NH2	2.54	0.40
1:A:2876:G:HO2'	1:A:2877:A:P	2.44	0.40
11:N:3:THR:C	11:N:5:VAL:H	2.24	0.40
1:A:2726:G:C6	1:A:2727:C:C4	3.09	0.40
1:A:322:A:O2'	1:A:342:C:H4'	2.21	0.40
1:A:817:G:OP1	31:7:10:ARG:NH1	2.52	0.40
1:A:1734:U:O2	1:A:1746:A:H8	2.04	0.40
1:A:816:G:O2'	1:A:1399:A:N1	2.49	0.40
1:A:2053:G:N1	1:A:2583:A:C8	2.89	0.40
1:A:1693:G:C8	1:A:1693:G:H5'	2.56	0.40
4:D:131:LEU:HD12	4:D:131:LEU:N	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:U:79:PHE:CE2	18:U:83:LEU:HD21	2.56	0.40
1:A:2722:A:OP1	1:A:2724:A:OP1	2.38	0.40
17:T:26:ASP:HB3	17:T:89:VAL:O	2.21	0.40
16:S:106:ARG:HD2	16:S:107:GLU:O	2.21	0.40
1:A:182:G:H2'	1:A:183:A:O4'	2.21	0.40
1:A:2241:G:H1'	25:1:45:ASN:CB	2.52	0.40
18:U:66:ASN:HD21	18:U:70:ARG:HE	1.68	0.40
1:A:199:A:H2'	1:A:200:G:O4'	2.20	0.40
8:H:121:ILE:HD11	8:H:140:LYS:HB3	2.04	0.40
1:A:1908:C:C3'	1:A:1909:G:H5'	2.51	0.40
1:A:295:U:OP2	1:A:295:U:C5	2.74	0.40
1:A:1006:G:H2'	1:A:1007:U:O4'	2.20	0.40
1:A:731:A:C2	1:A:735:A:C6	3.09	0.40
15:R:48:VAL:O	15:R:51:LEU:N	2.54	0.40
1:A:2082:G:N7	1:A:2512:C:H4'	2.36	0.40
15:R:20:LEU:HD21	15:R:40:LYS:HD3	2.01	0.40
1:A:2897:C:H2'	1:A:2898:C:H6	1.85	0.40
1:A:360:C:H2'	1:A:361:G:O4'	2.22	0.40
4:D:224:ALA:O	4:D:225:ALA:CB	2.69	0.40
17:T:48:ILE:O	17:T:63:VAL:HA	2.21	0.40
1:A:1373:G:H2'	1:A:1375:C:C5	2.56	0.40
1:A:1687:A:H2'	1:A:1688:G:O4'	2.22	0.40
15:R:63:ARG:HA	15:R:80:PHE:CZ	2.57	0.40
1:A:2328:C:H2'	1:A:2329:G:H5'	2.03	0.40
1:A:92:G:H21	26:2:47:ASN:HD22	1.68	0.40
7:G:111:LEU:HD13	7:G:120:LEU:HD21	2.03	0.40
1:A:906:U:C5	1:A:962:A:N7	2.85	0.40
5:E:33:VAL:HG11	5:E:88:GLY:HA2	2.03	0.40
1:A:2849:C:C5'	15:R:53:HIS:CD2	3.04	0.40
1:A:1789:A:C8	1:A:2707:U:O2	2.74	0.40
1:A:638:G:N2	6:F:44:ARG:O	2.53	0.40
1:A:2801:C:N3	1:A:2902:G:O6	2.54	0.40
1:A:1348:G:H1'	1:A:1687:A:N1	2.36	0.40
1:A:2513:G:H5''	1:A:2514:A:H5''	2.02	0.40
4:D:28:GLU:H	4:D:29:PRO:CD	2.34	0.40
4:D:28:GLU:H	4:D:29:PRO:HD2	1.87	0.40
1:A:2091:G:C2	1:A:2453:C:C2	3.09	0.40
9:I:82:ARG:O	9:I:89:TYR:HD1	2.04	0.40
16:S:54:LEU:HD23	16:S:58:LEU:O	2.21	0.40
1:A:2763:G:H2'	1:A:2763:G:N3	2.36	0.40
11:N:41:ASP:N	11:N:41:ASP:OD1	2.54	0.40
20:W:37:ARG:NH2	29:5:48:GLU:OE2	2.53	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:77:ALA:HB2	4:D:97:TYR:CG	2.56	0.40
1:A:1538:C:C5	1:A:2226:G:O2'	2.70	0.40
4:D:65:ILE:HG13	4:D:67:PHE:CE2	2.56	0.40
1:A:2345:G:H4'	1:A:2346:A:OP2	2.22	0.40
1:A:1808:U:H2'	1:A:1814:A:N6	2.37	0.40
1:A:2071:C:H2'	1:A:2072:A:O4'	2.21	0.40
5:E:77:ILE:HG22	5:E:78:LEU:H	1.86	0.40
1:A:386:G:C8	1:A:387:A:C8	3.10	0.40
1:A:1323:A:OP1	15:R:36:THR:HG22	2.22	0.40
2:B:100:A:C6	2:B:101:G:C5	3.09	0.40
12:O:43:VAL:HG23	12:O:56:ASP:O	2.22	0.40
13:P:92:GLU:HG3	13:P:123:LEU:HD23	2.02	0.40
1:A:1272:G:OP1	18:U:13:LYS:HD3	2.22	0.40
33:9:10:ILE:O	33:9:10:ILE:HG22	2.22	0.40
22:Y:44:ILE:O	22:Y:62:GLU:HB3	2.21	0.40
13:P:8:PRO:O	13:P:9:ASN:HB3	2.21	0.40
11:N:126:PRO:HB2	11:N:127:ASP:H	1.75	0.40
1:A:875:A:H5'	1:A:877:G:N7	2.36	0.40
11:N:46:VAL:HG13	11:N:48:MET:HG3	2.04	0.40
19:V:22:VAL:O	19:V:23:GLU:HB2	2.22	0.40
1:A:29:G:C5	1:A:30:C:C4	3.09	0.40
10:J:103:ALA:HA	10:J:107:ALA:HB3	2.04	0.40
1:A:1420:C:H2'	1:A:1421:C:H6	1.86	0.40
9:I:20:ASP:N	9:I:20:ASP:OD1	2.53	0.40
1:A:2329:G:C2'	1:A:2330:G:OP1	2.70	0.40
32:8:37:SER:OG	32:8:39:LYS:HB3	2.22	0.40
22:Y:14:LEU:HD11	22:Y:22:GLY:HA2	2.02	0.40
20:W:50:VAL:HG13	20:W:105:VAL:HG21	2.02	0.40
13:P:114:ILE:HG23	13:P:130:PHE:CD1	2.57	0.40
23:Z:127:LYS:HB2	23:Z:162:GLU:HG3	2.04	0.40
1:A:1488:G:H5''	1:A:1488:G:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	182/196 (93%)	115 (63%)	47 (26%)	20 (11%)	1	6
4	D	269/271 (99%)	217 (81%)	31 (12%)	21 (8%)	1	14
5	E	202/204 (99%)	152 (75%)	35 (17%)	15 (7%)	2	15
6	F	205/207 (99%)	163 (80%)	28 (14%)	14 (7%)	2	18
7	G	179/181 (99%)	137 (76%)	31 (17%)	11 (6%)	2	22
8	H	157/159 (99%)	116 (74%)	25 (16%)	16 (10%)	1	7
9	I	143/145 (99%)	110 (77%)	25 (18%)	8 (6%)	3	25
10	J	128/130 (98%)	72 (56%)	42 (33%)	14 (11%)	1	6
11	N	136/138 (99%)	108 (79%)	15 (11%)	13 (10%)	1	9
12	O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	27	78
13	P	144/146 (99%)	87 (60%)	28 (19%)	29 (20%)	0	1
14	Q	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	7	47
15	R	115/117 (98%)	92 (80%)	17 (15%)	6 (5%)	3	27
16	S	96/98 (98%)	63 (66%)	20 (21%)	13 (14%)	0	3
17	T	135/137 (98%)	89 (66%)	30 (22%)	16 (12%)	1	4
18	U	115/117 (98%)	92 (80%)	19 (16%)	4 (4%)	6	41
19	V	99/101 (98%)	72 (73%)	17 (17%)	10 (10%)	1	8
20	W	111/113 (98%)	96 (86%)	7 (6%)	8 (7%)	2	16
21	X	90/92 (98%)	75 (83%)	8 (9%)	7 (8%)	1	14
22	Y	98/100 (98%)	60 (61%)	19 (19%)	19 (19%)	0	1
23	Z	174/176 (99%)	130 (75%)	33 (19%)	11 (6%)	2	20
24	0	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	19	71
25	1	91/93 (98%)	74 (81%)	10 (11%)	7 (8%)	1	14
26	2	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	3	23
27	3	57/59 (97%)	53 (93%)	3 (5%)	1 (2%)	13	61
28	4	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	1	6
29	5	57/59 (97%)	48 (84%)	4 (7%)	5 (9%)	1	11
30	6	42/44 (96%)	23 (55%)	7 (17%)	12 (29%)	0	0
31	7	46/48 (96%)	45 (98%)	0	1 (2%)	10	55
32	8	61/63 (97%)	47 (77%)	8 (13%)	6 (10%)	1	8
33	9	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
All	All	3604/3678 (98%)	2737 (76%)	567 (16%)	300 (8%)	1	12

All (300) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	213	ALA
4	D	25	THR
4	D	33	LEU
4	D	242	ARG
4	D	271	ILE
5	E	66	HIS
5	E	72	VAL
5	E	131	ALA
6	F	3	GLU
6	F	21	ALA
6	F	89	VAL
6	F	167	ALA
7	G	87	PRO
7	G	97	ASP
7	G	115	ARG
8	H	45	VAL
8	H	137	ASP
8	H	138	LYS
8	H	154	PRO
8	H	155	SER
8	H	156	ALA
8	H	159	GLU
9	I	115	ALA
10	J	23	ALA
10	J	52	ALA
11	N	4	TYR
11	N	57	ALA
11	N	58	ASP
11	N	133	GLN
13	P	9	ASN
13	P	11	GLY
13	P	14	LYS
13	P	19	VAL
13	P	35	HIS
13	P	39	LYS
13	P	52	GLU
13	P	57	THR
13	P	58	THR
13	P	65	ARG
13	P	103	ALA
13	P	107	LYS
13	P	108	LYS

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Mol	Chain	Res	Type
13	P	111	ARG
14	Q	27	VAL
14	Q	135	ASP
16	S	53	SER
16	S	59	LYS
16	S	89	ARG
16	S	94	TYR
16	S	97	ARG
17	T	24	PRO
17	T	28	VAL
17	T	30	VAL
17	T	33	LYS
17	T	80	SER
17	T	129	ARG
17	T	131	ALA
19	V	23	GLU
19	V	46	VAL
19	V	49	THR
20	W	63	ASP
21	X	4	ALA
21	X	12	VAL
22	Y	3	VAL
22	Y	7	VAL
22	Y	17	SER
22	Y	24	VAL
22	Y	27	VAL
22	Y	38	ILE
22	Y	56	PRO
22	Y	77	PRO
22	Y	78	ALA
24	0	13	GLY
25	1	52	ARG
25	1	85	LEU
26	2	47	ASN
28	4	54	LYS
29	5	4	HIS
29	5	49	CYS
29	5	57	VAL
30	6	19	ARG
32	8	61	LEU
3	C	55	ASP
3	C	170	ALA

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Mol	Chain	Res	Type
3	C	202	ALA
3	C	209	ALA
3	C	211	ALA
3	C	216	ALA
4	D	32	SER
4	D	99	ASP
4	D	115	GLN
4	D	225	ALA
4	D	234	GLY
4	D	239	ARG
4	D	244	ARG
5	E	17	ASP
5	E	54	GLN
5	E	77	ILE
5	E	83	ASP
5	E	88	GLY
6	F	25	PRO
6	F	26	ALA
6	F	66	PRO
6	F	128	ALA
6	F	168	ARG
7	G	43	LEU
7	G	52	ILE
7	G	82	LEU
7	G	96	ARG
7	G	126	ASP
8	H	158	HIS
9	I	14	ASP
9	I	85	GLU
9	I	120	ILE
9	I	133	HIS
10	J	49	ALA
10	J	58	ALA
10	J	88	ALA
10	J	120	ALA
10	J	124	ALA
13	P	18	ARG
13	P	34	GLY
13	P	42	SER
13	P	46	LYS
13	P	47	ASP
13	P	49	ARG

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Mol	Chain	Res	Type
13	P	147	LEU
13	P	149	GLU
14	Q	2	LEU
15	R	45	ARG
15	R	117	VAL
16	S	102	ALA
17	T	12	SER
17	T	85	LYS
17	T	88	ILE
18	U	32	ALA
18	U	91	ASP
18	U	93	LYS
19	V	37	VAL
19	V	53	GLU
20	W	6	ILE
20	W	112	GLY
21	X	11	PRO
22	Y	29	GLU
23	Z	92	SER
25	1	28	GLY
25	1	58	ILE
25	1	84	GLY
26	2	44	LEU
27	3	13	ILE
28	4	61	VAL
30	6	16	CYS
30	6	28	ARG
30	6	31	PRO
30	6	33	LYS
30	6	44	ARG
32	8	31	HIS
32	8	34	TRP
3	C	126	ALA
3	C	171	ALA
3	C	173	ALA
3	C	178	ALA
3	C	198	ALA
3	C	205	ALA
4	D	23	GLU
4	D	27	THR
4	D	210	GLY
4	D	241	PRO

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Mol	Chain	Res	Type
5	E	60	ASN
5	E	89	ASP
5	E	118	LYS
6	F	11	VAL
6	F	54	ARG
7	G	50	ALA
8	H	55	PRO
8	H	56	SER
8	H	157	TYR
10	J	47	ALA
10	J	56	ALA
10	J	76	ALA
10	J	104	ALA
11	N	59	LYS
11	N	127	ASP
11	N	135	PRO
13	P	89	ALA
13	P	106	LEU
15	R	8	ARG
16	S	14	VAL
16	S	92	TYR
17	T	31	SER
17	T	92	GLY
17	T	107	ASP
19	V	79	VAL
20	W	11	ARG
20	W	65	LEU
20	W	93	ALA
21	X	13	LEU
22	Y	62	GLU
23	Z	42	VAL
23	Z	52	SER
23	Z	136	PHE
23	Z	165	VAL
23	Z	166	SER
23	Z	177	PRO
25	1	45	ASN
25	1	53	VAL
26	2	70	GLN
30	6	18	ARG
32	8	40	GLU
3	C	52	ARG

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Mol	Chain	Res	Type
3	C	125	ALA
3	C	167	ALA
3	C	177	ALA
4	D	3	VAL
4	D	202	LYS
5	E	70	ALA
5	E	90	THR
6	F	127	GLU
8	H	49	VAL
8	H	83	TYR
8	H	126	PRO
9	I	78	THR
10	J	7	ALA
10	J	29	ALA
11	N	8	GLN
11	N	47	ALA
11	N	126	PRO
15	R	102	GLU
15	R	105	ARG
17	T	35	LYS
17	T	83	ILE
19	V	18	LEU
20	W	12	ILE
20	W	35	ILE
21	X	10	ALA
21	X	36	LYS
22	Y	39	VAL
22	Y	81	LYS
29	5	36	CYS
30	6	17	LYS
32	8	35	GLN
4	D	28	GLU
4	D	35	LYS
4	D	127	VAL
5	E	45	THR
8	H	85	LYS
10	J	107	ALA
11	N	134	ARG
13	P	30	THR
13	P	104	GLY
16	S	100	ALA
16	S	107	GLU

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Mol	Chain	Res	Type
17	T	41	ARG
18	U	92	ARG
19	V	3	ALA
19	V	16	PRO
19	V	29	PRO
22	Y	37	VAL
22	Y	53	PRO
22	Y	67	LEU
22	Y	80	GLY
26	2	18	PRO
28	4	46	ASN
30	6	15	GLU
30	6	41	PRO
30	6	42	TRP
30	6	49	HIS
31	7	2	LYS
32	8	3	LYS
3	C	109	ALA
3	C	162	ALA
4	D	236	GLY
7	G	10	LYS
7	G	142	PRO
13	P	56	SER
14	Q	22	LYS
21	X	48	LYS
22	Y	31	LEU
23	Z	41	LEU
23	Z	168	GLU
29	5	37	LYS
9	I	7	GLU
12	O	48	PRO
13	P	122	PRO
15	R	58	GLY
23	Z	114	GLY
23	Z	147	GLY
11	N	5	VAL
16	S	85	VAL
3	C	64	LEU
8	H	92	ILE
9	I	15	VAL
11	N	129	PRO
6	F	14	PRO

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Mol	Chain	Res	Type
6	F	206	ILE
13	P	48	PRO
16	S	90	GLY
22	Y	66	PRO
5	E	53	PRO
16	S	35	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	61/66 (92%)	56 (92%)	5 (8%)	17	57
4	D	213/213 (100%)	176 (83%)	37 (17%)	3	14
5	E	165/165 (100%)	139 (84%)	26 (16%)	4	18
6	F	165/165 (100%)	149 (90%)	16 (10%)	12	45
7	G	155/155 (100%)	137 (88%)	18 (12%)	8	35
8	H	132/132 (100%)	120 (91%)	12 (9%)	14	49
9	I	122/122 (100%)	111 (91%)	11 (9%)	14	50
11	N	117/117 (100%)	94 (80%)	23 (20%)	2	9
12	O	100/100 (100%)	93 (93%)	7 (7%)	21	66
13	P	112/112 (100%)	86 (77%)	26 (23%)	1	5
14	Q	111/111 (100%)	101 (91%)	10 (9%)	14	50
15	R	100/100 (100%)	85 (85%)	15 (15%)	4	21
16	S	77/77 (100%)	67 (87%)	10 (13%)	6	29
17	T	120/120 (100%)	93 (78%)	27 (22%)	1	6
18	U	92/92 (100%)	82 (89%)	10 (11%)	9	38
19	V	82/82 (100%)	65 (79%)	17 (21%)	2	8
20	W	91/91 (100%)	80 (88%)	11 (12%)	7	33
21	X	74/74 (100%)	65 (88%)	9 (12%)	7	32
22	Y	84/84 (100%)	67 (80%)	17 (20%)	2	8
23	Z	155/155 (100%)	148 (96%)	7 (4%)	38	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	0	66/66 (100%)	60 (91%)	6 (9%)	14	49
25	1	78/78 (100%)	62 (80%)	16 (20%)	2	8
26	2	66/66 (100%)	60 (91%)	6 (9%)	14	49
27	3	51/51 (100%)	48 (94%)	3 (6%)	28	73
28	4	27/27 (100%)	24 (89%)	3 (11%)	9	37
29	5	51/51 (100%)	41 (80%)	10 (20%)	2	9
30	6	43/43 (100%)	36 (84%)	7 (16%)	3	17
31	7	41/41 (100%)	32 (78%)	9 (22%)	1	6
32	8	53/53 (100%)	43 (81%)	10 (19%)	2	11
33	9	33/33 (100%)	30 (91%)	3 (9%)	14	49
All	All	2837/2842 (100%)	2450 (86%)	387 (14%)	5	26

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	23	ASP
3	C	36	LYS
3	C	56	GLN
3	C	58	VAL
3	C	64	LEU
4	D	5	LYS
4	D	10	THR
4	D	13	ARG
4	D	20	ASP
4	D	24	ILE
4	D	25	THR
4	D	26	LYS
4	D	28	GLU
4	D	33	LEU
4	D	35	LYS
4	D	38	LYS
4	D	43	ARG
4	D	49	ILE
4	D	61	LEU
4	D	64	ILE
4	D	65	ILE
4	D	92	ILE
4	D	94	LEU

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Mol	Chain	Res	Type
4	D	98	VAL
4	D	103	ARG
4	D	106	ILE
4	D	131	LEU
4	D	155	LEU
4	D	157	ARG
4	D	166	GLN
4	D	171	ASP
4	D	173	VAL
4	D	192	THR
4	D	211	ARG
4	D	212	SER
4	D	221	VAL
4	D	229	VAL
4	D	242	ARG
4	D	257	LEU
4	D	260	ARG
4	D	267	SER
4	D	271	ILE
5	E	9	VAL
5	E	16	ARG
5	E	18	ASP
5	E	19	ARG
5	E	33	VAL
5	E	34	VAL
5	E	41	LYS
5	E	52	LEU
5	E	55	ASN
5	E	63	LEU
5	E	67	PHE
5	E	76	ARG
5	E	78	LEU
5	E	79	ARG
5	E	82	ARG
5	E	105	THR
5	E	113	PHE
5	E	119	ARG
5	E	144	ARG
5	E	152	LYS
5	E	163	GLU
5	E	179	GLU
5	E	181	LEU

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Mol	Chain	Res	Type
5	E	197	ILE
5	E	202	LYS
5	E	203	LYS
6	F	20	LEU
6	F	23	ASP
6	F	24	LEU
6	F	28	ILE
6	F	72	ARG
6	F	82	ILE
6	F	83	PHE
6	F	110	LEU
6	F	125	LEU
6	F	140	LEU
6	F	160	ASN
6	F	161	GLU
6	F	170	LEU
6	F	175	THR
6	F	199	TRP
6	F	200	GLU
7	G	5	VAL
7	G	22	ARG
7	G	47	LYS
7	G	49	ASP
7	G	59	GLU
7	G	67	LYS
7	G	74	LYS
7	G	97	ASP
7	G	113	ARG
7	G	116	ASP
7	G	125	PHE
7	G	126	ASP
7	G	130	ASN
7	G	136	ARG
7	G	143	GLU
7	G	155	MET
7	G	159	VAL
7	G	167	GLU
8	H	34	GLU
8	H	53	GLU
8	H	54	ARG
8	H	59	ARG
8	H	68	THR

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Mol	Chain	Res	Type
8	H	86	GLU
8	H	89	ILE
8	H	134	SER
8	H	143	GLN
8	H	153	LYS
8	H	155	SER
8	H	157	TYR
9	I	10	GLU
9	I	12	LEU
9	I	20	ASP
9	I	38	LEU
9	I	41	GLU
9	I	54	GLN
9	I	61	ARG
9	I	114	LEU
9	I	123	LEU
9	I	128	LEU
9	I	144	VAL
11	N	2	LYS
11	N	4	TYR
11	N	5	VAL
11	N	19	GLU
11	N	33	LEU
11	N	34	LEU
11	N	39	ARG
11	N	41	ASP
11	N	43	THR
11	N	45	ASN
11	N	48	MET
11	N	55	VAL
11	N	56	ASN
11	N	61	ARG
11	N	63	THR
11	N	87	LEU
11	N	106	MET
11	N	109	LYS
11	N	115	ARG
11	N	119	ARG
11	N	121	LYS
11	N	127	ASP
11	N	131	GLN
12	O	14	THR

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Mol	Chain	Res	Type
12	O	24	VAL
12	O	47	ILE
12	O	73	ASP
12	O	98	VAL
12	O	108	GLU
12	O	117	LEU
13	P	13	ASN
13	P	16	ARG
13	P	21	ARG
13	P	32	THR
13	P	35	HIS
13	P	36	LYS
13	P	39	LYS
13	P	40	SER
13	P	41	ARG
13	P	45	LEU
13	P	52	GLU
13	P	59	LEU
13	P	61	ARG
13	P	62	LEU
13	P	64	LYS
13	P	70	GLN
13	P	76	LYS
13	P	81	GLN
13	P	84	ASN
13	P	85	LEU
13	P	98	GLU
13	P	107	LYS
13	P	108	LYS
13	P	114	ILE
13	P	131	SER
13	P	135	LEU
14	Q	10	ARG
14	Q	16	ARG
14	Q	18	LYS
14	Q	45	GLN
14	Q	54	MET
14	Q	55	VAL
14	Q	58	PHE
14	Q	79	LEU
14	Q	110	THR
14	Q	135	ASP

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Mol	Chain	Res	Type
15	R	12	ARG
15	R	18	LEU
15	R	27	SER
15	R	28	LEU
15	R	29	LEU
15	R	57	ARG
15	R	67	LEU
15	R	71	GLN
15	R	74	LYS
15	R	79	LEU
15	R	95	THR
15	R	99	LYS
15	R	100	LEU
15	R	104	ARG
15	R	113	LEU
16	S	11	LYS
16	S	19	LYS
16	S	20	ARG
16	S	23	ARG
16	S	44	LYS
16	S	75	GLU
16	S	89	ARG
16	S	92	TYR
16	S	97	ARG
16	S	106	ARG
17	T	6	LEU
17	T	11	GLU
17	T	17	THR
17	T	18	ASP
17	T	24	PRO
17	T	29	ARG
17	T	32	TYR
17	T	38	ASN
17	T	41	ARG
17	T	51	ARG
17	T	54	ARG
17	T	58	ASN
17	T	59	THR
17	T	67	SER
17	T	74	ARG
17	T	78	LEU
17	T	82	LEU

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Mol	Chain	Res	Type
17	T	85	LYS
17	T	93	ARG
17	T	96	ARG
17	T	99	LEU
17	T	108	ARG
17	T	110	ILE
17	T	112	ARG
17	T	113	LYS
17	T	128	GLU
17	T	132	LYS
18	U	3	ARG
18	U	8	VAL
18	U	13	LYS
18	U	19	LYS
18	U	27	LEU
18	U	60	LEU
18	U	66	ASN
18	U	74	LEU
18	U	83	LEU
18	U	108	GLU
19	V	1	MET
19	V	2	PHE
19	V	13	ARG
19	V	15	GLU
19	V	18	LEU
19	V	19	LYS
19	V	20	LEU
19	V	21	ARG
19	V	39	LEU
19	V	40	LEU
19	V	46	VAL
19	V	49	THR
19	V	66	ARG
19	V	68	LYS
19	V	79	VAL
19	V	98	GLU
19	V	99	ILE
20	W	1	MET
20	W	11	ARG
20	W	15	ARG
20	W	24	ILE
20	W	30	GLU

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Mol	Chain	Res	Type
20	W	51	LEU
20	W	52	GLU
20	W	60	ASN
20	W	66	GLU
20	W	92	ARG
20	W	96	ILE
21	X	12	VAL
21	X	27	THR
21	X	41	ASN
21	X	48	LYS
21	X	52	VAL
21	X	57	LEU
21	X	63	LYS
21	X	68	ARG
21	X	80	ILE
22	Y	7	VAL
22	Y	8	LYS
22	Y	13	VAL
22	Y	28	LYS
22	Y	49	VAL
22	Y	50	ARG
22	Y	55	TYR
22	Y	56	PRO
22	Y	62	GLU
22	Y	63	LYS
22	Y	66	PRO
22	Y	71	LYS
22	Y	76	CYS
22	Y	77	PRO
22	Y	83	THR
22	Y	89	PHE
22	Y	97	ARG
23	Z	5	LEU
23	Z	6	LYS
23	Z	31	ARG
23	Z	53	ILE
23	Z	119	GLU
23	Z	155	LEU
23	Z	166	SER
24	0	3	HIS
24	0	19	LYS
24	0	20	ARG

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Mol	Chain	Res	Type
24	0	36	ILE
24	0	64	ASP
24	0	84	LEU
25	1	32	LYS
25	1	39	LYS
25	1	40	ARG
25	1	41	ARG
25	1	45	ASN
25	1	46	LEU
25	1	52	ARG
25	1	59	THR
25	1	61	ARG
25	1	69	LYS
25	1	72	GLU
25	1	80	LEU
25	1	82	LEU
25	1	88	LYS
25	1	92	LYS
25	1	94	LEU
26	2	2	LYS
26	2	17	SER
26	2	32	LEU
26	2	35	LEU
26	2	47	ASN
26	2	53	LEU
27	3	8	LEU
27	3	31	LEU
27	3	57	GLU
28	4	48	ILE
28	4	56	GLU
28	4	58	TYR
29	5	6	VAL
29	5	36	CYS
29	5	37	LYS
29	5	44	THR
29	5	46	CYS
29	5	48	GLU
29	5	49	CYS
29	5	51	TYR
29	5	52	TYR
29	5	56	LYS
30	6	18	ARG

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Mol	Chain	Res	Type
30	6	29	ASN
30	6	30	THR
30	6	33	LYS
30	6	42	TRP
30	6	43	CYS
30	6	47	THR
31	7	1	MET
31	7	2	LYS
31	7	4	THR
31	7	8	ASN
31	7	10	ARG
31	7	23	ARG
31	7	24	THR
31	7	41	ARG
31	7	48	LYS
32	8	8	LYS
32	8	16	ILE
32	8	30	ARG
32	8	31	HIS
32	8	32	LEU
32	8	33	ASN
32	8	34	TRP
32	8	44	LYS
32	8	49	VAL
32	8	61	LEU
33	9	9	ARG
33	9	26	ILE
33	9	27	CYS

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

Mol	Chain	Res	Type
3	C	56	GLN
4	D	58	HIS
4	D	126	GLN
4	D	198	ASN
5	E	192	ASN
6	F	69	HIS
6	F	75	HIS
6	F	133	ASN
6	F	160	ASN
6	F	169	ASN

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Mol	Chain	Res	Type
8	H	139	GLN
8	H	147	ASN
9	I	43	ASN
9	I	139	GLN
11	N	128	HIS
12	O	82	ASN
13	P	13	ASN
13	P	128	HIS
14	Q	45	GLN
15	R	23	ASN
15	R	53	HIS
15	R	71	GLN
16	S	34	HIS
17	T	38	ASN
17	T	43	GLN
17	T	58	ASN
17	T	90	GLN
18	U	14	HIS
18	U	49	HIS
18	U	66	ASN
20	W	34	ASN
20	W	57	ASN
20	W	102	HIS
21	X	41	ASN
21	X	55	ASN
23	Z	118	GLN
24	0	12	ASN
25	1	45	ASN
27	3	19	GLN
27	3	46	ASN
27	3	52	HIS
28	4	46	ASN
29	5	43	HIS
31	7	8	ASN
32	8	33	ASN
32	8	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2799/2915 (96%)	754 (26%)	122 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	118/119 (99%)	27 (22%)	4 (3%)
All	All	2917/3034 (96%)	781 (26%)	126 (4%)

All (781) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	G
1	A	14	G
1	A	33	C
1	A	34	G
1	A	35	G
1	A	40	C
1	A	44	C
1	A	47	A
1	A	48	U
1	A	52	G
1	A	53	G
1	A	57	U
1	A	67	C
1	A	69	A
1	A	70	U
1	A	72	A
1	A	73	G
1	A	80	G
1	A	81	G
1	A	82	A
1	A	86	G
1	A	88	U
1	A	89	A
1	A	91	C
1	A	93	G
1	A	98	G
1	A	99	G
1	A	110	G
1	A	115	A
1	A	116	A
1	A	117	U
1	A	125	C
1	A	126	C
1	A	136	G
1	A	138	A

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Mol	Chain	Res	Type
1	A	142	C
1	A	145	G
1	A	153	G
1	A	154	C
1	A	158	U
1	A	159	G
1	A	162	C
1	A	163	G
1	A	169	A
1	A	184	A
1	A	185	A
1	A	192	A
1	A	193	G
1	A	203	G
1	A	204	A
1	A	209	A
1	A	210	A
1	A	213	A
1	A	216	A
1	A	217	A
1	A	218	U
1	A	227	U
1	A	236	G
1	A	237	C
1	A	240	G
1	A	248	G
1	A	249	G
1	A	255	C
1	A	256	C
1	A	268	G
1	A	269	C
1	A	270	U
1	A	271	U
1	A	273	U
1	A	274	C
1	A	275	C
1	A	277	G
1	A	282	G
1	A	284	U
1	A	285	C
1	A	286	G
1	A	294	C

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Mol	Chain	Res	Type
1	A	295	U
1	A	296	C
1	A	297	G
1	A	298	G
1	A	321	G
1	A	322	A
1	A	333	A
1	A	334	A
1	A	335	G
1	A	347	A
1	A	350	G
1	A	352	G
1	A	353	A
1	A	355	A
1	A	356	G
1	A	375	G
1	A	376	G
1	A	381	U
1	A	385	U
1	A	386	G
1	A	388	G
1	A	389	G
1	A	392	A
1	A	393	C
1	A	394	C
1	A	397	A
1	A	398	G
1	A	412	G
1	A	413	U
1	A	414	G
1	A	422	G
1	A	431	U
1	A	432	G
1	A	433	G
1	A	437	G
1	A	440	C
1	A	444	G
1	A	454	A
1	A	466	U
1	A	469	C
1	A	473	U
1	A	480	C

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Mol	Chain	Res	Type
1	A	481	C
1	A	482	A
1	A	495	A
1	A	497	A
1	A	498	G
1	A	500	U
1	A	504	A
1	A	506	G
1	A	507	A
1	A	508	A
1	A	515	G
1	A	518	G
1	A	520	G
1	A	528	U
1	A	529	A
1	A	532	G
1	A	533	C
1	A	536	G
1	A	537	A
1	A	551	C
1	A	552	A
1	A	554	G
1	A	555	C
1	A	556	A
1	A	557	G
1	A	566	C
1	A	567	C
1	A	571	A
1	A	572	G
1	A	583	G
1	A	584	U
1	A	585	G
1	A	595	G
1	A	597	A
1	A	608	A
1	A	610	U
1	A	621	G
1	A	626	G
1	A	629	U
1	A	632	G
1	A	635	G
1	A	636	U

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Mol	Chain	Res	Type
1	A	637	U
1	A	638	G
1	A	640	G
1	A	646	G
1	A	648	C
1	A	650	U
1	A	651	A
1	A	652	G
1	A	661	A
1	A	669	C
1	A	670	A
1	A	674	C
1	A	675	G
1	A	676	C
1	A	703	U
1	A	710	C
1	A	715	G
1	A	716	A
1	A	717	C
1	A	719	C
1	A	731	A
1	A	732	G
1	A	747	G
1	A	753	G
1	A	754	C
1	A	755	U
1	A	763	G
1	A	768	A
1	A	776	C
1	A	784	G
1	A	786	U
1	A	792	A
1	A	793	U
1	A	799	C
1	A	804	C
1	A	808	U
1	A	810	A
1	A	811	G
1	A	821	G
1	A	822	G
1	A	828	A
1	A	830	A

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Mol	Chain	Res	Type
1	A	831	G
1	A	833	U
1	A	834	A
1	A	835	A
1	A	836	C
1	A	837	C
1	A	838	G
1	A	851	G
1	A	853	U
1	A	858	C
1	A	865	A
1	A	873	U
1	A	874	U
1	A	876	G
1	A	878	G
1	A	891	G
1	A	892	C
1	A	894	G
1	A	905	G
1	A	912	A
1	A	924	A
1	A	929	G
1	A	932	C
1	A	936	A
1	A	941	A
1	A	942	C
1	A	949	C
1	A	952	U
1	A	955	A
1	A	959	C
1	A	960	C
1	A	962	A
1	A	976	G
1	A	977	A
1	A	978	G
1	A	982	G
1	A	985	A
1	A	989	A
1	A	990	G
1	A	1002	U
1	A	1003	A
1	A	1005	C

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Mol	Chain	Res	Type
1	A	1008	C
1	A	1009	C
1	A	1017	A
1	A	1018	G
1	A	1025	A
1	A	1027	C
1	A	1028	A
1	A	1036	C
1	A	1041	A
1	A	1057	U
1	A	1058	C
1	A	1060	G
1	A	1067	G
1	A	1068	U
1	A	1070	G
1	A	1071	U
1	A	1072	A
1	A	1076	G
1	A	1077	A
1	A	1084	G
1	A	1085	C
1	A	1086	C
1	A	1087	G
1	A	1089	G
1	A	1090	A
1	A	1091	A
1	A	1092	G
1	A	1094	C
1	A	1097	C
1	A	1098	C
1	A	1155	G
1	A	1156	A
1	A	1157	G
1	A	1158	U
1	A	1159	G
1	A	1160	G
1	A	1161	C
1	A	1163	C
1	A	1167	G
1	A	1174	A
1	A	1175	U
1	A	1179	C

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Mol	Chain	Res	Type
1	A	1180	G
1	A	1184	C
1	A	1185	U
1	A	1186	U
1	A	1187	A
1	A	1189	G
1	A	1200	A
1	A	1216	G
1	A	1217	G
1	A	1218	A
1	A	1219	U
1	A	1220	G
1	A	1222	C
1	A	1223	C
1	A	1239	G
1	A	1249	U
1	A	1252	C
1	A	1254	A
1	A	1255	U
1	A	1256	G
1	A	1257	A
1	A	1262	C
1	A	1263	G
1	A	1264	A
1	A	1265	C
1	A	1287	A
1	A	1289	G
1	A	1293	G
1	A	1294	U
1	A	1295	G
1	A	1298	A
1	A	1301	G
1	A	1310	A
1	A	1314	A
1	A	1316	G
1	A	1317	A
1	A	1318	U
1	A	1326	G
1	A	1327	U
1	A	1331	A
1	A	1332	A
1	A	1345	U

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Mol	Chain	Res	Type
1	A	1346	A
1	A	1347	A
1	A	1351	C
1	A	1352	A
1	A	1358	U
1	A	1359	C
1	A	1364	G
1	A	1366	A
1	A	1374	U
1	A	1377	G
1	A	1383	G
1	A	1394	A
1	A	1404	A
1	A	1405	A
1	A	1410	A
1	A	1413	G
1	A	1415	C
1	A	1422	G
1	A	1424	A
1	A	1425	G
1	A	1429	A
1	A	1430	G
1	A	1431	C
1	A	1436	U
1	A	1447	C
1	A	1452	C
1	A	1453	C
1	A	1461	G
1	A	1462	C
1	A	1465	U
1	A	1466	G
1	A	1472	A
1	A	1473	C
1	A	1478	U
1	A	1482	C
1	A	1490	A
1	A	1494	G
1	A	1495	A
1	A	1496	G
1	A	1498	C
1	A	1499	A
1	A	1500	U

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Mol	Chain	Res	Type
1	A	1506	A
1	A	1507	G
1	A	1513	C
1	A	1517	A
1	A	1521	G
1	A	1522	C
1	A	1523	A
1	A	1524	G
1	A	1527	U
1	A	1528	G
1	A	1530	G
1	A	1535	A
1	A	1536	G
1	A	1538	C
1	A	1539	A
1	A	1540	A
1	A	1541	A
1	A	1542	U
1	A	1543	C
1	A	1546	C
1	A	1547	C
1	A	1550	C
1	A	1554	C
1	A	1555	A
1	A	1560	C
1	A	1567	G
1	A	1570	G
1	A	1575	G
1	A	1576	C
1	A	1577	C
1	A	1578	C
1	A	1579	G
1	A	1590	A
1	A	1591	A
1	A	1592	C
1	A	1595	C
1	A	1600	A
1	A	1601	G
1	A	1604	A
1	A	1605	G
1	A	1612	A
1	A	1615	A

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Mol	Chain	Res	Type
1	A	1621	C
1	A	1624	U
1	A	1625	A
1	A	1630	C
1	A	1631	A
1	A	1632	A
1	A	1633	C
1	A	1636	G
1	A	1638	G
1	A	1639	G
1	A	1647	U
1	A	1648	A
1	A	1653	A
1	A	1654	A
1	A	1655	A
1	A	1661	A
1	A	1662	C
1	A	1663	A
1	A	1670	C
1	A	1686	C
1	A	1691	G
1	A	1693	G
1	A	1694	C
1	A	1698	A
1	A	1699	G
1	A	1700	A
1	A	1713	G
1	A	1720	G
1	A	1724	G
1	A	1725	U
1	A	1727	G
1	A	1740	C
1	A	1741	G
1	A	1742	G
1	A	1744	A
1	A	1745	G
1	A	1746	A
1	A	1747	A
1	A	1765	G
1	A	1766	A
1	A	1767	U
1	A	1768	G

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Mol	Chain	Res	Type
1	A	1770	G
1	A	1772	C
1	A	1773	C
1	A	1775	G
1	A	1778	G
1	A	1783	G
1	A	1788	G
1	A	1793	G
1	A	1794	G
1	A	1803	A
1	A	1806	G
1	A	1810	A
1	A	1812	C
1	A	1816	A
1	A	1817	A
1	A	1821	A
1	A	1829	G
1	A	1830	C
1	A	1831	G
1	A	1832	A
1	A	1846	G
1	A	1849	A
1	A	1850	U
1	A	1851	A
1	A	1859	A
1	A	1865	G
1	A	1868	C
1	A	1869	G
1	A	1876	G
1	A	1877	A
1	A	1879	G
1	A	1888	G
1	A	1894	U
1	A	1896	C
1	A	1897	A
1	A	1898	A
1	A	1899	G
1	A	1902	C
1	A	1903	C
1	A	1906	A
1	A	1909	G
1	A	1910	A

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Mol	Chain	Res	Type
1	A	1917	G
1	A	1920	G
1	A	1921	A
1	A	1927	G
1	A	1930	C
1	A	1933	A
1	A	1934	A
1	A	1935	C
1	A	1937	A
1	A	1950	G
1	A	1951	G
1	A	1955	C
1	A	1956	G
1	A	1957	A
1	A	1959	A
1	A	1960	U
1	A	1961	U
1	A	1968	C
1	A	1976	U
1	A	1983	C
1	A	1984	U
1	A	1985	G
1	A	1988	C
1	A	1990	A
1	A	1991	A
1	A	1992	A
1	A	1993	A
1	A	2003	C
1	A	2008	G
1	A	2012	U
1	A	2014	U
1	A	2018	G
1	A	2041	A
1	A	2044	G
1	A	2047	C
1	A	2048	G
1	A	2052	A
1	A	2054	A
1	A	2055	U
1	A	2057	C
1	A	2060	C
1	A	2064	C

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Mol	Chain	Res	Type
1	A	2076	C
1	A	2077	G
1	A	2081	A
1	A	2082	G
1	A	2083	A
1	A	2084	C
1	A	2090	G
1	A	2091	G
1	A	2114	G
1	A	2115	G
1	A	2116	C
1	A	2117	U
1	A	2118	C
1	A	2120	U
1	A	2121	G
1	A	2124	C
1	A	2125	G
1	A	2129	C
1	A	2131	G
1	A	2137	G
1	A	2138	A
1	A	2140	A
1	A	2148	G
1	A	2149	C
1	A	2152	G
1	A	2154	G
1	A	2168	G
1	A	2170	G
1	A	2180	G
1	A	2193	U
1	A	2194	A
1	A	2198	C
1	A	2200	C
1	A	2201	U
1	A	2206	C
1	A	2208	G
1	A	2210	U
1	A	2212	G
1	A	2213	G
1	A	2214	G
1	A	2219	A
1	A	2220	A

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Mol	Chain	Res	Type
1	A	2221	C
1	A	2224	U
1	A	2227	G
1	A	2228	A
1	A	2230	G
1	A	2233	G
1	A	2236	A
1	A	2237	C
1	A	2249	G
1	A	2250	G
1	A	2256	U
1	A	2257	G
1	A	2286	C
1	A	2290	G
1	A	2291	G
1	A	2294	C
1	A	2298	A
1	A	2299	A
1	A	2300	G
1	A	2314	G
1	A	2316	A
1	A	2318	G
1	A	2319	G
1	A	2320	A
1	A	2322	A
1	A	2323	U
1	A	2324	C
1	A	2327	C
1	A	2330	G
1	A	2331	A
1	A	2332	G
1	A	2336	G
1	A	2338	A
1	A	2345	G
1	A	2347	A
1	A	2353	C
1	A	2357	A
1	A	2358	C
1	A	2361	C
1	A	2394	G
1	A	2395	G
1	A	2396	C

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Mol	Chain	Res	Type
1	A	2403	A
1	A	2410	G
1	A	2413	C
1	A	2417	U
1	A	2421	G
1	A	2422	A
1	A	2434	U
1	A	2436	A
1	A	2440	G
1	A	2441	A
1	A	2446	A
1	A	2450	A
1	A	2451	C
1	A	2452	C
1	A	2459	A
1	A	2460	U
1	A	2463	C
1	A	2476	C
1	A	2479	G
1	A	2480	A
1	A	2481	G
1	A	2482	C
1	A	2485	C
1	A	2487	A
1	A	2488	C
1	A	2489	A
1	A	2490	G
1	A	2493	G
1	A	2494	C
1	A	2495	G
1	A	2502	U
1	A	2509	C
1	A	2513	G
1	A	2516	G
1	A	2529	A
1	A	2535	G
1	A	2540	G
1	A	2542	A
1	A	2553	A
1	A	2554	G
1	A	2556	G
1	A	2565	U

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Mol	Chain	Res	Type
1	A	2577	A
1	A	2578	G
1	A	2584	C
1	A	2589	G
1	A	2593	G
1	A	2596	U
1	A	2597	C
1	A	2613	A
1	A	2615	U
1	A	2620	U
1	A	2621	C
1	A	2622	U
1	A	2623	C
1	A	2626	U
1	A	2632	A
1	A	2641	G
1	A	2664	U
1	A	2665	A
1	A	2666	G
1	A	2668	A
1	A	2669	C
1	A	2670	G
1	A	2671	A
1	A	2672	G
1	A	2673	A
1	A	2674	G
1	A	2677	C
1	A	2678	C
1	A	2683	G
1	A	2684	G
1	A	2690	A
1	A	2694	C
1	A	2701	C
1	A	2702	C
1	A	2704	A
1	A	2713	U
1	A	2714	C
1	A	2723	U
1	A	2724	A
1	A	2725	A
1	A	2732	U
1	A	2736	C

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Mol	Chain	Res	Type
1	A	2738	U
1	A	2742	C
1	A	2745	A
1	A	2746	A
1	A	2760	A
1	A	2763	G
1	A	2764	C
1	A	2770	A
1	A	2772	C
1	A	2774	G
1	A	2776	A
1	A	2777	A
1	A	2778	G
1	A	2782	G
1	A	2790	A
1	A	2791	U
1	A	2792	G
1	A	2799	C
1	A	2801	C
1	A	2802	A
1	A	2803	C
1	A	2804	G
1	A	2805	G
1	A	2806	C
1	A	2808	U
1	A	2809	C
1	A	2811	A
1	A	2812	G
1	A	2813	C
1	A	2814	C
1	A	2817	U
1	A	2827	G
1	A	2829	A
1	A	2830	A
1	A	2842	G
1	A	2843	G
1	A	2844	A
1	A	2853	G
1	A	2858	U
1	A	2859	A
1	A	2872	C
1	A	2881	G

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Mol	Chain	Res	Type
1	A	2888	C
1	A	2892	A
1	A	2901	G
1	A	2902	G
2	B	12	C
2	B	13	A
2	B	15	A
2	B	16	G
2	B	21	G
2	B	25	A
2	B	26	A
2	B	32	C
2	B	40	U
2	B	41	U
2	B	42	C
2	B	43	C
2	B	45	A
2	B	47	C
2	B	52	A
2	B	53	A
2	B	67	G
2	B	73	A
2	B	80	U
2	B	81	G
2	B	86	G
2	B	88	C
2	B	89	G
2	B	97	G
2	B	109	C
2	B	110	G
2	B	113	G

All (126) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	47	A
1	A	69	A
1	A	72	A
1	A	81	G
1	A	88	U
1	A	98	G
1	A	99	G

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Mol	Chain	Res	Type
1	A	116	A
1	A	125	C
1	A	158	U
1	A	165	G
1	A	187	A
1	A	200	G
1	A	209	A
1	A	284	U
1	A	333	A
1	A	354	A
1	A	355	A
1	A	379	G
1	A	392	A
1	A	413	U
1	A	416	A
1	A	473	U
1	A	497	A
1	A	499	G
1	A	506	G
1	A	527	A
1	A	566	C
1	A	609	C
1	A	625	A
1	A	639	A
1	A	715	G
1	A	731	A
1	A	732	G
1	A	792	A
1	A	798	A
1	A	810	A
1	A	822	G
1	A	836	C
1	A	904	U
1	A	912	A
1	A	1018	G
1	A	1067	G
1	A	1071	U
1	A	1085	C
1	A	1156	A
1	A	1254	A
1	A	1325	G
1	A	1326	G

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Mol	Chain	Res	Type
1	A	1331	A
1	A	1333	U
1	A	1345	U
1	A	1346	A
1	A	1410	A
1	A	1423	A
1	A	1424	A
1	A	1441	U
1	A	1465	U
1	A	1472	A
1	A	1498	C
1	A	1504	C
1	A	1535	A
1	A	1539	A
1	A	1542	U
1	A	1576	C
1	A	1590	A
1	A	1604	A
1	A	1647	U
1	A	1653	A
1	A	1655	A
1	A	1662	C
1	A	1698	A
1	A	1699	G
1	A	1740	C
1	A	1810	A
1	A	1829	G
1	A	1849	A
1	A	1850	U
1	A	1868	C
1	A	1869	G
1	A	1920	G
1	A	1921	A
1	A	1955	C
1	A	1960	U
1	A	1983	C
1	A	1984	U
1	A	1991	A
1	A	2005	G
1	A	2013	G
1	A	2052	A
1	A	2054	A

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Mol	Chain	Res	Type
1	A	2137	G
1	A	2147	A
1	A	2192	A
1	A	2193	U
1	A	2212	G
1	A	2236	A
1	A	2260	U
1	A	2293	G
1	A	2322	A
1	A	2329	G
1	A	2331	A
1	A	2346	A
1	A	2357	A
1	A	2416	G
1	A	2421	G
1	A	2433	A
1	A	2450	A
1	A	2459	A
1	A	2475	C
1	A	2492	G
1	A	2528	C
1	A	2673	A
1	A	2700	U
1	A	2792	G
1	A	2801	C
1	A	2803	C
1	A	2808	U
1	A	2812	G
1	A	2841	U
1	A	2842	G
1	A	2882	A
2	B	40	U
2	B	52	A
2	B	66	A
2	B	109	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2807/2915 (96%)	0.09	93 (3%) 44 10	24, 64, 168, 297	0
2	B	119/119 (100%)	0.60	6 (5%) 28 6	71, 112, 151, 191	0
3	C	190/196 (96%)	1.99	76 (40%) 1 0	109, 188, 240, 265	0
4	D	271/271 (100%)	-0.05	0 100 100	23, 56, 91, 127	0
5	E	204/204 (100%)	0.07	4 (1%) 62 19	28, 65, 120, 165	0
6	F	207/207 (100%)	0.12	0 100 100	31, 87, 149, 214	0
7	G	181/181 (100%)	0.59	11 (6%) 21 5	82, 128, 167, 210	0
8	H	159/159 (100%)	0.65	10 (6%) 19 5	70, 128, 180, 235	0
9	I	145/145 (100%)	-0.06	0 100 100	48, 101, 137, 159	0
10	J	130/130 (100%)	1.66	49 (37%) 1 0	122, 193, 233, 284	0
11	N	138/138 (100%)	0.21	2 (1%) 72 25	54, 90, 120, 133	0
12	O	122/122 (100%)	-0.00	1 (0%) 83 39	39, 64, 85, 92	0
13	P	146/146 (100%)	0.35	3 (2%) 60 17	39, 92, 134, 174	0
14	Q	141/141 (100%)	0.44	8 (5%) 23 5	58, 92, 125, 161	0
15	R	117/117 (100%)	0.06	0 100 100	40, 65, 100, 131	0
16	S	98/98 (100%)	0.47	1 (1%) 79 33	72, 110, 151, 181	0
17	T	137/137 (100%)	0.09	1 (0%) 84 42	43, 77, 135, 170	0
18	U	117/117 (100%)	0.24	3 (2%) 53 13	40, 80, 135, 155	0
19	V	101/101 (100%)	0.31	2 (1%) 62 19	61, 110, 143, 183	0
20	W	113/113 (100%)	0.03	2 (1%) 65 20	49, 66, 103, 147	0
21	X	92/92 (100%)	0.02	0 100 100	43, 77, 98, 114	0
22	Y	100/100 (100%)	0.38	2 (2%) 62 19	56, 100, 175, 209	0
23	Z	176/176 (100%)	1.24	33 (18%) 2 1	92, 149, 299, 353	0
24	0	84/84 (100%)	0.26	1 (1%) 75 29	58, 84, 105, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	1	93/93 (100%)	0.07	0 100 100	39, 63, 111, 153	0
26	2	71/71 (100%)	0.05	0 100 100	60, 90, 131, 150	0
27	3	59/59 (100%)	0.36	1 (1%) 67 21	65, 101, 135, 253	0
28	4	30/30 (100%)	0.48	2 (6%) 17 4	121, 142, 163, 173	0
29	5	59/59 (100%)	0.02	2 (3%) 43 10	42, 67, 130, 179	0
30	6	44/44 (100%)	0.44	2 (4%) 32 7	51, 90, 113, 121	0
31	7	48/48 (100%)	0.07	0 100 100	31, 49, 80, 98	0
32	8	63/63 (100%)	0.22	1 (1%) 68 22	50, 77, 112, 154	0
33	9	36/36 (100%)	0.53	2 (5%) 24 5	63, 91, 115, 125	0
All	All	6598/6712 (98%)	0.27	318 (4%) 29 7	23, 78, 188, 353	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	140	ALA	10.0
8	H	170	ARG	9.7
1	A	2812	G	9.2
3	C	78	ALA	8.3
3	C	141	ALA	8.2
23	Z	176	PRO	7.8
1	A	2146	G	7.7
1	A	2138	A	7.5
3	C	180	ALA	7.5
23	Z	173	ALA	7.4
3	C	95	GLY	7.3
23	Z	172	ALA	7.1
1	A	1158	U	7.0
10	J	54	ALA	6.8
3	C	184	ALA	6.7
23	Z	122	ARG	6.6
1	A	2143	U	6.4
3	C	134	ALA	6.3
3	C	139	ALA	6.3
10	J	19	ALA	6.0
3	C	85	GLU	5.9
23	Z	177	PRO	5.9
1	A	1093	A	5.9
14	Q	60	ARG	5.8
1	A	2803	C	5.3

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Mol	Chain	Res	Type	RSRZ
3	C	223	ALA	5.3
3	C	143	ALA	5.3
1	A	2144	G	5.3
3	C	59	ARG	5.2
10	J	15	ALA	5.2
23	Z	121	HIS	5.1
10	J	4	ALA	5.0
3	C	77	ILE	5.0
18	U	89	GLU	4.9
3	C	27	ARG	4.9
3	C	133	ALA	4.9
10	J	55	ALA	4.8
1	A	1157	G	4.8
23	Z	134	PRO	4.7
3	C	169	ALA	4.6
1	A	2137	G	4.6
10	J	81	ALA	4.6
7	G	2	PRO	4.5
1	A	2190	A	4.5
10	J	84	ALA	4.5
8	H	60	ARG	4.4
1	A	1554	C	4.4
3	C	190	ALA	4.4
1	A	1221	A	4.4
1	A	2811	A	4.4
23	Z	170	THR	4.4
23	Z	141	VAL	4.3
3	C	128	ALA	4.3
1	A	2151	U	4.3
1	A	2153	U	4.3
3	C	152	ALA	4.3
10	J	28	ALA	4.3
10	J	113	ALA	4.3
3	C	129	ALA	4.2
10	J	16	ALA	4.2
8	H	158	HIS	4.2
23	Z	175	VAL	4.1
7	G	86	MET	4.1
1	A	2154	G	4.1
3	C	185	ALA	4.1
3	C	121	ALA	4.1
10	J	72	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
3	C	142	ALA	4.0
1	A	941	A	4.0
1	A	2321	A	4.0
10	J	114	ALA	4.0
3	C	216	ALA	4.0
3	C	34	THR	4.0
3	C	38	ASP	3.9
7	G	137	GLU	3.9
1	A	1096	G	3.9
13	P	92	GLU	3.9
23	Z	171	ILE	3.8
11	N	1	MET	3.8
1	A	2212	G	3.8
3	C	124	ALA	3.8
23	Z	120	ILE	3.7
3	C	105	ALA	3.7
10	J	75	ALA	3.7
3	C	49	ILE	3.7
1	A	2139	U	3.7
1	A	2133	G	3.6
10	J	53	ALA	3.6
3	C	39	GLU	3.6
10	J	112	ALA	3.6
22	Y	58	GLY	3.6
1	A	976	G	3.6
14	Q	6	ARG	3.6
1	A	2804	G	3.6
3	C	222	ALA	3.6
5	E	204	ALA	3.6
3	C	37	PHE	3.5
3	C	136	ALA	3.5
10	J	20	ALA	3.5
7	G	138	GLN	3.5
1	A	2152	G	3.5
10	J	18	ALA	3.5
23	Z	149	SER	3.5
3	C	221	ALA	3.5
3	C	220	ALA	3.5
1	A	2147	A	3.4
3	C	187	ALA	3.4
1	A	1094	C	3.4
5	E	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	46	LYS	3.3
1	A	2671	A	3.3
3	C	76	ALA	3.3
1	A	2905	U	3.3
23	Z	123	ASP	3.3
1	A	2808	U	3.3
1	A	939	C	3.2
1	A	2809	C	3.2
10	J	101	ALA	3.2
23	Z	50	GLN	3.2
3	C	119	ALA	3.2
10	J	83	ALA	3.2
3	C	18	LYS	3.2
2	B	119	G	3.2
30	6	12	GLU	3.1
8	H	59	ARG	3.1
10	J	31	ALA	3.1
10	J	100	ALA	3.1
23	Z	115	GLY	3.1
3	C	215	ALA	3.1
8	H	58	GLU	3.1
3	C	189	ALA	3.1
1	A	2815	G	3.1
10	J	99	ALA	3.1
5	E	69	LYS	3.1
1	A	271	U	3.0
3	C	57	ASN	3.0
10	J	30	ALA	3.0
3	C	179	ALA	3.0
1	A	2805	G	3.0
10	J	14	ALA	3.0
23	Z	55	HIS	3.0
23	Z	147	GLY	3.0
7	G	3	LEU	2.9
23	Z	169	GLU	2.9
3	C	156	ALA	2.9
23	Z	148	ASP	2.9
14	Q	1	MET	2.9
23	Z	118	GLN	2.9
10	J	8	ALA	2.9
10	J	35	ALA	2.9
2	B	64	C	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	2902	G	2.9
3	C	202	ALA	2.9
10	J	67	ALA	2.9
10	J	111	ALA	2.9
1	A	2156	A	2.9
1	A	937	G	2.8
10	J	9	ALA	2.8
3	C	89	ALA	2.8
3	C	47	LEU	2.8
22	Y	91	GLU	2.8
14	Q	61	GLY	2.8
1	A	968	C	2.8
3	C	88	GLU	2.8
10	J	29	ALA	2.7
20	W	1	MET	2.7
1	A	2807	G	2.7
3	C	163	ALA	2.7
10	J	73	ALA	2.7
3	C	194	ALA	2.7
19	V	36	PRO	2.7
3	C	149	ALA	2.7
10	J	110	ALA	2.7
1	A	2195	C	2.7
1	A	2814	C	2.7
1	A	1227	G	2.7
1	A	933	A	2.6
1	A	945	A	2.6
23	Z	174	VAL	2.6
3	C	183	ALA	2.6
3	C	178	ALA	2.6
1	A	1086	C	2.6
23	Z	10	ARG	2.6
10	J	102	ALA	2.6
1	A	938	C	2.6
24	O	2	ALA	2.6
19	V	35	LEU	2.6
1	A	270	U	2.6
1	A	2083	A	2.6
1	A	2745	A	2.6
7	G	51	ARG	2.6
8	H	32	GLU	2.6
14	Q	128	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
28	4	61	VAL	2.5
3	C	195	ALA	2.5
1	A	570	A	2.5
1	A	1516	G	2.5
1	A	2132	C	2.5
3	C	172	ALA	2.5
10	J	7	ALA	2.5
1	A	2813	C	2.5
10	J	5	ALA	2.5
1	A	2142	G	2.5
2	B	5	C	2.5
2	B	65	C	2.5
20	W	113	ALA	2.4
1	A	5	A	2.4
1	A	965	G	2.4
1	A	1594	C	2.4
1	A	2177	G	2.4
1	A	2229	U	2.4
30	6	13	CYS	2.4
3	C	131	ALA	2.4
1	A	375	G	2.4
1	A	532	G	2.4
10	J	80	ALA	2.4
29	5	59	GLU	2.4
2	B	62	C	2.4
23	Z	56	VAL	2.4
3	C	73	ARG	2.4
3	C	25	ALA	2.4
14	Q	140	ALA	2.4
1	A	940	U	2.4
1	A	1089	G	2.4
7	G	55	LYS	2.4
1	A	380	A	2.4
7	G	17	PRO	2.4
1	A	1189	G	2.4
1	A	1091	A	2.4
23	Z	140	ASP	2.4
7	G	30	GLU	2.4
23	Z	119	GLU	2.4
1	A	936	A	2.4
1	A	1065	A	2.4
3	C	150	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	70	LYS	2.3
33	9	37	GLY	2.3
1	A	2315	G	2.3
1	A	2640	A	2.3
27	3	1	MET	2.3
23	Z	136	PHE	2.3
1	A	1934	A	2.3
23	Z	162	GLU	2.3
10	J	52	ALA	2.3
10	J	59	ALA	2.3
10	J	51	ALA	2.3
1	A	2191	A	2.3
1	A	676	C	2.3
3	C	84	LYS	2.3
10	J	50	ALA	2.3
10	J	60	ALA	2.3
1	A	1160	G	2.3
1	A	149	C	2.2
1	A	1161	C	2.2
8	H	17	VAL	2.2
3	C	94	VAL	2.2
23	Z	143	GLY	2.2
1	A	2763	G	2.2
10	J	82	ALA	2.2
32	8	64	TYR	2.2
11	N	80	GLY	2.2
3	C	19	VAL	2.2
16	S	80	LEU	2.2
18	U	90	VAL	2.2
23	Z	37	VAL	2.2
8	H	168	PRO	2.2
1	A	1095	A	2.2
3	C	170	ALA	2.2
33	9	36	GLN	2.2
3	C	197	ALA	2.2
7	G	128	ARG	2.2
1	A	2136	G	2.2
1	A	2777	A	2.2
1	A	2901	G	2.2
3	C	177	ALA	2.2
29	5	60	VAL	2.2
7	G	21	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	88	C	2.2
1	A	2135	A	2.2
13	P	35	HIS	2.2
14	Q	18	LYS	2.2
1	A	2130	U	2.2
14	Q	59	ARG	2.2
10	J	21	ALA	2.1
10	J	91	ALA	2.1
3	C	58	VAL	2.1
5	E	203	LYS	2.1
1	A	157	U	2.1
8	H	169	VAL	2.1
13	P	117	GLU	2.1
23	Z	25	PRO	2.1
3	C	148	ALA	2.1
18	U	73	GLY	2.1
12	O	48	PRO	2.1
23	Z	152	ALA	2.1
1	A	2140	A	2.1
10	J	88	ALA	2.1
1	A	1062	G	2.1
23	Z	97	GLU	2.1
1	A	1593	C	2.1
17	T	113	LYS	2.1
3	C	191	ALA	2.1
3	C	79	LYS	2.1
1	A	1078	U	2.1
10	J	17	ALA	2.1
10	J	70	ALA	2.1
1	A	944	A	2.0
10	J	87	ALA	2.0
3	C	35	ALA	2.0
3	C	144	ALA	2.0
10	J	6	ALA	2.0
1	A	934	C	2.0
3	C	86	ALA	2.0
3	C	188	ALA	2.0
8	H	167	GLU	2.0
28	4	60	GLU	2.0
1	A	1088	C	2.0
3	C	127	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.